



Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 11:47 AM JST

PDB ID : 8XQX / pdb_00008xqx
EMDB ID : EMD-38590
Title : Cryo-EM structure of the Ycf2-FtsHi motor complex from *Chlamydomonas reinhardtii* in apo state
Authors : Liang, K.; Zhan, X.; Wu, J.; Yan, Z.
Deposited on : 2024-01-05
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

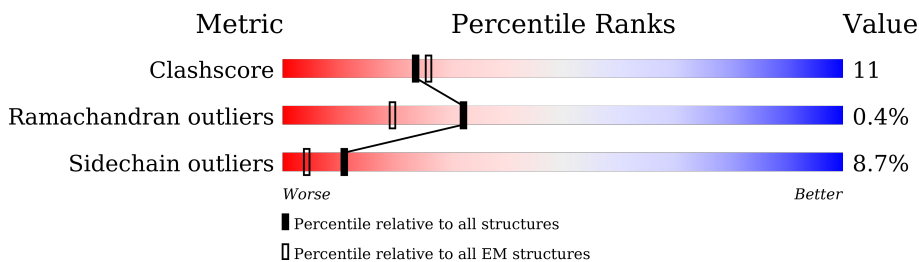
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1182	
2	B	1112	
2	C	1112	
3	D	2971	
4	E	982	
5	F	1024	
6	G	495	
7	H	555	

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Mol	Chain	Length	Quality of chain
8	I	366	
9	J	117	
10	K	255	
11	L	303	
12	M	682	
13	N	137	
14	O	471	
15	P	691	
16	Q	365	
17	R	462	
18	S	324	
19	T	299	
20	U	156	
21	V	86	

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 73189 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fhl1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	988	Total	C	N	O	S	0	0
			7627	4839	1342	1410	36		

- Molecule 2 is a protein called Fhl3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	751	Total	C	N	O	P	S	0	0
			5844	3675	1037	1094	3	35		
2	C	690	Total	C	N	O	S		0	0
			5324	3359	949	985	31			

- Molecule 3 is a protein called Ycf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1539	Total	C	N	O	S	0	0
			12719	8252	2175	2266	26		

- Molecule 4 is a protein called Ctap1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	868	Total	C	N	O	S	0	0
			6221	3881	1143	1183	14		

- Molecule 5 is a protein called Ctap6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	701	Total	C	N	O	S	0	0
			5333	3344	963	1007	19		

- Molecule 6 is a protein called ARHL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	394	Total	C	N	O	S	0	0
			2931	1839	539	549	4		

- Molecule 7 is a protein called PcyA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	406	Total	C	N	O	S	0	0
			3246	2061	547	617	21		

- Molecule 8 is a protein called CrTam39.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	272	Total	C	N	O	S	0	0
			2119	1336	394	374	15		

- Molecule 9 is a protein called ACP.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	85	Total	C	N	O	P	S	0	0
			651	404	101	141	1	4		

- Molecule 10 is a protein called CrTam29.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	189	Total	C	N	O	S	0	0
			1567	1032	271	257	7		

- Molecule 11 is a protein called CrTam34.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	151	Total	C	N	O	S	0	0
			1254	844	210	196	4		

- Molecule 12 is a protein called FADL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	390	Total	C	N	O	S	0	0
			3000	1958	510	516	16		

- Molecule 13 is a protein called CrTam15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	115	Total	C	N	O	S	0	0
			921	585	172	161	3		

- Molecule 14 is a protein called CrTam49.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	318	Total	C	N	O	S	0	0
			1718	1044	335	337	2		

- Molecule 15 is a protein called Ctap7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	617	Total	C	N	O	S	0	0
			4510	2802	829	868	11		

- Molecule 16 is a protein called Tic22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	262	Total	C	N	O	S	0	0
			2078	1316	365	388	9		

- Molecule 17 is a protein called DnaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	401	Total	C	N	O	P S	0	0
			3160	1981	571	585	2 21		

- Molecule 18 is a protein called CrTam35.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	117	Total	C	N	O	P S	0	0
			951	588	169	190	3 1		

- Molecule 19 is a protein called CrTam31.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	110	Total	C	N	O	P S	0	0
			868	535	147	182	2 2		

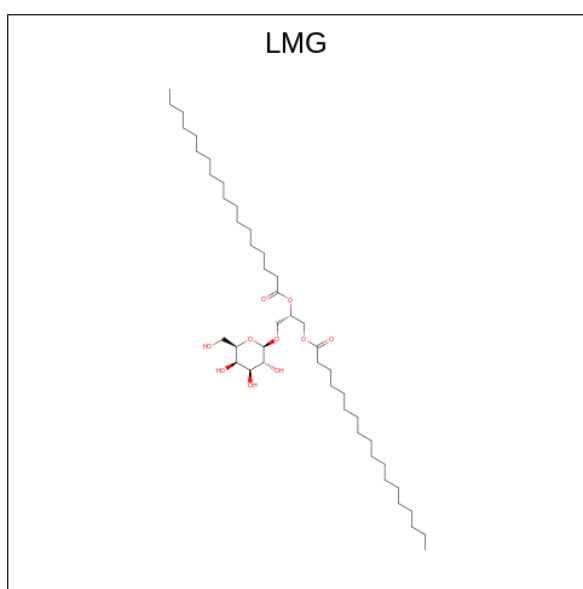
- Molecule 20 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	U	36	Total	C	N	O	1	0
			188	115	36	37		

- Molecule 21 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	68	Total	C	N	O	0	0
			340	204	68	68		

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

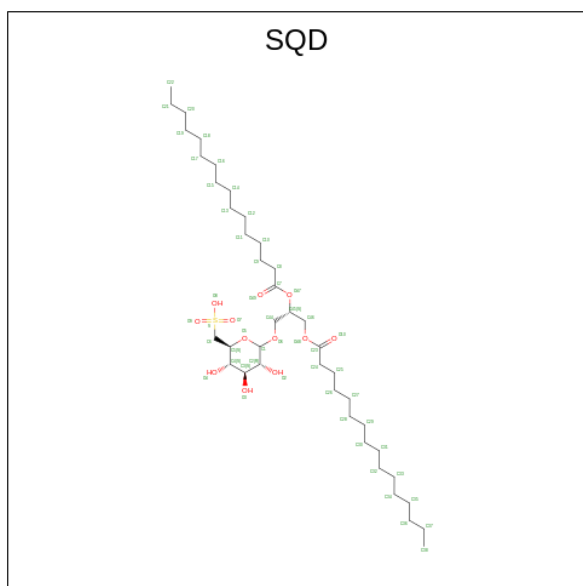


Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			46	36	10	
22	C	1	Total	C	O	0
			25	20	5	
22	I	1	Total	C	O	0
			32	22	10	
22	K	1	Total	C	O	0
			41	31	10	
22	M	1	Total	C	O	0
			48	38	10	

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

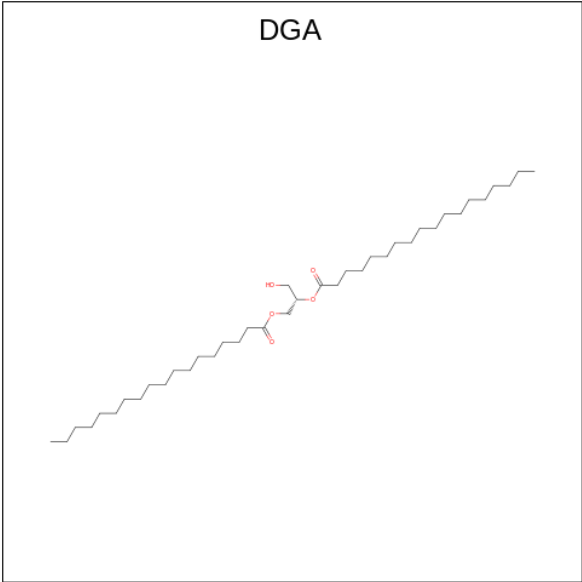
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Mg	0
			1	1	

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



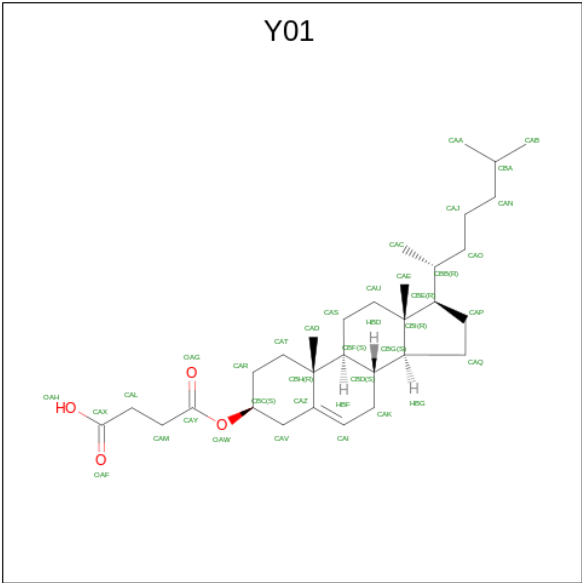
Mol	Chain	Residues	Atoms				AltConf
24	B	1	Total	C	O	S	0
			46	33	12	1	
24	I	1	Total	C	O	S	0
			49	36	12	1	
24	K	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 25 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



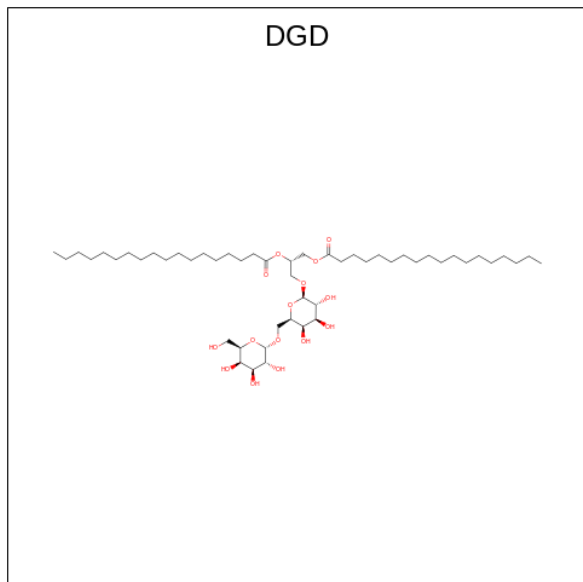
Mol	Chain	Residues	Atoms			AltConf
25	D	1	Total	C	O	0
			39	34	5	
25	L	1	Total	C	O	0
			34	29	5	

- Molecule 26 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



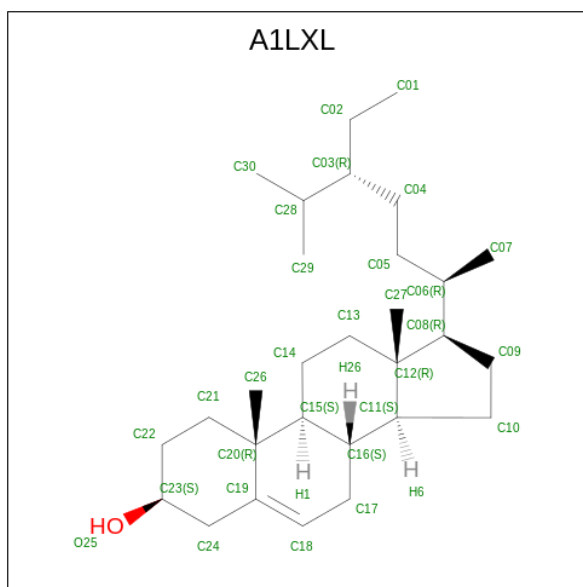
Mol	Chain	Residues	Atoms			AltConf
26	D	1	Total	C	O	0
			35	31	4	
26	M	1	Total	C	O	0
			35	31	4	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
27	I	1	Total	C	O	0
			40	25	15	
27	N	1	Total	C	O	0
			41	26	15	

- Molecule 28 is Beta-Sitosterol (CCD ID: A1LXL) (formula: $C_{29}H_{50}O$).



Mol	Chain	Residues	Atoms			AltConf
28	P	1	Total	C	O	0
			30	29	1	
28	P	1	Total	C	O	0
			30	29	1	

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
29	R	2	Total	Zn	0
			2	2	

- Molecule 2: Fhl3

Chain B:

[illegible]

ARG	ALA	ALA	ASN	VAL	ARG	THR	LEU	ALA	ALA	THR	SER	ARG	GLY	GLU	GLN	PRO	GLN	ASP	SER	GLY	PRO	SER	THR	SER	GLY	ALA	ALA	GLU	LEU	PRO	LEU	ASP	SER	GLY	ILE	GLY	LYS	LEU	ILE	SER	THR	THR	ALA	LYS	ALA	ILE	ILE	GLY	LEU	VAL	VAL	GLY	LEU	MET	LEU	SER	LEU	GLY	PRO
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THR	ARG	ALA	ALA	HIS	ALA	ASP	ARG	LEU	SER	ALA	GLN	PRO	ALA	GLY	GLU	ALA	ALA	ILE	HIS	HIS	GLN	GLN	PRO	Tyr	GLN	GLN	GLN	PRO	HIS	HIS	HIS	GLN	GLN	Gly	VAL	ALA	ASN	ALA	VAL	PRO	LEU	SER	ASP	LEU	ALA	ALA	ALA	PRO	THR	Leu	GLU	Pro	ALA
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THR	LEU	GLU	PRO	ALA	THR	SER	THR	THR	SER	SER	ALA	LEU	T193	T199	S200	A201	Y202	L203	R204	R205	Y210	L211	A212	E213	E214	P215	Q216	M217	H222	A223	H224	A225	V226	V229	V230	R231	T237	P238	F241	D242	E243	L244	M245	R246	P250	A251	E254	V255	P256	N257	R258
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S260
R261
V264
A265
E266
Z267
V268
L271
L272
Y275
ASP
ARG
GLU
ASP
PHE
ASP
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GLY
ILE
LYS
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PRO
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TYR
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GIU
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LEU
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GIU

PHE	ALA	ALA	GLU	GLY	ALA	ALA	PRO	LYS	GLU	K334	K335	K336	T337	E338	D339	M340	T346	T347	A353	M354	A355	L356	F357	G358	D359	A360	K364	K367	R368	T369	Q370	E371	V372	L373	V390	V393	R394	N401	K402	V403	K419	V420	V421	L422	D425	D430	H431
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M435	M439	M443	M446	M449	M453	M454	M457	M458	M468	M469	M470	M473	M474	M475	M476	M477	M478	M479	M480	PRO	LEU	LEU	ASN	LYS	PHE	ARG	ARG	GLN	GLU	PHE	ILE	ARG	M494	M495	M496	M497	M498	M501	F507	F508	F509	P510	M514	R515	M524	M525
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V526	V527	V528	V529	V530	V531	V532		V535	V536	V539	V540	V541	V542	V543	V544	V545	V546	V547		V551	V552	V563		V566	V569	V570	V571		V575	V579		V583	V586	V587	V588	V589	V590	V591	V592	V593	V594	V595	V596	V597	V598	V599	V600	V601	V602	V603	V604		V607	V608
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[illegible]

K702	K703	M704	Q705	V706	H707	A708		K711	A712	V713		M716		R719	Y720		R724	A725	M726		T730		D733	V734	M735		R740		M744		G749	R750	H751		D757		A760	A761	M762	E763		N764	K765	V766	M767		GIU	ALA	THR	LEU	GLU	ALA	ALA	SER	THR	ALA	ALA	GLY	ASP	GLY	GLY	GLY	GLY	LEU
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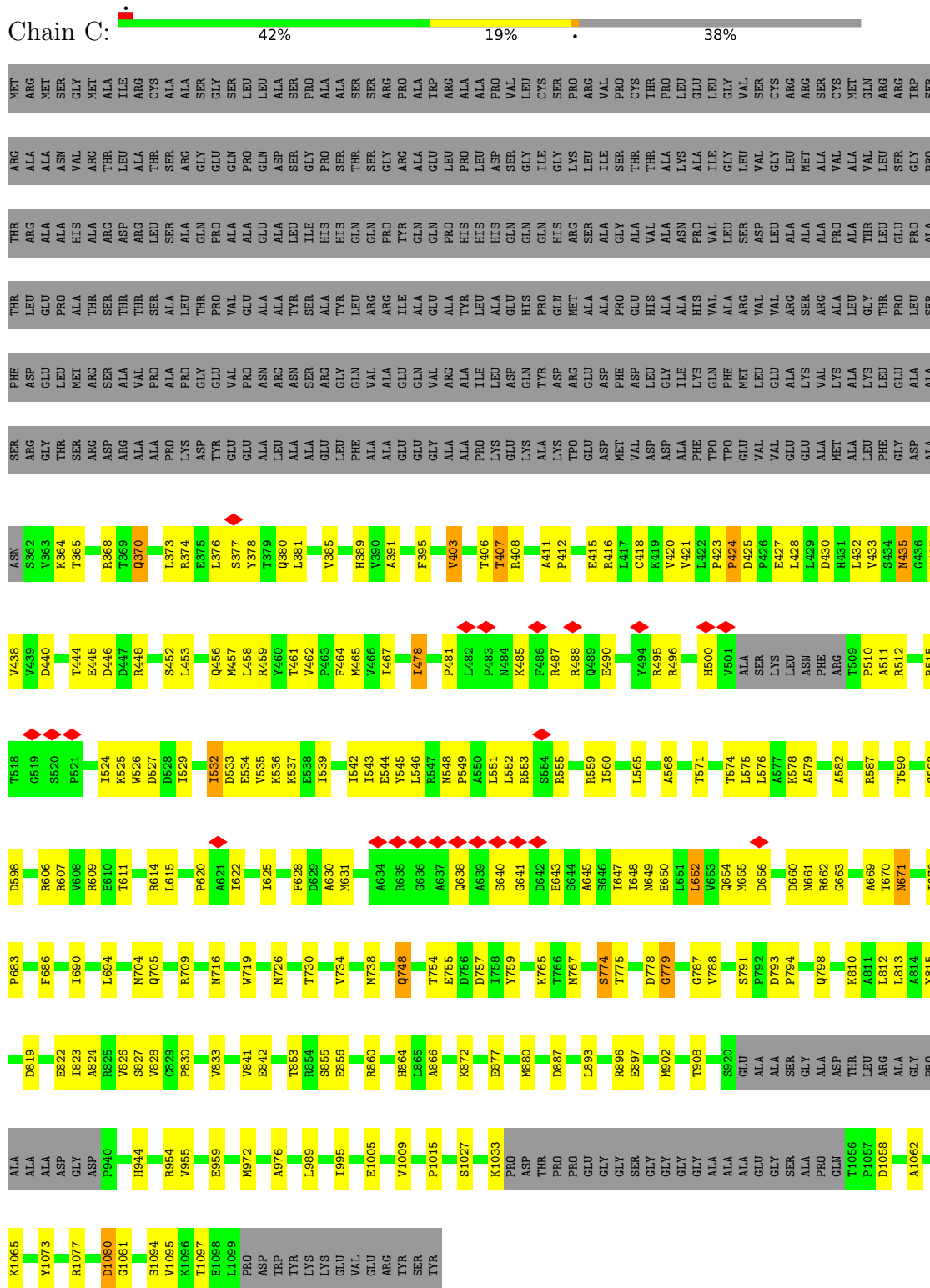
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R907
T908
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D912
L913
E921
ALA
ALA
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GLY
ALA
ASP
THR
LEU
ARG
ALA
GLY
PRO
ALA
ALA
ALA
ASP
G938
T946
S949
T950
E959
D965
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A976
T977
N978
T986
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V1000
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S1006
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SER
LEU
PER

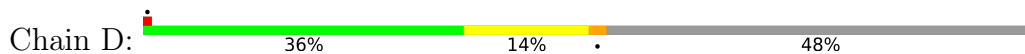
TYR	PRO	PHE	LYS	PRO	ASP	THR	PRO	PRO	PRO	GLU	GLY	GLY	SER	GLY	GLY	GLY	ALA	ALA	ALA	ALA	GLU	GLY	GLY	SER	ALA	PRO	GLN	THR	PRO	ASP	LEU	SER	GLY	ARG	ALA	GLY	LYS	THR	TRP	PHE	ALA	ALA	GLY	THR	ALA	TYR	ASP	ASP	ALA	ASP	GLY	THR	PHE	LYS	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290	1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315	1316	1317	1318	1319	1320	1321	1322	1323	1324	1325	1326	1327	1328	1329	1330	1331	1332	1333	1334	1335	1336	1337	1338	1339	1340	1341	1342	1343	1344	1345	1346	1347	1348	1349	1350	1351	1352	1353	1354	1355	1356	1357	1358	1359	1360	1361	1362	1363	1364	1365	1366	1367	1368	1369	1370	1371	1372	1373	1374	1375	1376	1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390	1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415	1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440	1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490	1491	1492	1493	1494	1495	1496	1497	1498	1499	1500
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Y1103	E1106	E1108	R1109	Y1110	S1111	Y1112
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Chain C:

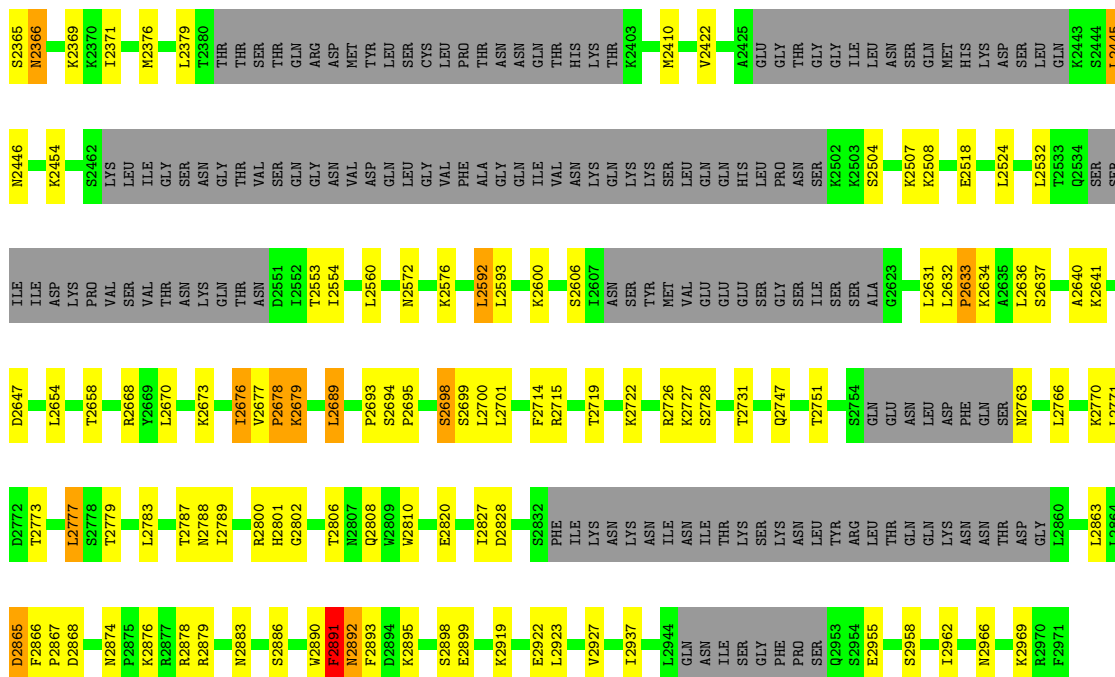


Chain D:

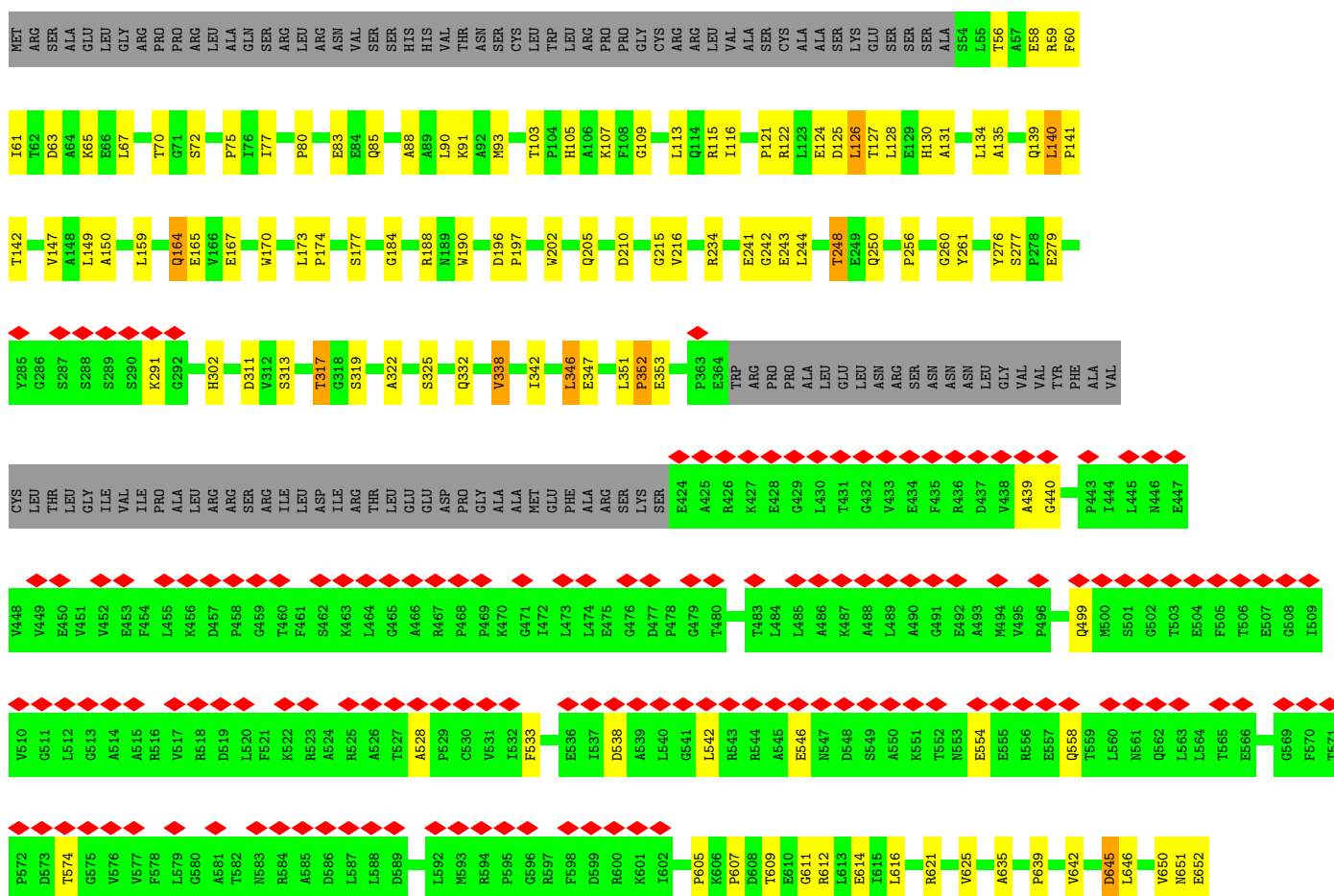


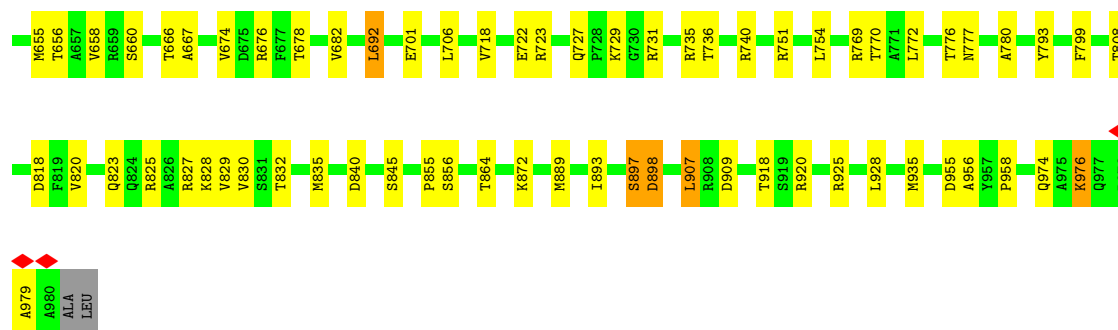




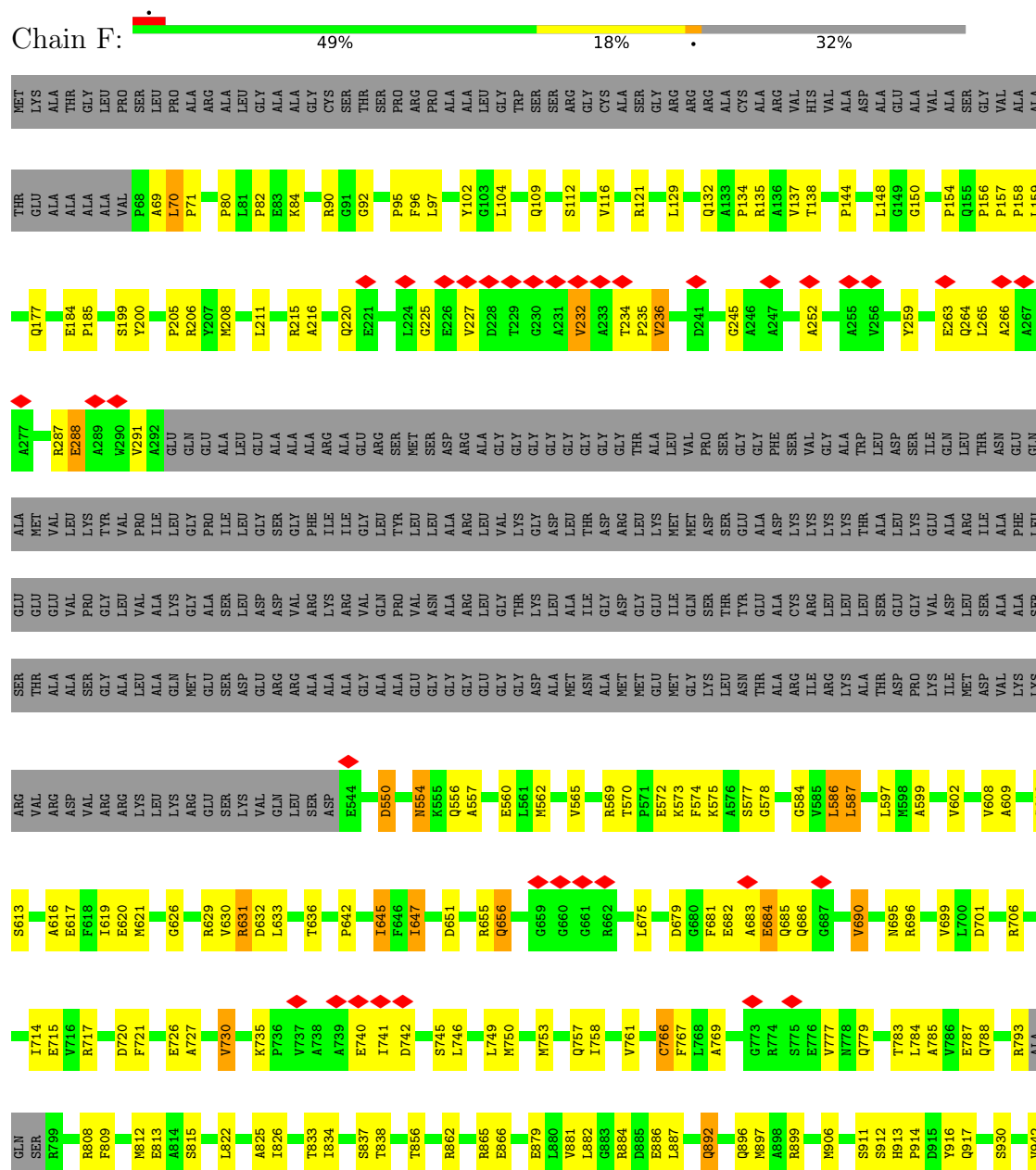


• Molecule 4: Ctap1

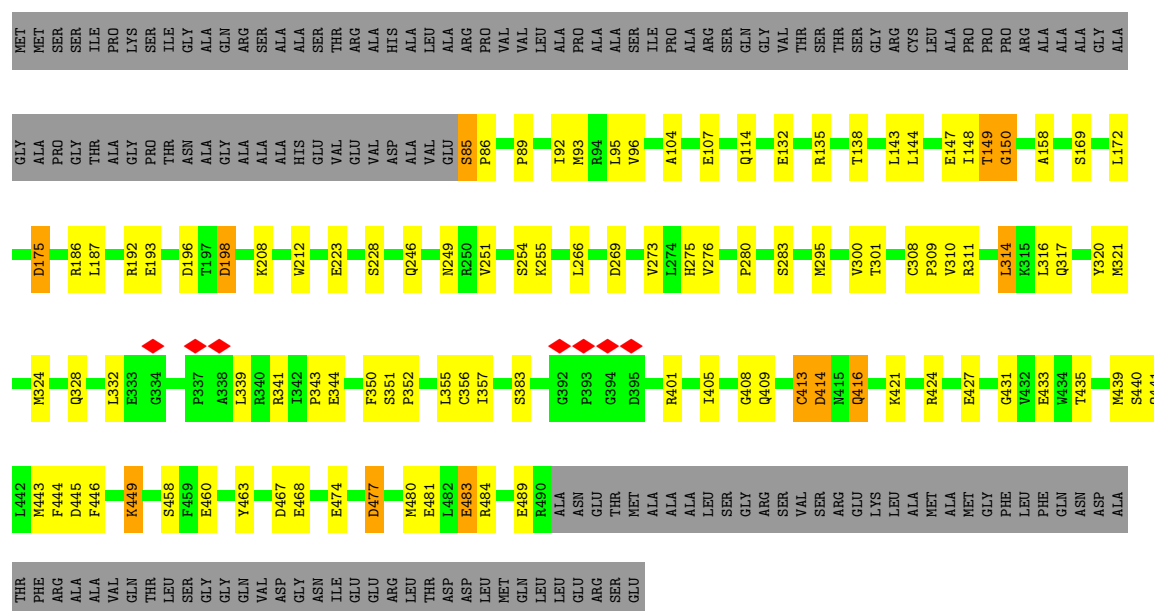


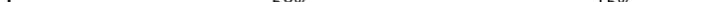


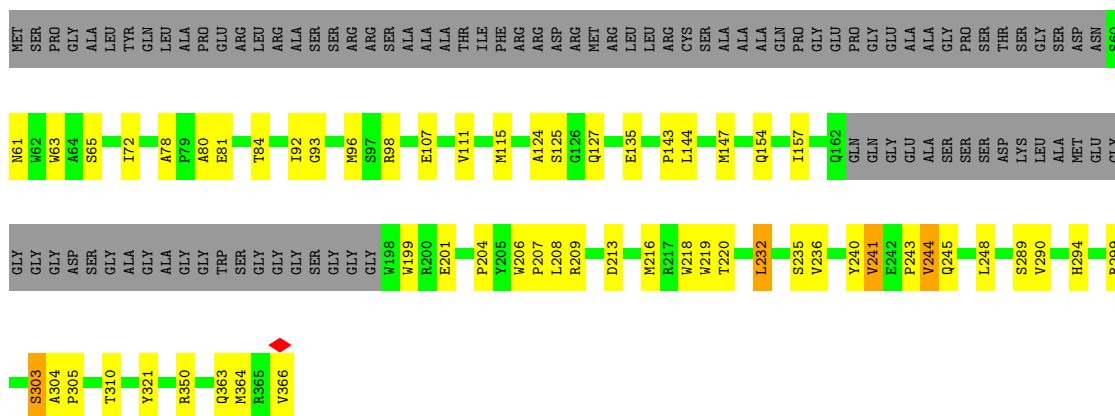
• Molecule 5: Ctap6



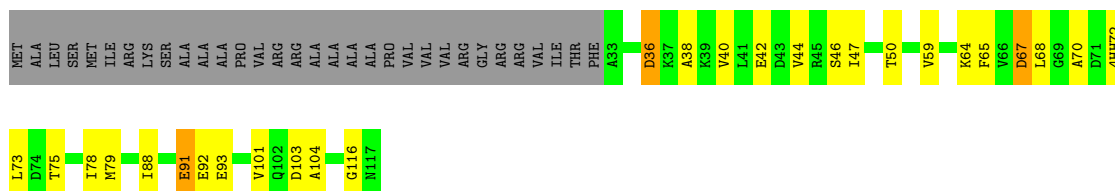
Chain G:



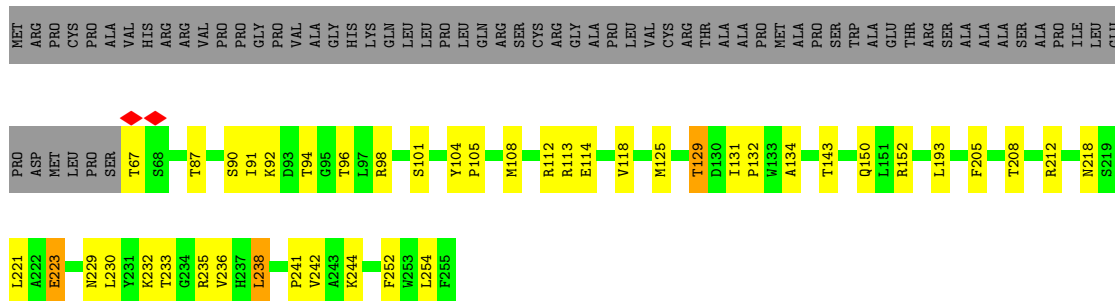
Chain I:  58% 15% 26%



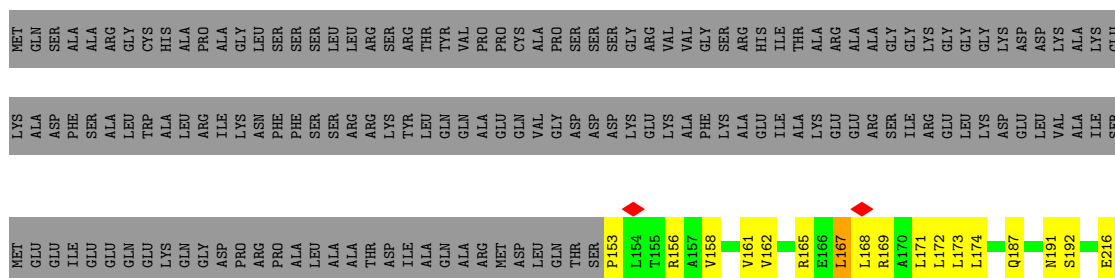
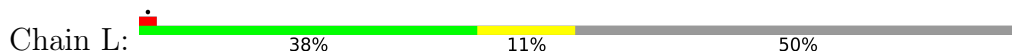
- Molecule 9: ACP



- Molecule 10: CrTam29

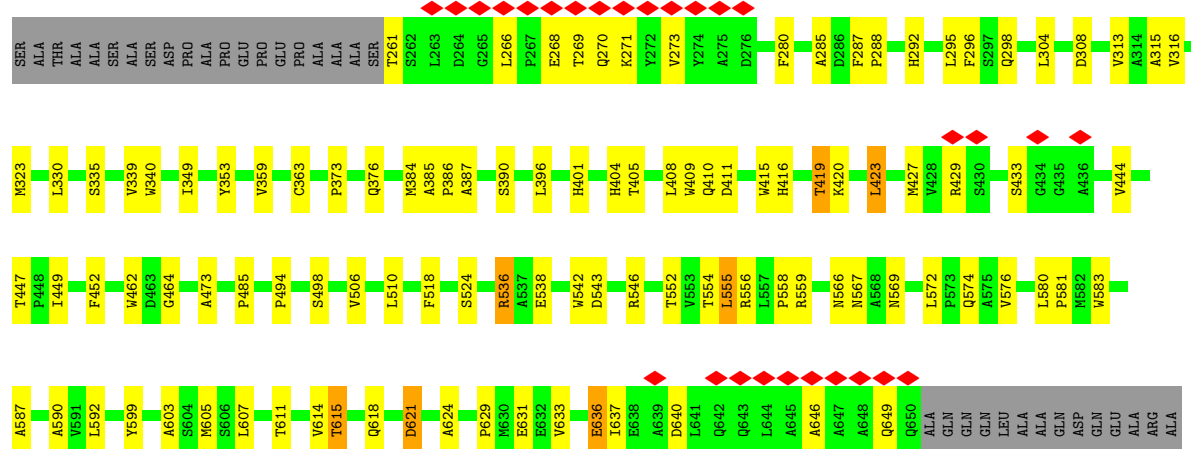
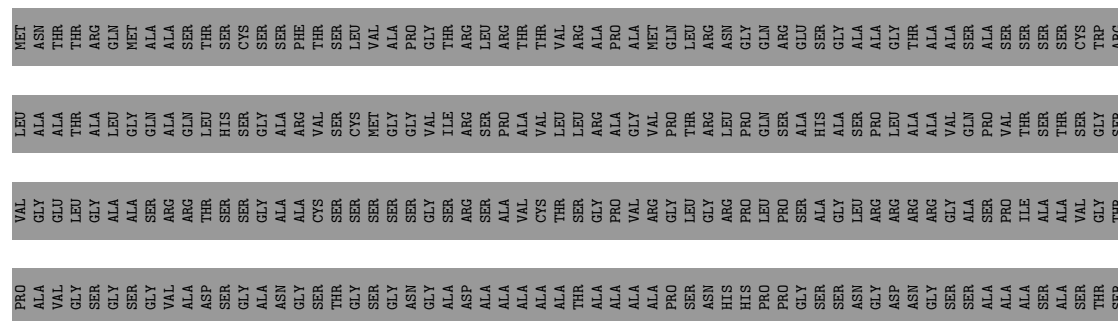


- Molecule 11: CrTam34

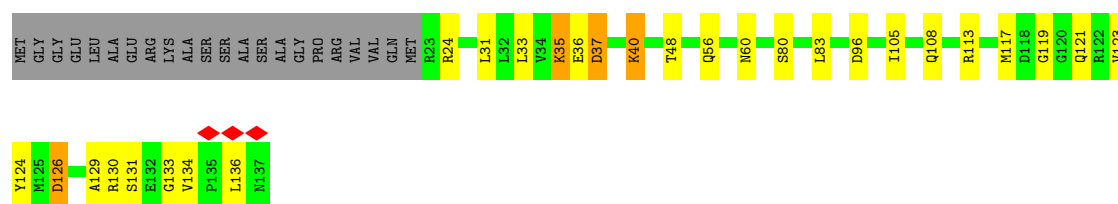




• Molecule 12: FADL



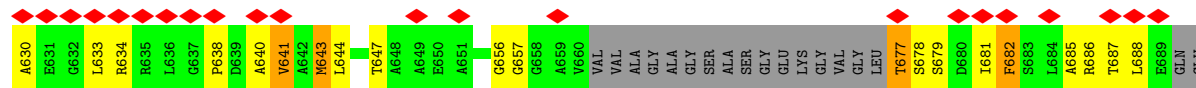
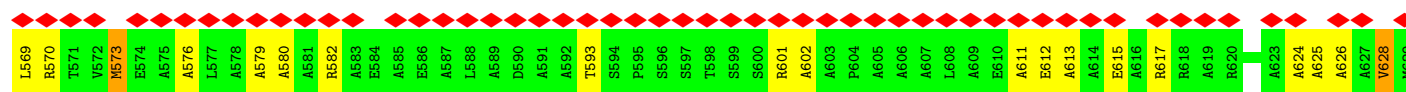
• Molecule 13: CrTam15



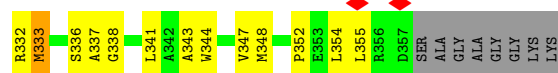
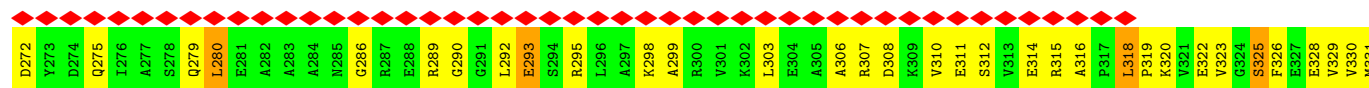
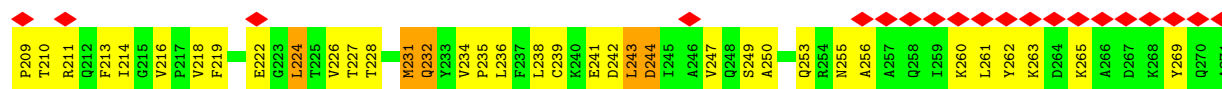
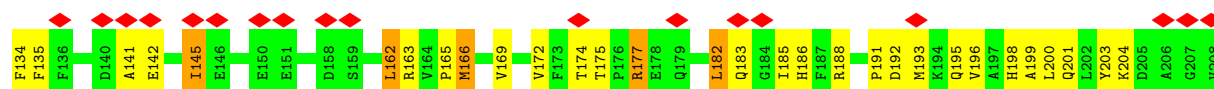
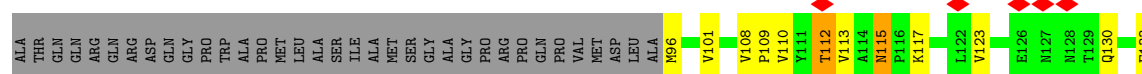
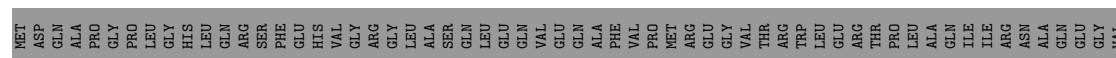
• Molecule 14: CrTam49





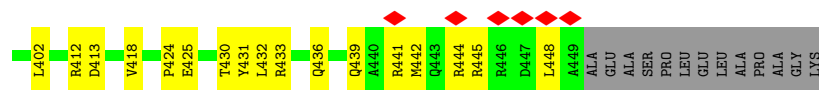


• Molecule 16: Tic22

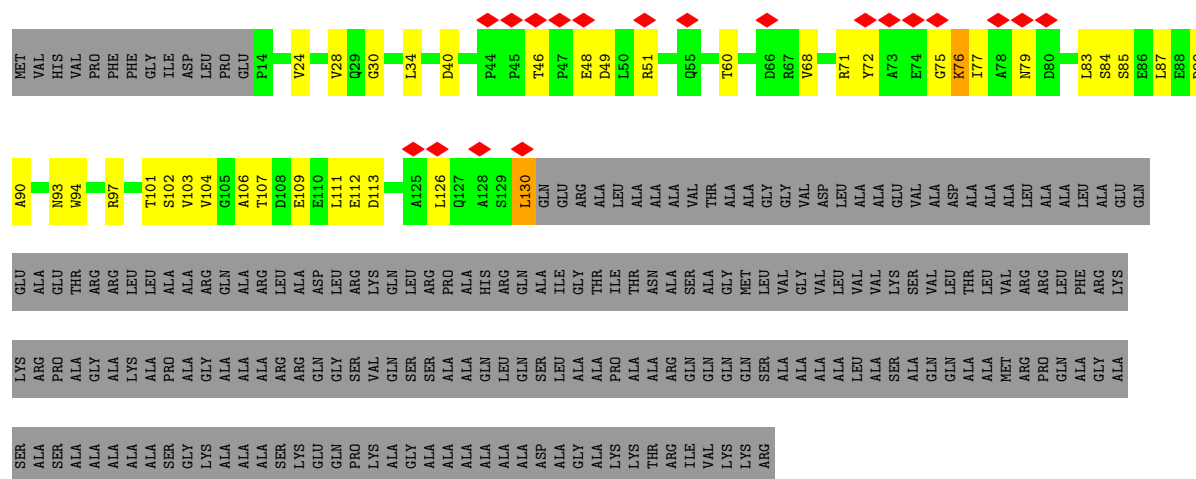


• Molecule 17: DnaJ

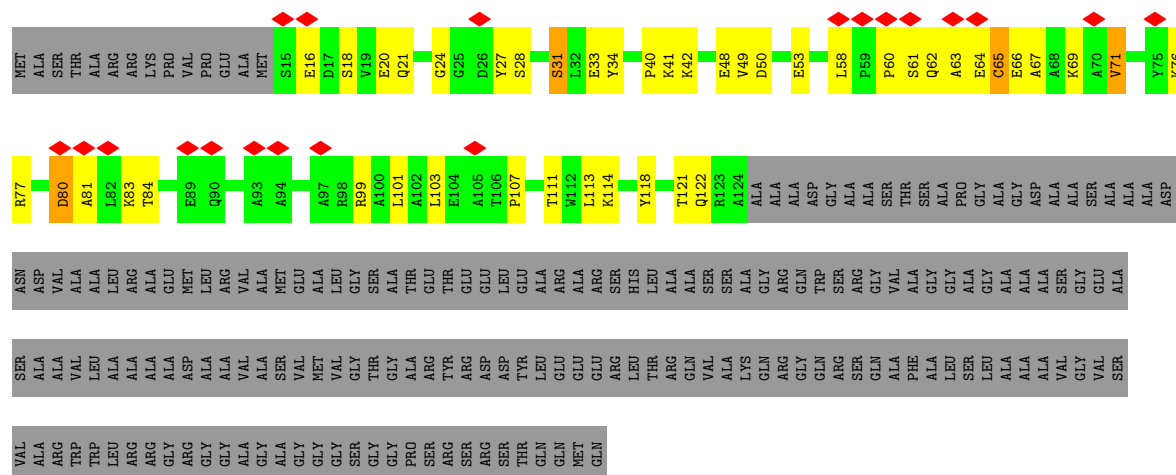




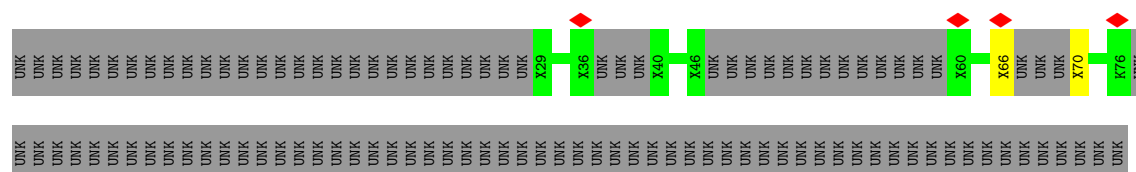
• Molecule 18: CrTam35



• Molecule 19: CrTam31

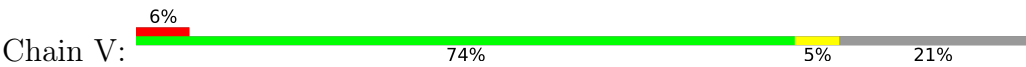


• Molecule 20: UNK





● Molecule 21: UNK



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	461334	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.356	Depositor
Minimum map value	-2.856	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DGA, SEP, Y01, A1LXL, MG, SQD, LMG, DGD, TPO, ZN, 4HH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/7792	0.51	3/10575 (0.0%)
2	B	0.37	1/5925 (0.0%)	0.57	2/8024 (0.0%)
2	C	0.33	0/5432	0.50	0/7359
3	D	0.36	0/12978	0.60	14/17507 (0.1%)
4	E	0.35	0/6350	0.56	2/8655 (0.0%)
5	F	0.31	0/5432	0.49	0/7366
6	G	0.36	0/2999	0.60	2/4087 (0.0%)
7	H	0.36	0/3324	0.48	0/4515
8	I	0.36	0/2177	0.51	0/2958
9	J	0.32	0/625	0.55	0/839
10	K	0.34	0/1627	0.54	0/2223
11	L	0.32	0/1303	0.48	0/1786
12	M	0.23	0/3103	0.47	0/4258
13	N	0.29	0/945	0.50	0/1280
14	O	0.19	0/1731	0.46	0/2391
15	P	0.23	0/4601	0.53	0/6273
16	Q	0.25	0/2115	0.53	0/2857
17	R	0.29	1/3224 (0.0%)	0.53	1/4379 (0.0%)
18	S	0.17	0/936	0.47	0/1267
19	T	0.20	0/862	0.51	0/1164
20	U	0.12	0/45	0.23	0/58
All	All	0.32	2/73526 (0.0%)	0.54	24/99821 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	2
4	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	794	PRO	C-O	-6.48	1.15	1.24
17	R	290	ASP	C-N	-5.46	1.23	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2891	PHE	CA-CB-CG	-18.73	95.08	113.80
3	D	2678	PRO	N-CA-CB	-10.37	92.36	103.25
3	D	2678	PRO	N-CD-CG	-9.34	89.18	103.20
4	E	546	GLU	CB-CA-C	-8.47	100.80	111.22
3	D	971	PRO	N-CA-C	-7.59	96.84	112.47
3	D	2891	PHE	CB-CA-C	6.96	124.27	110.42
3	D	971	PRO	N-CA-CB	-6.75	96.17	103.25
3	D	2867	PRO	N-CA-CB	-6.62	94.71	102.86
1	A	740	PRO	N-CA-CB	-6.42	97.60	103.31
17	R	385	GLU	N-CA-C	-6.22	105.73	113.38
1	A	1163	PRO	N-CA-CB	6.19	110.07	103.39
6	G	253	GLU	N-CA-C	-5.78	105.33	112.38
3	D	2893	PHE	CA-CB-CG	5.77	119.57	113.80
3	D	2891	PHE	N-CA-CB	5.68	120.09	110.49
6	G	263	SER	N-CA-C	-5.50	107.14	112.97
3	D	2866	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	1132	ALA	N-CA-C	-5.30	106.66	113.23
4	E	955	ASP	N-CA-C	-5.29	105.13	113.02
3	D	2892	ASN	CB-CA-C	-5.29	104.08	111.80
3	D	2676	ILE	N-CA-C	-5.26	105.87	113.07
3	D	2676	ILE	CA-C-N	5.25	123.55	120.24
3	D	2676	ILE	C-N-CA	5.25	123.55	120.24
2	B	443	VAL	CA-C-N	5.15	131.37	121.54
2	B	443	VAL	C-N-CA	5.15	131.37	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	962	ARG	Sidechain
3	D	979	ARG	Sidechain
4	E	676	ARG	Sidechain
6	G	257	ARG	Sidechain
6	G	265	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7627	0	7581	148	0
2	B	5844	0	5785	168	0
2	C	5324	0	5301	147	0
3	D	12719	0	13029	315	0
4	E	6221	0	5650	114	0
5	F	5333	0	5318	132	0
6	G	2931	0	2867	67	0
7	H	3246	0	3152	61	0
8	I	2119	0	2069	46	0
9	J	651	0	657	18	0
10	K	1567	0	1558	24	0
11	L	1254	0	1246	22	0
12	M	3000	0	2945	63	0
13	N	921	0	917	21	0
14	O	1718	0	1100	9	0
15	P	4510	0	4451	175	0
16	Q	2078	0	2090	94	0
17	R	3160	0	3001	91	0
18	S	951	0	924	27	0
19	T	868	0	824	30	0
20	U	188	0	60	2	0
21	V	340	0	76	3	0
22	A	46	0	62	3	0
22	C	25	0	31	0	0
22	I	32	0	34	2	0
22	K	41	0	52	1	0
22	M	48	0	66	1	0
23	A	1	0	0	0	0
24	B	46	0	55	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	I	49	0	65	5	0
24	K	45	0	53	0	0
25	D	39	0	63	1	0
25	L	34	0	50	1	0
26	D	35	0	49	0	0
26	M	35	0	49	4	0
27	I	40	0	38	2	0
27	N	41	0	40	0	0
28	P	60	0	0	9	0
29	R	2	0	0	0	0
All	All	73189	0	71308	1549	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:ALA:O	2:B:763:GLU:HB2	1.68	0.94
16:Q:286:GLY:H	16:Q:289:ARG:HG2	1.31	0.93
15:P:472:THR:OG1	28:P:701:A1LXL:C17	2.22	0.88
3:D:881:LEU:HD11	3:D:990:LYS:HA	1.55	0.85
4:E:439:ALA:HB1	4:E:614:GLU:HG3	1.58	0.85
15:P:108:GLU:HB2	15:P:113:ASN:HB2	1.60	0.83
16:Q:200:LEU:HD11	16:Q:213:PHE:HB2	1.60	0.82
17:R:195:LYS:HB2	19:T:27:TYR:HE1	1.44	0.81
3:D:1993:LEU:HD11	3:D:2338:ILE:HG23	1.62	0.80
28:P:701:A1LXL:C09	28:P:702:A1LXL:C26	2.58	0.80
15:P:455:VAL:HG13	15:P:471:LEU:HB2	1.63	0.80
15:P:68:ARG:N	15:P:348:THR:HG21	1.97	0.79
4:E:347:GLU:HA	4:E:351:LEU:HB2	1.63	0.79
3:D:2572:ASN:HD22	3:D:2576:LYS:HG2	1.49	0.78
3:D:59:THR:C	3:D:61:TYR:H	1.90	0.78
4:E:322:ALA:HB3	4:E:325:SER:HB3	1.66	0.76
11:L:168:LEU:HA	11:L:171:LEU:HD12	1.67	0.76
16:Q:177:ARG:HB3	16:Q:182:LEU:HD22	1.66	0.76
17:R:351:ASP:HB2	17:R:354:ARG:HH12	1.50	0.76
2:B:245:MET:HE2	18:S:126:LEU:HD11	1.67	0.76
16:Q:227:THR:HA	16:Q:232:GLN:HA	1.67	0.76
4:E:134:LEU:HD11	4:E:149:LEU:HG	1.67	0.75
2:B:601:SER:HA	2:B:643:GLU:OE2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:165:GLN:O	15:P:169:ASN:HB3	1.87	0.75
12:M:285:ALA:H	12:M:599:TYR:HA	1.52	0.75
7:H:92:ILE:HD11	12:M:288:PRO:HG2	1.68	0.74
2:C:641:GLY:O	2:C:645:ALA:HB3	1.86	0.74
6:G:364:LEU:O	6:G:368:ASN:ND2	2.20	0.74
16:Q:262:TYR:CZ	16:Q:307:ARG:HB3	2.22	0.74
16:Q:269:TYR:HE1	16:Q:299:ALA:HB1	1.53	0.74
15:P:557:ALA:HB3	16:Q:325:SER:H	1.51	0.74
2:B:498:MET:HG3	3:D:1811:ILE:HD11	1.68	0.74
6:G:250:TYR:C	6:G:252:ALA:H	1.96	0.74
15:P:138:LEU:O	15:P:141:GLN:NE2	2.21	0.73
5:F:619:ILE:HG22	5:F:621:MET:HE1	1.70	0.73
4:E:740:ARG:NH2	4:E:829:VAL:O	2.21	0.73
7:H:341:ARG:NH1	7:H:356:CYS:SG	2.62	0.73
1:A:905:ARG:NH1	1:A:961:GLU:OE1	2.21	0.73
3:D:40:ARG:HA	3:D:43:LYS:HE3	1.71	0.72
3:D:947:ILE:HA	3:D:950:LYS:HD2	1.70	0.72
5:F:746:LEU:HD12	5:F:750:MET:HE2	1.72	0.72
5:F:617:GLU:OE2	5:F:629:ARG:NH1	2.22	0.71
10:K:92:LYS:HG3	10:K:105:PRO:HG3	1.71	0.71
15:P:677:THR:OG1	15:P:678:SER:N	2.23	0.71
2:B:431:HIS:O	2:B:435:ASN:ND2	2.25	0.70
11:L:242:VAL:HG13	11:L:248:TRP:HB3	1.73	0.70
5:F:617:GLU:O	5:F:629:ARG:NH1	2.24	0.70
15:P:443:VAL:HG21	28:P:701:A1LXL:C01	2.21	0.70
2:B:610:GLU:OE2	13:N:113:ARG:NH1	2.25	0.70
3:D:566:LEU:HD12	15:P:268:GLN:HA	1.72	0.70
1:A:444:LYS:HA	1:A:451:MET:HB3	1.72	0.70
2:B:762:MET:SD	2:B:762:MET:N	2.65	0.70
3:D:2298:ASP:HA	3:D:2301:VAL:HG12	1.73	0.70
4:E:956:ALA:O	5:F:949:ARG:NH1	2.24	0.70
2:C:660:ASP:OD2	2:C:662:ARG:NH2	2.24	0.70
2:C:536:LYS:HA	2:C:539:ILE:HG12	1.72	0.70
5:F:206:ARG:O	5:F:215:ARG:NH2	2.24	0.69
2:C:748:GLN:HG3	10:K:113:ARG:HG2	1.72	0.69
2:B:494:TYR:N	2:B:497:GLU:OE2	2.25	0.69
4:E:241:GLU:HB2	4:E:261:TYR:CZ	2.28	0.69
3:D:2124:ARG:O	4:E:827:ARG:NH2	2.25	0.69
4:E:167:GLU:OE2	4:E:170:TRP:NE1	2.23	0.69
2:C:376:LEU:HB2	2:C:420:VAL:HG22	1.75	0.69
15:P:100:LEU:HD13	15:P:105:LEU:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:449:LYS:H	7:H:449:LYS:HD3	1.57	0.69
12:M:555:LEU:O	12:M:569:ASN:ND2	2.26	0.69
2:C:810:LYS:NZ	2:C:887:ASP:OD2	2.26	0.68
3:D:1308:ASN:ND2	3:D:1318:SER:OG	2.26	0.68
3:D:560:ILE:HD11	15:P:298:LEU:HD11	1.75	0.68
3:D:904:LYS:NZ	18:S:106:ALA:O	2.26	0.68
5:F:991:ARG:NH1	5:F:998:GLU:OE1	2.27	0.68
7:H:440:SER:OG	7:H:441:GLN:OE1	2.12	0.68
15:P:143:VAL:HG22	15:P:148:MET:HE1	1.76	0.68
1:A:325:SER:OG	1:A:327:GLN:NE2	2.26	0.68
1:A:693:LEU:HG	1:A:694:PRO:HD3	1.76	0.68
2:B:510:PRO:HD3	2:B:607:ARG:HE	1.59	0.68
3:D:750:PRO:HG3	15:P:215:HIS:CE1	2.29	0.68
3:D:1326:HIS:HD2	17:R:225:MET:HE3	1.59	0.68
3:D:2059:VAL:HG21	3:D:2293:LEU:HG	1.76	0.68
5:F:825:ALA:HB3	5:F:866:GLU:HG3	1.75	0.68
6:G:182:ARG:HG2	6:G:491:LEU:HD13	1.76	0.68
12:M:558:PRO:HD3	12:M:605:MET:SD	2.34	0.68
3:D:550:LYS:HB2	15:P:353:VAL:HG21	1.75	0.67
8:I:218:TRP:NE1	24:I:401:SQD:O2	2.23	0.67
15:P:554:LEU:HD21	15:P:562:GLU:HG2	1.77	0.67
3:D:1328:SER:O	3:D:1330:TRP:N	2.27	0.67
3:D:2376:MET:HB2	12:M:473:ALA:HB1	1.76	0.67
5:F:70:LEU:HD22	5:F:71:PRO:HD2	1.76	0.67
4:E:135:ALA:HB1	4:E:139:GLN:HG2	1.76	0.67
1:A:380:ARG:NH1	2:B:478:ILE:O	2.24	0.67
4:E:131:ALA:HA	4:E:149:LEU:O	1.95	0.67
12:M:420:LYS:HA	12:M:423:LEU:HD23	1.75	0.67
12:M:427:MET:HE1	12:M:433:SER:HB2	1.77	0.67
16:Q:307:ARG:NH1	16:Q:308:ASP:OD1	2.28	0.67
2:C:511:ALA:HB2	2:C:611:THR:HG22	1.77	0.67
2:C:525:LYS:HZ3	2:C:527:ASP:HB2	1.59	0.67
3:D:988:ARG:NH1	17:R:212:ALA:O	2.26	0.67
9:J:92:GLU:HB3	10:K:208:THR:HG23	1.77	0.67
15:P:562:GLU:HA	15:P:565:LEU:HG	1.75	0.67
15:P:557:ALA:HB2	16:Q:329:VAL:HG13	1.78	0.67
1:A:981:ILE:HD11	1:A:1066:LEU:HD21	1.77	0.66
6:G:477:GLU:HA	6:G:480:VAL:HG12	1.77	0.66
13:N:126:ASP:O	13:N:130:ARG:N	2.28	0.66
3:D:2600:LYS:NZ	3:D:2637:SER:OG	2.28	0.66
17:R:9:PHE:HB3	17:R:15:VAL:HG11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASN:HA	17:R:413:ASP:HA	1.76	0.66
2:B:545:TYR:HB2	2:B:552:LEU:HD22	1.77	0.66
1:A:802:VAL:HG22	3:D:2789:ILE:HD13	1.78	0.66
19:T:31:SER:HA	19:T:34:TYR:HB3	1.78	0.66
8:I:248:LEU:HD12	12:M:494:PRO:HG3	1.78	0.65
18:S:48:GLU:OE1	18:S:51:ARG:NH1	2.29	0.65
2:C:412:PRO:O	2:C:416:ARG:NH1	2.28	0.65
4:E:242:GLY:H	4:E:260:GLY:HA3	1.62	0.65
15:P:202:SER:O	15:P:205:ASP:N	2.28	0.65
16:Q:96:MET:N	16:Q:336:SER:O	2.29	0.65
2:B:340:MET:HE1	3:D:956:GLN:HE22	1.62	0.65
3:D:2878:ARG:NH1	4:E:855:PRO:O	2.29	0.65
5:F:656:GLN:HA	5:F:701:ASP:HB3	1.78	0.65
7:H:149:THR:OG1	7:H:150:GLY:N	2.22	0.65
16:Q:186:HIS:HB3	16:Q:188:ARG:HH11	1.62	0.65
17:R:213:ASN:OD1	17:R:214:LEU:N	2.30	0.65
2:C:391:ALA:HB2	2:C:408:ARG:HB3	1.78	0.65
3:D:743:ASN:OD1	15:P:458:GLN:NE2	2.30	0.65
15:P:165:GLN:O	15:P:169:ASN:CB	2.44	0.65
15:P:536:GLY:N	16:Q:348:MET:SD	2.70	0.65
2:B:257:ASN:O	2:B:258:ARG:NH1	2.25	0.65
4:E:141:PRO:O	4:E:142:THR:OG1	2.14	0.65
15:P:569:LEU:HD12	15:P:640:ALA:HB1	1.78	0.65
2:B:353:ALA:HB1	3:D:891:LEU:HD11	1.78	0.64
3:D:547:LEU:HD21	3:D:635:TYR:HE1	1.60	0.64
2:C:641:GLY:O	2:C:645:ALA:CB	2.46	0.64
18:S:109:GLU:HG2	18:S:113:ASP:HB2	1.79	0.64
8:I:218:TRP:HE1	24:I:401:SQD:HO2	1.44	0.64
16:Q:112:THR:OG1	16:Q:113:VAL:N	2.25	0.64
3:D:59:THR:C	3:D:61:TYR:N	2.54	0.64
4:E:80:PRO:HG2	4:E:85:GLN:HG2	1.80	0.64
2:B:892:ASN:HD22	2:B:896:ARG:HH12	1.44	0.64
3:D:816:TYR:O	3:D:820:ASN:ND2	2.31	0.64
16:Q:123:VAL:HA	20:U:151:UNK:HA	1.78	0.64
1:A:573:ASP:HB3	1:A:576:SER:HB3	1.80	0.64
15:P:557:ALA:HB1	16:Q:328:GLU:HB3	1.80	0.64
16:Q:306:ALA:O	16:Q:310:VAL:HG23	1.98	0.64
1:A:296:ASP:OD2	17:R:293:LYS:NZ	2.30	0.63
5:F:245:GLY:HA3	19:T:114:LYS:HD3	1.80	0.63
17:R:243:LEU:O	17:R:267:ARG:NH1	2.31	0.63
19:T:20:GLU:HG2	19:T:24:GLY:HA2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:855:SER:HB2	2:C:1015:PRO:HG2	1.80	0.63
3:D:1126:ASN:ND2	3:D:1129:ASP:OD1	2.30	0.63
2:B:267:GLN:OE1	3:D:1251:ARG:NH1	2.31	0.63
3:D:1372:ASN:OD1	3:D:1392:GLN:NE2	2.30	0.63
5:F:573:LYS:H	5:F:573:LYS:HD3	1.63	0.63
15:P:485:MET:SD	15:P:486:SER:OG	2.56	0.63
16:Q:201:GLN:HA	16:Q:204:LYS:HZ3	1.62	0.63
3:D:2033:ASN:HD22	3:D:2317:THR:HB	1.63	0.63
5:F:70:LEU:HD23	19:T:101:LEU:HD11	1.81	0.63
16:Q:312:SER:O	16:Q:316:ALA:N	2.32	0.63
17:R:144:LYS:HE2	17:R:214:LEU:HD23	1.79	0.63
2:B:761:ALA:O	2:B:764:ASN:ND2	2.32	0.63
3:D:348:THR:HG23	3:D:1374:LYS:HB3	1.81	0.63
11:L:254:LEU:O	11:L:258:THR:HG23	1.98	0.63
2:B:369:THR:O	2:B:373:LEU:HB2	1.99	0.63
2:B:510:PRO:HG2	2:B:596:PHE:CZ	2.34	0.63
3:D:736:ASN:O	28:P:701:A1LXL:C26	2.47	0.63
3:D:2678:PRO:HG2	3:D:2891:PHE:CE2	2.34	0.63
5:F:569:ARG:HG3	5:F:570:THR:HG23	1.81	0.63
12:M:462:TRP:O	12:M:464:GLY:N	2.32	0.62
2:C:374:ARG:HH12	2:C:376:LEU:HD21	1.62	0.62
2:C:490:GLU:OE1	2:C:512:ARG:NH2	2.32	0.62
5:F:232:VAL:HG11	5:F:259:TYR:HB3	1.80	0.62
15:P:279:PRO:HB3	15:P:507:LEU:HD11	1.81	0.62
6:G:351:ASP:OD1	6:G:352:VAL:N	2.33	0.62
18:S:77:ILE:HD12	18:S:77:ILE:H	1.64	0.62
3:D:1364:ASN:ND2	17:R:317:SER:OG	2.32	0.62
17:R:424:PRO:O	17:R:433:ARG:NH2	2.32	0.62
3:D:566:LEU:HD22	15:P:656:GLY:HA2	1.80	0.62
16:Q:260:LYS:HA	16:Q:263:LYS:HD3	1.81	0.62
11:L:187:GLN:O	11:L:191:ASN:ND2	2.33	0.62
5:F:809:PHE:O	5:F:813:GLU:HG2	2.00	0.62
10:K:212:ARG:NH2	10:K:218:ASN:OD1	2.32	0.62
1:A:322:ASP:OD2	1:A:325:SER:HB3	2.00	0.62
13:N:113:ARG:HE	14:O:470:ARG:HH12	1.48	0.62
15:P:171:PRO:HB2	18:S:130:LEU:HD13	1.81	0.62
2:B:508:ARG:NH2	3:D:1781:ASP:OD1	2.33	0.61
3:D:473:ASN:HA	3:D:476:LEU:HB2	1.81	0.61
4:E:840:ASP:O	5:F:892:GLN:NE2	2.31	0.61
6:G:473:GLU:OE1	6:G:476:ARG:NH2	2.32	0.61
15:P:101:SER:OG	15:P:102:ALA:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:424:LEU:HD12	15:P:430:VAL:HG21	1.82	0.61
2:B:598:ASP:HB3	2:B:600:TYR:CE1	2.35	0.61
3:D:739:LYS:HA	15:P:469:TYR:HA	1.82	0.61
4:E:65:LYS:NZ	19:T:121:THR:O	2.32	0.61
15:P:346:ASP:O	15:P:349:ASP:N	2.31	0.61
3:D:1363:ILE:HG21	17:R:317:SER:HB2	1.83	0.61
2:B:528:ASP:O	2:B:530:ASN:ND2	2.33	0.61
3:D:951:ARG:HH22	17:R:167:TPO:HB	1.66	0.61
17:R:385:GLU:HA	17:R:389:GLY:HA2	1.82	0.61
1:A:782:THR:O	1:A:793:ASP:N	2.34	0.61
2:B:251:ALA:HB3	2:B:254:GLU:HG2	1.82	0.61
12:M:633:VAL:O	12:M:637:ILE:HG13	2.00	0.61
1:A:144:THR:O	1:A:161:TRP:NE1	2.29	0.61
3:D:756:LYS:HE3	15:P:520:ARG:HD3	1.83	0.61
3:D:2699:SER:O	3:D:2699:SER:OG	2.13	0.61
4:E:93:MET:HB3	5:F:80:PRO:HG3	1.82	0.61
4:E:173:LEU:HD12	4:E:174:PRO:HD2	1.82	0.61
2:B:593:GLY:HA2	2:B:631:MET:HE1	1.82	0.61
2:C:549:PRO:O	2:C:553:ARG:HB2	2.01	0.61
2:C:757:ASP:OD1	10:K:113:ARG:NH1	2.33	0.61
5:F:651:ASP:OD2	5:F:695:ASN:ND2	2.34	0.61
7:H:311:ARG:NH2	7:H:317:GLN:OE1	2.33	0.61
16:Q:308:ASP:O	16:Q:312:SER:HB3	2.00	0.61
1:A:851:PRO:HG2	1:A:1049:ILE:HG21	1.83	0.60
7:H:439:MET:HA	7:H:443:MET:HB2	1.83	0.60
6:G:182:ARG:HB3	6:G:491:LEU:HB2	1.83	0.60
6:G:328:CYS:HB2	6:G:452:LEU:HB2	1.83	0.60
15:P:119:ASP:O	15:P:123:GLN:HG2	2.01	0.60
1:A:137:LYS:HE3	1:A:138:GLN:HG3	1.84	0.60
2:B:536:LYS:O	2:B:540:ASN:ND2	2.33	0.60
3:D:2454:LYS:HD3	7:H:480:MET:HG3	1.83	0.60
3:D:2800:ARG:O	3:D:2802:GLY:N	2.34	0.60
2:C:428:LEU:O	2:C:432:LEU:HD12	2.02	0.60
3:D:449:LEU:HA	3:D:452:ILE:HG22	1.84	0.60
15:P:517:ASN:ND2	15:P:519:GLU:OE2	2.34	0.60
1:A:911:ARG:NE	1:A:949:GLU:OE2	2.30	0.60
2:B:535:VAL:HG12	2:B:690:ILE:HG22	1.81	0.60
6:G:134:ARG:NH2	6:G:400:HIS:O	2.34	0.60
17:R:365:GLY:HA2	17:R:368:ARG:HB2	1.84	0.60
1:A:542:SER:O	1:A:546:ASN:ND2	2.35	0.60
4:E:128:LEU:HD21	5:F:104:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:243:VAL:HG13	6:G:244:PRO:HD3	1.84	0.60
2:C:568:ALA:O	2:C:571:THR:OG1	2.20	0.60
3:D:970:PHE:N	3:D:971:PRO:HD3	2.16	0.60
18:S:68:VAL:O	18:S:72:TYR:N	2.35	0.60
2:B:199:TYR:O	2:B:203:LEU:HD12	2.02	0.59
7:H:175:ASP:OD1	7:H:175:ASP:N	2.35	0.59
17:R:442:MET:HA	17:R:445:ARG:HB2	1.83	0.59
16:Q:172:VAL:O	16:Q:175:THR:OG1	2.20	0.59
3:D:2055:ARG:NH2	3:D:2056:TYR:OH	2.34	0.59
7:H:89:PRO:HB3	12:M:288:PRO:HG3	1.83	0.59
15:P:580:ALA:HB2	15:P:625:ALA:HB2	1.82	0.59
3:D:2962:ILE:HG23	8:I:144:LEU:HD11	1.84	0.59
17:R:1:MET:N	17:R:25:GLU:OE1	2.35	0.59
8:I:235:SER:HB2	8:I:243:PRO:HG2	1.83	0.59
8:I:294:HIS:NE2	27:I:403:DGD:O5E	2.34	0.59
11:L:217:ARG:NH2	13:N:96:ASP:OD1	2.36	0.59
15:P:633:LEU:HB3	15:P:641:VAL:HG12	1.85	0.59
1:A:855:SER:O	1:A:855:SER:OG	2.19	0.59
2:B:446:ASP:OD1	2:B:446:ASP:N	2.36	0.59
2:C:755:GLU:HG3	6:G:258:HIS:CD2	2.38	0.59
4:E:126:LEU:HA	5:F:104:LEU:HD23	1.85	0.59
4:E:751:ARG:NH1	4:E:793:TYR:OH	2.36	0.59
5:F:70:LEU:HD12	13:N:24:ARG:HG2	1.84	0.59
7:H:431:GLY:O	7:H:435:THR:OG1	2.20	0.59
15:P:630:ALA:O	15:P:634:ARG:HB2	2.02	0.59
2:C:705:GLN:O	2:C:709:ARG:NH1	2.36	0.59
7:H:96:VAL:HG12	12:M:295:LEU:HD11	1.85	0.59
2:C:525:LYS:HD3	2:C:527:ASP:H	1.66	0.59
3:D:621:HIS:HD2	15:P:57:ASP:HB3	1.65	0.59
4:E:655:MET:HA	4:E:658:VAL:HG12	1.84	0.59
4:E:439:ALA:HB1	4:E:614:GLU:CG	2.33	0.59
5:F:822:LEU:HD22	5:F:1011:ASP:HB3	1.85	0.59
2:B:635:ARG:NH1	3:D:2055:ARG:O	2.36	0.58
1:A:496:ILE:HB	1:A:625:VAL:HG23	1.85	0.58
1:A:948:GLY:HA2	1:A:951:LEU:HB2	1.85	0.58
3:D:557:LEU:HA	3:D:560:ILE:HD12	1.85	0.58
3:D:1224:SER:O	3:D:1228:ILE:HG13	2.02	0.58
6:G:250:TYR:C	6:G:252:ALA:N	2.61	0.58
6:G:311:THR:HG23	6:G:314:GLY:H	1.68	0.58
3:D:1363:ILE:C	3:D:1365:SER:H	2.11	0.58
3:D:2152:ASP:O	3:D:2154:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:413:CYS:SG	7:H:414:ASP:N	2.76	0.58
2:C:778:ASP:O	2:C:779:GLY:C	2.46	0.58
2:B:629:ASP:N	2:B:629:ASP:OD1	2.37	0.58
6:G:112:LYS:NZ	6:G:329:GLY:O	2.36	0.58
3:D:448:ASP:OD1	3:D:448:ASP:N	2.34	0.58
9:J:75:THR:O	9:J:79:MET:HG2	2.03	0.58
2:B:256:PRO:HB2	2:B:258:ARG:HH12	1.68	0.58
4:E:59:ARG:HH22	19:T:122:GLN:HE22	1.50	0.58
7:H:317:GLN:HB2	7:H:320:TYR:HD2	1.69	0.58
12:M:614:VAL:O	12:M:618:GLN:NE2	2.37	0.58
16:Q:109:PRO:HA	16:Q:165:PRO:HA	1.85	0.58
2:B:635:ARG:HD2	3:D:2055:ARG:HH11	1.68	0.58
16:Q:256:ALA:O	16:Q:260:LYS:HD2	2.03	0.58
2:B:601:SER:HA	2:B:643:GLU:CD	2.28	0.58
3:D:2330:ARG:HD3	3:D:2333:ARG:HH21	1.68	0.58
4:E:93:MET:HE2	5:F:96:PHE:HE2	1.69	0.58
5:F:234:THR:HG23	19:T:99:ARG:HG3	1.86	0.58
12:M:621:ASP:OD1	12:M:624:ALA:N	2.37	0.58
3:D:977:ARG:HD3	17:R:153:TRP:CD1	2.39	0.57
4:E:740:ARG:HE	4:E:835:MET:HE1	1.69	0.57
6:G:111:ASP:HA	6:G:114:VAL:HG12	1.86	0.57
1:A:364:GLY:O	1:A:367:GLU:HG3	2.05	0.57
2:C:430:ASP:OD1	2:C:430:ASP:N	2.36	0.57
2:C:593:GLY:HA3	2:C:630:ALA:HB3	1.86	0.57
4:E:727:GLN:O	4:E:735:ARG:NH2	2.30	0.57
12:M:574:GLN:NE2	12:M:580:LEU:O	2.29	0.57
2:B:1002:HIS:O	2:B:1006:SER:OG	2.22	0.57
12:M:462:TRP:HH2	12:M:485:PRO:HB2	1.69	0.57
15:P:203:GLY:O	15:P:207:SER:OG	2.21	0.57
2:B:679:ALA:O	2:B:685:ARG:NH1	2.37	0.57
2:B:757:ASP:O	2:B:760:ALA:HB3	2.04	0.57
3:D:545:SER:HB3	15:P:226:LEU:HA	1.86	0.57
3:D:784:HIS:HE1	17:R:60:ARG:NH1	2.02	0.57
9:J:91:GLU:OE2	9:J:92:GLU:N	2.38	0.57
12:M:611:THR:O	12:M:615:THR:OG1	2.22	0.57
16:Q:280:LEU:HD21	16:Q:293:GLU:HB2	1.86	0.57
5:F:84:LYS:NZ	5:F:92:GLY:O	2.35	0.57
3:D:2865:ASP:OD1	3:D:2865:ASP:N	2.36	0.57
11:L:258:THR:HG22	11:L:264:LEU:HA	1.85	0.57
13:N:105:ILE:O	13:N:108:GLN:NE2	2.37	0.57
19:T:50:ASP:HB2	19:T:53:GLU:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:MET:SD	2:B:222:HIS:NE2	2.78	0.57
5:F:584:GLY:HA3	5:F:710:PHE:HA	1.86	0.57
18:S:68:VAL:HA	18:S:71:ARG:HB2	1.87	0.57
2:C:425:ASP:OD1	2:C:427:GLU:HG2	2.05	0.57
2:C:822:GLU:HB2	2:C:841:VAL:HG13	1.87	0.57
2:C:1062:ALA:N	7:H:223:GLU:OE2	2.38	0.57
4:E:722:GLU:OE1	4:E:723:ARG:NH1	2.37	0.57
15:P:320:TRP:CH2	28:P:701:A1LXL:C02	2.87	0.57
16:Q:193:MET:HA	16:Q:196:VAL:HG12	1.86	0.57
1:A:647:LYS:NZ	5:F:578:GLY:O	2.32	0.56
2:C:485:LYS:HD2	2:C:488:ARG:HH22	1.70	0.56
5:F:745:SER:O	5:F:749:LEU:HB2	2.05	0.56
15:P:624:ALA:O	15:P:628:VAL:HG22	2.04	0.56
2:B:897:GLU:O	2:B:901:SER:HB2	2.05	0.56
2:B:906:ARG:NH1	2:C:1094:SER:OG	2.31	0.56
4:E:538:ASP:O	4:E:542:LEU:N	2.38	0.56
7:H:138:THR:HG22	7:H:143:LEU:HD21	1.87	0.56
10:K:125:MET:HA	10:K:129:THR:OG1	2.06	0.56
15:P:626:ALA:HB2	15:P:687:THR:HB	1.88	0.56
16:Q:307:ARG:HH21	16:Q:311:GLU:HG3	1.70	0.56
1:A:1073:ARG:NH2	2:B:873:LEU:O	2.38	0.56
3:D:894:LEU:HD13	3:D:975:TRP:CZ3	2.40	0.56
5:F:684:GLU:OE1	5:F:685:GLN:N	2.34	0.56
12:M:308:ASP:OD1	12:M:583:TRP:NE1	2.39	0.56
2:C:645:ALA:O	2:C:649:ASN:ND2	2.39	0.56
3:D:2632:LEU:O	3:D:2634:LYS:N	2.39	0.56
16:Q:130:GLN:HB2	16:Q:185:ILE:HG13	1.87	0.56
1:A:390:THR:HG23	2:B:495:ARG:HE	1.71	0.56
6:G:221:ARG:NH2	6:G:471:GLU:OE1	2.38	0.56
12:M:415:TRP:NE1	12:M:524:SER:OG	2.38	0.56
3:D:813:TYR:O	3:D:817:VAL:HG22	2.05	0.56
5:F:266:ALA:HA	19:T:83:LYS:HD3	1.88	0.56
16:Q:262:TYR:OH	16:Q:303:LEU:HG	2.06	0.56
3:D:2376:MET:HE1	8:I:124:ALA:HB2	1.88	0.56
15:P:144:ALA:HB1	15:P:160:LEU:HB2	1.87	0.56
16:Q:198:HIS:O	16:Q:201:GLN:HG3	2.06	0.56
5:F:150:GLY:HA2	17:R:268:SER:HB3	1.88	0.55
12:M:315:ALA:O	12:M:566:ASN:ND2	2.30	0.55
8:I:144:LEU:H	8:I:144:LEU:HD22	1.71	0.55
10:K:112:ARG:HH12	10:K:114:GLU:HB2	1.69	0.55
13:N:56:GLN:NE2	13:N:60:ASN:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:119:GLY:HA3	17:R:8:GLU:HG2	1.88	0.55
4:E:121:PRO:O	4:E:122:ARG:NH1	2.39	0.55
4:E:612:ARG:NH1	4:E:635:ALA:O	2.39	0.55
15:P:361:ARG:HB3	15:P:362:PRO:HD3	1.87	0.55
1:A:740:PRO:HD2	1:A:760:ILE:HD11	1.89	0.55
7:H:481:GLU:OE2	7:H:484:ARG:NH2	2.39	0.55
10:K:229:ASN:OD1	10:K:235:ARG:NH2	2.40	0.55
5:F:574:PHE:HA	5:F:577:SER:HB3	1.87	0.55
10:K:233:THR:OG1	10:K:235:ARG:NE	2.38	0.55
12:M:296:PHE:HB2	12:M:576:VAL:HG21	1.88	0.55
1:A:775:THR:HA	1:A:778:MET:HE3	1.89	0.55
4:E:184:GLY:O	4:E:188:ARG:NH1	2.39	0.55
4:E:701:GLU:OE2	4:E:736:THR:OG1	2.21	0.55
5:F:184:GLU:HG2	5:F:185:PRO:HD2	1.89	0.55
15:P:118:LYS:HA	15:P:121:LYS:HB2	1.89	0.55
2:C:896:ARG:HH11	2:C:944:HIS:HD2	1.54	0.55
5:F:227:VAL:HG23	5:F:236:VAL:HB	1.88	0.55
5:F:554:ASN:HB2	5:F:557:ALA:HB3	1.87	0.55
10:K:101:SER:HG	10:K:104:TYR:C	2.13	0.55
15:P:337:PRO:HB3	15:P:385:VAL:HG23	1.89	0.55
16:Q:110:VAL:HG21	16:Q:134:PHE:HB3	1.89	0.55
19:T:77:ARG:HH12	19:T:81:ALA:HB2	1.71	0.55
3:D:1917:ILE:HD13	14:O:448:ALA:HB1	1.88	0.55
6:G:397:LEU:HD22	6:G:411:SER:HB2	1.89	0.55
11:L:169:ARG:NH2	21:V:13:UNK:O	2.39	0.55
15:P:84:TRP:NE1	15:P:100:LEU:HB2	2.22	0.55
15:P:149:PHE:CG	15:P:157:LYS:HB3	2.42	0.55
3:D:1781:ASP:O	3:D:1785:THR:HG23	2.06	0.55
1:A:493:LYS:HA	1:A:601:LEU:HD23	1.88	0.55
2:C:976:ALA:HB1	8:I:63:TRP:HB3	1.89	0.55
4:E:134:LEU:HB2	4:E:147:VAL:HG13	1.89	0.55
5:F:556:GLN:O	5:F:560:GLU:HG2	2.06	0.55
6:G:265:ARG:C	6:G:267:ASP:N	2.62	0.55
15:P:237:TRP:HA	15:P:253:LYS:HA	1.89	0.55
2:C:370:GLN:H	8:I:290:VAL:HG13	1.71	0.54
2:C:374:ARG:NH1	2:C:418:CYS:SG	2.80	0.54
3:D:2962:ILE:HD12	8:I:144:LEU:HD21	1.89	0.54
6:G:150:TRP:NE1	6:G:152:TYR:O	2.40	0.54
6:G:239:ASP:OD1	6:G:242:LYS:N	2.26	0.54
15:P:355:TRP:CD1	15:P:356:PRO:HD3	2.42	0.54
19:T:65:CYS:O	19:T:69:LYS:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PRO:HA	1:A:278:TRP:CD2	2.42	0.54
1:A:329:ILE:HD13	2:B:238:PRO:HA	1.89	0.54
3:D:1415:GLN:OE1	3:D:1415:GLN:N	2.37	0.54
3:D:1417:ARG:NH1	3:D:1761:PRO:O	2.40	0.54
4:E:276:TYR:CD1	4:E:302:HIS:HB3	2.43	0.54
4:E:656:THR:O	4:E:660:SER:OG	2.24	0.54
24:I:401:SQD:H311	26:M:802:Y01:HAR1	1.89	0.54
15:P:89:ASP:HB3	15:P:92:LYS:HG2	1.89	0.54
2:B:977:ILE:HG13	2:B:978:ASN:ND2	2.22	0.54
2:C:385:VAL:O	2:C:435:ASN:ND2	2.40	0.54
5:F:608:VAL:HG12	5:F:609:ALA:H	1.72	0.54
16:Q:195:GLN:HE21	16:Q:239:CYS:HA	1.73	0.54
12:M:404:HIS:HD2	12:M:410:GLN:HB3	1.72	0.54
5:F:715:GLU:OE1	5:F:717:ARG:NE	2.39	0.54
12:M:580:LEU:HD12	12:M:581:PRO:HD2	1.90	0.54
15:P:367:HIS:HD2	15:P:611:ALA:HB1	1.72	0.54
16:Q:192:ASP:OD1	16:Q:192:ASP:N	2.39	0.54
1:A:481:ASP:N	1:A:481:ASP:OD1	2.40	0.54
1:A:583:LEU:HD11	1:A:616:LEU:HD21	1.87	0.54
2:B:260:SER:O	2:B:264:VAL:HG13	2.08	0.54
2:C:456:GLN:HE22	2:C:459:ARG:HH21	1.56	0.54
2:C:755:GLU:CG	6:G:258:HIS:CD2	2.90	0.54
3:D:738:THR:HG23	15:P:470:LEU:HB3	1.89	0.54
5:F:225:GLY:O	5:F:236:VAL:N	2.29	0.54
9:J:36:ASP:N	9:J:36:ASP:OD1	2.38	0.54
12:M:646:ALA:HA	12:M:649:GLN:OE1	2.07	0.54
17:R:368:ARG:O	17:R:368:ARG:NH2	2.41	0.54
2:C:628:PHE:HB3	2:C:670:THR:HB	1.90	0.54
2:C:652:LEU:O	2:C:656:ASP:N	2.41	0.54
3:D:969:PHE:HB2	3:D:971:PRO:HG3	1.89	0.54
4:E:346:LEU:O	4:E:351:LEU:N	2.40	0.54
16:Q:242:ASP:HB3	16:Q:355:LEU:HD23	1.90	0.54
16:Q:318:LEU:HD22	16:Q:319:PRO:HD2	1.90	0.54
6:G:460:GLU:H	6:G:460:GLU:CD	2.15	0.54
11:L:172:LEU:HD12	11:L:173:LEU:HG	1.90	0.54
1:A:718:LYS:NZ	1:A:927:GLU:OE2	2.36	0.54
3:D:272:LYS:HE3	8:I:135:GLU:HG3	1.88	0.54
3:D:2827:ILE:HG13	3:D:2828:ASP:H	1.73	0.54
1:A:134:ASN:O	1:A:137:LYS:HG3	2.08	0.53
2:C:872:LYS:HG3	2:C:877:GLU:HG3	1.90	0.53
3:D:461:ASN:ND2	16:Q:174:THR:HG22	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:38:ALA:O	9:J:42:GLU:HG2	2.08	0.53
1:A:656:LEU:O	1:A:660:THR:HG22	2.07	0.53
2:B:526:TRP:CZ2	2:B:536:LYS:HG3	2.43	0.53
3:D:1696:LEU:HD23	13:N:83:LEU:HD21	1.90	0.53
16:Q:244:ASP:HA	16:Q:247:VAL:HB	1.89	0.53
3:D:1363:ILE:O	3:D:1365:SER:N	2.39	0.53
3:D:2262:GLU:OE2	3:D:2263:GLN:N	2.41	0.53
3:D:2727:LYS:HG3	3:D:2728:SER:O	2.08	0.53
3:D:2966:ASN:ND2	7:H:460:GLU:OE2	2.22	0.53
4:E:116:ILE:HG22	5:F:97:LEU:HD21	1.90	0.53
6:G:258:HIS:O	6:G:259:ALA:HB3	2.08	0.53
1:A:289:GLU:OE1	2:B:364:LYS:N	2.41	0.53
1:A:875:ARG:HB3	3:D:2185:ASN:HD21	1.74	0.53
11:L:299:LEU:HD21	15:P:246:LEU:HD23	1.90	0.53
2:B:222:HIS:HB3	2:B:225:HIS:HB3	1.90	0.53
2:B:498:MET:HA	2:B:501:VAL:HG22	1.91	0.53
2:C:793:ASP:HB2	2:C:794:PRO:HD3	1.91	0.53
6:G:295:GLU:CD	6:G:295:GLU:H	2.16	0.53
12:M:462:TRP:HB2	26:M:802:Y01:HAD2	1.89	0.53
15:P:71:GLU:HA	15:P:74:VAL:HG23	1.91	0.53
3:D:884:SER:HA	17:R:431:TYR:HE2	1.73	0.53
2:B:598:ASP:HB3	2:B:600:TYR:HE1	1.72	0.53
3:D:964:LYS:HZ2	3:D:965:LYS:H	1.55	0.53
5:F:685:GLN:HG2	5:F:686:GLN:H	1.74	0.53
7:H:198:ASP:OD1	7:H:198:ASP:N	2.42	0.53
9:J:103:ASP:OD1	9:J:104:ALA:N	2.42	0.53
1:A:647:LYS:HD3	1:A:680:ALA:HB2	1.89	0.53
1:A:696:VAL:O	1:A:700:VAL:HG13	2.09	0.53
2:C:421:VAL:O	2:C:423:PRO:HD3	2.09	0.53
6:G:251:LEU:HD21	6:G:273:PRO:HD3	1.91	0.53
12:M:353:TYR:HE2	12:M:387:ALA:HB2	1.73	0.53
15:P:236:LEU:O	15:P:254:ASP:N	2.42	0.53
3:D:457:ASN:OD1	16:Q:175:THR:HA	2.08	0.53
3:D:561:THR:HG21	15:P:373:GLU:HG2	1.90	0.53
3:D:2820:GLU:HG3	4:E:845:SER:HB3	1.91	0.53
17:R:70:PRO:HA	17:R:73:LEU:HG	1.89	0.53
1:A:279:PHE:HZ	17:R:388:VAL:HG12	1.73	0.52
4:E:61:ILE:O	4:E:147:VAL:HA	2.08	0.52
2:C:456:GLN:NE2	2:C:459:ARG:HH21	2.07	0.52
3:D:2763:ASN:OD1	3:D:2763:ASN:N	2.40	0.52
3:D:2958:SER:O	3:D:2962:ILE:HG12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:946:ASN:OD1	5:F:946:ASN:N	2.42	0.52
7:H:424:ARG:HA	7:H:427:GLU:HG2	1.91	0.52
1:A:580:GLU:O	1:A:584:LEU:HG	2.10	0.52
13:N:121:GLN:O	13:N:124:TYR:HB3	2.09	0.52
15:P:679:SER:HA	15:P:682:PHE:CD2	2.44	0.52
1:A:261:ARG:N	17:R:412:ARG:O	2.38	0.52
3:D:1259:LYS:NZ	3:D:1263:GLN:OE1	2.36	0.52
3:D:2259:LEU:HB2	3:D:2264:LEU:HD13	1.91	0.52
16:Q:108:VAL:HG23	16:Q:352:PRO:HD3	1.91	0.52
2:B:600:TYR:CE1	2:B:603:VAL:HG21	2.45	0.52
2:B:702:LYS:O	2:B:706:VAL:HG12	2.10	0.52
5:F:287:ARG:NH2	19:T:60:PRO:O	2.43	0.52
7:H:343:PRO:HD2	7:H:350:PHE:HE2	1.73	0.52
2:C:533:ASP:O	2:C:537:LYS:HG2	2.10	0.52
7:H:295:MET:HE2	7:H:300:VAL:HG22	1.92	0.52
9:J:116:GLY:HA3	10:K:118:VAL:HG11	1.91	0.52
12:M:574:GLN:HG3	12:M:580:LEU:HB3	1.91	0.52
15:P:162:ASP:OD1	15:P:162:ASP:N	2.37	0.52
1:A:586:MET:O	1:A:590:MET:HG2	2.08	0.52
2:B:535:VAL:HG11	2:B:692:MET:HE2	1.92	0.52
5:F:271:ASP:O	5:F:274:GLN:HG3	2.10	0.52
7:H:328:GLN:HG2	7:H:332:LEU:HD12	1.90	0.52
15:P:288:TYR:OH	15:P:503:ARG:O	2.28	0.52
1:A:162:ASP:HB3	22:A:1201:LMG:H111	1.92	0.52
2:B:241:PHE:HE2	18:S:126:LEU:HD22	1.75	0.52
2:B:616:ARG:NH1	2:B:654:GLN:OE1	2.38	0.52
2:C:488:ARG:HG2	3:D:2079:LEU:HD22	1.91	0.52
3:D:352:LEU:HD21	3:D:1370:SER:HB2	1.90	0.52
6:G:265:ARG:C	6:G:267:ASP:H	2.18	0.52
15:P:148:MET:SD	15:P:347:PRO:HB3	2.49	0.52
15:P:685:ALA:O	15:P:688:LEU:HB2	2.10	0.52
1:A:486:ARG:CZ	2:B:751:HIS:HB3	2.40	0.52
2:B:272:LEU:HD22	17:R:148:PRO:HB2	1.91	0.52
2:C:524:ILE:HG13	2:C:578:LYS:HB2	1.91	0.52
3:D:269:PHE:CZ	3:D:273:LEU:HD11	2.45	0.52
3:D:975:TRP:HB2	3:D:979:ARG:HH22	1.75	0.52
4:E:616:LEU:HD21	4:E:635:ALA:HB2	1.92	0.52
5:F:742:ASP:H	5:F:779:GLN:HE21	1.58	0.52
18:S:24:VAL:O	18:S:28:VAL:HG12	2.10	0.52
1:A:945:ASP:OD1	1:A:945:ASP:N	2.43	0.51
3:D:2126:GLU:HA	4:E:830:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:440:GLY:CA	4:E:611:GLY:HA2	2.40	0.51
4:E:607:PRO:HB2	4:E:611:GLY:HA3	1.92	0.51
5:F:216:ALA:O	5:F:220:GLN:HB2	2.10	0.51
11:L:158:VAL:O	11:L:162:VAL:HG23	2.09	0.51
1:A:324:ALA:HB3	2:B:231:ARG:HE	1.74	0.51
2:B:1106:GLU:OE2	2:B:1109:ARG:NH1	2.43	0.51
3:D:739:LYS:HB3	15:P:469:TYR:CE2	2.46	0.51
7:H:317:GLN:HB2	7:H:320:TYR:CD2	2.44	0.51
8:I:199:TRP:HE1	8:I:201:GLU:HB3	1.75	0.51
10:K:101:SER:OG	10:K:104:TYR:O	2.20	0.51
11:L:161:VAL:O	11:L:165:ARG:HG3	2.10	0.51
1:A:252:PRO:HG3	1:A:261:ARG:HH21	1.75	0.51
2:B:908:THR:HG23	2:B:959:GLU:OE1	2.11	0.51
2:B:1111:SER:O	2:B:1111:SER:OG	2.28	0.51
3:D:944:ARG:HA	3:D:947:ILE:HG12	1.91	0.51
8:I:65:SER:O	8:I:65:SER:OG	2.27	0.51
15:P:122:GLN:HA	15:P:125:SER:HB3	1.92	0.51
16:Q:238:LEU:HD12	16:Q:352:PRO:HG3	1.92	0.51
17:R:352:PRO:HB2	17:R:358:LEU:HD13	1.92	0.51
18:S:30:GLY:O	18:S:34:LEU:HG	2.09	0.51
1:A:966:GLU:OE1	1:A:966:GLU:N	2.42	0.51
2:B:354:MET:O	2:B:358:GLY:N	2.43	0.51
2:C:403:VAL:HG23	2:C:420:VAL:HB	1.92	0.51
2:C:458:LEU:O	2:C:461:THR:HG22	2.09	0.51
2:C:598:ASP:N	2:C:643:GLU:OE2	2.41	0.51
3:D:2068:LYS:HD2	3:D:2071:ARG:HG2	1.92	0.51
3:D:2175:ILE:O	3:D:2895:LYS:NZ	2.37	0.51
24:I:401:SQD:H342	26:M:802:Y01:HAU1	1.92	0.51
12:M:270:GLN:HA	12:M:273:VAL:HG22	1.93	0.51
16:Q:236:LEU:HD21	16:Q:347:VAL:HB	1.93	0.51
16:Q:289:ARG:HG3	16:Q:290:GLY:N	2.26	0.51
2:C:565:LEU:HB2	2:C:669:ALA:HA	1.93	0.51
3:D:794:LEU:H	5:F:134:PRO:HG2	1.76	0.51
3:D:1311:THR:OG1	3:D:1312:SER:N	2.43	0.51
3:D:2255:PRO:C	3:D:2257:THR:H	2.19	0.51
12:M:506:VAL:HG13	12:M:510:LEU:HD23	1.92	0.51
12:M:543:ASP:HB3	12:M:546:ARG:HB3	1.92	0.51
15:P:355:TRP:CG	15:P:356:PRO:HD3	2.46	0.51
15:P:544:ALA:HB1	16:Q:227:THR:O	2.10	0.51
16:Q:199:ALA:HB1	16:Q:323:VAL:HG21	1.92	0.51
16:Q:204:LYS:HB2	16:Q:209:PRO:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LEU:HG	1:A:571:GLY:H	1.75	0.51
1:A:576:SER:O	1:A:580:GLU:HG2	2.10	0.51
3:D:882:ARG:HG3	3:D:883:GLY:O	2.10	0.51
3:D:1126:ASN:HD22	3:D:1129:ASP:CG	2.18	0.51
16:Q:218:VAL:O	16:Q:323:VAL:HA	2.11	0.51
1:A:323:PRO:HG2	15:P:188:PRO:HG3	1.93	0.51
2:B:740:ARG:O	2:B:744:MET:HG3	2.10	0.51
1:A:300:ASP:OD1	1:A:300:ASP:N	2.44	0.51
2:B:430:ASP:N	2:B:430:ASP:OD1	2.43	0.51
5:F:681:PHE:C	5:F:683:ALA:H	2.18	0.51
5:F:769:ALA:HB2	5:F:777:VAL:HG22	1.92	0.51
16:Q:222:GLU:HG2	16:Q:320:LYS:HB3	1.93	0.51
2:C:524:ILE:HG22	2:C:579:ALA:HB2	1.92	0.51
2:C:552:LEU:HA	2:C:555:ARG:HB2	1.92	0.51
4:E:63:ASP:O	4:E:67:LEU:HD12	2.11	0.51
8:I:241:VAL:O	8:I:245:GLN:HG3	2.11	0.51
15:P:147:ARG:O	15:P:348:THR:HG22	2.11	0.51
16:Q:201:GLN:HA	16:Q:204:LYS:NZ	2.26	0.51
16:Q:210:THR:HG22	16:Q:211:ARG:H	1.74	0.51
1:A:1028:ASP:OD1	1:A:1028:ASP:N	2.43	0.51
2:B:241:PHE:CE1	15:P:176:LEU:HD21	2.46	0.51
2:B:831:LEU:HD21	3:D:2770:LYS:HG3	1.92	0.51
2:C:529:ILE:HB	2:C:532:ILE:HG12	1.92	0.51
4:E:872:LYS:HD2	4:E:935:MET:HB3	1.91	0.51
5:F:135:ARG:HD2	5:F:157:PRO:O	2.11	0.51
5:F:982:ASP:HA	5:F:985:THR:HG22	1.93	0.51
6:G:316:ASP:OD2	6:G:355:THR:OG1	2.28	0.51
8:I:199:TRP:CG	10:K:232:LYS:HZ1	2.29	0.51
15:P:255:TRP:CE3	15:P:305:LEU:HG	2.45	0.51
16:Q:226:VAL:HG12	16:Q:235:PRO:HD3	1.92	0.51
2:B:535:VAL:HG12	2:B:690:ILE:CG2	2.41	0.50
2:B:541:GLU:OE2	2:B:688:ARG:NH1	2.44	0.50
3:D:1326:HIS:CD2	17:R:225:MET:HE3	2.43	0.50
3:D:2022:PRO:HG3	3:D:2342:ASN:HB2	1.92	0.50
3:D:2352:THR:O	3:D:2356:GLU:HG2	2.11	0.50
5:F:613:SER:O	5:F:647:ILE:HA	2.11	0.50
5:F:879:GLU:HB2	5:F:887:LEU:HD21	1.92	0.50
6:G:239:ASP:OD1	6:G:241:LEU:N	2.44	0.50
2:B:214:HIS:HB3	2:B:216:GLN:HE22	1.75	0.50
4:E:646:LEU:O	4:E:650:VAL:HG23	2.11	0.50
7:H:321:MET:HE1	7:H:352:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:430:ASP:HA	2:C:433:VAL:HG12	1.92	0.50
2:C:444:THR:OG1	2:C:446:ASP:OD1	2.28	0.50
3:D:1414:SER:HB2	3:D:1763:THR:HG23	1.93	0.50
7:H:401:ARG:O	7:H:405:ILE:HG12	2.11	0.50
16:Q:320:LYS:NZ	16:Q:322:GLU:OE1	2.31	0.50
2:B:837:PHE:HB3	3:D:2783:LEU:HD23	1.93	0.50
3:D:58:ILE:O	3:D:61:TYR:HB3	2.11	0.50
15:P:320:TRP:CZ3	28:P:701:A1LXL:C02	2.94	0.50
2:B:563:VAL:HG13	2:B:688:ARG:HB2	1.92	0.50
3:D:973:PRO:HB3	3:D:975:TRP:CD1	2.46	0.50
4:E:893:ILE:O	4:E:897:SER:OG	2.29	0.50
10:K:230:LEU:HD21	10:K:236:VAL:HA	1.94	0.50
1:A:1125:ASP:N	1:A:1125:ASP:OD1	2.45	0.50
2:C:643:GLU:O	2:C:647:ILE:HG12	2.12	0.50
5:F:779:GLN:O	5:F:783:THR:HG23	2.12	0.50
12:M:423:LEU:HD11	12:M:637:ILE:HG12	1.93	0.50
1:A:477:MET:HG2	1:A:491:CYS:SG	2.51	0.50
1:A:586:MET:HE2	1:A:590:MET:SD	2.51	0.50
2:B:510:PRO:HG2	2:B:596:PHE:CE2	2.47	0.50
3:D:618:PRO:HB2	15:P:173:LEU:HD21	1.93	0.50
3:D:620:ASN:OD1	3:D:620:ASN:N	2.44	0.50
3:D:2366:ASN:HB2	3:D:2369:LYS:HG3	1.93	0.50
2:C:765:LYS:HG2	3:D:2149:PHE:HE1	1.76	0.50
3:D:894:LEU:HD13	3:D:975:TRP:HZ3	1.77	0.50
3:D:2668:ARG:HG2	3:D:2670:LEU:HD13	1.94	0.50
4:E:141:PRO:C	4:E:142:THR:HG1	2.17	0.50
8:I:350:ARG:HD2	8:I:364:MET:HE2	1.94	0.50
12:M:419:THR:HG22	12:M:420:LYS:H	1.75	0.50
3:D:2140:HIS:HD2	3:D:2144:HIS:ND1	2.10	0.50
5:F:675:LEU:O	5:F:709:ARG:NH2	2.45	0.50
15:P:77:ALA:HA	15:P:80:ASP:HB2	1.94	0.50
18:S:90:ALA:HA	18:S:93:ASN:HD21	1.77	0.50
3:D:630:ASN:ND2	3:D:742:LEU:HD13	2.26	0.49
4:E:93:MET:HE1	5:F:95:PRO:HD2	1.92	0.49
4:E:215:GLY:H	4:E:332:GLN:HE21	1.60	0.49
12:M:268:GLU:HA	12:M:271:LYS:HG2	1.92	0.49
15:P:70:ASP:O	15:P:72:ALA:N	2.44	0.49
15:P:135:LEU:O	15:P:139:VAL:HG12	2.11	0.49
1:A:640:LEU:HB3	1:A:657:LEU:HD22	1.94	0.49
2:C:819:ASP:OD1	6:G:134:ARG:NH1	2.44	0.49
3:D:452:ILE:HA	3:D:455:CYS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1955:TYR:O	3:D:1972:PHE:HA	2.11	0.49
12:M:444:VAL:HA	12:M:449:ILE:HD11	1.93	0.49
16:Q:182:LEU:HD12	16:Q:185:ILE:H	1.77	0.49
16:Q:195:GLN:NE2	16:Q:241:GLU:OE2	2.45	0.49
2:B:241:PHE:CZ	15:P:172:GLU:HB3	2.47	0.49
2:B:751:HIS:CD2	2:B:751:HIS:H	2.29	0.49
2:C:526:TRP:CZ2	2:C:536:LYS:HE2	2.48	0.49
2:C:535:VAL:HA	2:C:690:ILE:HD11	1.93	0.49
3:D:739:LYS:HB3	15:P:469:TYR:CD2	2.47	0.49
3:D:2677:VAL:N	3:D:2678:PRO:HD3	2.27	0.49
5:F:727:ALA:HA	5:F:730:VAL:HG12	1.94	0.49
7:H:187:LEU:HD23	7:H:276:VAL:HG21	1.94	0.49
15:P:514:THR:O	15:P:524:HIS:NE2	2.45	0.49
1:A:530:GLU:OE2	1:A:539:ARG:NH2	2.45	0.49
1:A:568:SER:OG	1:A:569:THR:N	2.45	0.49
2:B:700:ARG:O	2:B:703:ILE:HG22	2.13	0.49
3:D:1770:GLU:O	3:D:1773:THR:HG22	2.12	0.49
16:Q:269:TYR:CG	16:Q:303:LEU:HD22	2.48	0.49
2:B:696:ASP:N	2:B:696:ASP:OD1	2.45	0.49
2:C:793:ASP:H	8:I:93:GLY:HA3	1.77	0.49
3:D:473:ASN:ND2	15:P:647:THR:HB	2.28	0.49
3:D:2061:ARG:HH21	3:D:2063:PHE:HD2	1.60	0.49
4:E:190:TRP:CZ3	17:R:357:GLN:HB2	2.47	0.49
17:R:229:VAL:O	17:R:232:MET:N	2.43	0.49
17:R:240:PRO:HD2	17:R:243:LEU:HD12	1.95	0.49
1:A:308:GLN:NE2	2:B:425:ASP:OD1	2.39	0.49
3:D:895:PHE:HD2	18:S:103:VAL:HG11	1.77	0.49
3:D:983:ASN:O	3:D:987:GLU:HG2	2.12	0.49
17:R:56:HIS:CD2	17:R:317:SER:HB3	2.48	0.49
2:C:765:LYS:HG2	3:D:2149:PHE:CE1	2.48	0.49
6:G:182:ARG:CB	6:G:491:LEU:HB2	2.42	0.49
7:H:421:LYS:O	7:H:424:ARG:HG3	2.11	0.49
13:N:37:ASP:HB2	13:N:40:LYS:HB2	1.94	0.49
15:P:681:ILE:HD12	15:P:681:ILE:H	1.77	0.49
1:A:737:GLY:HA3	1:A:801:HIS:HE1	1.77	0.49
7:H:343:PRO:HD2	7:H:350:PHE:CE2	2.48	0.49
13:N:126:ASP:HA	13:N:129:ALA:HB3	1.95	0.49
15:P:477:GLN:HB3	15:P:480:LEU:HD12	1.95	0.49
1:A:744:VAL:HB	1:A:929:ILE:HG22	1.95	0.49
3:D:59:THR:O	3:D:61:TYR:N	2.45	0.49
4:E:124:GLU:N	4:E:124:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:130:HIS:O	4:E:150:ALA:HA	2.13	0.49
1:A:909:GLN:HE21	1:A:946:LEU:HD21	1.78	0.49
2:B:900:MET:HG2	2:B:913:LEU:HD12	1.95	0.49
3:D:2275:ARG:HH11	3:D:2275:ARG:HB2	1.78	0.49
8:I:208:LEU:HD21	10:K:221:LEU:HD23	1.94	0.49
15:P:105:LEU:HD21	15:P:116:THR:HG23	1.94	0.49
17:R:7:ARG:O	17:R:7:ARG:NE	2.46	0.49
1:A:332:TYR:HA	1:A:335:GLN:NE2	2.28	0.48
2:B:453:LEU:HD23	2:B:454:LEU:HD23	1.95	0.48
2:C:368:ARG:NH2	8:I:303:SER:O	2.46	0.48
3:D:1243:ASN:HA	3:D:1325:PHE:CD2	2.48	0.48
5:F:629:ARG:HA	5:F:632:ASP:OD2	2.13	0.48
5:F:741:ILE:HA	5:F:779:GLN:HE21	1.78	0.48
2:B:475:HIS:CE1	2:B:476:THR:HG23	2.48	0.48
2:B:600:TYR:CD1	2:B:603:VAL:HG21	2.48	0.48
3:D:1371:ILE:HD13	3:D:1395:LEU:HD22	1.95	0.48
3:D:2269:ARG:NH1	3:D:2272:TYR:OH	2.46	0.48
1:A:715:SER:HB2	1:A:717:ALA:H	1.78	0.48
2:B:812:LEU:HD22	2:B:975:LEU:HD23	1.94	0.48
4:E:210:ASP:HB2	4:E:317:THR:O	2.12	0.48
6:G:250:TYR:O	6:G:252:ALA:N	2.46	0.48
16:Q:255:ASN:ND2	16:Q:314:GLU:HG2	2.28	0.48
2:B:595:ASP:O	2:B:607:ARG:NH2	2.47	0.48
8:I:98:ARG:H	8:I:98:ARG:HG2	1.45	0.48
12:M:404:HIS:CD2	12:M:410:GLN:HB3	2.47	0.48
17:R:317:SER:OG	17:R:317:SER:O	2.30	0.48
1:A:465:GLU:HA	1:A:468:VAL:HG22	1.95	0.48
2:B:659:GLU:OE2	8:I:363:GLN:HG2	2.13	0.48
2:B:1087:TRP:HA	2:B:1087:TRP:CE3	2.48	0.48
2:C:828:VAL:HG13	2:C:989:LEU:HD22	1.95	0.48
3:D:1415:GLN:HE21	17:R:38:GLU:CD	2.21	0.48
4:E:440:GLY:HA3	4:E:611:GLY:HA2	1.94	0.48
9:J:40:VAL:O	9:J:44:VAL:HG23	2.13	0.48
2:B:526:TRP:CH2	2:B:539:ILE:HD11	2.48	0.48
3:D:898:GLN:HE22	3:D:975:TRP:CD1	2.32	0.48
3:D:1325:PHE:O	3:D:1327:ASN:N	2.47	0.48
5:F:784:LEU:O	5:F:787:GLU:HG3	2.13	0.48
6:G:254:THR:O	6:G:255:THR:C	2.57	0.48
6:G:260:SER:O	6:G:268:ARG:NH2	2.46	0.48
17:R:203:ARG:NH2	19:T:41:LYS:HA	2.29	0.48
17:R:425:GLU:H	17:R:425:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:HIS:O	2:B:226:VAL:HG12	2.13	0.48
3:D:1443:ASN:HA	3:D:1446:GLN:HB2	1.96	0.48
6:G:297:LEU:O	6:G:301:VAL:HG13	2.13	0.48
6:G:459:PRO:HD2	6:G:462:TRP:CE3	2.47	0.48
17:R:141:TYR:CZ	17:R:214:LEU:HD12	2.48	0.48
2:B:497:GLU:O	2:B:501:VAL:HG13	2.14	0.48
2:B:826:VAL:HG22	2:B:838:THR:HG23	1.96	0.48
2:C:625:ILE:HD12	2:C:631:MET:HE1	1.94	0.48
2:C:902:MET:HG2	4:E:780:ALA:HB2	1.95	0.48
3:D:900:MET:HG3	18:S:104:VAL:HG21	1.95	0.48
3:D:1182:TRP:HE3	3:D:1230:LEU:HD22	1.77	0.48
3:D:2033:ASN:OD1	3:D:2033:ASN:N	2.47	0.48
5:F:587:LEU:HD22	5:F:714:ILE:HD11	1.95	0.48
19:T:77:ARG:NH1	19:T:81:ALA:HB2	2.28	0.48
1:A:481:ASP:C	1:A:483:ALA:H	2.22	0.48
2:C:1080:ASP:OD1	2:C:1080:ASP:N	2.44	0.48
2:B:271:ILE:HD11	3:D:1310:MET:HE1	1.95	0.48
5:F:696:ARG:HB3	5:F:699:VAL:HG23	1.96	0.48
15:P:555:LEU:HD13	16:Q:344:TRP:CE3	2.48	0.48
1:A:1114:ALA:HB2	2:B:1013:PRO:HB2	1.96	0.47
2:C:542:ILE:HD13	2:C:560:ILE:HG21	1.96	0.47
2:C:824:ALA:O	6:G:259:ALA:HB1	2.14	0.47
3:D:547:LEU:HD12	3:D:548:TYR:H	1.79	0.47
3:D:1776:TRP:HZ3	17:R:17:LEU:HD13	1.79	0.47
24:I:401:SQD:H131	24:I:401:SQD:H101	1.50	0.47
2:B:996:THR:O	2:B:1000:VAL:HG23	2.14	0.47
2:C:395:PHE:CZ	4:E:256:PRO:HG2	2.49	0.47
2:C:638:GLN:HG3	2:C:640:SER:HB3	1.95	0.47
5:F:112:SER:O	5:F:116:VAL:HG23	2.14	0.47
7:H:416:GLN:HB3	7:H:444:PHE:CZ	2.49	0.47
7:H:445:ASP:OD1	7:H:446:PHE:N	2.47	0.47
9:J:72:4HH:HP3	9:J:72:4HH:HS2	1.65	0.47
13:N:113:ARG:NE	14:O:470:ARG:HH12	2.11	0.47
16:Q:326:PHE:O	16:Q:330:VAL:HG23	2.14	0.47
17:R:390:LYS:HZ2	17:R:392:PRO:HB3	1.78	0.47
2:B:401:ASN:OD1	2:B:401:ASN:N	2.44	0.47
2:B:403:VAL:HG13	2:B:422:LEU:HD11	1.94	0.47
2:C:496:ARG:HH22	13:N:136:LEU:HD23	1.80	0.47
2:C:798:GLN:NE2	8:I:81:GLU:O	2.47	0.47
3:D:334:TYR:O	3:D:338:PRO:HD2	2.14	0.47
3:D:566:LEU:H	15:P:268:GLN:HE22	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:616:SER:O	3:D:616:SER:OG	2.31	0.47
3:D:963:GLN:O	3:D:964:LYS:HB2	2.14	0.47
5:F:911:SER:OG	5:F:912:SER:N	2.47	0.47
19:T:61:SER:OG	19:T:62:GLN:N	2.47	0.47
1:A:1143:ASP:OD1	1:A:1161:PRO:HD3	2.13	0.47
6:G:128:ALA:O	6:G:222:ARG:NH2	2.44	0.47
8:I:218:TRP:HH2	26:M:802:Y01:HAM1	1.79	0.47
15:P:517:ASN:HD21	15:P:519:GLU:HG2	1.79	0.47
19:T:67:ALA:O	19:T:71:VAL:HG13	2.14	0.47
1:A:442:MET:HE2	1:A:517:GLU:HA	1.96	0.47
5:F:550:ASP:N	5:F:550:ASP:OD1	2.47	0.47
6:G:184:VAL:O	6:G:303:ARG:NE	2.41	0.47
7:H:192:ARG:O	7:H:196:ASP:HB3	2.15	0.47
15:P:302:THR:HA	15:P:445:VAL:O	2.15	0.47
15:P:657:GLY:O	15:P:686:ARG:NH2	2.48	0.47
1:A:588:VAL:O	1:A:592:GLY:N	2.47	0.47
1:A:1073:ARG:NH1	1:A:1092:PRO:O	2.47	0.47
2:C:1062:ALA:HA	2:C:1065:LYS:HE3	1.96	0.47
3:D:1669:SER:HB3	13:N:117:MET:HG2	1.97	0.47
4:E:645:ASP:OD1	4:E:645:ASP:N	2.47	0.47
15:P:402:ALA:HB2	15:P:479:ALA:HB3	1.97	0.47
1:A:714:ASP:N	1:A:714:ASP:OD1	2.48	0.47
2:B:259:ASN:ND2	3:D:1251:ARG:HH22	2.13	0.47
2:B:566:ALA:HA	2:B:670:THR:O	2.14	0.47
2:B:1091:MET:HE1	2:C:1073:TYR:HB3	1.96	0.47
2:C:378:TYR:CZ	2:C:423:PRO:HD2	2.50	0.47
2:C:435:ASN:OD1	2:C:435:ASN:N	2.48	0.47
3:D:450:ILE:H	3:D:450:ILE:HD12	1.80	0.47
3:D:961:ARG:HE	3:D:961:ARG:HB2	1.56	0.47
3:D:1292:PHE:CE1	18:S:83:LEU:HD11	2.50	0.47
5:F:288:GLU:HA	5:F:291:VAL:HG12	1.97	0.47
7:H:463:TYR:CD2	8:I:115:MET:HE1	2.49	0.47
25:L:3001:DGA:HA22	25:L:3001:DGA:HB21	1.96	0.47
15:P:100:LEU:HA	15:P:104:GLU:OE1	2.14	0.47
15:P:257:LEU:HA	15:P:305:LEU:HA	1.96	0.47
15:P:562:GLU:HG2	15:P:643:MET:HE1	1.97	0.47
16:Q:333:MET:SD	16:Q:344:TRP:HB3	2.54	0.47
1:A:721:LEU:HD22	5:F:856:THR:HB	1.95	0.47
1:A:747:TRP:CD1	1:A:749:GLY:H	2.33	0.47
2:B:243:GLU:O	2:B:246:ARG:HG2	2.15	0.47
5:F:225:GLY:N	5:F:236:VAL:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:250:ALA:O	16:Q:253:GLN:HG2	2.15	0.47
16:Q:326:PHE:HA	16:Q:329:VAL:HG22	1.96	0.47
1:A:332:TYR:HD1	1:A:335:GLN:HE22	1.63	0.47
1:A:588:VAL:HA	1:A:591:ASP:HB2	1.97	0.47
1:A:693:LEU:HA	1:A:696:VAL:HG12	1.96	0.47
1:A:1088:PRO:C	1:A:1090:PHE:H	2.23	0.47
2:C:559:ARG:NE	2:C:661:ASN:HB3	2.29	0.47
3:D:743:ASN:OD1	15:P:468:SER:OG	2.31	0.47
3:D:2777:LEU:O	3:D:2779:THR:N	2.42	0.47
4:E:277:SER:OG	4:E:279:GLU:OE2	2.24	0.47
4:E:351:LEU:C	4:E:353:GLU:N	2.73	0.47
5:F:632:ASP:OD1	5:F:633:LEU:N	2.48	0.47
5:F:645:ILE:HB	5:F:690:VAL:HG13	1.97	0.47
5:F:681:PHE:HD1	5:F:682:GLU:H	1.62	0.47
15:P:118:LYS:O	15:P:122:GLN:HG2	2.15	0.47
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.75	0.47
2:C:485:LYS:HD2	2:C:488:ARG:NH2	2.29	0.47
3:D:545:SER:HA	15:P:228:TRP:CE3	2.50	0.47
3:D:2250:ILE:HG13	3:D:2715:ARG:HD3	1.97	0.47
3:D:2504:SER:OG	3:D:2508:LYS:NZ	2.48	0.47
5:F:834:ILE:HG23	5:F:988:LEU:HD22	1.96	0.47
5:F:862:ARG:O	5:F:866:GLU:HG2	2.15	0.47
7:H:269:ASP:OD1	7:H:269:ASP:N	2.48	0.47
8:I:310:THR:HG22	27:I:403:DGD:O2E	2.14	0.47
12:M:538:GLU:HG3	12:M:542:TRP:HB3	1.97	0.47
14:O:390:SER:O	14:O:394:TYR:N	2.41	0.47
15:P:68:ARG:H	15:P:348:THR:HG21	1.75	0.47
1:A:641:ARG:HH21	1:A:654:GLN:HG3	1.80	0.46
2:B:615:LEU:HD11	2:B:623:LEU:HB2	1.97	0.46
4:E:244:LEU:O	17:R:342:LYS:NZ	2.48	0.46
7:H:212:TRP:O	7:H:249:ASN:ND2	2.48	0.46
1:A:1108:PRO:O	3:D:2606:SER:OG	2.32	0.46
2:B:949:SER:OG	3:D:2899:GLU:OE1	2.32	0.46
3:D:953:ALA:HA	3:D:956:GLN:CD	2.40	0.46
5:F:199:SER:OG	5:F:200:TYR:N	2.48	0.46
6:G:345:LEU:HD12	6:G:345:LEU:HA	1.79	0.46
6:G:448:LEU:HA	6:G:451:THR:HG22	1.97	0.46
16:Q:312:SER:HA	16:Q:315:ARG:HB2	1.96	0.46
2:C:510:PRO:HA	2:C:512:ARG:HH11	1.81	0.46
2:C:525:LYS:NZ	2:C:527:ASP:HB2	2.28	0.46
3:D:2335:ASP:OD1	3:D:2335:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:244:LEU:HG	17:R:343:TYR:CE1	2.50	0.46
15:P:127:LEU:HD21	15:P:135:LEU:HD23	1.97	0.46
15:P:138:LEU:HA	15:P:141:GLN:HE22	1.80	0.46
15:P:236:LEU:HD22	15:P:254:ASP:HB2	1.97	0.46
15:P:304:VAL:HG22	15:P:444:TRP:CG	2.50	0.46
2:B:708:ALA:HB1	2:B:713:VAL:HG11	1.98	0.46
3:D:910:LYS:HG3	3:D:921:LYS:HG3	1.96	0.46
3:D:988:ARG:NH1	17:R:141:TYR:HB2	2.30	0.46
2:B:661:ASN:HB3	2:B:664:ILE:HB	1.98	0.46
2:B:701:ALA:O	2:B:705:GLN:HG3	2.16	0.46
2:C:524:ILE:HG21	2:C:575:LEU:O	2.16	0.46
2:C:813:LEU:HG	2:C:866:ALA:HB2	1.98	0.46
3:D:64:MET:SD	3:D:64:MET:N	2.86	0.46
3:D:1335:ILE:O	3:D:1339:VAL:HG23	2.16	0.46
4:E:291:LYS:HA	4:E:291:LYS:HD3	1.65	0.46
4:E:754:LEU:HD23	4:E:793:TYR:HD2	1.80	0.46
5:F:144:PRO:HB3	5:F:148:LEU:HD12	1.98	0.46
15:P:159:SER:OG	15:P:162:ASP:OD1	2.32	0.46
3:D:2069:LEU:O	3:D:2073:VAL:HG13	2.14	0.46
3:D:2073:VAL:O	3:D:2077:ILE:HG12	2.16	0.46
5:F:273:TYR:CZ	19:T:76:LYS:HE2	2.50	0.46
5:F:753:MET:HE2	5:F:757:GLN:HB3	1.98	0.46
12:M:587:ALA:O	12:M:590:ALA:HB3	2.15	0.46
15:P:325:GLY:O	15:P:329:GLN:HG2	2.16	0.46
16:Q:234:VAL:HB	16:Q:347:VAL:HG12	1.98	0.46
1:A:890:LYS:HD2	1:A:1148:ASP:HA	1.97	0.46
2:B:261:ARG:O	2:B:264:VAL:HG22	2.16	0.46
5:F:616:ALA:HA	5:F:619:ILE:HG12	1.96	0.46
14:O:447:PHE:O	14:O:451:THR:HG23	2.16	0.46
17:R:60:ARG:NH2	17:R:67:MET:HG3	2.30	0.46
17:R:248:THR:OG1	17:R:259:THR:HG22	2.15	0.46
1:A:444:LYS:HB2	1:A:444:LYS:HE2	1.58	0.46
1:A:745:THR:HG22	1:A:747:TRP:H	1.79	0.46
3:D:2327:ALA:O	3:D:2333:ARG:NE	2.48	0.46
3:D:2422:VAL:HG21	7:H:148:ILE:HD13	1.96	0.46
3:D:2631:LEU:HD12	3:D:2636:LEU:HD13	1.97	0.46
4:E:777:ASN:O	4:E:780:ALA:HB3	2.16	0.46
17:R:154:TYR:O	17:R:158:LEU:HB2	2.15	0.46
19:T:63:ALA:HA	19:T:66:GLU:OE2	2.16	0.46
1:A:930:THR:HG23	1:A:933:ARG:H	1.81	0.46
3:D:951:ARG:NH2	17:R:167:TPO:HB	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1729:LYS:HB2	3:D:1730:MET:SD	2.56	0.46
3:D:2969:LYS:HB2	3:D:2969:LYS:HE2	1.55	0.46
12:M:340:TRP:H	12:M:340:TRP:CD1	2.33	0.46
15:P:422:TRP:HB3	15:P:424:LEU:HD23	1.98	0.46
17:R:133:GLY:HA2	17:R:136:GLU:OE1	2.15	0.46
17:R:436:GLN:O	17:R:439:GLN:HG3	2.16	0.46
2:B:393:VAL:HG21	2:B:432:LEU:HD13	1.98	0.46
2:B:579:ALA:O	2:B:583:GLU:HG2	2.16	0.46
2:B:843:ASP:OD1	2:B:844:GLU:N	2.49	0.46
2:B:965:ASP:OD1	2:B:966:ALA:N	2.48	0.46
3:D:557:LEU:HD12	3:D:560:ILE:HB	1.98	0.46
3:D:885:LYS:NZ	17:R:413:ASP:OD2	2.33	0.46
6:G:241:LEU:HB2	6:G:242:LYS:HD3	1.97	0.46
15:P:409:LEU:HB3	15:P:410:PRO:HD3	1.97	0.46
15:P:601:ARG:HG2	15:P:602:ALA:N	2.31	0.46
16:Q:214:ILE:O	16:Q:325:SER:HB2	2.16	0.46
16:Q:224:LEU:HD21	16:Q:235:PRO:HG2	1.98	0.46
3:D:811:ASN:OD1	3:D:811:ASN:N	2.48	0.45
3:D:2632:LEU:C	3:D:2634:LYS:N	2.73	0.45
3:D:2922:GLU:OE2	7:H:208:LYS:NZ	2.49	0.45
4:E:499:GLN:HA	4:E:533:PHE:O	2.16	0.45
4:E:976:LYS:HD2	4:E:979:ALA:HB3	1.98	0.45
5:F:572:GLU:O	5:F:575:LYS:HE2	2.16	0.45
5:F:750:MET:HB2	5:F:753:MET:SD	2.56	0.45
8:I:241:VAL:HB	12:M:498:SER:HB2	1.98	0.45
12:M:554:THR:OG1	12:M:572:LEU:HD23	2.16	0.45
15:P:612:GLU:HA	15:P:615:GLU:HB2	1.97	0.45
1:A:1119:TRP:CE2	3:D:2640:ALA:HB3	2.52	0.45
2:B:831:LEU:HD11	3:D:2770:LYS:HG3	1.99	0.45
2:C:438:VAL:HG22	2:C:440:ASP:OD1	2.17	0.45
2:C:734:VAL:O	2:C:738:MET:HG2	2.16	0.45
3:D:974:VAL:HG11	17:R:194:LYS:HG3	1.98	0.45
3:D:1746:ARG:HD3	3:D:1746:ARG:HA	1.77	0.45
3:D:1761:PRO:HD3	14:O:471:ALA:HB3	1.99	0.45
4:E:729:LYS:HB2	4:E:729:LYS:HE3	1.53	0.45
5:F:911:SER:O	5:F:917:GLN:HG3	2.16	0.45
7:H:344:GLU:H	7:H:344:GLU:CD	2.24	0.45
12:M:452:PHE:CE2	12:M:518:PHE:HB2	2.51	0.45
2:B:702:LYS:HA	2:B:702:LYS:HD3	1.76	0.45
3:D:2883:ASN:HA	3:D:2886:SER:O	2.16	0.45
4:E:75:PRO:HD3	5:F:245:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:88:ALA:HA	4:E:91:LYS:HG2	1.97	0.45
7:H:93:MET:O	7:H:96:VAL:HG22	2.15	0.45
7:H:254:SER:OG	7:H:255:LYS:N	2.50	0.45
8:I:78:ALA:O	8:I:80:ALA:N	2.49	0.45
15:P:58:LEU:HD23	15:P:58:LEU:HA	1.82	0.45
2:B:539:ILE:O	2:B:543:ILE:HG13	2.16	0.45
2:B:608:VAL:HA	2:B:611:THR:HG22	1.98	0.45
2:B:793:ASP:OD2	2:B:800:ARG:NH1	2.49	0.45
3:D:951:ARG:O	3:D:955:LYS:HG2	2.16	0.45
3:D:1228:ILE:HG22	17:R:271:ASP:HB3	1.98	0.45
3:D:1310:MET:HG3	3:D:1311:THR:HG22	1.98	0.45
5:F:906:MET:SD	5:F:911:SER:HB2	2.57	0.45
7:H:309:PRO:HG3	7:H:314:LEU:HG	1.99	0.45
8:I:143:PRO:O	8:I:147:MET:HG3	2.16	0.45
10:K:132:PRO:C	10:K:134:ALA:H	2.24	0.45
22:M:801:LMG:O5	22:M:801:LMG:O4	2.27	0.45
15:P:83:GLY:C	15:P:117:TRP:HB2	2.41	0.45
15:P:638:PRO:O	15:P:641:VAL:HG22	2.16	0.45
1:A:856:LEU:HD13	1:A:1136:LEU:HD12	1.99	0.45
2:C:694:LEU:HD23	2:C:694:LEU:HA	1.82	0.45
3:D:1308:ASN:HB2	3:D:1316:VAL:HG11	1.98	0.45
5:F:626:GLY:O	5:F:630:VAL:HG23	2.17	0.45
6:G:316:ASP:O	6:G:320:VAL:HG22	2.15	0.45
6:G:319:HIS:CE1	6:G:352:VAL:HG13	2.51	0.45
11:L:169:ARG:HD2	21:V:14:UNK:HA	1.98	0.45
15:P:242:THR:HG22	15:P:250:ASP:CG	2.42	0.45
15:P:313:LEU:H	15:P:313:LEU:HD23	1.81	0.45
16:Q:200:LEU:HA	16:Q:203:TYR:HB2	1.97	0.45
1:A:333:ARG:HB3	17:R:387:VAL:O	2.17	0.45
2:B:243:GLU:H	2:B:243:GLU:HG2	1.53	0.45
12:M:313:VAL:HA	12:M:316:VAL:HG12	1.98	0.45
12:M:373:PRO:HA	12:M:376:GLN:HG2	1.99	0.45
15:P:277:ARG:HB2	15:P:282:VAL:HG23	1.98	0.45
1:A:258:ALA:O	1:A:260:ASN:N	2.48	0.45
2:B:600:TYR:HD1	2:B:600:TYR:H	1.64	0.45
2:B:670:THR:HG22	2:B:672:ARG:H	1.82	0.45
2:C:578:LYS:O	2:C:582:ALA:N	2.50	0.45
3:D:976:LEU:HG	3:D:977:ARG:N	2.31	0.45
3:D:1922:GLU:HA	3:D:1925:PHE:CZ	2.51	0.45
4:E:751:ARG:HD2	4:E:799:PHE:HB3	1.99	0.45
5:F:121:ARG:NE	17:R:363:GLU:OE2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:199:TRP:CZ3	8:I:204:PRO:HB3	2.51	0.45
10:K:238:LEU:HD23	10:K:238:LEU:HA	1.74	0.45
11:L:216:GLU:OE1	11:L:216:GLU:N	2.39	0.45
16:Q:289:ARG:HG3	16:Q:290:GLY:H	1.82	0.45
1:A:457:ARG:HD2	1:A:515:GLU:HG3	1.98	0.45
2:B:258:ARG:HD3	2:B:360:ALA:HA	1.99	0.45
2:B:357:PHE:HB2	3:D:891:LEU:HD13	1.99	0.45
2:B:514:VAL:HG12	2:B:588:MET:HB3	1.99	0.45
2:C:880:MET:HB3	2:C:880:MET:HE2	1.75	0.45
3:D:1303:LYS:HD3	3:D:1303:LYS:HA	1.66	0.45
3:D:2252:GLU:HG2	3:D:2253:GLU:H	1.82	0.45
15:P:506:LEU:C	15:P:509:PRO:HD2	2.41	0.45
15:P:576:ALA:HA	15:P:628:VAL:HG21	1.98	0.45
1:A:466:PHE:O	1:A:470:GLU:HG2	2.17	0.45
2:C:645:ALA:O	2:C:648:ILE:HG13	2.16	0.45
3:D:975:TRP:O	3:D:979:ARG:HG2	2.16	0.45
4:E:115:ARG:NH2	4:E:125:ASP:OD1	2.50	0.45
4:E:828:LYS:HE3	4:E:828:LYS:HB3	1.77	0.45
5:F:586:LEU:HD23	5:F:586:LEU:HA	1.81	0.45
6:G:262:SER:HB2	6:G:399:PHE:HZ	1.82	0.45
8:I:235:SER:CB	8:I:244:VAL:HB	2.47	0.45
12:M:637:ILE:HA	12:M:640:ASP:OD2	2.17	0.45
1:A:300:ASP:OD1	17:R:68:THR:OG1	2.35	0.45
1:A:527:GLU:O	1:A:539:ARG:NH1	2.50	0.45
1:A:561:ASP:OD1	1:A:561:ASP:N	2.50	0.45
2:B:726:MET:HB3	2:B:726:MET:HE2	1.74	0.45
2:C:774:SER:OG	2:C:775:THR:N	2.50	0.45
3:D:325:GLN:O	3:D:326:LEU:HB2	2.16	0.45
3:D:2410:MET:HE2	3:D:2410:MET:HB3	1.78	0.45
4:E:898:ASP:OD1	4:E:898:ASP:N	2.48	0.45
14:O:292:VAL:O	15:P:500:ALA:HB1	2.17	0.45
15:P:570:ARG:HA	15:P:573:MET:HB2	1.99	0.45
1:A:133:LYS:HA	1:A:133:LYS:HD2	1.80	0.44
1:A:176:ASN:C	1:A:176:ASN:HD22	2.25	0.44
2:B:616:ARG:HA	2:B:664:ILE:HD11	1.99	0.44
3:D:51:THR:O	3:D:55:GLU:HG2	2.16	0.44
3:D:469:LEU:HD21	16:Q:332:ARG:HG2	1.99	0.44
3:D:2016:ASN:HB3	3:D:2334:LEU:HD23	1.99	0.44
3:D:2255:PRO:O	3:D:2256:TRP:HB2	2.17	0.44
4:E:105:HIS:ND1	4:E:107:LYS:HG2	2.31	0.44
4:E:159:LEU:HD22	5:F:177:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:164:GLN:HE21	4:E:164:GLN:HB3	1.42	0.44
5:F:608:VAL:HG11	5:F:642:PRO:HG2	1.98	0.44
15:P:495:ASP:O	15:P:498:LEU:HD23	2.17	0.44
19:T:42:LYS:HG2	19:T:48:GLU:HG3	1.99	0.44
19:T:99:ARG:O	19:T:103:LEU:HD12	2.16	0.44
2:B:543:ILE:O	2:B:547:ARG:HG3	2.18	0.44
3:D:979:ARG:HA	3:D:982:LEU:HD12	1.99	0.44
3:D:1296:ILE:O	3:D:1300:VAL:HG22	2.17	0.44
3:D:1981:PHE:CD2	3:D:2043:GLU:HG3	2.52	0.44
3:D:2325:ASP:OD1	3:D:2325:ASP:N	2.42	0.44
3:D:2348:ILE:HD12	8:I:96:MET:HG2	2.00	0.44
4:E:165:GLU:CD	4:E:205:GLN:HE22	2.25	0.44
6:G:111:ASP:OD1	6:G:111:ASP:N	2.49	0.44
19:T:107:PRO:O	19:T:111:THR:HG22	2.18	0.44
1:A:450:LYS:HG3	1:A:451:MET:N	2.32	0.44
2:B:475:HIS:HB3	17:R:34:ILE:HG21	1.98	0.44
2:B:906:ARG:HD2	2:C:1094:SER:OG	2.18	0.44
2:C:432:LEU:HD23	2:C:437:VAL:HG11	2.00	0.44
10:K:220:PRO:O	10:K:223:GLU:HG3	2.18	0.44
17:R:182:ARG:HG2	17:R:186:HIS:CE1	2.53	0.44
1:A:1144:LEU:HD23	1:A:1144:LEU:HA	1.84	0.44
2:C:716:ASN:OD1	2:C:716:ASN:N	2.50	0.44
3:D:2298:ASP:OD1	3:D:2298:ASP:N	2.51	0.44
3:D:2694:SER:HB2	3:D:2695:PRO:HD2	1.98	0.44
3:D:2876:LYS:HE3	5:F:947:GLN:HB3	2.00	0.44
4:E:311:ASP:OD1	4:E:311:ASP:N	2.50	0.44
4:E:651:ASN:OD1	4:E:652:GLU:N	2.50	0.44
5:F:184:GLU:CG	5:F:185:PRO:HD2	2.47	0.44
5:F:562:MET:HA	5:F:565:VAL:HG22	1.99	0.44
6:G:206:VAL:HG11	6:G:214:SER:H	1.83	0.44
6:G:317:ALA:O	6:G:321:VAL:HG12	2.17	0.44
11:L:238:TRP:NE1	11:L:253:PRO:HG3	2.32	0.44
15:P:100:LEU:HA	15:P:100:LEU:HD23	1.77	0.44
15:P:471:LEU:HD13	28:P:701:A1LXL:C27	2.47	0.44
16:Q:135:PHE:CD1	16:Q:141:ALA:HB2	2.52	0.44
21:V:12:UNK:O	21:V:16:UNK:N	2.51	0.44
2:C:704:MET:HG3	2:C:719:TRP:CE3	2.53	0.44
3:D:2770:LYS:O	3:D:2773:THR:HB	2.18	0.44
4:E:351:LEU:N	4:E:352:PRO:HD2	2.33	0.44
5:F:785:ALA:O	5:F:788:GLN:HG3	2.17	0.44
7:H:310:VAL:O	7:H:408:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:316:LEU:HB2	7:H:321:MET:HG2	2.00	0.44
12:M:269:THR:O	12:M:273:VAL:HG13	2.17	0.44
17:R:441:ARG:HA	17:R:444:ARG:HE	1.82	0.44
18:S:72:TYR:HA	18:S:77:ILE:HG13	2.00	0.44
1:A:385:VAL:HG12	1:A:386:ILE:HD13	2.00	0.44
2:C:380:GLN:H	2:C:380:GLN:CD	2.17	0.44
3:D:2282:ALA:HB2	3:D:2701:LEU:HD21	2.00	0.44
3:D:2679:LYS:HB2	3:D:2679:LYS:HE2	1.51	0.44
5:F:742:ASP:H	5:F:779:GLN:NE2	2.14	0.44
12:M:323:MET:HG2	12:M:349:ILE:HG23	1.99	0.44
15:P:106:GLN:O	15:P:109:VAL:HG12	2.17	0.44
15:P:443:VAL:CG2	28:P:701:A1LXL:C01	2.94	0.44
1:A:336:LYS:HA	1:A:336:LYS:HD3	1.90	0.44
1:A:922:LEU:HD23	1:A:922:LEU:HA	1.84	0.44
2:B:346:TPO:HB	3:D:899:LYS:NZ	2.33	0.44
2:C:526:TRP:HH2	2:C:539:ILE:HG13	1.82	0.44
3:D:790:ASN:OD1	3:D:790:ASN:N	2.50	0.44
5:F:679:ASP:OD2	5:F:706:ARG:NH2	2.48	0.44
5:F:913:HIS:CD2	5:F:914:PRO:HD2	2.52	0.44
7:H:339:LEU:HD23	7:H:357:ILE:HG23	2.00	0.44
12:M:552:THR:HG21	12:M:572:LEU:HG	1.99	0.44
16:Q:269:TYR:HA	16:Q:272:ASP:HB3	2.00	0.44
17:R:448:LEU:HD12	17:R:448:LEU:HA	1.90	0.44
2:B:457:MET:HB2	25:D:3101:DGA:HA91	1.99	0.44
2:C:537:LYS:HA	2:C:537:LYS:HD3	1.89	0.44
2:C:680:LEU:HG	2:C:686:PHE:CD2	2.53	0.44
3:D:969:PHE:C	3:D:971:PRO:HD3	2.42	0.44
3:D:1239:LYS:HD2	3:D:1239:LYS:HA	1.74	0.44
5:F:943:MET:HE3	5:F:943:MET:HB3	1.82	0.44
6:G:218:LEU:O	6:G:218:LEU:HD12	2.18	0.44
9:J:64:LYS:O	9:J:68:LEU:HG	2.17	0.44
9:J:91:GLU:OE2	9:J:93:GLU:HG3	2.17	0.44
10:K:112:ARG:HH11	10:K:112:ARG:HB3	1.81	0.44
15:P:116:THR:HG22	15:P:117:TRP:H	1.83	0.44
15:P:304:VAL:HG22	15:P:444:TRP:CD1	2.53	0.44
1:A:481:ASP:OD2	1:A:484:TYR:HB2	2.18	0.44
2:B:643:GLU:O	2:B:647:ILE:HG23	2.17	0.44
2:B:806:TYR:OH	2:B:887:ASP:OD2	2.35	0.44
2:C:511:ALA:HB3	2:C:614:ARG:HH11	1.82	0.44
3:D:330:THR:OG1	3:D:331:PHE:N	2.51	0.44
3:D:1303:LYS:O	3:D:1307:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2336:GLU:CD	3:D:2336:GLU:H	2.25	0.44
5:F:236:VAL:HG21	5:F:252:ALA:HA	2.00	0.44
16:Q:177:ARG:HH12	16:Q:186:HIS:HA	1.82	0.44
16:Q:226:VAL:H	16:Q:235:PRO:HD3	1.83	0.44
19:T:118:TYR:O	19:T:121:THR:HG22	2.18	0.44
22:A:1201:LMG:H171	22:A:1201:LMG:H142	1.80	0.43
2:C:620:PRO:HB3	2:C:663:GLY:HA3	1.99	0.43
4:E:242:GLY:N	4:E:260:GLY:HA3	2.29	0.43
4:E:338:VAL:O	4:E:342:ILE:HG12	2.18	0.43
5:F:758:ILE:HA	5:F:761:VAL:HG12	2.00	0.43
9:J:92:GLU:HG2	10:K:212:ARG:HG3	2.00	0.43
14:O:383:VAL:O	14:O:386:ALA:HB3	2.18	0.43
15:P:149:PHE:CB	15:P:157:LYS:HB3	2.48	0.43
15:P:231:VAL:O	15:P:505:VAL:HG11	2.18	0.43
15:P:446:THR:OG1	15:P:454:LEU:HB2	2.19	0.43
1:A:495:ILE:HD13	1:A:624:VAL:HB	2.00	0.43
2:C:815:TYR:OH	2:C:1005:GLU:OE2	2.31	0.43
3:D:2689:LEU:HD12	3:D:2689:LEU:HA	1.74	0.43
4:E:109:GLY:O	4:E:113:LEU:HG	2.17	0.43
5:F:235:PRO:HG3	19:T:103:LEU:HG	2.00	0.43
6:G:128:ALA:HA	6:G:439:PRO:HG3	2.01	0.43
7:H:95:LEU:HD22	12:M:298:GLN:HE22	1.83	0.43
7:H:198:ASP:OD2	7:H:254:SER:OG	2.36	0.43
11:L:277:TYR:O	11:L:281:TYR:HB3	2.18	0.43
16:Q:109:PRO:HG3	16:Q:163:ARG:HH21	1.82	0.43
16:Q:191:PRO:HB3	16:Q:216:VAL:HG13	2.00	0.43
18:S:94:TRP:CD1	18:S:97:ARG:HH21	2.36	0.43
3:D:2174:SER:HB2	3:D:2895:LYS:HE3	1.99	0.43
3:D:2249:LYS:NZ	3:D:2249:LYS:HB3	2.32	0.43
3:D:2747:GLN:O	3:D:2751:THR:OG1	2.22	0.43
5:F:740:GLU:CD	5:F:740:GLU:H	2.27	0.43
12:M:330:LEU:HD12	12:M:330:LEU:HA	1.84	0.43
15:P:104:GLU:HA	15:P:107:GLU:HG2	2.00	0.43
15:P:455:VAL:HG22	15:P:471:LEU:HD12	1.99	0.43
15:P:486:SER:O	15:P:490:GLY:HA3	2.18	0.43
18:S:75:GLY:C	18:S:77:ILE:HD12	2.43	0.43
1:A:260:ASN:OD1	17:R:413:ASP:HB3	2.18	0.43
1:A:479:LYS:HD2	1:A:479:LYS:HA	1.60	0.43
1:A:655:ARG:O	1:A:659:LYS:HG2	2.18	0.43
2:B:625:ILE:HD13	2:B:628:PHE:HD1	1.83	0.43
3:D:954:LYS:NZ	3:D:959:GLU:O	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:957:MET:HE2	5:F:957:MET:HB3	1.83	0.43
12:M:261:THR:O	12:M:536:ARG:NH2	2.52	0.43
15:P:313:LEU:HD21	15:P:435:ARG:HA	2.01	0.43
1:A:168:ARG:HA	1:A:168:ARG:HD3	1.85	0.43
2:B:241:PHE:HE1	15:P:176:LEU:HD21	1.84	0.43
2:B:799:LEU:O	2:B:803:VAL:HG23	2.19	0.43
2:B:906:ARG:HB3	3:D:2641:LYS:HE2	2.01	0.43
2:C:445:GLU:OE1	2:C:448:ARG:NH1	2.42	0.43
2:C:515:ARG:NH1	2:C:515:ARG:HA	2.34	0.43
2:C:606:ARG:HA	2:C:606:ARG:HD2	1.78	0.43
2:C:972:MET:HE1	8:I:72:ILE:HD13	1.99	0.43
3:D:1992:ILE:HD11	3:D:2339:CYS:HB2	2.00	0.43
5:F:129:LEU:HA	5:F:199:SER:O	2.19	0.43
16:Q:218:VAL:HG12	16:Q:238:LEU:HD23	2.00	0.43
1:A:243:SER:HB2	1:A:245:LEU:HG	2.00	0.43
1:A:797:GLY:C	1:A:799:PHE:H	2.26	0.43
2:B:526:TRP:HB2	2:B:583:GLU:HG3	2.00	0.43
2:C:478:ILE:O	2:C:481:PRO:HD3	2.18	0.43
4:E:554:GLU:O	4:E:558:GLN:CB	2.67	0.43
5:F:137:VAL:HA	5:F:156:PRO:HG2	2.00	0.43
7:H:439:MET:HE3	7:H:439:MET:HB3	1.91	0.43
16:Q:115:ASN:OD1	16:Q:115:ASN:N	2.52	0.43
1:A:477:MET:HA	1:A:481:ASP:HB3	2.00	0.43
2:C:378:TYR:CE2	2:C:423:PRO:HD2	2.54	0.43
2:C:726:MET:HE1	2:C:734:VAL:HG12	2.00	0.43
2:C:755:GLU:HG2	6:G:258:HIS:CD2	2.54	0.43
3:D:2129:GLU:OE1	4:E:731:ARG:NH1	2.48	0.43
3:D:2693:PRO:HB2	3:D:2698:SER:HB3	2.01	0.43
6:G:371:GLN:NE2	6:G:418:LEU:O	2.50	0.43
7:H:280:PRO:O	7:H:409:GLN:NE2	2.51	0.43
8:I:213:ASP:O	22:I:402:LMG:O3	2.34	0.43
8:I:216:MET:HE3	8:I:216:MET:HB3	1.73	0.43
15:P:116:THR:O	15:P:119:ASP:HB2	2.19	0.43
15:P:413:LEU:HD23	15:P:413:LEU:HA	1.79	0.43
17:R:317:SER:O	17:R:318:PHE:HB3	2.18	0.43
1:A:235:GLU:HG2	1:A:292:ARG:HG2	2.00	0.43
2:B:535:VAL:HG11	2:B:692:MET:HG3	2.01	0.43
2:B:847:ASN:OD1	2:B:847:ASN:N	2.47	0.43
2:C:893:LEU:O	2:C:897:GLU:HG2	2.18	0.43
3:D:1294:LYS:HA	3:D:1294:LYS:HD3	1.86	0.43
3:D:1696:LEU:HD12	3:D:1696:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:666:THR:HG22	4:E:667:ALA:N	2.34	0.43
4:E:907:LEU:HD23	4:E:907:LEU:HA	1.67	0.43
5:F:132:GLN:OE1	5:F:158:PRO:HG2	2.19	0.43
6:G:172:LEU:O	6:G:176:THR:HG23	2.18	0.43
17:R:290:ASP:HB3	17:R:330:ARG:HH21	1.83	0.43
18:S:97:ARG:O	18:S:101:THR:HG23	2.19	0.43
1:A:248:PRO:HB2	17:R:418:VAL:HG23	2.00	0.43
1:A:487:VAL:HG12	2:B:711:LYS:NZ	2.33	0.43
1:A:908:ALA:O	1:A:911:ARG:NH2	2.52	0.43
3:D:1760:GLN:NE2	14:O:468:THR:H	2.16	0.43
3:D:2678:PRO:HG2	3:D:2891:PHE:CZ	2.54	0.43
4:E:828:LYS:HD2	4:E:829:VAL:O	2.18	0.43
6:G:275:ASP:OD1	6:G:309:HIS:NE2	2.48	0.43
7:H:187:LEU:CD2	7:H:276:VAL:HG21	2.48	0.43
15:P:169:ASN:O	15:P:171:PRO:HD3	2.18	0.43
16:Q:337:ALA:HA	16:Q:341:LEU:HD22	2.01	0.43
17:R:230:TRP:O	17:R:234:GLN:NE2	2.40	0.43
2:C:908:THR:OG1	2:C:959:GLU:OE2	2.30	0.43
3:D:1179:GLN:HA	3:D:1182:TRP:HD1	1.82	0.43
3:D:2632:LEU:C	3:D:2634:LYS:H	2.27	0.43
4:E:823:GLN:HG3	4:E:825:ARG:HH12	1.84	0.43
8:I:235:SER:HB3	8:I:244:VAL:HB	2.01	0.43
9:J:59:VAL:HG23	9:J:59:VAL:O	2.18	0.43
15:P:238:ARG:HB3	15:P:252:VAL:HG22	2.01	0.43
17:R:193:ASP:OD1	17:R:193:ASP:N	2.51	0.43
18:S:76:LYS:O	18:S:76:LYS:HD3	2.19	0.43
19:T:16:GLU:OE1	19:T:21:GLN:HG2	2.17	0.43
2:B:644:SER:O	2:B:648:ILE:HG13	2.20	0.42
2:B:733:ASP:OD1	2:B:733:ASP:N	2.52	0.42
2:C:510:PRO:HD3	2:C:607:ARG:HB3	2.01	0.42
2:C:545:TYR:HB2	2:C:552:LEU:HD11	2.01	0.42
3:D:2096:ARG:HA	3:D:2325:ASP:HB3	1.99	0.42
3:D:2263:GLN:O	3:D:2266:THR:HG22	2.19	0.42
5:F:69:ALA:O	19:T:113:LEU:HD21	2.20	0.42
6:G:257:ARG:HB3	6:G:268:ARG:NH2	2.34	0.42
12:M:287:PHE:HA	12:M:288:PRO:HD3	1.92	0.42
12:M:304:LEU:HD23	12:M:304:LEU:HA	1.83	0.42
15:P:108:GLU:HA	15:P:111:LYS:HB2	2.01	0.42
1:A:178:PRO:HB3	18:S:28:VAL:HG11	2.01	0.42
2:B:600:TYR:OH	2:B:607:ARG:NH1	2.52	0.42
2:B:1004:LEU:HD23	2:B:1004:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:739:LYS:HB2	3:D:739:LYS:HE3	1.76	0.42
3:D:824:PHE:HB2	4:E:60:PHE:CZ	2.54	0.42
3:D:1447:LYS:HB3	3:D:1447:LYS:HE3	1.82	0.42
5:F:655:ARG:H	5:F:655:ARG:HG2	1.67	0.42
5:F:976:ARG:NH1	5:F:1011:ASP:OD1	2.52	0.42
15:P:152:LEU:HD13	15:P:156:SER:HB3	2.00	0.42
15:P:231:VAL:HG22	15:P:259:ALA:C	2.44	0.42
16:Q:328:GLU:HA	16:Q:331:MET:HG2	2.01	0.42
3:D:1776:TRP:O	3:D:1780:ALA:HB3	2.20	0.42
3:D:1804:GLN:O	3:D:1808:ILE:HG12	2.20	0.42
3:D:1805:ASN:OD1	3:D:1805:ASN:N	2.50	0.42
3:D:2243:LYS:HB2	3:D:2243:LYS:HE2	1.69	0.42
5:F:109:GLN:N	5:F:109:GLN:OE1	2.52	0.42
15:P:262:HIS:CD2	15:P:264:PRO:HD2	2.54	0.42
15:P:346:ASP:O	15:P:347:PRO:C	2.62	0.42
15:P:505:VAL:O	15:P:509:PRO:HD3	2.19	0.42
16:Q:113:VAL:HG21	16:Q:145:ILE:CD1	2.49	0.42
18:S:46:THR:HG21	18:S:49:ASP:HB2	2.00	0.42
18:S:89:ASP:O	18:S:93:ASN:ND2	2.52	0.42
19:T:61:SER:O	19:T:64:GLU:HB3	2.19	0.42
1:A:429:GLN:O	1:A:433:LEU:HB2	2.20	0.42
1:A:1090:PHE:CE1	2:B:986:THR:HG21	2.54	0.42
2:C:376:LEU:HG	2:C:418:CYS:HB3	2.01	0.42
3:D:1220:ILE:HD12	3:D:1224:SER:OG	2.18	0.42
5:F:575:LYS:HE3	5:F:575:LYS:HB2	1.89	0.42
5:F:865:ARG:HH11	5:F:865:ARG:HG3	1.84	0.42
16:Q:292:LEU:HA	16:Q:295:ARG:HB2	2.02	0.42
17:R:53:LEU:O	17:R:321:ASN:HB3	2.19	0.42
17:R:432:LEU:HD23	17:R:432:LEU:HA	1.89	0.42
19:T:80:ASP:O	19:T:84:THR:HG22	2.19	0.42
2:B:705:GLN:HG2	2:B:719:TRP:CZ2	2.54	0.42
2:B:1087:TRP:HA	2:B:1087:TRP:HE3	1.84	0.42
2:C:606:ARG:NH1	2:C:609:ARG:HB2	2.34	0.42
3:D:1126:ASN:HD21	3:D:1128:ARG:HB3	1.83	0.42
3:D:1699:ILE:HD13	3:D:1699:ILE:HA	1.88	0.42
3:D:2592:LEU:HA	3:D:2592:LEU:HD12	1.81	0.42
4:E:439:ALA:HB1	4:E:614:GLU:CB	2.49	0.42
4:E:639:PRO:HD2	4:E:828:LYS:HD3	2.02	0.42
4:E:920:ARG:NH1	4:E:925:ARG:HG2	2.34	0.42
5:F:82:PRO:HD2	13:N:36:GLU:OE1	2.19	0.42
5:F:205:PRO:HB3	5:F:211:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:265:ARG:HE	6:G:265:ARG:N	2.18	0.42
7:H:275:HIS:NE2	7:H:443:MET:HE1	2.34	0.42
7:H:474:GLU:O	7:H:474:GLU:HG2	2.18	0.42
8:I:107:GLU:O	8:I:111:VAL:HG23	2.19	0.42
13:N:35:LYS:HE2	13:N:35:LYS:HB3	1.74	0.42
15:P:293:LEU:HD11	15:P:486:SER:HA	2.01	0.42
15:P:513:PHE:HB3	15:P:524:HIS:CD2	2.55	0.42
16:Q:112:THR:HG23	16:Q:162:LEU:HD11	2.00	0.42
16:Q:311:GLU:O	16:Q:315:ARG:HD2	2.20	0.42
16:Q:338:GLY:H	16:Q:341:LEU:HB2	1.84	0.42
17:R:351:ASP:HB2	17:R:354:ARG:NH1	2.25	0.42
1:A:264:MET:HE3	1:A:264:MET:HB3	1.93	0.42
1:A:786:THR:HG23	1:A:787:ASN:H	1.85	0.42
3:D:1228:ILE:CG2	17:R:271:ASP:HB3	2.49	0.42
3:D:2264:LEU:HD12	3:D:2264:LEU:HA	1.72	0.42
3:D:2654:LEU:O	3:D:2658:THR:HG23	2.19	0.42
4:E:976:LYS:HD2	4:E:976:LYS:HA	1.78	0.42
7:H:172:LEU:HD23	7:H:172:LEU:HA	1.80	0.42
12:M:385:ALA:HB3	12:M:386:PRO:HD3	2.00	0.42
16:Q:228:THR:OG1	16:Q:231:MET:O	2.34	0.42
16:Q:241:GLU:HG2	16:Q:242:ASP:H	1.85	0.42
17:R:184:ALA:O	17:R:188:ARG:HG3	2.20	0.42
17:R:319:PHE:HA	17:R:320:PRO:HD3	1.79	0.42
1:A:168:ARG:HG3	1:A:184:LYS:HG3	2.02	0.42
2:B:473:MET:HB3	2:B:473:MET:HE3	1.72	0.42
2:B:604:GLY:O	2:B:608:VAL:HG22	2.19	0.42
2:C:1033:LYS:HE3	2:C:1033:LYS:HB3	1.85	0.42
3:D:563:LYS:NZ	15:P:382:GLU:O	2.38	0.42
3:D:2306:VAL:HG23	3:D:2306:VAL:O	2.19	0.42
3:D:2632:LEU:O	3:D:2633:PRO:C	2.63	0.42
4:E:528:ALA:HB1	4:E:574:THR:O	2.20	0.42
4:E:920:ARG:HE	4:E:928:LEU:HD12	1.84	0.42
5:F:565:VAL:O	5:F:569:ARG:HG2	2.20	0.42
5:F:808:ARG:HH22	5:F:886:GLU:HB3	1.84	0.42
6:G:206:VAL:HG21	6:G:213:SER:HA	2.02	0.42
6:G:247:ALA:O	6:G:251:LEU:HG	2.20	0.42
15:P:190:ASP:N	15:P:191:PRO:HD3	2.34	0.42
16:Q:295:ARG:O	16:Q:298:LYS:HB3	2.20	0.42
1:A:476:ARG:HA	1:A:476:ARG:HD3	1.77	0.42
1:A:1039:LEU:HA	1:A:1039:LEU:HD12	1.86	0.42
2:C:364:LYS:HA	8:I:240:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:955:VAL:O	2:C:959:GLU:HG3	2.19	0.42
5:F:881:VAL:HG12	5:F:882:LEU:HD23	2.02	0.42
6:G:265:ARG:H	6:G:265:ARG:HG2	1.55	0.42
15:P:558:GLY:O	16:Q:203:TYR:OH	2.36	0.42
16:Q:332:ARG:O	16:Q:336:SER:OG	2.37	0.42
17:R:126:SEP:O1P	17:R:397:ARG:NH2	2.42	0.42
17:R:130:GLU:O	17:R:134:GLU:HG3	2.20	0.42
20:U:66:UNK:O	20:U:70:UNK:N	2.53	0.42
1:A:523:SER:HB2	1:A:527:GLU:OE2	2.20	0.42
1:A:524:VAL:HG23	1:A:526:SER:H	1.85	0.42
1:A:747:TRP:CD1	1:A:747:TRP:C	2.98	0.42
2:C:389:HIS:HB3	2:C:411:ALA:HB2	2.02	0.42
2:C:546:LEU:HG	2:C:622:ILE:HD11	2.00	0.42
3:D:267:TYR:O	3:D:271:GLN:HG3	2.19	0.42
3:D:2445:LEU:HD23	3:D:2445:LEU:HA	1.79	0.42
4:E:692:LEU:HD23	4:E:692:LEU:HA	1.82	0.42
6:G:116:CYS:SG	6:G:117:LEU:N	2.93	0.42
6:G:142:ARG:HG3	6:G:146:VAL:HG22	2.01	0.42
7:H:477:ASP:OD1	7:H:477:ASP:N	2.50	0.42
12:M:633:VAL:O	12:M:636:GLU:HG3	2.19	0.42
13:N:40:LYS:HE3	13:N:40:LYS:HB3	1.63	0.42
15:P:311:LEU:HB2	15:P:437:TRP:HB3	2.02	0.42
15:P:555:LEU:HD23	15:P:555:LEU:HA	1.83	0.42
18:S:90:ALA:HA	18:S:93:ASN:ND2	2.34	0.42
2:B:496:ARG:HG2	2:B:496:ARG:HH21	1.85	0.42
2:C:683:PRO:HB3	4:E:651:ASN:ND2	2.35	0.42
3:D:1170:ASN:OD1	17:R:226:GLY:HA3	2.20	0.42
4:E:140:LEU:HG	4:E:141:PRO:HD2	2.02	0.42
4:E:250:GLN:HB3	17:R:349:VAL:HG22	2.02	0.42
6:G:193:LEU:HB3	6:G:231:MET:SD	2.60	0.42
13:N:131:SER:C	13:N:133:GLY:N	2.78	0.42
17:R:223:ALA:HB3	17:R:228:ASN:HD21	1.84	0.42
2:B:201:ALA:O	2:B:205:ARG:HG3	2.20	0.41
2:C:496:ARG:NH2	13:N:136:LEU:HD23	2.35	0.41
2:C:533:ASP:HB3	2:C:534:GLU:OE2	2.19	0.41
3:D:546:PRO:HD2	15:P:228:TRP:CE3	2.54	0.41
3:D:989:ASN:C	3:D:991:TYR:H	2.28	0.41
3:D:1245:PHE:HD2	17:R:221:PRO:HG2	1.85	0.41
3:D:2132:GLN:HG2	4:E:731:ARG:O	2.19	0.41
5:F:135:ARG:HB2	5:F:159:LEU:HG	2.02	0.41
7:H:158:ALA:HB3	7:H:193:GLU:HG3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:206:TRP:CG	8:I:207:PRO:HD3	2.55	0.41
8:I:350:ARG:NH1	8:I:366:VAL:HG21	2.35	0.41
15:P:613:ALA:O	15:P:617:ARG:HG3	2.20	0.41
17:R:442:MET:HG2	17:R:445:ARG:HD2	2.02	0.41
2:B:1091:MET:HE2	2:B:1091:MET:HB3	1.66	0.41
2:C:415:GLU:HG3	8:I:299:ARG:HA	2.02	0.41
2:C:767:MET:HG3	2:C:830:PRO:HG2	2.03	0.41
2:C:856:GLU:O	2:C:860:ARG:HG3	2.20	0.41
2:C:872:LYS:HB2	2:C:872:LYS:HE3	1.72	0.41
3:D:1392:GLN:O	3:D:1396:MET:HG3	2.20	0.41
3:D:1671:PHE:O	3:D:1674:ILE:HG12	2.20	0.41
3:D:1917:ILE:HG12	3:D:1921:PHE:HE2	1.85	0.41
3:D:2827:ILE:O	3:D:2828:ASP:HB3	2.20	0.41
4:E:77:ILE:HD12	5:F:102:TYR:CE1	2.55	0.41
5:F:84:LYS:HE2	5:F:84:LYS:HB2	1.94	0.41
5:F:599:ALA:O	5:F:602:VAL:HG12	2.20	0.41
5:F:896:GLN:NE2	5:F:899:ARG:HH21	2.18	0.41
6:G:263:SER:O	6:G:264:ASP:C	2.62	0.41
7:H:186:ARG:HD2	7:H:186:ARG:HA	1.83	0.41
8:I:232:LEU:HA	8:I:244:VAL:HG23	2.03	0.41
15:P:147:ARG:HA	15:P:147:ARG:HD3	1.80	0.41
15:P:431:ASP:OD2	15:P:436:ASN:HB2	2.20	0.41
15:P:557:ALA:CB	16:Q:328:GLU:HB3	2.48	0.41
15:P:564:LYS:HA	15:P:564:LYS:HD3	1.77	0.41
16:Q:96:MET:HE2	16:Q:341:LEU:HD12	2.02	0.41
1:A:593:ILE:O	1:A:596:LYS:NZ	2.48	0.41
2:B:515:ARG:HH11	2:B:515:ARG:HA	1.86	0.41
2:B:848:VAL:HB	3:D:2218:GLN:HB3	2.02	0.41
2:B:1103:TYR:O	2:B:1107:VAL:HG23	2.21	0.41
2:C:759:TYR:HE2	6:G:258:HIS:CD2	2.39	0.41
3:D:569:LEU:O	3:D:573:LEU:HD12	2.20	0.41
3:D:637:ASN:OD1	3:D:637:ASN:N	2.52	0.41
3:D:2275:ARG:HB2	3:D:2275:ARG:NH1	2.35	0.41
3:D:2647:ASP:OD1	3:D:2647:ASP:N	2.51	0.41
3:D:2923:LEU:O	3:D:2927:VAL:HG23	2.20	0.41
5:F:906:MET:HE3	5:F:906:MET:HB3	1.87	0.41
10:K:252:PHE:C	10:K:254:LEU:H	2.28	0.41
12:M:280:PHE:HD1	12:M:603:ALA:HB2	1.84	0.41
12:M:408:LEU:HD12	12:M:408:LEU:HA	1.87	0.41
16:Q:186:HIS:HB3	16:Q:188:ARG:NH1	2.32	0.41
17:R:123:ASP:N	17:R:123:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TYR:OH	1:A:287:ASP:OD2	2.30	0.41
2:B:210:TYR:HA	2:B:213:GLU:OE1	2.21	0.41
3:D:757:LYS:HD3	3:D:757:LYS:HA	1.87	0.41
3:D:825:ILE:HG13	3:D:826:GLN:N	2.35	0.41
3:D:2140:HIS:CD2	3:D:2144:HIS:ND1	2.88	0.41
4:E:248:THR:O	4:E:248:THR:OG1	2.33	0.41
5:F:632:ASP:O	5:F:636:THR:HG23	2.21	0.41
18:S:79:ASN:OD1	18:S:79:ASN:N	2.53	0.41
1:A:610:GLN:HG2	1:A:611:GLU:HG2	2.03	0.41
1:A:1067:HIS:ND1	1:A:1069:GLU:OE1	2.51	0.41
2:B:199:TYR:CZ	2:B:203:LEU:HD11	2.56	0.41
2:B:479:LEU:HD11	17:R:31:GLN:HG3	2.01	0.41
2:B:529:ILE:H	2:B:529:ILE:HG13	1.67	0.41
2:C:453:LEU:HG	2:C:457:MET:HE3	2.03	0.41
2:C:464:PHE:O	2:C:467:ILE:HG13	2.21	0.41
2:C:1077:ARG:NH2	2:C:1081:GLY:O	2.54	0.41
3:D:1163:ASP:OD1	3:D:1163:ASP:N	2.54	0.41
3:D:2262:GLU:H	3:D:2262:GLU:HG3	1.62	0.41
5:F:208:MET:HE2	5:F:211:LEU:HG	2.02	0.41
22:I:402:LMG:H292	10:K:221:LEU:HD21	2.01	0.41
12:M:409:TRP:H	12:M:416:HIS:HE1	1.68	0.41
15:P:390:GLN:HE22	15:P:395:ALA:HA	1.84	0.41
15:P:393:LYS:HA	15:P:393:LYS:HD2	1.71	0.41
17:R:224:SER:HB3	17:R:227:GLU:HG3	2.02	0.41
2:B:852:LEU:HD11	3:D:2218:GLN:HE21	1.85	0.41
2:C:423:PRO:HA	2:C:424:PRO:HD3	1.92	0.41
2:C:671:ASN:OD1	2:C:671:ASN:N	2.50	0.41
2:C:730:THR:O	2:C:734:VAL:HG13	2.20	0.41
3:D:784:HIS:HE1	17:R:60:ARG:CZ	2.33	0.41
3:D:1693:THR:O	3:D:1693:THR:OG1	2.35	0.41
4:E:674:VAL:C	4:E:678:THR:HG1	2.28	0.41
6:G:278:ALA:HB2	6:G:309:HIS:CG	2.56	0.41
7:H:144:LEU:HD23	7:H:144:LEU:HA	1.93	0.41
8:I:220:THR:OG1	8:I:321:TYR:OH	2.22	0.41
13:N:123:VAL:O	13:N:124:TYR:C	2.64	0.41
15:P:311:LEU:O	15:P:437:TRP:N	2.43	0.41
15:P:332:ALA:HB1	15:P:333:PRO:HD2	2.01	0.41
17:R:359:LEU:HD13	17:R:360:PRO:HD2	2.02	0.41
1:A:527:GLU:HA	5:F:631:ARG:HH21	1.85	0.41
1:A:543:LEU:HA	1:A:546:ASN:HD21	1.85	0.41
1:A:697:LEU:O	1:A:701:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:938:GLY:N	3:D:2722:LYS:HZ2	2.18	0.41
2:C:381:LEU:HD22	2:C:420:VAL:HG11	2.01	0.41
2:C:615:LEU:HD12	2:C:615:LEU:HA	1.80	0.41
2:C:860:ARG:O	2:C:864:HIS:HD2	2.03	0.41
3:D:986:THR:O	3:D:990:LYS:HG3	2.21	0.41
3:D:2359:LYS:HD2	3:D:2359:LYS:HA	1.78	0.41
4:E:196:ASP:HA	4:E:197:PRO:HD3	1.93	0.41
4:E:872:LYS:HB2	4:E:935:MET:SD	2.60	0.41
8:I:219:TRP:CE2	22:K:301:LMG:H131	2.56	0.41
9:J:65:PHE:O	9:J:70:ALA:HB3	2.20	0.41
12:M:556:ARG:HG2	12:M:603:ALA:O	2.20	0.41
12:M:592:LEU:HD23	12:M:592:LEU:HA	1.93	0.41
15:P:555:LEU:HD11	16:Q:343:ALA:HB1	2.01	0.41
15:P:679:SER:HA	15:P:682:PHE:HD2	1.84	0.41
1:A:145:TYR:CZ	2:B:394:ARG:HD2	2.55	0.41
1:A:424:GLU:O	1:A:428:SER:HB2	2.20	0.41
2:B:202:TYR:HA	2:B:205:ARG:NH2	2.36	0.41
2:B:265:ALA:O	2:B:268:VAL:HG12	2.21	0.41
2:C:374:ARG:NH1	2:C:376:LEU:HD21	2.33	0.41
2:C:524:ILE:HG13	2:C:578:LYS:CB	2.51	0.41
3:D:888:LEU:HD13	3:D:888:LEU:HA	1.90	0.41
3:D:957:ARG:HB2	3:D:959:GLU:OE1	2.21	0.41
3:D:1135:ASN:OD1	3:D:1162:ARG:NH1	2.54	0.41
5:F:265:LEU:HD11	19:T:83:LYS:HA	2.03	0.41
5:F:913:HIS:HB3	5:F:916:TYR:HB2	2.02	0.41
7:H:135:ARG:HE	7:H:135:ARG:HB3	1.73	0.41
11:L:242:VAL:O	11:L:242:VAL:HG12	2.21	0.41
15:P:280:ARG:HE	15:P:280:ARG:HB2	1.77	0.41
1:A:444:LYS:HA	1:A:451:MET:CB	2.46	0.41
1:A:516:ALA:O	1:A:518:VAL:HG13	2.20	0.41
1:A:1088:PRO:O	1:A:1090:PHE:N	2.52	0.41
2:B:199:TYR:CE2	2:B:203:LEU:HD11	2.55	0.41
2:B:360:ALA:HB3	3:D:1311:THR:HA	2.03	0.41
2:B:551:LEU:HD11	7:H:483:GLU:HG3	2.03	0.41
2:C:609:ARG:HE	2:C:654:GLN:NE2	2.18	0.41
2:C:826:VAL:HB	2:C:995:ILE:HG22	2.03	0.41
3:D:637:ASN:HD22	15:P:473:HIS:CG	2.39	0.41
3:D:1225:LYS:HB3	3:D:1225:LYS:HE2	1.75	0.41
3:D:1297:ILE:HA	3:D:1300:VAL:HG22	2.02	0.41
3:D:1957:SER:C	3:D:1959:HIS:H	2.29	0.41
3:D:2254:LEU:HA	3:D:2255:PRO:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2879:ARG:HB3	3:D:2890:TRP:HB3	2.03	0.41
4:E:83:GLU:OE1	4:E:83:GLU:N	2.53	0.41
5:F:897:MET:HE2	5:F:897:MET:HB2	1.86	0.41
8:I:235:SER:OG	8:I:240:TYR:O	2.34	0.41
9:J:47:ILE:HD13	9:J:47:ILE:HA	1.91	0.41
10:K:252:PHE:C	10:K:254:LEU:N	2.79	0.41
11:L:233:LEU:HD23	11:L:233:LEU:HA	1.91	0.41
12:M:268:GLU:H	12:M:268:GLU:CD	2.28	0.41
12:M:401:HIS:HA	12:M:411:ASP:OD1	2.20	0.41
12:M:631:GLU:OE2	12:M:631:GLU:N	2.49	0.41
15:P:317:ALA:HB2	15:P:413:LEU:HD12	2.02	0.41
15:P:368:ALA:O	15:P:371:GLU:HG3	2.20	0.41
15:P:502:ALA:HA	15:P:505:VAL:HG12	2.03	0.41
16:Q:219:PHE:HB3	16:Q:243:LEU:HD13	2.01	0.41
17:R:195:LYS:HB2	19:T:27:TYR:CE1	2.36	0.41
1:A:778:MET:HG2	1:A:784:PHE:CE2	2.55	0.41
1:A:846:ASN:O	3:D:2726:ARG:HG2	2.21	0.41
22:A:1201:LMG:H331	22:A:1201:LMG:H302	1.25	0.41
2:B:367:TRP:CD1	2:B:368:ARG:HG2	2.56	0.41
2:B:532:ILE:O	2:B:536:LYS:HB2	2.21	0.41
2:B:893:LEU:HA	2:B:893:LEU:HD12	1.82	0.41
3:D:1172:THR:O	3:D:1172:THR:HG22	2.21	0.41
3:D:2891:PHE:O	3:D:2892:ASN:C	2.64	0.41
6:G:256:ARG:O	6:G:257:ARG:C	2.63	0.41
9:J:78:ILE:HG13	9:J:79:MET:HE2	2.02	0.41
12:M:629:PRO:O	12:M:633:VAL:HG23	2.20	0.41
15:P:152:LEU:HD12	15:P:152:LEU:H	1.85	0.41
1:A:257:SER:HA	18:S:111:LEU:HD12	2.02	0.40
1:A:300:ASP:CG	17:R:68:THR:HG1	2.30	0.40
1:A:798:GLU:HG3	3:D:2787:THR:OG1	2.20	0.40
2:B:474:ILE:HG13	2:B:475:HIS:N	2.35	0.40
2:B:507:PHE:CE1	2:B:600:TYR:HE2	2.39	0.40
2:C:656:ASP:N	2:C:656:ASP:OD1	2.53	0.40
3:D:938:GLU:H	3:D:938:GLU:HG2	1.50	0.40
3:D:2070:LEU:HA	3:D:2070:LEU:HD23	1.70	0.40
3:D:2237:LEU:HA	3:D:2240:LYS:HB3	2.03	0.40
6:G:134:ARG:HH22	6:G:400:HIS:HB3	1.87	0.40
7:H:85:SER:N	7:H:86:PRO:HD2	2.36	0.40
8:I:304:ALA:HA	8:I:305:PRO:HD3	1.94	0.40
17:R:154:TYR:HB2	17:R:206:HIS:CE1	2.56	0.40
1:A:257:SER:OG	18:S:112:GLU:OE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:787:GLY:HA2	2:C:793:ASP:OD1	2.21	0.40
3:D:454:TYR:O	3:D:458:ASN:ND2	2.50	0.40
3:D:554:ASP:OD2	15:P:353:VAL:HB	2.22	0.40
3:D:572:LYS:HE2	3:D:572:LYS:HB3	1.89	0.40
3:D:1437:ILE:O	3:D:1441:LEU:HG	2.21	0.40
3:D:1664:LEU:HD21	17:R:4:PHE:CE1	2.56	0.40
9:J:93:GLU:HG3	9:J:93:GLU:H	1.60	0.40
11:L:264:LEU:HD12	11:L:265:PRO:HD2	2.04	0.40
11:L:274:MET:HE3	11:L:274:MET:HB3	1.88	0.40
15:P:265:LEU:O	15:P:269:LEU:HD12	2.22	0.40
17:R:223:ALA:HB1	17:R:227:GLU:OE1	2.21	0.40
1:A:744:VAL:HG13	1:A:757:VAL:HG22	2.03	0.40
1:A:1045:VAL:O	1:A:1049:ILE:HG12	2.21	0.40
2:C:897:GLU:HG2	2:C:897:GLU:H	1.68	0.40
3:D:449:LEU:H	3:D:449:LEU:HD12	1.86	0.40
3:D:1249:SER:OG	3:D:1250:LYS:N	2.53	0.40
3:D:1249:SER:OG	3:D:1251:ARG:N	2.55	0.40
4:E:958:PRO:HD3	5:F:949:ARG:NH1	2.36	0.40
9:J:67:ASP:OD1	9:J:67:ASP:N	2.33	0.40
10:K:131:ILE:HA	10:K:132:PRO:HD3	1.79	0.40
15:P:202:SER:O	15:P:204:LEU:N	2.54	0.40
15:P:279:PRO:O	15:P:283:VAL:HG12	2.22	0.40
15:P:405:LEU:O	28:P:702:A1LXL:C21	2.69	0.40
15:P:579:ALA:HA	15:P:582:ARG:HG2	2.02	0.40
16:Q:275:GLN:O	16:Q:279:GLN:NE2	2.54	0.40
1:A:842:TYR:OH	3:D:2788:ASN:HB2	2.21	0.40
1:A:875:ARG:H	3:D:2185:ASN:HD21	1.69	0.40
2:C:389:HIS:O	2:C:407:THR:HG22	2.20	0.40
2:C:535:VAL:O	2:C:539:ILE:HG23	2.21	0.40
3:D:2695:PRO:HD3	3:D:2700:LEU:O	2.22	0.40
3:D:2962:ILE:HG12	3:D:2962:ILE:H	1.72	0.40
4:E:90:LEU:HA	4:E:90:LEU:HD23	1.84	0.40
5:F:746:LEU:O	5:F:750:MET:HG2	2.21	0.40
7:H:320:TYR:O	7:H:324:MET:HG3	2.21	0.40
11:L:153:PRO:HA	11:L:156:ARG:HE	1.85	0.40
15:P:143:VAL:HA	15:P:146:GLU:OE2	2.21	0.40
16:Q:236:LEU:HD13	16:Q:236:LEU:HA	1.96	0.40
2:B:607:ARG:O	2:B:611:THR:HG22	2.22	0.40
2:C:377:SER:OG	2:C:378:TYR:N	2.53	0.40
3:D:2349:LEU:HD23	3:D:2349:LEU:HA	1.87	0.40
4:E:190:TRP:CH2	17:R:357:GLN:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:770:THR:HG23	4:E:889:MET:HE1	2.04	0.40
5:F:720:ASP:CG	5:F:721:PHE:H	2.30	0.40
5:F:735:LYS:HD2	5:F:766:CYS:HB2	2.04	0.40
6:G:238:THR:OG1	6:G:239:ASP:N	2.54	0.40
7:H:104:ALA:O	7:H:107:GLU:HG3	2.22	0.40
11:L:167:LEU:HD13	11:L:171:LEU:HD11	2.03	0.40
11:L:300:MET:N	11:L:300:MET:SD	2.94	0.40
15:P:84:TRP:CG	15:P:100:LEU:HD12	2.57	0.40
16:Q:166:MET:HA	16:Q:169:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	982/1182 (83%)	912 (93%)	70 (7%)	0	100	100
2	B	736/1112 (66%)	683 (93%)	51 (7%)	2 (0%)	37	67
2	C	682/1112 (61%)	622 (91%)	58 (8%)	2 (0%)	37	67
3	D	1471/2971 (50%)	1341 (91%)	116 (8%)	14 (1%)	13	39
4	E	864/982 (88%)	798 (92%)	64 (7%)	2 (0%)	44	73
5	F	695/1024 (68%)	646 (93%)	48 (7%)	1 (0%)	48	77
6	G	392/495 (79%)	359 (92%)	30 (8%)	3 (1%)	16	44
7	H	404/555 (73%)	384 (95%)	19 (5%)	1 (0%)	44	73
8	I	268/366 (73%)	243 (91%)	25 (9%)	0	100	100
9	J	82/117 (70%)	78 (95%)	4 (5%)	0	100	100
10	K	187/255 (73%)	167 (89%)	17 (9%)	3 (2%)	8	27
11	L	149/303 (49%)	135 (91%)	14 (9%)	0	100	100
12	M	388/682 (57%)	357 (92%)	31 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	113/137 (82%)	107 (95%)	6 (5%)	0	100	100
14	O	312/471 (66%)	288 (92%)	24 (8%)	0	100	100
15	P	613/691 (89%)	558 (91%)	53 (9%)	2 (0%)	37	67
16	Q	260/365 (71%)	245 (94%)	15 (6%)	0	100	100
17	R	393/462 (85%)	356 (91%)	35 (9%)	2 (0%)	25	56
18	S	112/324 (35%)	101 (90%)	11 (10%)	0	100	100
19	T	106/299 (36%)	95 (90%)	10 (9%)	1 (1%)	14	42
20	U	6/156 (4%)	5 (83%)	1 (17%)	0	100	100
All	All	9215/14061 (66%)	8480 (92%)	702 (8%)	33 (0%)	32	61

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	971	PRO
3	D	2777	LEU
3	D	2801	HIS
3	D	2891	PHE
3	D	60	ASN
3	D	964	LYS
3	D	1329	TRP
3	D	1364	ASN
6	G	251	LEU
6	G	260	SER
6	G	261	SER
10	K	90	SER
15	P	71	GLU
2	C	779	GLY
3	D	2251	VAL
17	R	333	TRP
2	B	449	LEU
3	D	965	LYS
3	D	1326	HIS
4	E	605	PRO
10	K	241	PRO
19	T	40	PRO
2	C	424	PRO
3	D	2153	TYR
2	B	250	PRO
4	E	352	PRO

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Mol	Chain	Res	Type
3	D	2250	ILE
7	H	150	GLY
3	D	2633	PRO
15	P	203	GLY
5	F	154	PRO
10	K	91	ILE
17	R	387	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	774/936 (83%)	724 (94%)	50 (6%)	14	40
2	B	599/858 (70%)	538 (90%)	61 (10%)	6	19
2	C	548/858 (64%)	501 (91%)	47 (9%)	8	27
3	D	1443/2762 (52%)	1316 (91%)	127 (9%)	8	26
4	E	536/774 (69%)	491 (92%)	45 (8%)	9	28
5	F	542/773 (70%)	498 (92%)	44 (8%)	9	29
6	G	283/358 (79%)	251 (89%)	32 (11%)	4	16
7	H	346/451 (77%)	315 (91%)	31 (9%)	8	25
8	I	204/263 (78%)	190 (93%)	14 (7%)	13	37
9	J	64/87 (74%)	56 (88%)	8 (12%)	3	12
10	K	163/215 (76%)	147 (90%)	16 (10%)	6	21
11	L	124/243 (51%)	118 (95%)	6 (5%)	21	53
12	M	298/492 (61%)	276 (93%)	22 (7%)	11	33
13	N	92/107 (86%)	83 (90%)	9 (10%)	6	21
14	O	37/340 (11%)	34 (92%)	3 (8%)	9	29
15	P	431/485 (89%)	383 (89%)	48 (11%)	5	16
16	Q	218/296 (74%)	192 (88%)	26 (12%)	4	14
17	R	312/345 (90%)	290 (93%)	22 (7%)	12	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S	97/226 (43%)	91 (94%)	6 (6%)	15	43
19	T	83/198 (42%)	76 (92%)	7 (8%)	9	28
20	U	1/7 (14%)	1 (100%)	0	100	100
All	All	7195/11074 (65%)	6571 (91%)	624 (9%)	11	26

All (624) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	173	VAL
1	A	250	THR
1	A	300	ASP
1	A	320	VAL
1	A	374	CYS
1	A	385	VAL
1	A	428	SER
1	A	444	LYS
1	A	446	GLU
1	A	476	ARG
1	A	487	VAL
1	A	512	ILE
1	A	522	SER
1	A	529	VAL
1	A	560	ILE
1	A	561	ASP
1	A	569	THR
1	A	576	SER
1	A	581	SER
1	A	595	ASN
1	A	601	LEU
1	A	607	ASN
1	A	617	LEU
1	A	637	MET
1	A	675	LEU
1	A	682	LEU
1	A	708	GLN
1	A	714	ASP
1	A	738	LEU
1	A	775	THR
1	A	782	THR
1	A	791	VAL

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Mol	Chain	Res	Type
1	A	796	LEU
1	A	826	SER
1	A	833	LEU
1	A	855	SER
1	A	904	LEU
1	A	907	VAL
1	A	941	THR
1	A	943	LEU
1	A	968	LEU
1	A	978	VAL
1	A	1031	THR
1	A	1040	MET
1	A	1043	LEU
1	A	1098	GLU
1	A	1104	SER
1	A	1131	SER
1	A	1136	LEU
2	B	211	LEU
2	B	229	VAL
2	B	237	THR
2	B	243	GLU
2	B	245	MET
2	B	268	VAL
2	B	336	LYS
2	B	339	ASP
2	B	356	LEU
2	B	371	GLU
2	B	373	LEU
2	B	390	VAL
2	B	419	LYS
2	B	421	VAL
2	B	430	ASP
2	B	439	VAL
2	B	446	ASP
2	B	458	LEU
2	B	468	SER
2	B	470	LEU
2	B	498	MET
2	B	524	ILE
2	B	552	LEU
2	B	563	VAL
2	B	571	THR

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Mol	Chain	Res	Type
2	B	575	LEU
2	B	586	VAL
2	B	588	MET
2	B	590	THR
2	B	600	TYR
2	B	622	ILE
2	B	625	ILE
2	B	629	ASP
2	B	647	ILE
2	B	678	SER
2	B	689	ILE
2	B	690	ILE
2	B	692	MET
2	B	696	ASP
2	B	707	HIS
2	B	713	VAL
2	B	720	TYR
2	B	730	THR
2	B	735	MET
2	B	792	PRO
2	B	813	LEU
2	B	817	THR
2	B	839	LEU
2	B	880	MET
2	B	881	THR
2	B	885	SER
2	B	893	LEU
2	B	901	SER
2	B	911	ILE
2	B	946	THR
2	B	949	SER
2	B	950	THR
2	B	1006	SER
2	B	1012	PHE
2	B	1085	HIS
2	B	1111	SER
2	C	365	THR
2	C	370	GLN
2	C	373	LEU
2	C	403	VAL
2	C	406	THR
2	C	407	THR

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Mol	Chain	Res	Type
2	C	435	ASN
2	C	452	SER
2	C	462	VAL
2	C	465	MET
2	C	478	ILE
2	C	487	ARG
2	C	495	ARG
2	C	500	HIS
2	C	517	ASP
2	C	532	ILE
2	C	543	ILE
2	C	544	GLU
2	C	548	ASN
2	C	551	LEU
2	C	574	THR
2	C	576	LEU
2	C	587	ARG
2	C	590	THR
2	C	650	GLU
2	C	652	LEU
2	C	655	MET
2	C	671	ASN
2	C	676	ILE
2	C	748	GLN
2	C	754	THR
2	C	774	SER
2	C	788	VAL
2	C	791	SER
2	C	812	LEU
2	C	823	ILE
2	C	827	SER
2	C	833	VAL
2	C	842	GLU
2	C	853	THR
2	C	954	ARG
2	C	1009	VAL
2	C	1027	SER
2	C	1058	ASP
2	C	1080	ASP
2	C	1095	VAL
2	C	1097	THR
3	D	266	THR

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Mol	Chain	Res	Type
3	D	325	GLN
3	D	332	LEU
3	D	333	SER
3	D	336	LEU
3	D	350	LEU
3	D	356	SER
3	D	448	ASP
3	D	455	CYS
3	D	469	LEU
3	D	471	THR
3	D	553	ILE
3	D	554	ASP
3	D	565	THR
3	D	569	LEU
3	D	615	ASN
3	D	620	ASN
3	D	629	ILE
3	D	637	ASN
3	D	747	THR
3	D	754	LEU
3	D	787	VAL
3	D	793	LEU
3	D	809	ARG
3	D	810	LEU
3	D	905	THR
3	D	906	LEU
3	D	938	GLU
3	D	964	LYS
3	D	976	LEU
3	D	988	ARG
3	D	1246	THR
3	D	1249	SER
3	D	1312	SER
3	D	1314	LEU
3	D	1331	THR
3	D	1372	ASN
3	D	1374	LYS
3	D	1397	SER
3	D	1398	SER
3	D	1407	ILE
3	D	1409	SER
3	D	1412	SER

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Mol	Chain	Res	Type
3	D	1424	LEU
3	D	1426	LEU
3	D	1445	LEU
3	D	1665	VAL
3	D	1666	GLU
3	D	1675	ILE
3	D	1763	THR
3	D	1770	GLU
3	D	1773	THR
3	D	1788	ASP
3	D	1811	ILE
3	D	1814	ASP
3	D	1815	PHE
3	D	1959	HIS
3	D	2006	SER
3	D	2013	ILE
3	D	2019	LEU
3	D	2024	THR
3	D	2031	ASP
3	D	2033	ASN
3	D	2035	LEU
3	D	2058	LEU
3	D	2065	ILE
3	D	2127	VAL
3	D	2129	GLU
3	D	2153	TYR
3	D	2155	LEU
3	D	2165	ASP
3	D	2183	ASN
3	D	2212	ASN
3	D	2235	SER
3	D	2239	LEU
3	D	2251	VAL
3	D	2258	SER
3	D	2262	GLU
3	D	2264	LEU
3	D	2266	THR
3	D	2283	GLU
3	D	2289	LEU
3	D	2293	LEU
3	D	2299	LEU
3	D	2303	ILE

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Mol	Chain	Res	Type
3	D	2320	ILE
3	D	2337	THR
3	D	2343	ILE
3	D	2345	THR
3	D	2364	THR
3	D	2365	SER
3	D	2366	ASN
3	D	2371	ILE
3	D	2379	LEU
3	D	2445	LEU
3	D	2446	ASN
3	D	2507	LYS
3	D	2518	GLU
3	D	2524	LEU
3	D	2532	LEU
3	D	2553	THR
3	D	2554	ILE
3	D	2560	LEU
3	D	2592	LEU
3	D	2593	LEU
3	D	2673	LYS
3	D	2676	ILE
3	D	2679	LYS
3	D	2689	LEU
3	D	2698	SER
3	D	2714	PHE
3	D	2719	THR
3	D	2731	THR
3	D	2766	LEU
3	D	2771	LEU
3	D	2806	THR
3	D	2808	GLN
3	D	2810	TRP
3	D	2863	LEU
3	D	2865	ASP
3	D	2868	ASP
3	D	2874	ASN
3	D	2891	PHE
3	D	2898	SER
3	D	2919	LYS
3	D	2937	ILE
3	D	2955	GLU

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Mol	Chain	Res	Type
4	E	56	THR
4	E	58	GLU
4	E	70	THR
4	E	72	SER
4	E	103	THR
4	E	126	LEU
4	E	127	THR
4	E	140	LEU
4	E	164	GLN
4	E	177	SER
4	E	202	TRP
4	E	216	VAL
4	E	234	ARG
4	E	243	GLU
4	E	248	THR
4	E	313	SER
4	E	317	THR
4	E	319	SER
4	E	338	VAL
4	E	346	LEU
4	E	609	THR
4	E	621	ARG
4	E	625	VAL
4	E	642	VAL
4	E	645	ASP
4	E	682	VAL
4	E	692	LEU
4	E	706	LEU
4	E	718	VAL
4	E	769	ARG
4	E	772	LEU
4	E	776	THR
4	E	808	THR
4	E	818	ASP
4	E	820	VAL
4	E	832	THR
4	E	856	SER
4	E	864	THR
4	E	897	SER
4	E	898	ASP
4	E	907	LEU
4	E	909	ASP

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Mol	Chain	Res	Type
4	E	918	THR
4	E	974	GLN
4	E	976	LYS
5	F	70	LEU
5	F	90	ARG
5	F	138	THR
5	F	232	VAL
5	F	236	VAL
5	F	263	GLU
5	F	264	GLN
5	F	288	GLU
5	F	550	ASP
5	F	554	ASN
5	F	586	LEU
5	F	587	LEU
5	F	597	LEU
5	F	612	SER
5	F	620	GLU
5	F	631	ARG
5	F	645	ILE
5	F	647	ILE
5	F	656	GLN
5	F	684	GLU
5	F	690	VAL
5	F	726	GLU
5	F	730	VAL
5	F	766	CYS
5	F	767	PHE
5	F	793	ARG
5	F	812	MET
5	F	815	SER
5	F	826	ILE
5	F	833	THR
5	F	837	SER
5	F	838	THR
5	F	884	ARG
5	F	892	GLN
5	F	930	SER
5	F	942	VAL
5	F	946	ASN
5	F	947	GLN
5	F	948	THR

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Mol	Chain	Res	Type
5	F	949	ARG
5	F	998	GLU
5	F	1001	GLN
5	F	1014	ARG
5	F	1023	LEU
6	G	110	GLU
6	G	116	CYS
6	G	117	LEU
6	G	126	LEU
6	G	163	GLN
6	G	172	LEU
6	G	174	VAL
6	G	177	SER
6	G	215	SER
6	G	231	MET
6	G	234	VAL
6	G	239	ASP
6	G	243	VAL
6	G	246	LEU
6	G	253	GLU
6	G	257	ARG
6	G	262	SER
6	G	264	ASP
6	G	265	ARG
6	G	267	ASP
6	G	276	LEU
6	G	298	LEU
6	G	345	LEU
6	G	355	THR
6	G	369	LEU
6	G	400	HIS
6	G	402	LEU
6	G	420	SER
6	G	443	GLN
6	G	466	LEU
6	G	477	GLU
6	G	490	GLU
7	H	85	SER
7	H	114	GLN
7	H	132	GLU
7	H	147	GLU
7	H	149	THR

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Mol	Chain	Res	Type
7	H	169	SER
7	H	175	ASP
7	H	198	ASP
7	H	228	SER
7	H	246	GLN
7	H	251	VAL
7	H	266	LEU
7	H	273	VAL
7	H	283	SER
7	H	301	THR
7	H	308	CYS
7	H	314	LEU
7	H	351	SER
7	H	355	LEU
7	H	383	SER
7	H	413	CYS
7	H	414	ASP
7	H	416	GLN
7	H	433	GLU
7	H	449	LYS
7	H	458	SER
7	H	467	ASP
7	H	468	GLU
7	H	477	ASP
7	H	483	GLU
7	H	489	GLU
8	I	61	ASN
8	I	84	THR
8	I	92	ILE
8	I	125	SER
8	I	127	GLN
8	I	154	GLN
8	I	157	ILE
8	I	209	ARG
8	I	232	LEU
8	I	236	VAL
8	I	241	VAL
8	I	244	VAL
8	I	289	SER
8	I	303	SER
9	J	36	ASP
9	J	46	SER

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Mol	Chain	Res	Type
9	J	50	THR
9	J	67	ASP
9	J	73	LEU
9	J	88	ILE
9	J	91	GLU
9	J	101	VAL
10	K	67	THR
10	K	87	THR
10	K	94	THR
10	K	96	THR
10	K	98	ARG
10	K	108	MET
10	K	129	THR
10	K	143	THR
10	K	150	GLN
10	K	152	ARG
10	K	193	LEU
10	K	205	PHE
10	K	223	GLU
10	K	238	LEU
10	K	242	VAL
10	K	244	LYS
11	L	167	LEU
11	L	174	LEU
11	L	192	SER
11	L	234	VAL
11	L	292	LEU
11	L	296	VAL
12	M	266	LEU
12	M	292	HIS
12	M	335	SER
12	M	339	VAL
12	M	359	VAL
12	M	363	CYS
12	M	384	MET
12	M	390	SER
12	M	396	LEU
12	M	405	THR
12	M	419	THR
12	M	423	LEU
12	M	429	ARG
12	M	447	THR

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Mol	Chain	Res	Type
12	M	536	ARG
12	M	555	LEU
12	M	559	ARG
12	M	567	ASN
12	M	607	LEU
12	M	615	THR
12	M	621	ASP
12	M	636	GLU
13	N	31	LEU
13	N	33	LEU
13	N	35	LYS
13	N	37	ASP
13	N	40	LYS
13	N	48	THR
13	N	80	SER
13	N	126	ASP
13	N	134	VAL
14	O	432	ASP
14	O	440	VAL
14	O	465	SER
15	P	65	LEU
15	P	75	GLN
15	P	85	VAL
15	P	87	THR
15	P	109	VAL
15	P	116	THR
15	P	122	GLN
15	P	124	VAL
15	P	133	GLU
15	P	141	GLN
15	P	162	ASP
15	P	189	GLU
15	P	196	LEU
15	P	216	MET
15	P	246	LEU
15	P	252	VAL
15	P	257	LEU
15	P	302	THR
15	P	313	LEU
15	P	324	LEU
15	P	328	LEU
15	P	330	ARG

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Mol	Chain	Res	Type
15	P	340	VAL
15	P	347	PRO
15	P	350	LEU
15	P	371	GLU
15	P	385	VAL
15	P	390	GLN
15	P	398	SER
15	P	408	SER
15	P	413	LEU
15	P	428	LYS
15	P	472	THR
15	P	485	MET
15	P	498	LEU
15	P	506	LEU
15	P	507	LEU
15	P	519	GLU
15	P	564	LYS
15	P	568	GLU
15	P	573	MET
15	P	593	THR
15	P	628	VAL
15	P	641	VAL
15	P	643	MET
15	P	644	LEU
15	P	677	THR
15	P	682	PHE
16	Q	101	VAL
16	Q	112	THR
16	Q	115	ASN
16	Q	117	LYS
16	Q	133	PHE
16	Q	142	GLU
16	Q	145	ILE
16	Q	162	LEU
16	Q	166	MET
16	Q	177	ARG
16	Q	182	LEU
16	Q	183	GLN
16	Q	224	LEU
16	Q	231	MET
16	Q	232	GLN
16	Q	243	LEU

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Mol	Chain	Res	Type
16	Q	244	ASP
16	Q	249	SER
16	Q	261	LEU
16	Q	265	LYS
16	Q	280	LEU
16	Q	293	GLU
16	Q	318	LEU
16	Q	325	SER
16	Q	333	MET
16	Q	354	LEU
17	R	33	VAL
17	R	44	ASP
17	R	49	THR
17	R	66	VAL
17	R	114	ARG
17	R	115	VAL
17	R	137	SER
17	R	149	LEU
17	R	158	LEU
17	R	163	LEU
17	R	214	LEU
17	R	217	GLN
17	R	238	SER
17	R	251	LEU
17	R	289	GLN
17	R	304	VAL
17	R	324	VAL
17	R	342	LYS
17	R	359	LEU
17	R	395	THR
17	R	402	LEU
17	R	430	THR
18	S	40	ASP
18	S	60	THR
18	S	76	LYS
18	S	87	LEU
18	S	102	SER
18	S	130	LEU
19	T	31	SER
19	T	33	GLU
19	T	49	VAL
19	T	58	LEU

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Mol	Chain	Res	Type
19	T	65	CYS
19	T	71	VAL
19	T	80	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	138	GLN
1	A	176	ASN
1	A	190	GLN
1	A	308	GLN
1	A	314	GLN
1	A	327	GLN
1	A	335	GLN
1	A	340	GLN
1	A	541	ASN
1	A	546	ASN
1	A	665	GLN
1	A	687	ASN
1	A	771	HIS
1	A	801	HIS
1	A	909	GLN
2	B	257	ASN
2	B	259	ASN
2	B	274	GLN
2	B	475	HIS
2	B	506	ASN
2	B	530	ASN
2	B	548	ASN
2	B	661	ASN
2	B	751	HIS
2	B	764	ASN
2	B	832	ASN
2	B	892	ASN
2	B	952	GLN
2	C	456	GLN
2	C	638	GLN
2	C	649	ASN
2	C	661	ASN
2	C	710	ASN
2	C	764	ASN

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Mol	Chain	Res	Type
2	C	832	ASN
2	C	864	HIS
2	C	944	HIS
2	C	952	GLN
3	D	38	ASN
3	D	355	GLN
3	D	473	ASN
3	D	574	ASN
3	D	615	ASN
3	D	621	HIS
3	D	630	ASN
3	D	638	ASN
3	D	735	GLN
3	D	782	ASN
3	D	784	HIS
3	D	818	ASN
3	D	826	GLN
3	D	909	HIS
3	D	994	ASN
3	D	1126	ASN
3	D	1137	ASN
3	D	1138	ASN
3	D	1290	ASN
3	D	1308	ASN
3	D	1326	HIS
3	D	1364	ASN
3	D	1448	ASN
3	D	1728	GLN
3	D	1760	GLN
3	D	1915	ASN
3	D	1956	GLN
3	D	1976	HIS
3	D	1983	HIS
3	D	1994	GLN
3	D	2054	GLN
3	D	2080	ASN
3	D	2140	HIS
3	D	2173	GLN
3	D	2180	ASN
3	D	2183	ASN
3	D	2185	ASN
3	D	2194	HIS

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Mol	Chain	Res	Type
3	D	2218	GLN
3	D	2248	ASN
3	D	2263	GLN
3	D	2344	HIS
3	D	2377	GLN
3	D	2416	ASN
3	D	2446	ASN
3	D	2529	ASN
3	D	2572	ASN
3	D	2628	GLN
3	D	2653	ASN
3	D	2725	GLN
3	D	2729	GLN
3	D	2763	ASN
3	D	2780	ASN
3	D	2784	GLN
3	D	2817	HIS
3	D	2874	ASN
3	D	2941	ASN
3	D	2953	GLN
4	E	130	HIS
4	E	139	GLN
4	E	164	GLN
4	E	205	GLN
4	E	263	HIS
4	E	270	GLN
4	E	332	GLN
4	E	619	HIS
4	E	633	GLN
4	E	824	GLN
4	E	886	GLN
4	E	964	GLN
5	F	152	GLN
5	F	153	GLN
5	F	177	GLN
5	F	279	GLN
5	F	664	ASN
5	F	779	GLN
5	F	867	GLN
5	F	893	HIS
5	F	896	GLN
5	F	907	ASN

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Mol	Chain	Res	Type
5	F	913	HIS
5	F	938	GLN
5	F	947	GLN
5	F	1001	GLN
5	F	1008	HIS
5	F	1017	GLN
6	G	157	GLN
6	G	160	GLN
6	G	258	HIS
6	G	271	HIS
6	G	400	HIS
7	H	114	GLN
7	H	145	GLN
7	H	246	GLN
7	H	249	ASN
7	H	406	GLN
7	H	415	ASN
8	I	61	ASN
8	I	138	GLN
8	I	355	GLN
9	J	117	ASN
10	K	106	GLN
10	K	121	GLN
10	K	150	GLN
11	L	191	ASN
11	L	193	GLN
11	L	293	GLN
12	M	270	GLN
12	M	400	HIS
12	M	404	HIS
12	M	416	HIS
12	M	517	HIS
12	M	528	HIS
12	M	567	ASN
13	N	108	GLN
15	P	141	GLN
15	P	165	GLN
15	P	215	HIS
15	P	268	GLN
15	P	367	HIS
15	P	403	GLN
15	P	517	ASN

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Mol	Chain	Res	Type
16	Q	152	ASN
16	Q	195	GLN
16	Q	253	GLN
16	Q	255	ASN
16	Q	270	GLN
16	Q	279	GLN
17	R	45	HIS
17	R	186	HIS
17	R	228	ASN
17	R	237	ASN
17	R	260	GLN
17	R	321	ASN
18	S	32	HIS
18	S	39	HIS
18	S	55	GLN
18	S	127	GLN
19	T	74	ASN
19	T	122	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPO	B	337	2	8,10,11	1.60	1 (12%)	10,14,16	1.64	2 (20%)
17	SEP	R	126	17	8,9,10	1.52	1 (12%)	8,12,14	1.35	1 (12%)
19	SEP	T	28	19	8,9,10	1.55	1 (12%)	8,12,14	1.49	2 (25%)
18	SEP	S	85	18	8,9,10	1.54	1 (12%)	8,12,14	1.41	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	TPO	R	167	17	8,10,11	1.04	0	10,14,16	2.04	1 (10%)
18	TPO	S	107	18	8,10,11	1.57	1 (12%)	10,14,16	1.73	1 (10%)
2	TPO	B	347	2	8,10,11	1.08	0	10,14,16	2.02	1 (10%)
19	SEP	T	18	19	8,9,10	1.54	1 (12%)	8,12,14	1.76	2 (25%)
18	SEP	S	84	18	8,9,10	1.56	1 (12%)	8,12,14	1.68	2 (25%)
9	4HH	J	72	9	21,26,27	0.38	0	27,35,37	0.59	0
2	TPO	B	346	2	8,10,11	1.58	1 (12%)	10,14,16	1.73	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	B	337	2	-	3/9/11/13	-
17	SEP	R	126	17	-	0/5/8/10	-
19	SEP	T	28	19	-	1/5/8/10	-
18	SEP	S	85	18	-	2/5/8/10	-
17	TPO	R	167	17	-	2/9/11/13	-
18	TPO	S	107	18	-	1/9/11/13	-
2	TPO	B	347	2	-	4/9/11/13	-
19	SEP	T	18	19	-	0/5/8/10	-
18	SEP	S	84	18	-	1/5/8/10	-
9	4HH	J	72	9	-	5/32/35/37	-
2	TPO	B	346	2	-	3/9/11/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	S	84	SEP	P-O1P	3.39	1.61	1.50
2	B	337	TPO	P-O1P	3.37	1.61	1.50
2	B	346	TPO	P-O1P	3.37	1.61	1.50
19	T	18	SEP	P-O1P	3.36	1.61	1.50
19	T	28	SEP	P-O1P	3.36	1.61	1.50
18	S	85	SEP	P-O1P	3.36	1.61	1.50
18	S	107	TPO	P-O1P	3.33	1.61	1.50
17	R	126	SEP	P-O1P	3.32	1.61	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	167	TPO	P-OG1-CB	-5.94	105.28	123.21
2	B	347	TPO	P-OG1-CB	-5.79	105.72	123.21
2	B	346	TPO	P-OG1-CB	-5.00	108.09	123.21
18	S	107	TPO	P-OG1-CB	-4.97	108.21	123.21
2	B	337	TPO	P-OG1-CB	-4.19	110.55	123.21
19	T	18	SEP	OG-CB-CA	3.31	111.36	108.14
18	S	84	SEP	P-OG-CB	-3.12	109.69	118.30
19	T	18	SEP	P-OG-CB	-3.12	109.70	118.30
18	S	85	SEP	P-OG-CB	-2.99	110.05	118.30
18	S	84	SEP	OG-CB-CA	2.96	111.03	108.14
17	R	126	SEP	P-OG-CB	-2.93	110.24	118.30
19	T	28	SEP	P-OG-CB	-2.60	111.13	118.30
19	T	28	SEP	OG-CB-CA	2.53	110.61	108.14
2	B	337	TPO	CG2-CB-CA	-2.19	108.83	113.16

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	R	167	TPO	CB-OG1-P-O1P
18	S	84	SEP	N-CA-CB-OG
18	S	85	SEP	N-CA-CB-OG
18	S	107	TPO	O-C-CA-CB
2	B	337	TPO	C-CA-CB-CG2
2	B	346	TPO	N-CA-CB-OG1
2	B	346	TPO	C-CA-CB-CG2
2	B	347	TPO	N-CA-CB-OG1
2	B	347	TPO	O-C-CA-CB
2	B	347	TPO	CB-OG1-P-O1P
19	T	28	SEP	CA-CB-OG-P
9	J	72	4HH	CP-CQ-NR-CS
9	J	72	4HH	OR-CQ-NR-CS
2	B	346	TPO	CB-OG1-P-O3P
2	B	347	TPO	C-CA-CB-CG2
18	S	85	SEP	CB-OG-P-O1P
9	J	72	4HH	CB-OG-P-O3P
9	J	72	4HH	CL2-CK-CM-OM
17	R	167	TPO	CB-OG1-P-O2P
2	B	337	TPO	CB-OG1-P-O2P
9	J	72	4HH	CB-OG-P-O2P
2	B	337	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	R	126	SEP	1	0
17	R	167	TPO	2	0
9	J	72	4HH	1	0
2	B	346	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	SQD	I	401	-	48,49,54	1.03	5 (10%)	57,60,65	1.62	11 (19%)
22	LMG	A	1201	-	46,46,55	0.85	2 (4%)	54,54,63	1.34	8 (14%)
22	LMG	I	402	-	32,32,55	0.99	2 (6%)	40,40,63	1.30	6 (15%)
22	LMG	M	801	-	48,48,55	0.84	2 (4%)	56,56,63	1.40	7 (12%)
25	DGA	L	3001	-	33,33,43	1.21	3 (9%)	35,35,45	1.72	3 (8%)
28	A1LXL	P	702	-	33,33,33	4.63	15 (45%)	51,51,51	2.17	16 (31%)
26	Y01	D	3102	-	38,38,38	0.46	0	57,57,57	0.62	0
24	SQD	K	302	-	44,45,54	1.09	6 (13%)	53,56,65	1.73	10 (18%)
28	A1LXL	P	701	-	33,33,33	4.56	14 (42%)	51,51,51	2.28	13 (25%)
26	Y01	M	802	-	38,38,38	0.46	0	57,57,57	0.62	0
27	DGD	N	201	-	42,42,67	1.11	3 (7%)	56,56,81	1.38	6 (10%)
25	DGA	D	3101	-	38,38,43	1.13	3 (7%)	40,40,45	1.68	3 (7%)
22	LMG	K	301	-	41,41,55	0.82	0	49,49,63	1.27	5 (10%)
27	DGD	I	403	-	41,41,67	1.21	4 (9%)	55,55,81	1.44	7 (12%)
24	SQD	B	1201	-	45,46,54	1.08	6 (13%)	54,57,65	1.71	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMG	C	1201	-	24,24,55	0.71	0	26,26,63	1.07	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	SQD	I	401	-	-	21/44/64/69	0/1/1/1
22	LMG	A	1201	-	-	15/41/61/70	0/1/1/1
22	LMG	I	402	-	-	13/27/47/70	0/1/1/1
22	LMG	M	801	-	-	21/43/63/70	0/1/1/1
25	DGA	L	3001	-	-	22/35/35/45	-
28	A1LXL	P	702	-	-	6/15/73/73	0/4/4/4
26	Y01	D	3102	-	-	6/19/77/77	0/4/4/4
24	SQD	K	302	-	-	20/40/60/69	0/1/1/1
28	A1LXL	P	701	-	-	10/15/73/73	0/4/4/4
26	Y01	M	802	-	-	4/19/77/77	0/4/4/4
27	DGD	N	201	-	-	11/30/70/95	0/2/2/2
25	DGA	D	3101	-	-	28/40/40/45	-
22	LMG	K	301	-	-	14/36/56/70	0/1/1/1
27	DGD	I	403	-	-	12/29/69/95	0/2/2/2
24	SQD	B	1201	-	-	17/41/61/69	0/1/1/1
22	LMG	C	1201	-	-	11/26/26/70	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P	702	A1LXL	C18-C19	15.17	1.66	1.33
28	P	701	A1LXL	C18-C19	14.13	1.64	1.33
28	P	702	A1LXL	C06-C08	-10.39	1.36	1.54
28	P	701	A1LXL	C06-C08	-8.93	1.38	1.54
28	P	701	A1LXL	C09-C08	8.66	1.72	1.54
28	P	701	A1LXL	C17-C16	8.65	1.67	1.53
28	P	702	A1LXL	C17-C16	8.44	1.67	1.53
28	P	702	A1LXL	C09-C08	8.22	1.71	1.54
28	P	701	A1LXL	C13-C12	-8.01	1.39	1.54
28	P	701	A1LXL	C12-C08	7.24	1.68	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P	702	A1LXL	C13-C12	-7.22	1.41	1.54
28	P	702	A1LXL	C12-C08	6.60	1.67	1.55
28	P	702	A1LXL	C13-C14	6.26	1.66	1.53
28	P	701	A1LXL	C13-C14	6.18	1.66	1.53
28	P	701	A1LXL	C20-C15	5.34	1.65	1.56
28	P	702	A1LXL	C20-C15	4.71	1.63	1.56
28	P	701	A1LXL	C05-C06	4.43	1.65	1.54
28	P	702	A1LXL	C05-C06	4.42	1.65	1.54
28	P	701	A1LXL	C10-C11	3.83	1.62	1.54
25	L	3001	DGA	OG2-CB1	3.43	1.44	1.34
25	D	3101	DGA	OG2-CB1	3.41	1.43	1.34
25	L	3001	DGA	OG1-CA1	3.38	1.43	1.33
28	P	702	A1LXL	C10-C11	3.34	1.61	1.54
25	D	3101	DGA	OG1-CA1	3.20	1.42	1.33
28	P	701	A1LXL	C07-C06	3.15	1.60	1.53
28	P	702	A1LXL	C07-C06	3.14	1.60	1.53
24	I	401	SQD	O48-C23	3.13	1.42	1.33
24	K	302	SQD	O48-C23	2.99	1.42	1.33
24	I	401	SQD	O47-C7	2.94	1.42	1.34
27	I	403	DGD	O2G-C2G	-2.90	1.39	1.46
27	N	201	DGD	O2G-C2G	-2.83	1.39	1.46
24	B	1201	SQD	O48-C23	2.82	1.41	1.33
22	M	801	LMG	O8-C9	-2.69	1.39	1.45
24	K	302	SQD	O47-C7	2.57	1.41	1.34
24	B	1201	SQD	O47-C7	2.55	1.41	1.34
24	K	302	SQD	O2-C2	-2.52	1.37	1.43
27	N	201	DGD	O1G-C1G	-2.37	1.39	1.45
22	A	1201	LMG	O7-C8	-2.37	1.40	1.46
28	P	701	A1LXL	C22-C23	-2.36	1.46	1.51
24	B	1201	SQD	O2-C2	-2.33	1.37	1.43
24	B	1201	SQD	O3-C3	-2.30	1.37	1.43
22	A	1201	LMG	O4-C4	-2.27	1.37	1.43
28	P	702	A1LXL	C24-C19	2.27	1.56	1.51
24	B	1201	SQD	O4-C4	-2.27	1.37	1.43
24	I	401	SQD	O2-C2	-2.24	1.37	1.43
27	I	403	DGD	O1G-C1G	-2.24	1.40	1.45
28	P	702	A1LXL	C10-C09	2.23	1.60	1.54
27	I	403	DGD	O3G-C3G	-2.22	1.39	1.43
25	L	3001	DGA	OG2-CG2	-2.22	1.41	1.46
24	K	302	SQD	O4-C4	-2.18	1.37	1.43
27	I	403	DGD	O6D-C5D	-2.18	1.39	1.44
24	K	302	SQD	O3-C3	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	M	801	LMG	O7-C8	-2.17	1.41	1.46
28	P	701	A1LXL	C24-C19	2.16	1.56	1.51
24	I	401	SQD	O3-C3	-2.14	1.37	1.43
24	I	401	SQD	O4-C4	-2.13	1.38	1.43
22	I	402	LMG	O8-C9	-2.12	1.40	1.45
22	I	402	LMG	O7-C8	-2.12	1.41	1.46
24	K	302	SQD	O47-C45	-2.11	1.41	1.46
24	B	1201	SQD	O47-C45	-2.11	1.41	1.46
25	D	3101	DGA	OG2-CG2	-2.08	1.41	1.46
28	P	701	A1LXL	C10-C09	2.06	1.59	1.54
28	P	702	A1LXL	C12-C11	2.05	1.58	1.55
28	P	702	A1LXL	C22-C23	-2.03	1.46	1.51
27	N	201	DGD	O6D-C5D	-2.00	1.39	1.44

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	701	A1LXL	C17-C18-C19	-7.67	110.91	125.06
25	L	3001	DGA	CDB-CCB-CBB	-6.75	80.14	114.42
25	D	3101	DGA	CDB-CCB-CBB	-6.65	80.64	114.42
28	P	701	A1LXL	C27-C12-C13	-5.80	101.42	110.59
28	P	701	A1LXL	C20-C19-C18	-5.73	114.14	122.90
28	P	702	A1LXL	C13-C12-C08	5.19	124.34	116.57
28	P	702	A1LXL	C17-C18-C19	-5.15	115.56	125.06
25	D	3101	DGA	OG2-CB1-CB2	5.00	122.28	111.50
28	P	702	A1LXL	C27-C12-C13	-4.98	102.73	110.59
27	I	403	DGD	O3G-C3G-C2G	-4.40	100.28	110.90
24	B	1201	SQD	O6-C1-C2	4.37	115.12	108.30
24	B	1201	SQD	O7-S-C6	4.32	112.08	106.94
24	I	401	SQD	O7-S-C6	4.22	111.96	106.94
27	N	201	DGD	O3G-C3G-C2G	-4.18	100.81	110.90
25	L	3001	DGA	OG2-CB1-CB2	4.09	120.31	111.50
24	B	1201	SQD	O8-S-C6	4.02	112.14	105.74
24	K	302	SQD	O9-S-O7	-4.00	100.09	113.95
24	K	302	SQD	O6-C1-C2	3.98	114.51	108.30
24	B	1201	SQD	O9-S-O7	-3.97	100.21	113.95
28	P	701	A1LXL	C13-C12-C08	3.91	122.42	116.57
24	I	401	SQD	O9-S-O7	-3.78	100.88	113.95
24	K	302	SQD	O47-C7-C8	3.74	119.55	111.50
24	K	302	SQD	O7-S-C6	3.69	111.32	106.94
24	K	302	SQD	C3-C4-C5	3.63	116.71	110.24
28	P	701	A1LXL	C13-C12-C11	3.60	112.86	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	I	401	SQD	O9-S-C6	3.57	111.18	106.94
24	B	1201	SQD	O47-C7-C8	3.56	119.17	111.50
28	P	701	A1LXL	C17-C16-C15	3.54	114.01	109.71
24	I	401	SQD	O5-C5-C4	3.53	116.10	109.69
24	K	302	SQD	O5-C5-C4	3.52	116.09	109.69
24	I	401	SQD	O6-C1-C2	3.49	113.75	108.30
28	P	702	A1LXL	C24-C19-C20	-3.47	111.81	116.42
27	I	403	DGD	O6D-C1D-O3G	-3.39	101.95	109.97
28	P	701	A1LXL	C07-C06-C08	3.29	117.96	112.92
24	I	401	SQD	O47-C7-C8	3.29	118.58	111.50
28	P	702	A1LXL	C20-C15-C16	-3.24	107.88	112.73
28	P	702	A1LXL	C20-C19-C18	-3.22	117.97	122.90
24	K	302	SQD	O8-S-C6	3.18	110.81	105.74
28	P	702	A1LXL	C22-C23-C24	3.18	114.67	110.31
24	B	1201	SQD	O9-S-C6	3.17	110.71	106.94
27	N	201	DGD	O6D-C1D-O3G	-3.15	102.52	109.97
28	P	701	A1LXL	C24-C19-C20	-3.13	112.26	116.42
28	P	702	A1LXL	C26-C20-C15	-2.99	108.12	111.68
24	K	302	SQD	C4-C3-C2	2.99	116.04	110.82
28	P	701	A1LXL	C21-C20-C19	2.98	114.22	108.75
28	P	702	A1LXL	C13-C12-C11	2.97	111.88	107.27
28	P	702	A1LXL	C16-C17-C18	-2.90	108.56	112.73
27	I	403	DGD	C4E-C3E-C2E	-2.84	105.87	110.82
28	P	702	A1LXL	C07-C06-C08	-2.78	108.67	112.92
28	P	701	A1LXL	C17-C16-C11	-2.77	106.89	110.91
22	M	801	LMG	O1-C7-C8	-2.76	104.23	110.90
24	I	401	SQD	O8-S-C6	2.75	110.12	105.74
25	D	3101	DGA	OG1-CA1-CA2	2.73	120.49	111.91
28	P	702	A1LXL	C21-C22-C23	2.71	113.94	110.47
27	N	201	DGD	O5D-C6D-C5D	-2.70	104.05	109.05
27	I	403	DGD	C1D-C2D-C3D	-2.70	104.38	110.00
24	K	302	SQD	O9-S-C6	2.70	110.14	106.94
22	I	402	LMG	O6-C1-O1	-2.62	103.76	109.97
28	P	702	A1LXL	C04-C03-C28	-2.61	106.11	112.36
24	I	401	SQD	O48-C23-C24	2.60	120.08	111.91
25	L	3001	DGA	OG1-CA1-CA2	2.60	120.07	111.91
22	I	402	LMG	O3-C3-C2	-2.60	104.34	110.35
27	N	201	DGD	C3G-C2G-C1G	-2.60	105.64	111.79
24	B	1201	SQD	O5-C5-C4	2.60	114.41	109.69
22	K	301	LMG	O6-C1-O1	-2.56	103.91	109.97
24	I	401	SQD	C3-C4-C5	2.56	114.81	110.24
22	M	801	LMG	C1-C2-C3	-2.55	104.69	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1201	LMG	O3-C3-C2	-2.55	104.46	110.35
22	M	801	LMG	C38-C37-C36	-2.54	101.55	114.42
28	P	702	A1LXL	C17-C16-C11	2.53	114.58	110.91
22	A	1201	LMG	O2-C2-C1	-2.52	103.93	110.05
24	K	302	SQD	O48-C23-C24	2.52	119.80	111.91
22	M	801	LMG	C40-C39-C38	-2.44	102.02	114.42
22	A	1201	LMG	C1-C2-C3	-2.42	104.96	110.00
27	I	403	DGD	C3G-C2G-C1G	-2.40	106.10	111.79
22	A	1201	LMG	O6-C1-O1	-2.38	104.33	109.97
22	K	301	LMG	C1-C2-C3	-2.37	105.07	110.00
22	A	1201	LMG	C38-C37-C36	-2.35	102.48	114.42
27	N	201	DGD	O6E-C1E-O5D	-2.35	104.40	109.97
28	P	702	A1LXL	C27-C12-C08	-2.35	107.34	111.71
27	I	403	DGD	O6E-C1E-O5D	-2.33	104.46	109.97
22	C	1201	LMG	O1-C7-C8	-2.28	105.74	111.78
24	I	401	SQD	C4-C3-C2	2.27	114.79	110.82
22	A	1201	LMG	O7-C10-O9	-2.27	118.22	123.70
24	B	1201	SQD	O48-C23-O10	-2.27	117.87	123.59
24	I	401	SQD	C44-O6-C1	2.26	118.16	113.74
22	I	402	LMG	O2-C2-C1	-2.25	104.58	110.05
28	P	702	A1LXL	C10-C11-C12	2.25	106.55	103.84
24	B	1201	SQD	O47-C7-O49	-2.23	118.32	123.70
24	B	1201	SQD	C4-C3-C2	2.21	114.69	110.82
22	I	402	LMG	O1-C1-C2	-2.18	104.91	108.30
27	I	403	DGD	O2D-C2D-C1D	-2.16	104.79	110.05
24	B	1201	SQD	C3-C4-C5	2.16	114.09	110.24
22	A	1201	LMG	O1-C1-C2	-2.16	104.93	108.30
22	M	801	LMG	O3-C3-C2	-2.14	105.41	110.35
22	I	402	LMG	O1-C7-C8	-2.12	105.79	110.90
22	K	301	LMG	O1-C7-C8	-2.12	105.79	110.90
28	P	701	A1LXL	C14-C13-C12	2.11	116.40	112.78
24	B	1201	SQD	O48-C23-C24	2.10	118.50	111.91
27	N	201	DGD	C3D-C4D-C5D	-2.08	106.52	110.24
22	A	1201	LMG	O8-C28-O10	-2.08	118.34	123.59
22	K	301	LMG	O3-C3-C2	-2.08	105.54	110.35
28	P	701	A1LXL	C04-C05-C06	-2.07	109.93	115.34
22	I	402	LMG	C1-C2-C3	-2.06	105.71	110.00
22	K	301	LMG	O2-C2-C1	-2.04	105.09	110.05
22	M	801	LMG	O1-C1-C2	-2.03	105.13	108.30
28	P	701	A1LXL	C14-C15-C16	-2.02	108.85	111.75
22	M	801	LMG	O6-C1-O1	-2.02	105.19	109.97

There are no chirality outliers.

All (231) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	C	1201	LMG	O1-C7-C8-O7
22	I	402	LMG	O6-C1-O1-C7
22	M	801	LMG	C2-C1-O1-C7
22	M	801	LMG	O6-C1-O1-C7
24	B	1201	SQD	O47-C45-C46-O48
24	I	401	SQD	C8-C7-O47-C45
24	I	401	SQD	C5-C6-S-O7
24	I	401	SQD	C5-C6-S-O8
24	I	401	SQD	C5-C6-S-O9
24	K	302	SQD	O49-C7-O47-C45
24	K	302	SQD	C8-C7-O47-C45
24	K	302	SQD	C5-C6-S-O7
24	K	302	SQD	C5-C6-S-O8
25	D	3101	DGA	CB2-CB1-OG2-CG2
25	D	3101	DGA	CG1-CG2-CG3-OXT
25	D	3101	DGA	OG2-CG2-CG3-OXT
25	L	3001	DGA	CB2-CB1-OG2-CG2
25	L	3001	DGA	CG1-CG2-CG3-OXT
25	L	3001	DGA	OG2-CG2-CG3-OXT
28	P	701	A1LXL	C28-C03-C04-C05
28	P	701	A1LXL	C03-C04-C05-C06
28	P	702	A1LXL	C02-C03-C04-C05
28	P	702	A1LXL	C03-C04-C05-C06
24	B	1201	SQD	O10-C23-O48-C46
24	I	401	SQD	O49-C7-O47-C45
25	D	3101	DGA	OB1-CB1-OG2-CG2
25	L	3001	DGA	OB1-CB1-OG2-CG2
22	A	1201	LMG	O10-C28-O8-C9
22	A	1201	LMG	C29-C28-O8-C9
24	B	1201	SQD	C24-C23-O48-C46
22	I	402	LMG	O6-C5-C6-O5
22	A	1201	LMG	C11-C10-O7-C8
22	A	1201	LMG	C30-C31-C32-C33
22	K	301	LMG	O6-C5-C6-O5
22	I	402	LMG	C4-C5-C6-O5
27	I	403	DGD	O6D-C1D-O3G-C3G
27	N	201	DGD	O6D-C1D-O3G-C3G
25	D	3101	DGA	CA2-CA1-OG1-CG1
22	I	402	LMG	O1-C7-C8-O7
22	K	301	LMG	C4-C5-C6-O5
28	P	701	A1LXL	C05-C06-C08-C12
27	I	403	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
24	I	401	SQD	C10-C11-C12-C13
25	D	3101	DGA	OA1-CA1-OG1-CG1
25	D	3101	DGA	CB1-CB2-CB3-CB4
25	L	3001	DGA	CB1-CB2-CB3-CB4
27	I	403	DGD	O6E-C5E-C6E-O5E
28	P	701	A1LXL	C05-C06-C08-C09
24	K	302	SQD	O5-C1-O6-C44
28	P	701	A1LXL	C04-C05-C06-C08
22	I	402	LMG	C11-C10-O7-C8
25	L	3001	DGA	CA2-CA1-OG1-CG1
27	I	403	DGD	C2A-C1A-O1G-C1G
22	M	801	LMG	O9-C10-O7-C8
22	A	1201	LMG	C19-C20-C21-C22
22	M	801	LMG	C29-C28-O8-C9
24	K	302	SQD	C11-C12-C13-C14
25	D	3101	DGA	CB5-CB6-CB7-CB8
25	L	3001	DGA	CB3-CB4-CB5-CB6
22	C	1201	LMG	O9-C10-O7-C8
22	I	402	LMG	C10-C11-C12-C13
24	I	401	SQD	C9-C10-C11-C12
24	K	302	SQD	C26-C27-C28-C29
25	L	3001	DGA	CA6-CA7-CA8-CA9
22	I	402	LMG	C28-C29-C30-C31
27	I	403	DGD	C2D-C1D-O3G-C3G
27	N	201	DGD	C2D-C1D-O3G-C3G
22	A	1201	LMG	C18-C19-C20-C21
25	L	3001	DGA	CA2-CA3-CA4-CA5
25	L	3001	DGA	OA1-CA1-OG1-CG1
22	A	1201	LMG	O6-C5-C6-O5
24	I	401	SQD	C12-C13-C14-C15
25	L	3001	DGA	CB2-CB3-CB4-CB5
22	M	801	LMG	C13-C14-C15-C16
25	D	3101	DGA	CBB-CCB-CDB-CEB
22	C	1201	LMG	C31-C32-C33-C34
28	P	701	A1LXL	C07-C06-C08-C09
22	C	1201	LMG	C30-C31-C32-C33
25	L	3001	DGA	CA4-CA5-CA6-CA7
22	A	1201	LMG	C31-C32-C33-C34
22	K	301	LMG	C18-C19-C20-C21
25	D	3101	DGA	CA9-CAA-CBA-CCA
25	D	3101	DGA	CAB-CBB-CCB-CDB
25	L	3001	DGA	CB9-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
25	D	3101	DGA	CB6-CB7-CB8-CB9
22	A	1201	LMG	C32-C33-C34-C35
22	M	801	LMG	C18-C19-C20-C21
24	I	401	SQD	C11-C12-C13-C14
28	P	701	A1LXL	C01-C02-C03-C04
22	C	1201	LMG	C13-C14-C15-C16
22	M	801	LMG	C11-C12-C13-C14
25	L	3001	DGA	CA5-CA6-CA7-CA8
22	A	1201	LMG	C29-C30-C31-C32
22	C	1201	LMG	C32-C33-C34-C35
24	K	302	SQD	C9-C10-C11-C12
25	D	3101	DGA	CA7-CA8-CA9-CAA
25	L	3001	DGA	CA7-CA8-CA9-CAA
22	M	801	LMG	C11-C10-O7-C8
22	I	402	LMG	C11-C12-C13-C14
27	I	403	DGD	C1A-C2A-C3A-C4A
22	K	301	LMG	C16-C17-C18-C19
22	K	301	LMG	C13-C14-C15-C16
24	I	401	SQD	C27-C28-C29-C30
24	I	401	SQD	C32-C33-C34-C35
22	M	801	LMG	C12-C13-C14-C15
26	D	3102	Y01	CAM-CAY-OAW-CBC
24	B	1201	SQD	C11-C10-C9-C8
22	C	1201	LMG	C28-C29-C30-C31
22	M	801	LMG	C10-C11-C12-C13
25	D	3101	DGA	CB4-CB5-CB6-CB7
24	K	302	SQD	C25-C26-C27-C28
22	I	402	LMG	O9-C10-O7-C8
24	K	302	SQD	C7-C8-C9-C10
24	B	1201	SQD	C12-C13-C14-C15
25	D	3101	DGA	CA2-CA3-CA4-CA5
26	M	802	Y01	CAJ-CAN-CBA-CAB
22	C	1201	LMG	C11-C10-O7-C8
24	B	1201	SQD	C8-C7-O47-C45
27	I	403	DGD	C2B-C1B-O2G-C2G
22	A	1201	LMG	O9-C10-O7-C8
24	I	401	SQD	C34-C35-C36-C37
26	D	3102	Y01	OAG-CAY-OAW-CBC
25	L	3001	DGA	CBB-CAB-CB9-CB8
27	N	201	DGD	C1B-C2B-C3B-C4B
27	N	201	DGD	C4E-C5E-C6E-O5E
22	M	801	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	L	3001	DGA	CB7-CB8-CB9-CAB
24	K	302	SQD	C44-C45-C46-O48
25	D	3101	DGA	CB9-CAB-CBB-CCB
27	N	201	DGD	O1G-C1G-C2G-C3G
24	B	1201	SQD	C9-C10-C11-C12
24	B	1201	SQD	C28-C29-C30-C31
25	D	3101	DGA	CB2-CB3-CB4-CB5
22	M	801	LMG	C31-C32-C33-C34
24	I	401	SQD	O5-C1-O6-C44
27	I	403	DGD	C1B-C2B-C3B-C4B
24	K	302	SQD	C24-C25-C26-C27
22	A	1201	LMG	C37-C38-C39-C40
26	M	802	Y01	CAJ-CAN-CBA-CAA
27	N	201	DGD	C2A-C3A-C4A-C5A
25	L	3001	DGA	CCB-CDB-CEB-CFB
28	P	701	A1LXL	C04-C05-C06-C07
27	I	403	DGD	C4E-C5E-C6E-O5E
22	A	1201	LMG	C33-C34-C35-C36
25	L	3001	DGA	CB5-CB6-CB7-CB8
22	K	301	LMG	C32-C33-C34-C35
22	M	801	LMG	C28-C29-C30-C31
22	I	402	LMG	C29-C28-O8-C9
24	B	1201	SQD	C44-C45-C46-O48
27	N	201	DGD	C1G-C2G-C3G-O3G
22	K	301	LMG	C11-C12-C13-C14
22	K	301	LMG	C28-C29-C30-C31
24	B	1201	SQD	C14-C15-C16-C17
24	K	302	SQD	C12-C13-C14-C15
24	K	302	SQD	O47-C45-C46-O48
27	N	201	DGD	O1G-C1G-C2G-O2G
24	K	302	SQD	C28-C29-C30-C31
22	C	1201	LMG	O1-C7-C8-C9
22	M	801	LMG	C33-C34-C35-C36
25	D	3101	DGA	CEB-CFB-CGB-CHB
22	K	301	LMG	C30-C31-C32-C33
24	I	401	SQD	C26-C27-C28-C29
25	D	3101	DGA	CA5-CA6-CA7-CA8
24	I	401	SQD	C30-C31-C32-C33
27	N	201	DGD	O6E-C5E-C6E-O5E
22	I	402	LMG	O1-C7-C8-C9
22	M	801	LMG	O10-C28-O8-C9
28	P	702	A1LXL	C04-C05-C06-C07

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Mol	Chain	Res	Type	Atoms
27	N	201	DGD	O2G-C2G-C3G-O3G
22	K	301	LMG	C15-C16-C17-C18
27	I	403	DGD	O1B-C1B-O2G-C2G
24	B	1201	SQD	C5-C6-S-O8
25	L	3001	DGA	CB4-CB5-CB6-CB7
27	I	403	DGD	C3B-C4B-C5B-C6B
26	D	3102	Y01	CAV-CBC-OAW-CAY
25	D	3101	DGA	CA4-CA5-CA6-CA7
24	B	1201	SQD	C5-C6-S-O9
24	K	302	SQD	C5-C6-S-O9
24	I	401	SQD	C7-C8-C9-C10
24	K	302	SQD	C30-C31-C32-C33
22	M	801	LMG	C7-C8-O7-C10
26	D	3102	Y01	CAR-CBC-OAW-CAY
22	I	402	LMG	O7-C8-C9-O8
24	B	1201	SQD	C25-C26-C27-C28
25	D	3101	DGA	CDB-CEB-CFB-CGB
22	M	801	LMG	C30-C31-C32-C33
24	K	302	SQD	C31-C32-C33-C34
24	B	1201	SQD	O6-C44-C45-O47
28	P	702	A1LXL	C01-C02-C03-C04
28	P	702	A1LXL	C28-C03-C04-C05
26	D	3102	Y01	CAM-CAL-CAX-OAF
25	D	3101	DGA	CA3-CA4-CA5-CA6
24	K	302	SQD	C32-C33-C34-C35
28	P	701	A1LXL	C01-C02-C03-C28
22	I	402	LMG	C7-C8-C9-O8
22	M	801	LMG	C32-C33-C34-C35
24	I	401	SQD	C24-C25-C26-C27
24	B	1201	SQD	C10-C11-C12-C13
22	K	301	LMG	C31-C32-C33-C34
26	M	802	Y01	CAM-CAL-CAX-OAH
25	D	3101	DGA	CBB-CAB-CB9-CB8
24	I	401	SQD	C11-C10-C9-C8
22	C	1201	LMG	C14-C15-C16-C17
22	C	1201	LMG	C12-C13-C14-C15
25	D	3101	DGA	CB7-CB8-CB9-CAB
24	I	401	SQD	C25-C26-C27-C28
24	B	1201	SQD	O6-C44-C45-C46
26	M	802	Y01	CAM-CAL-CAX-OAF
22	M	801	LMG	C38-C39-C40-C41
26	D	3102	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
22	M	801	LMG	C19-C20-C21-C22
27	N	201	DGD	O2G-C1B-C2B-C3B
25	D	3101	DGA	CA8-CA9-CAA-CBA
22	M	801	LMG	C17-C18-C19-C20
22	A	1201	LMG	C35-C36-C37-C38
28	P	701	A1LXL	C02-C03-C04-C05
22	K	301	LMG	O1-C7-C8-C9
22	K	301	LMG	O7-C8-C9-O8
24	B	1201	SQD	O48-C23-C24-C25
25	D	3101	DGA	OG1-CA1-CA2-CA3
25	L	3001	DGA	OG1-CA1-CA2-CA3
27	I	403	DGD	O2G-C1B-C2B-C3B
28	P	702	A1LXL	C01-C02-C03-C28
25	D	3101	DGA	CA6-CA7-CA8-CA9
24	I	401	SQD	O49-C7-C8-C9
24	K	302	SQD	C10-C11-C12-C13
25	L	3001	DGA	OA1-CA1-CA2-CA3
22	A	1201	LMG	C34-C35-C36-C37
22	K	301	LMG	C20-C21-C22-C23
25	D	3101	DGA	OA1-CA1-CA2-CA3
24	I	401	SQD	O47-C7-C8-C9

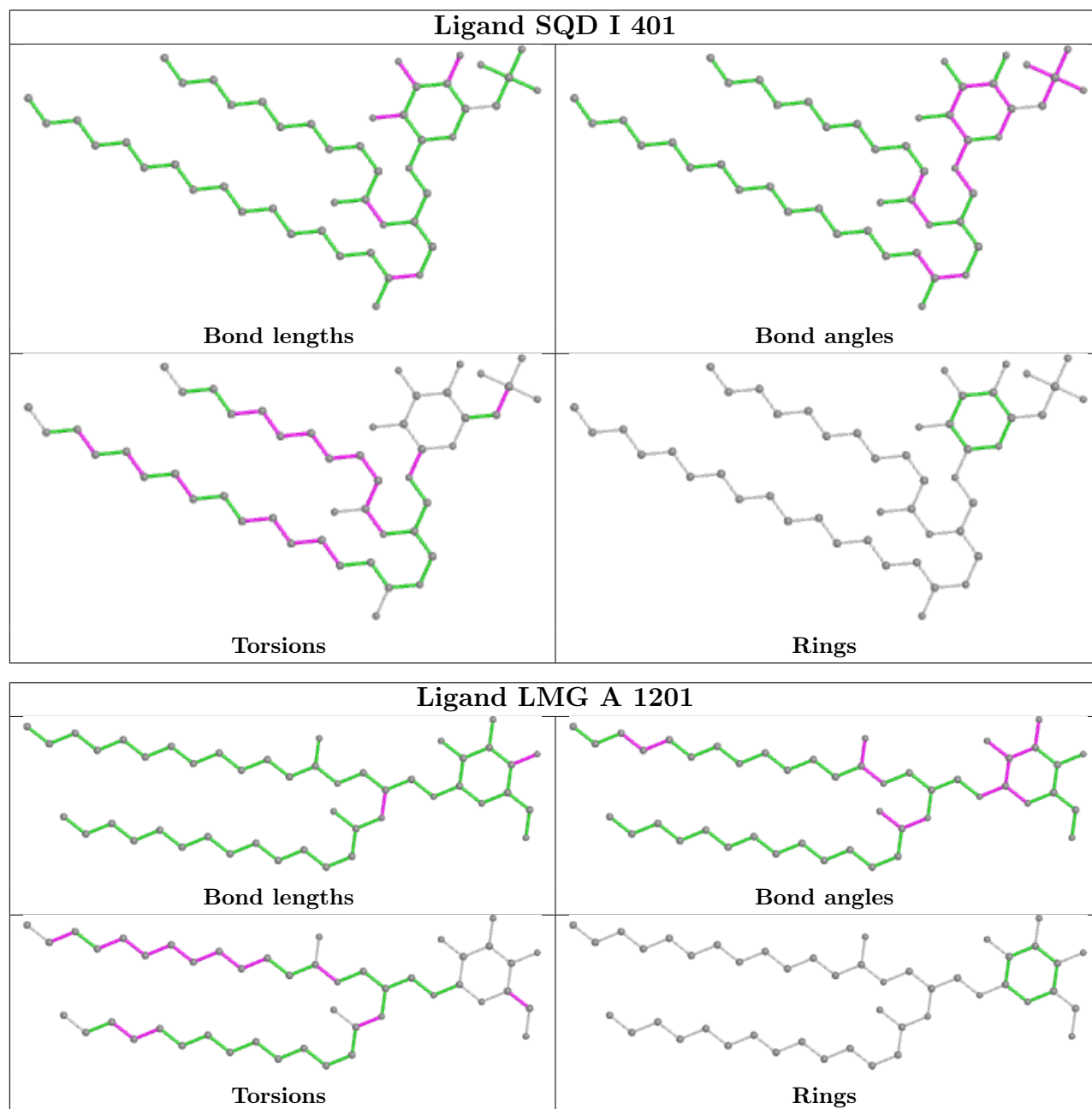
There are no ring outliers.

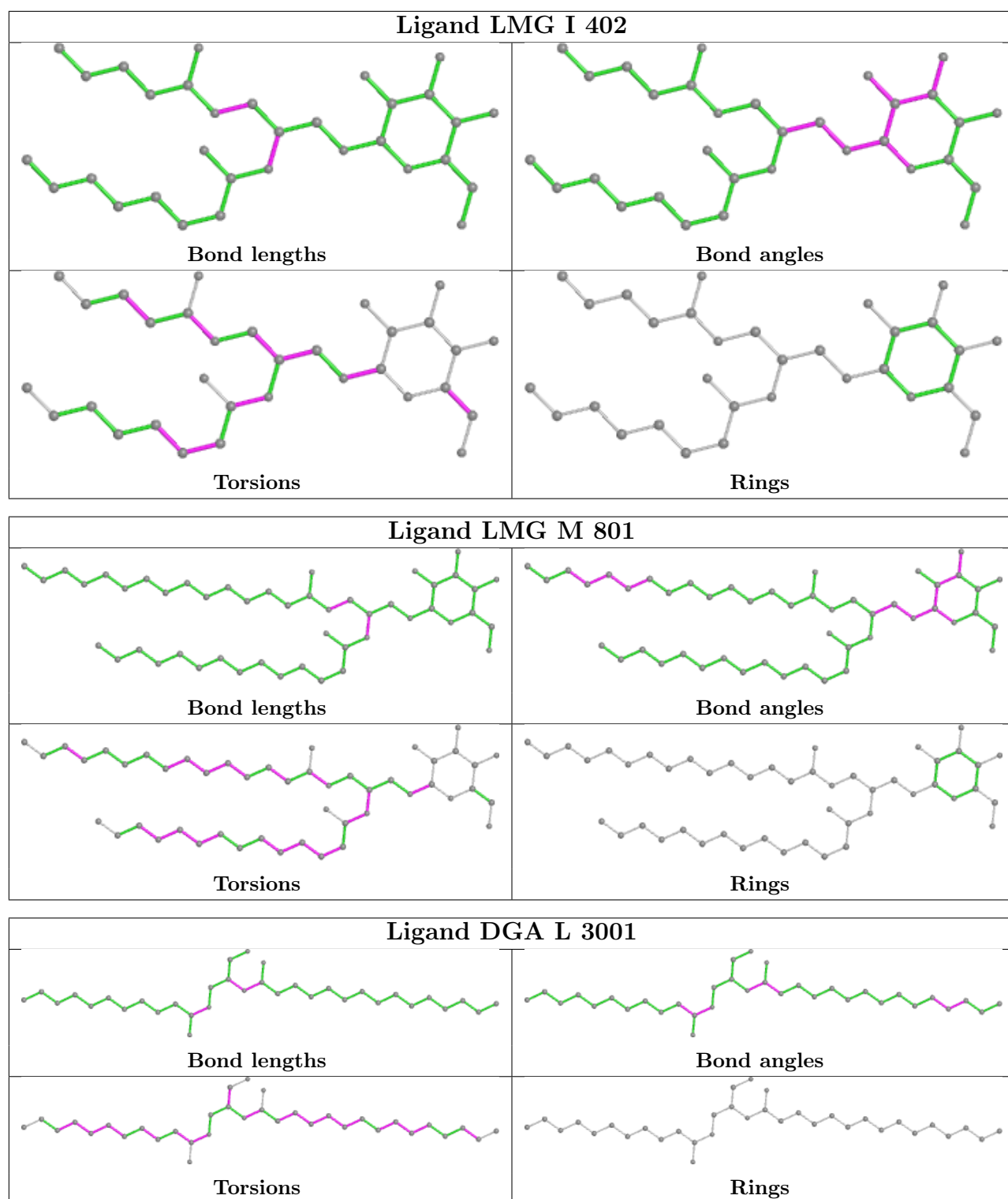
11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	I	401	SQD	5	0
22	A	1201	LMG	3	0
22	I	402	LMG	2	0
22	M	801	LMG	1	0
25	L	3001	DGA	1	0
28	P	702	A1LXL	2	0
28	P	701	A1LXL	8	0
26	M	802	Y01	4	0
25	D	3101	DGA	1	0
22	K	301	LMG	1	0
27	I	403	DGD	2	0

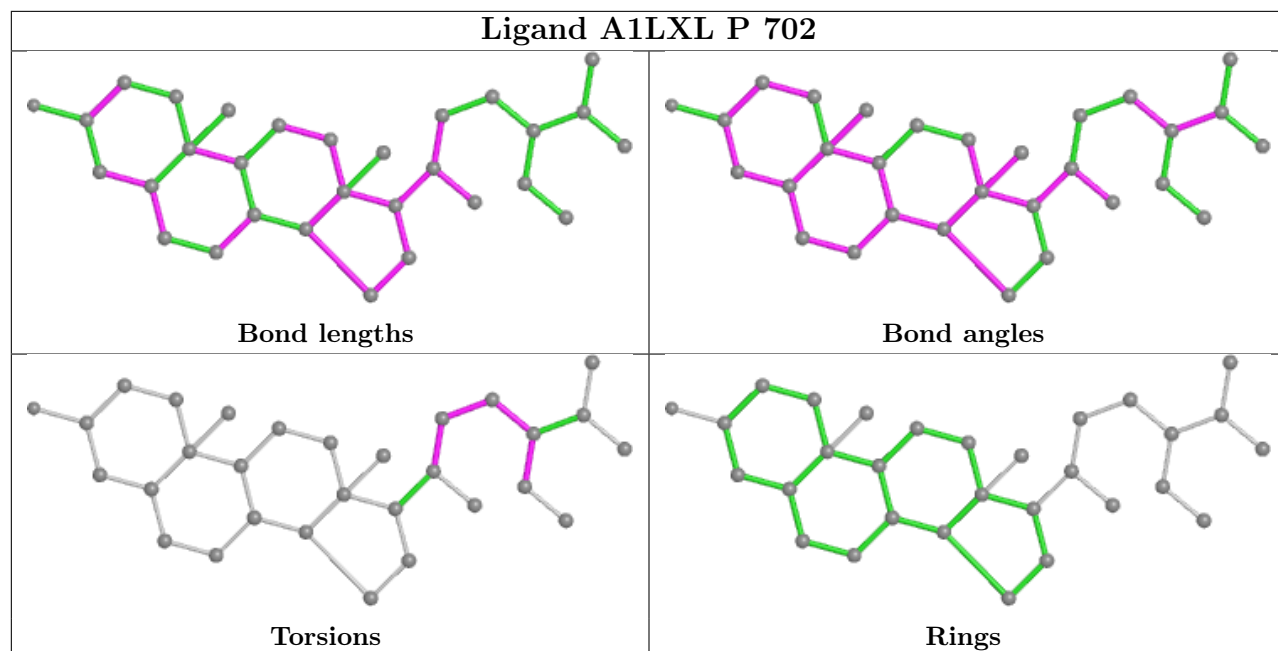
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

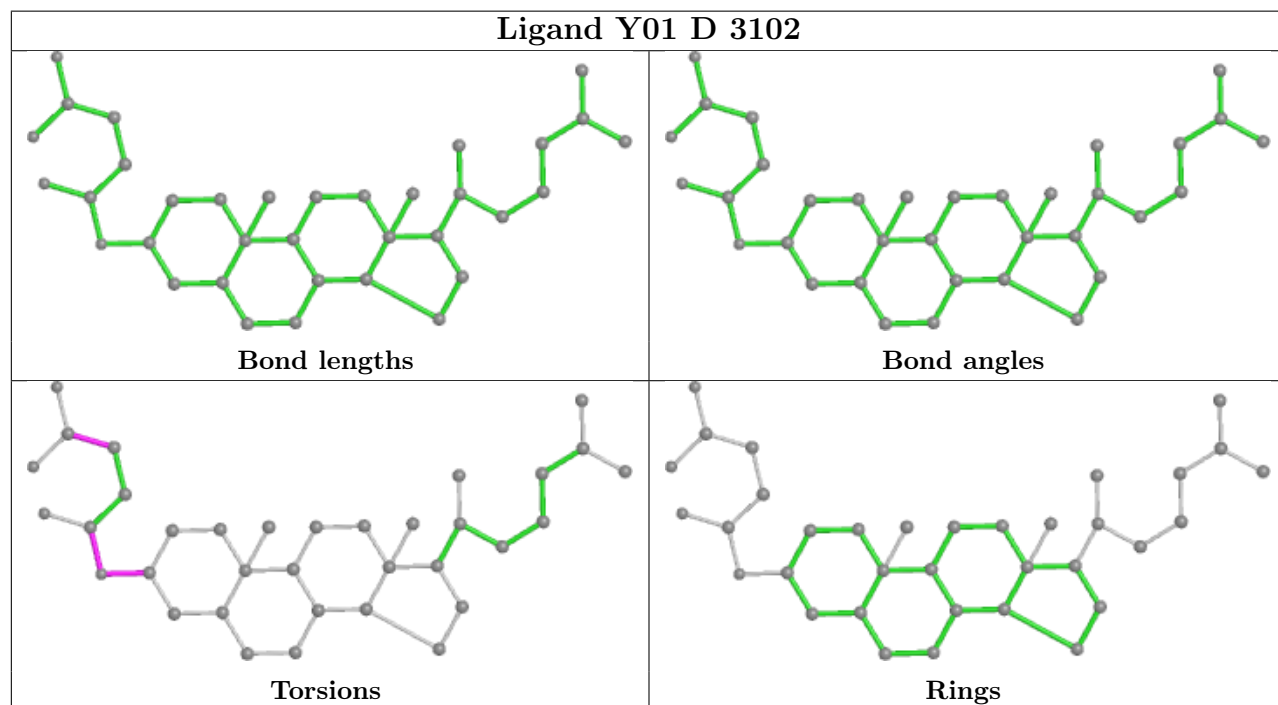


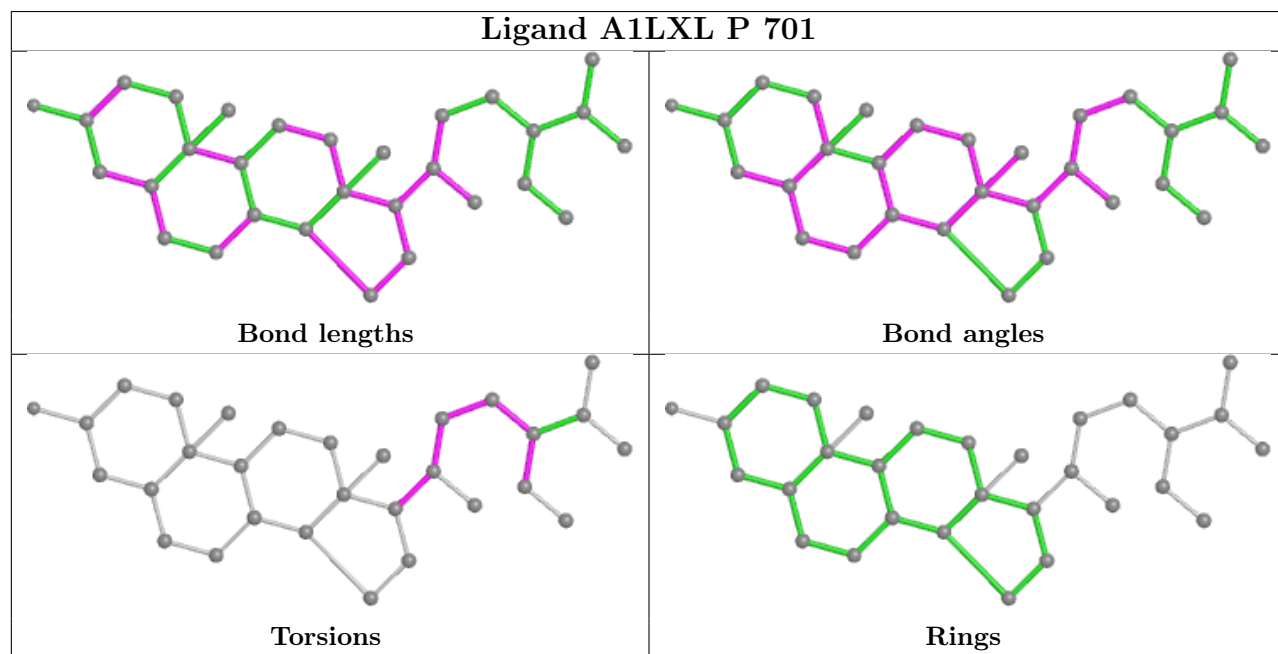
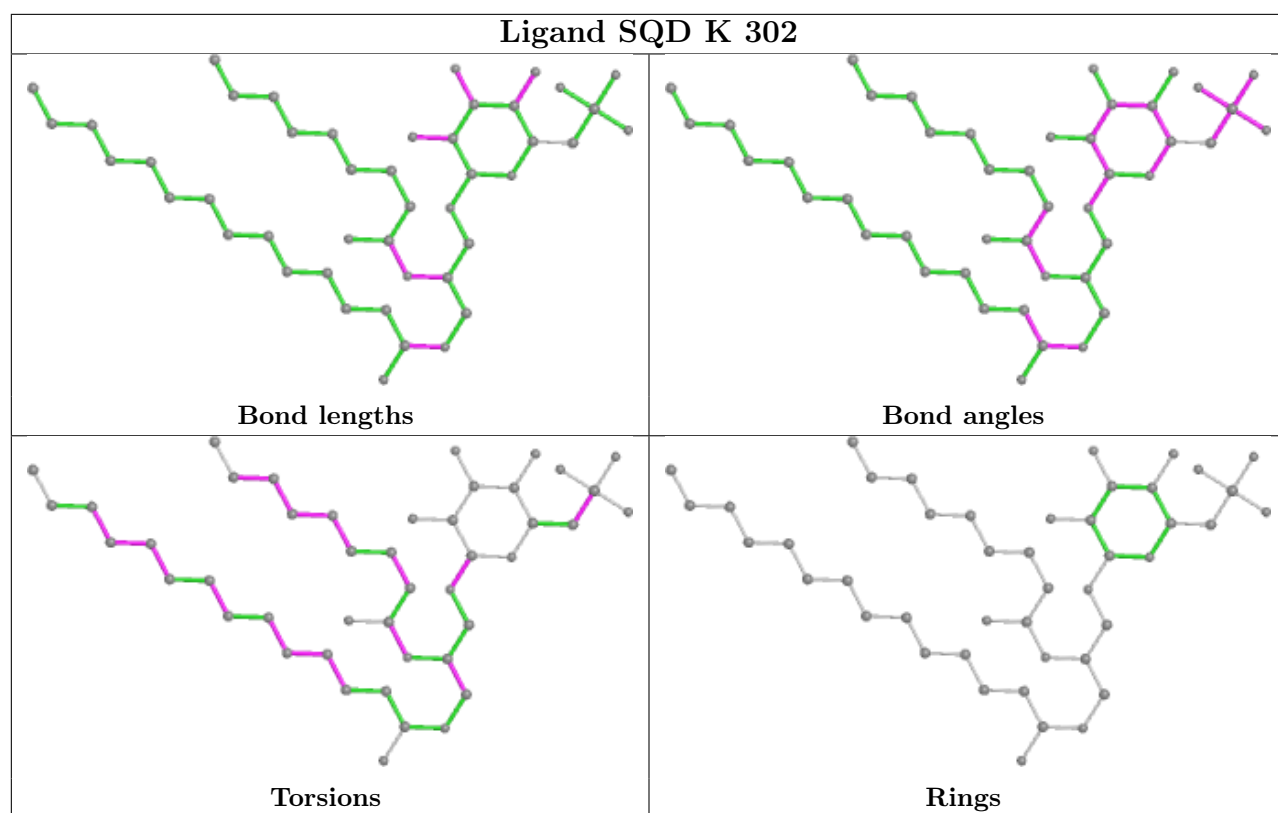


Ligand A1LXL P 702

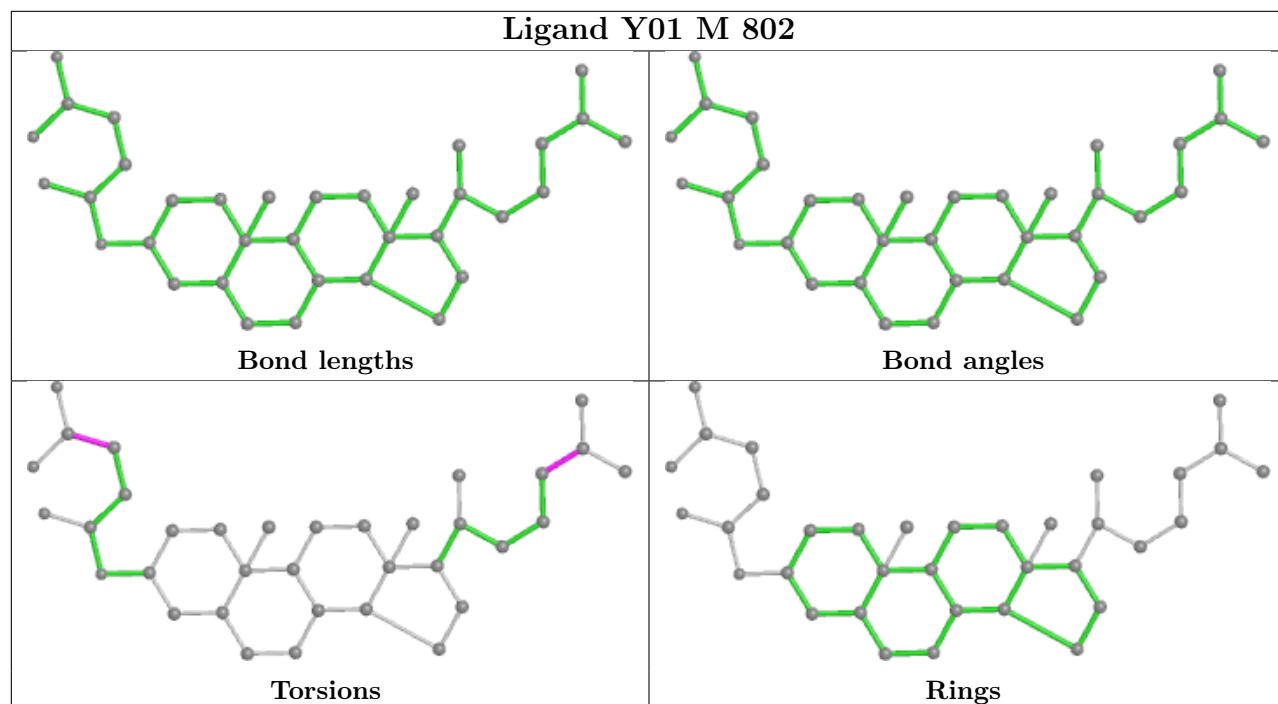


Ligand Y01 D 3102

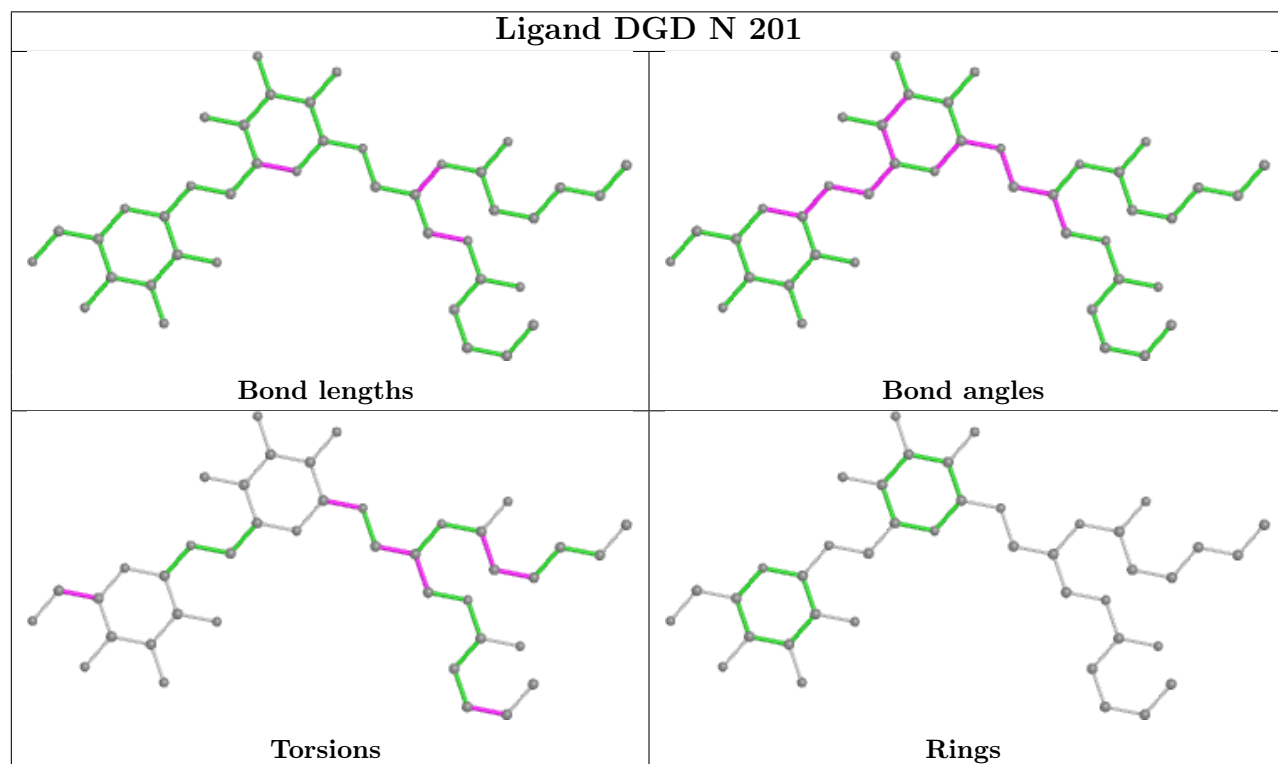




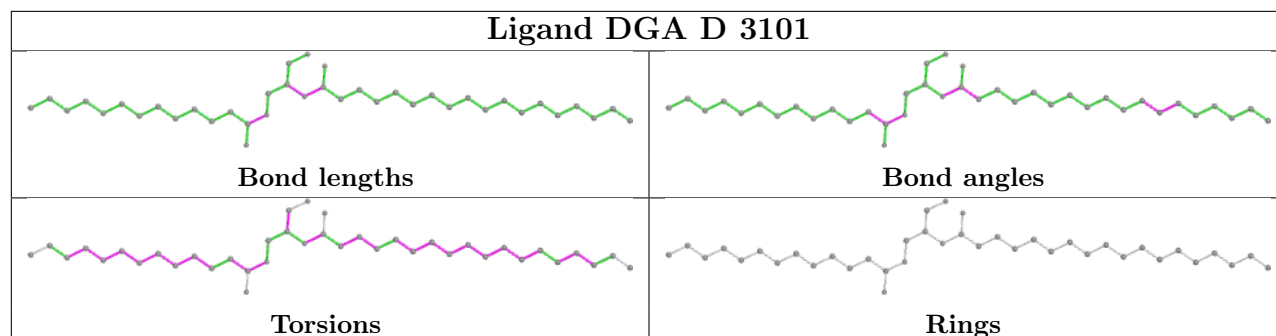
Ligand Y01 M 802



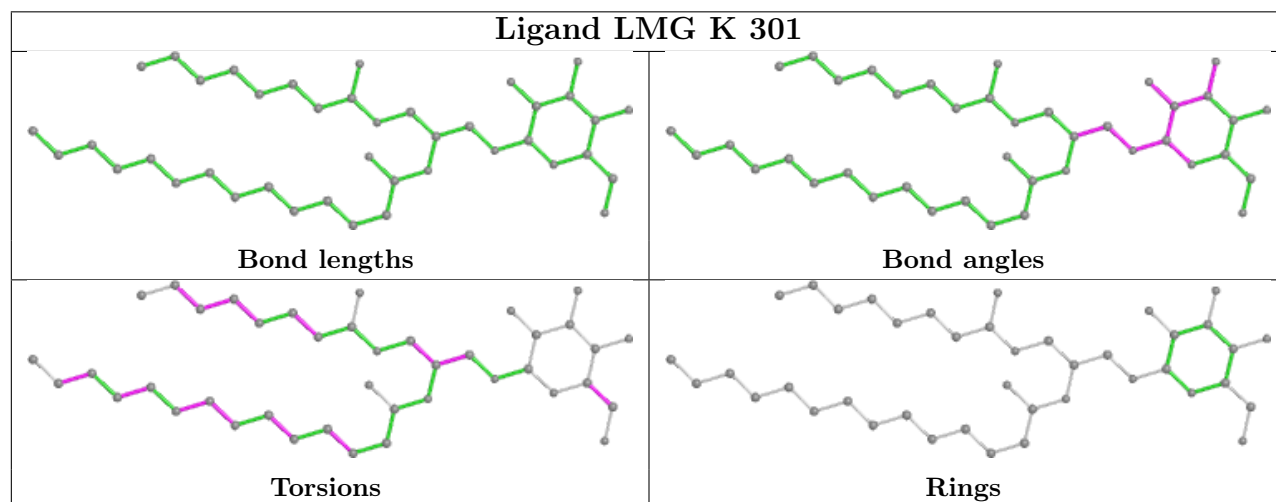
Ligand DGD N 201



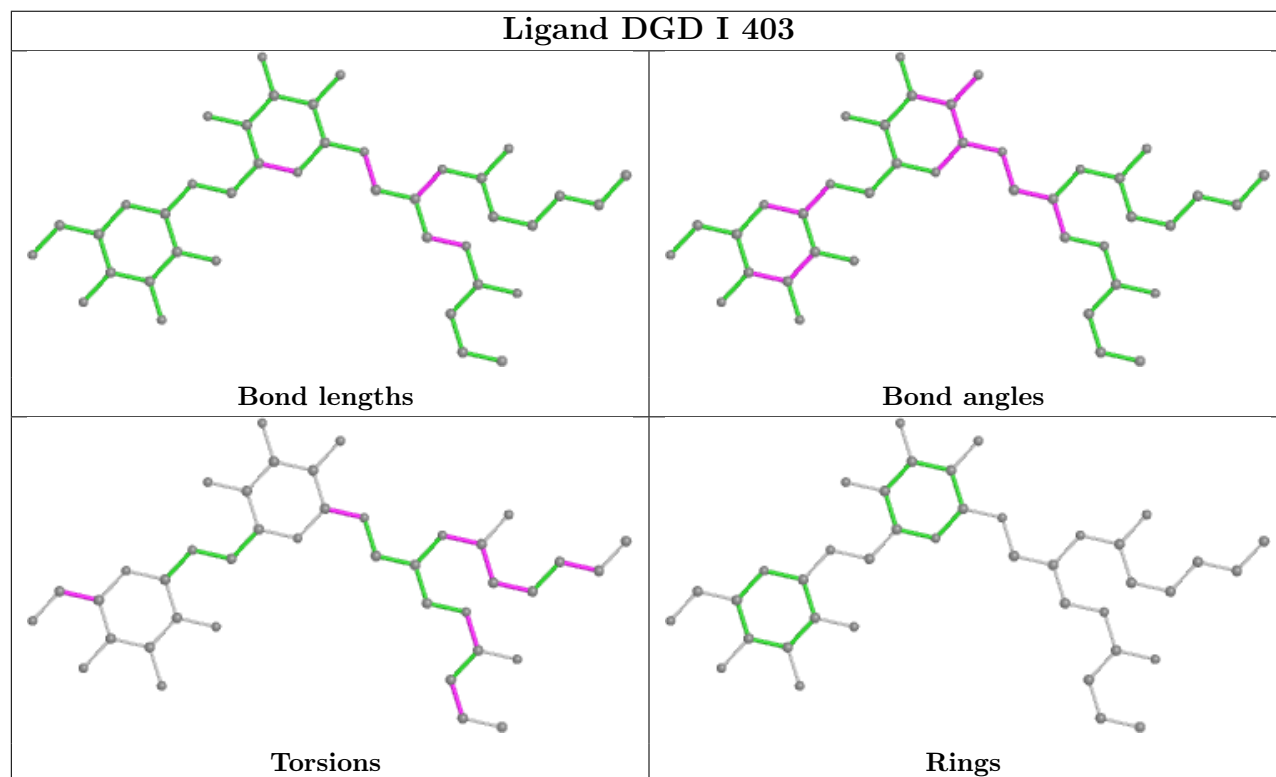
Ligand DGA D 3101

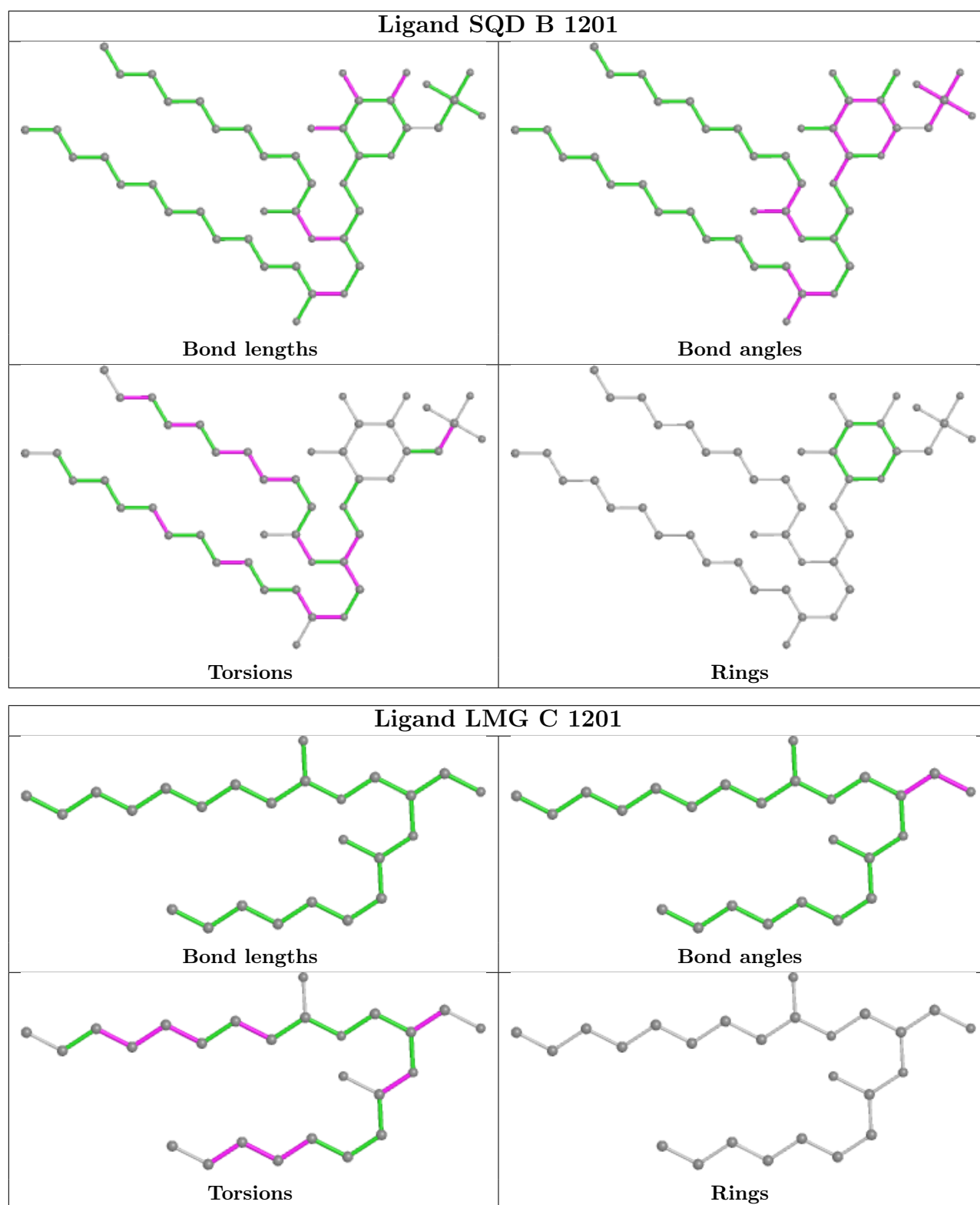


Ligand LMG K 301



Ligand DGD I 403





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

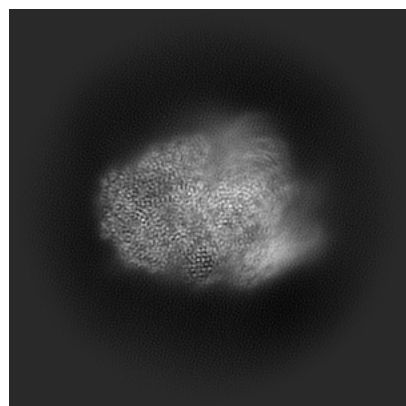
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38590. These allow visual inspection of the internal detail of the map and identification of artifacts.

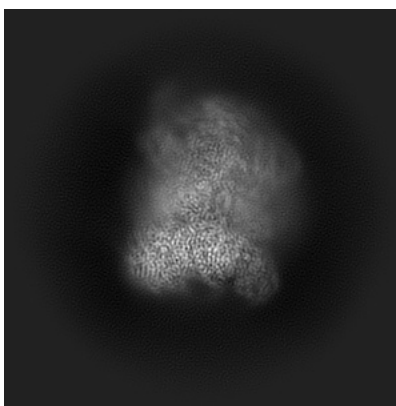
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

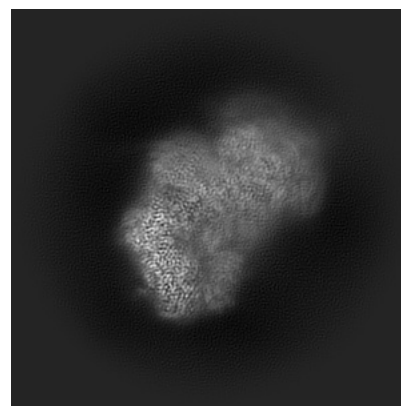
6.1.1 Primary map



X

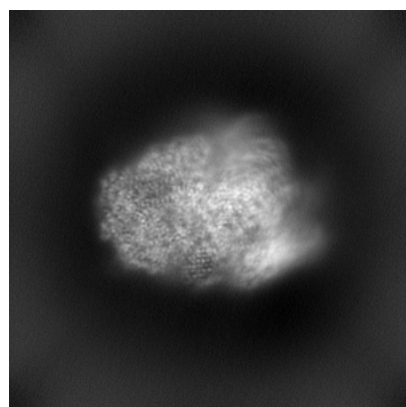


Y

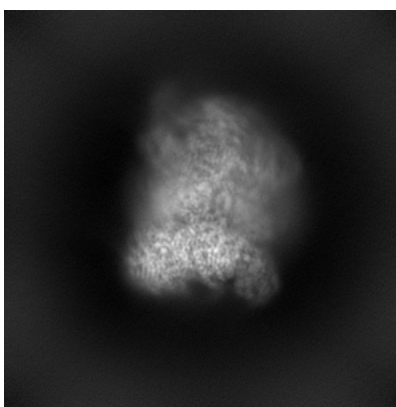


Z

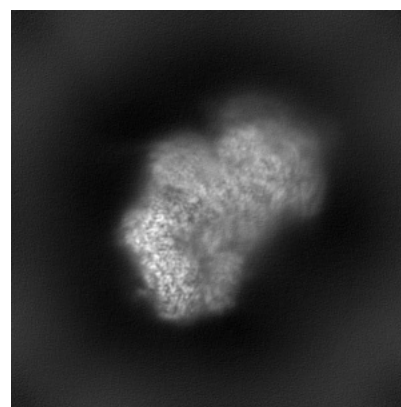
6.1.2 Raw map



X



Y

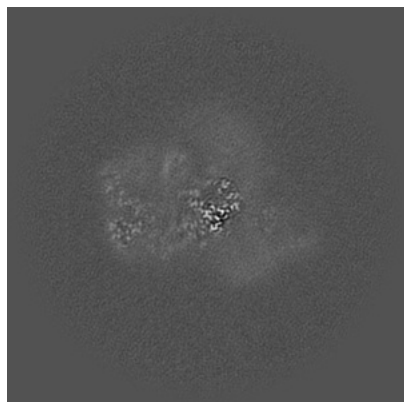


Z

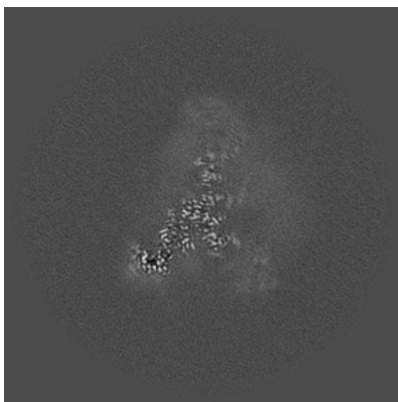
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

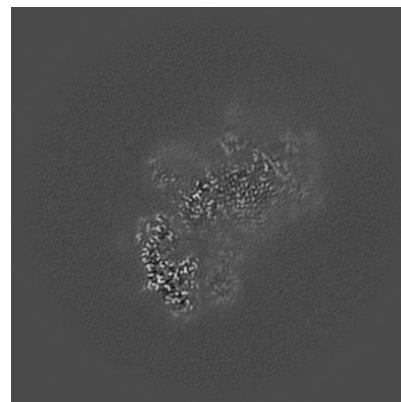
6.2.1 Primary map



X Index: 180

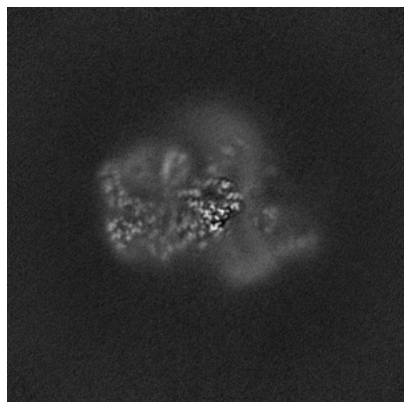


Y Index: 180

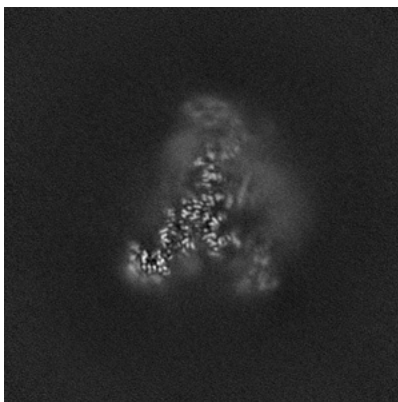


Z Index: 180

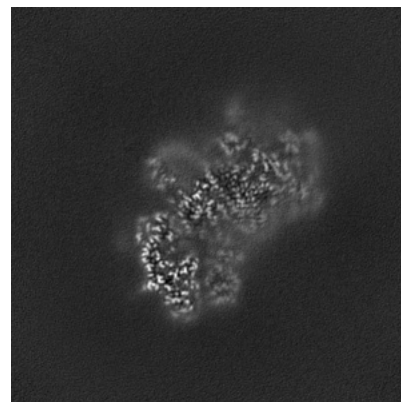
6.2.2 Raw map



X Index: 180



Y Index: 180

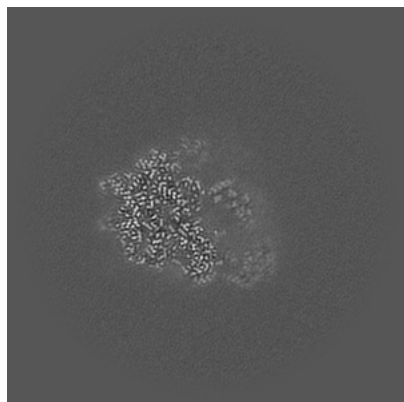


Z Index: 180

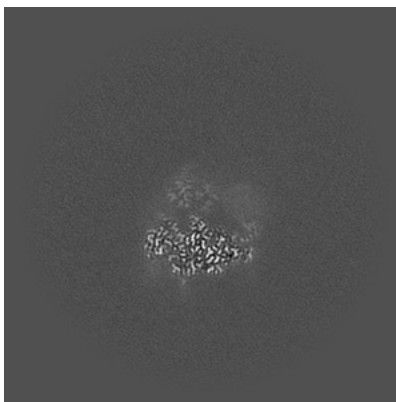
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

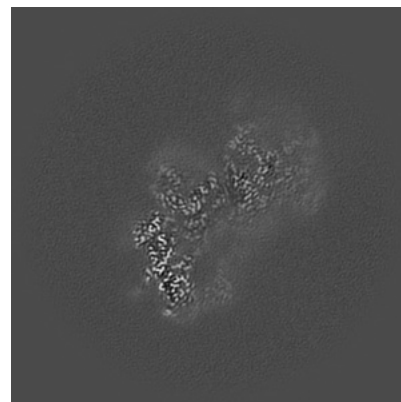
6.3.1 Primary map



X Index: 135

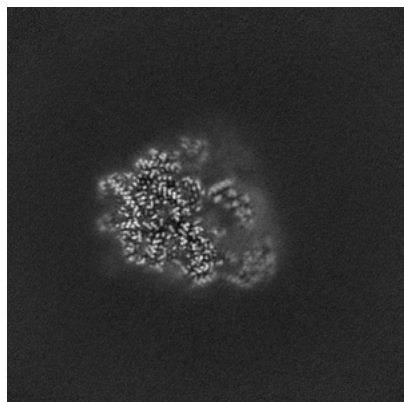


Y Index: 120

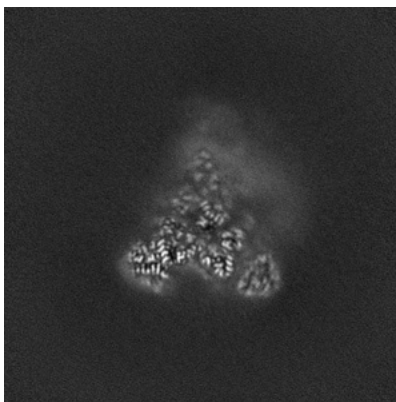


Z Index: 188

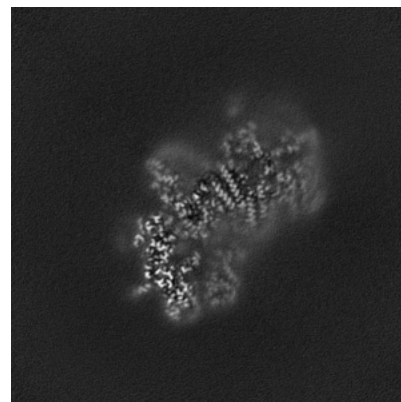
6.3.2 Raw map



X Index: 135



Y Index: 170

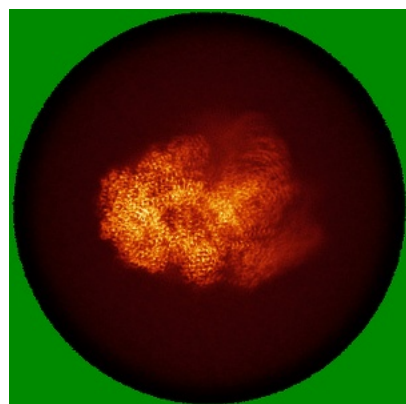


Z Index: 184

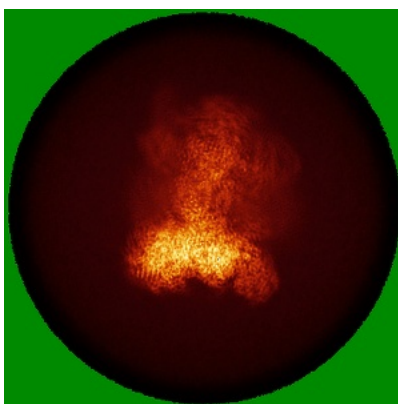
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

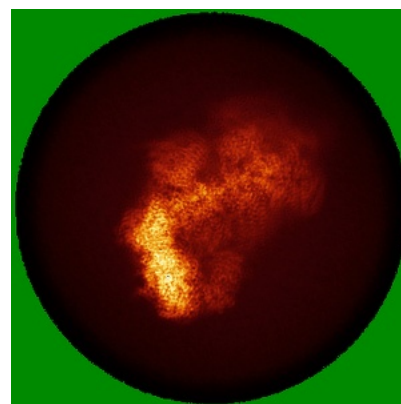
6.4.1 Primary map



X

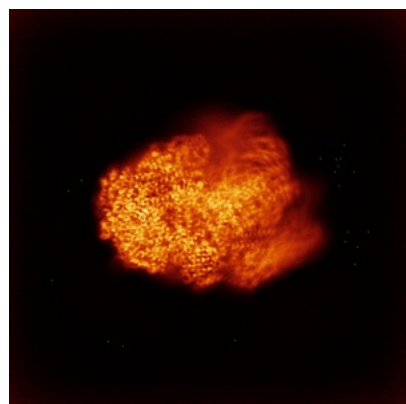


Y

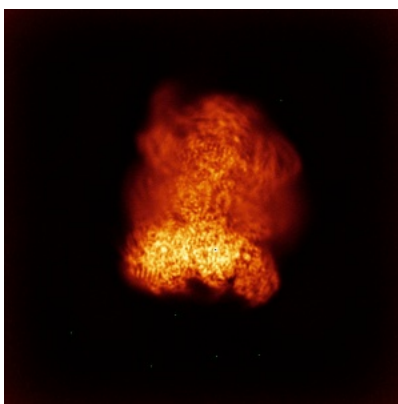


Z

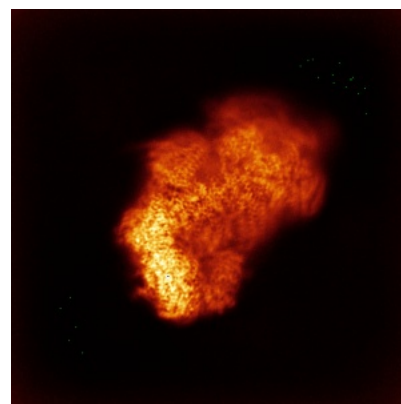
6.4.2 Raw map



X



Y

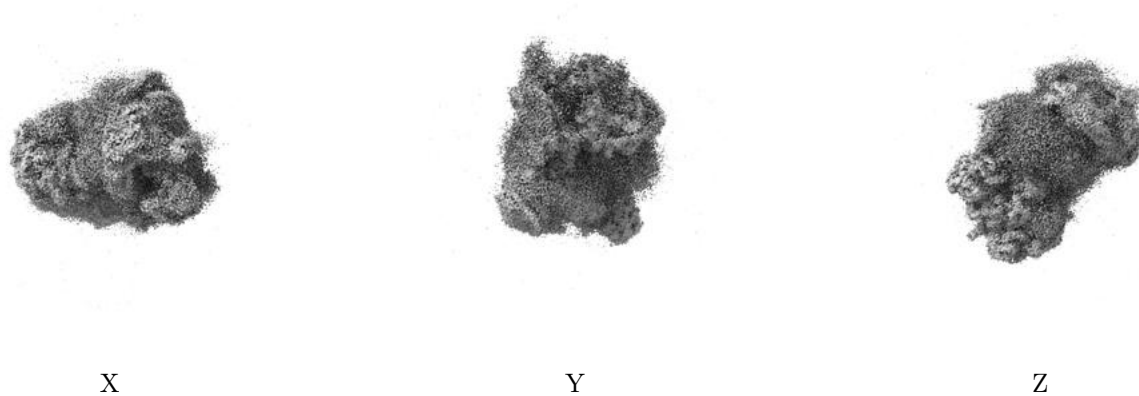


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

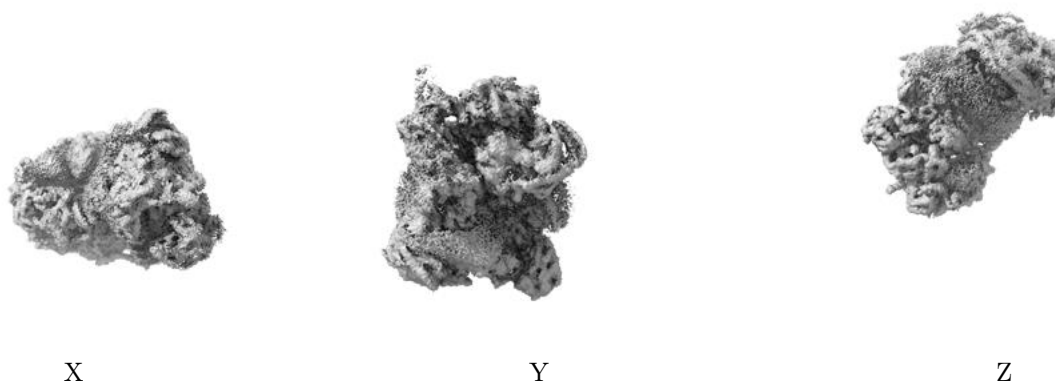
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

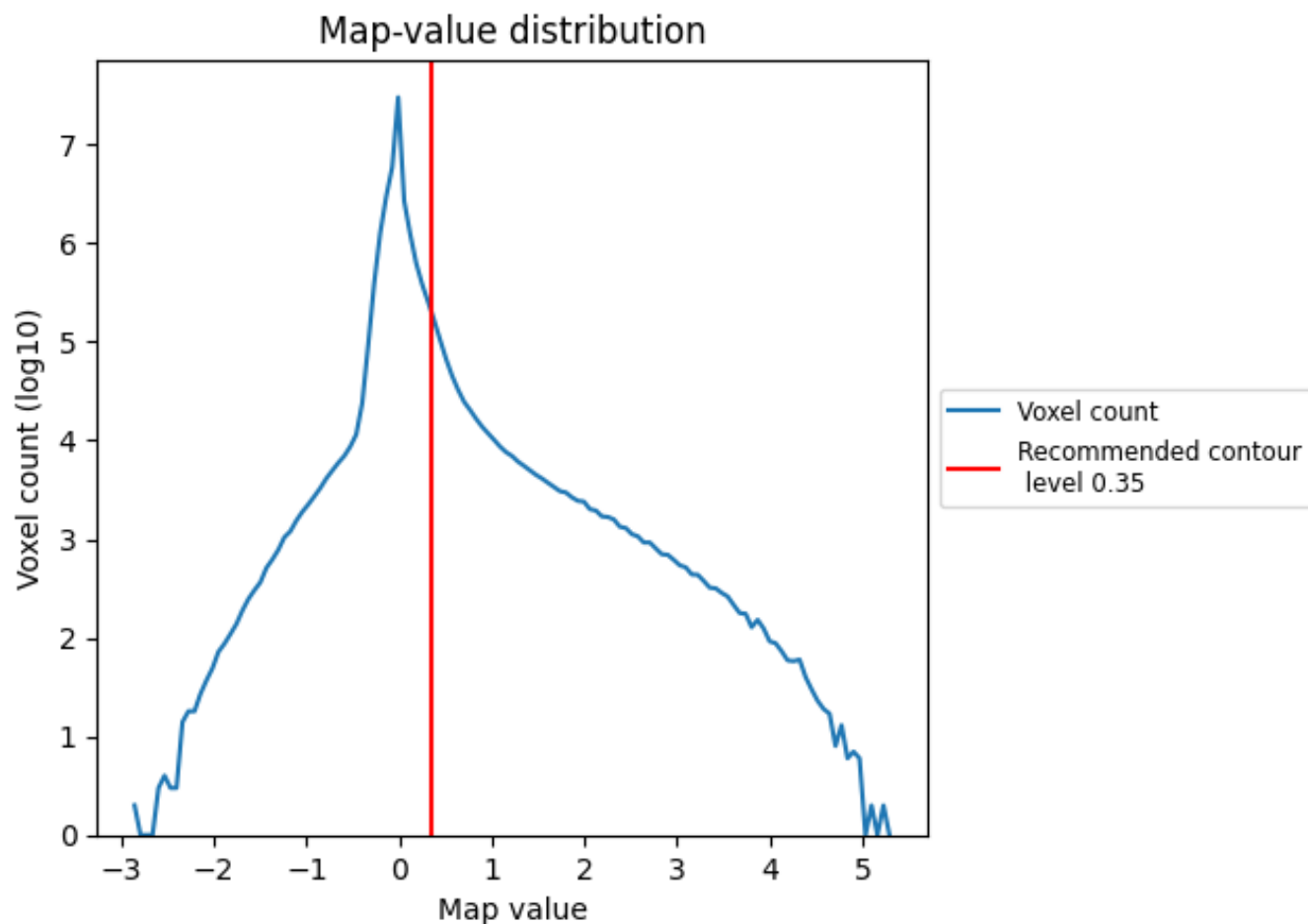
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

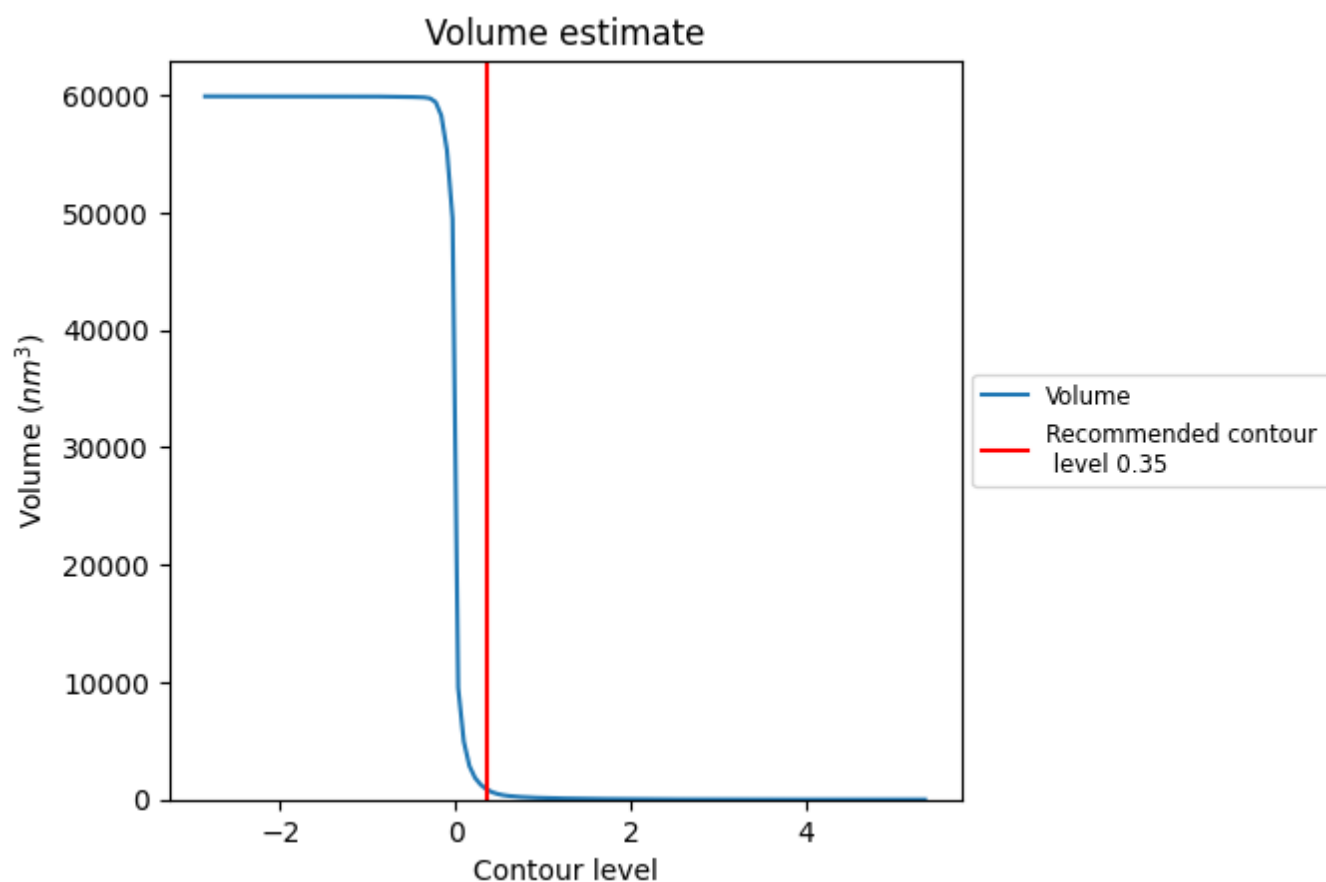
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

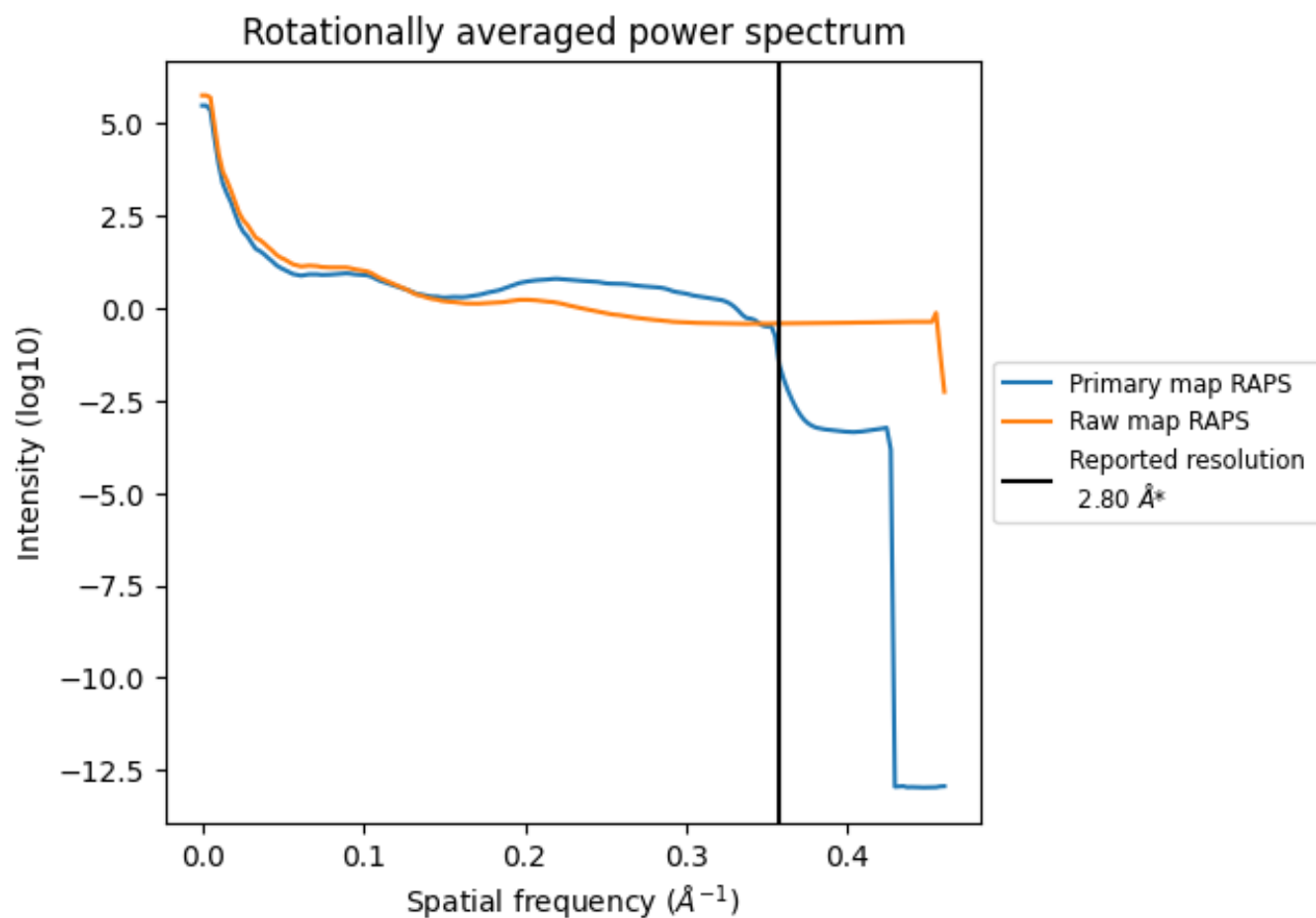
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 901 nm^3 ; this corresponds to an approximate mass of 814 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

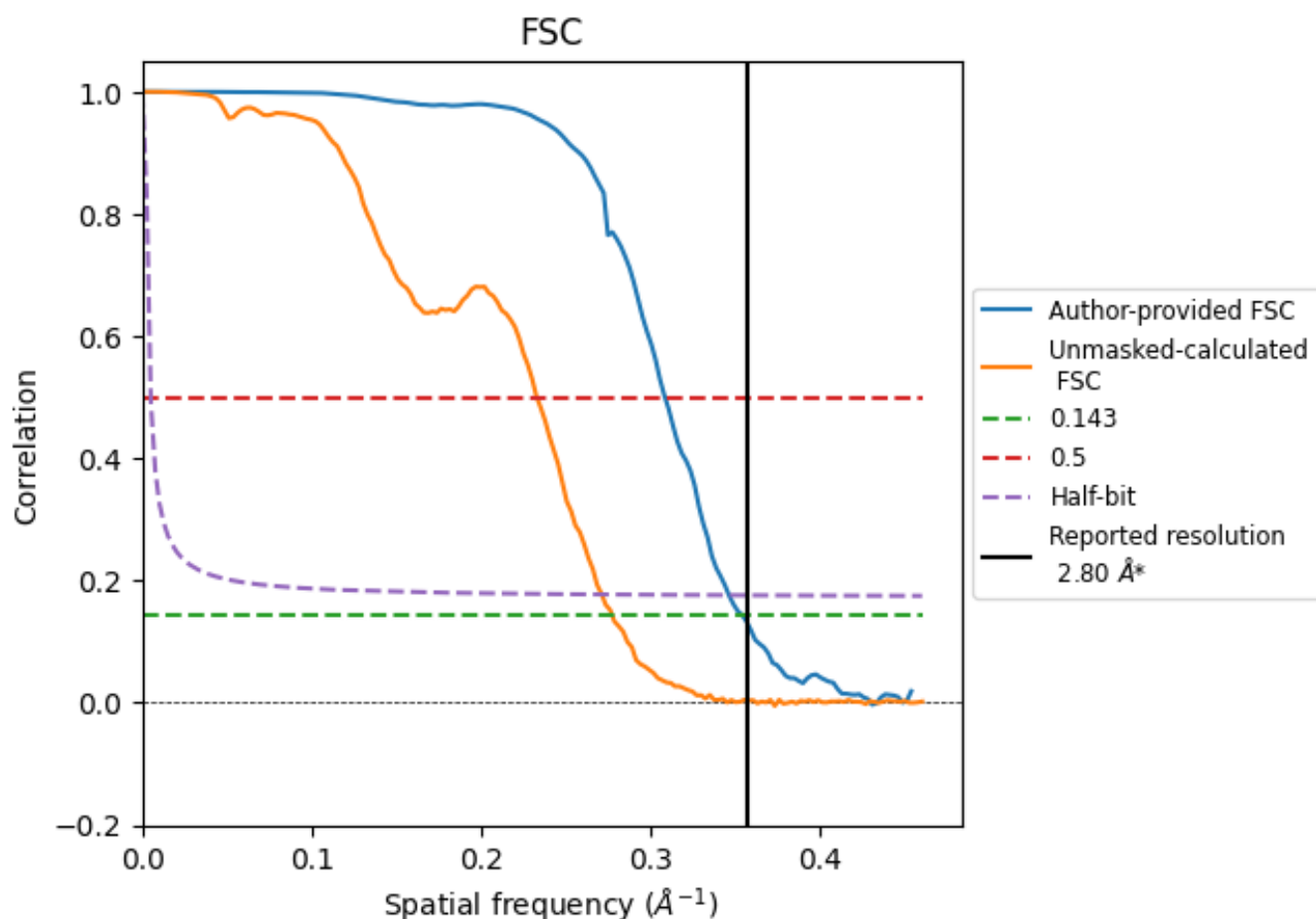


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

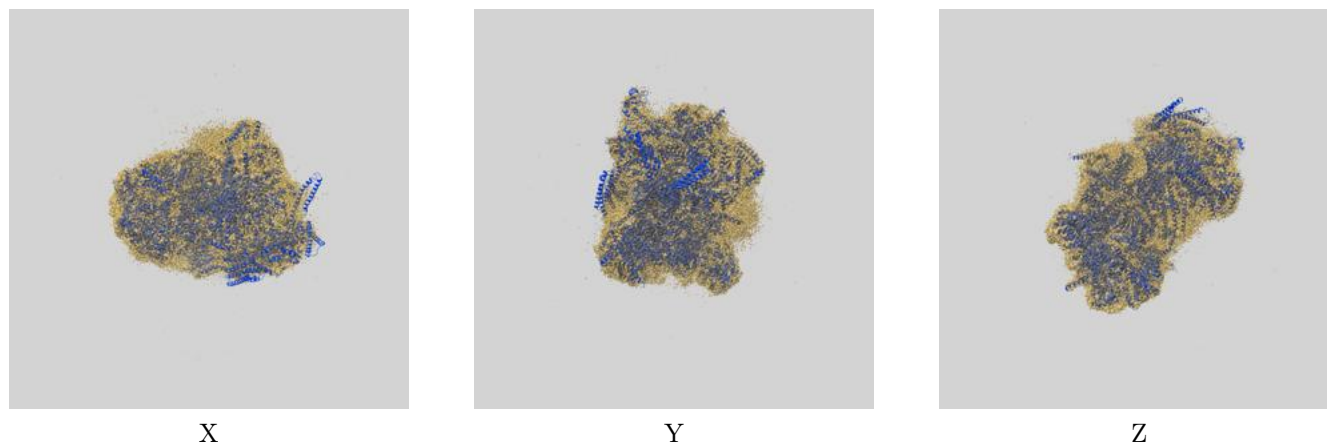
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.24	2.89
Unmasked-calculated*	3.61	4.30	3.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

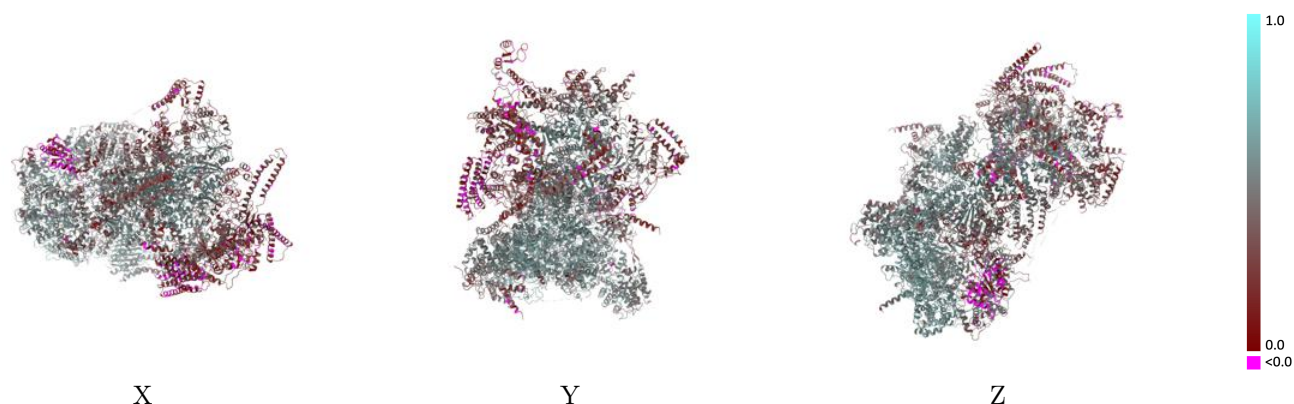
This section contains information regarding the fit between EMDB map EMD-38590 and PDB model 8XQX. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



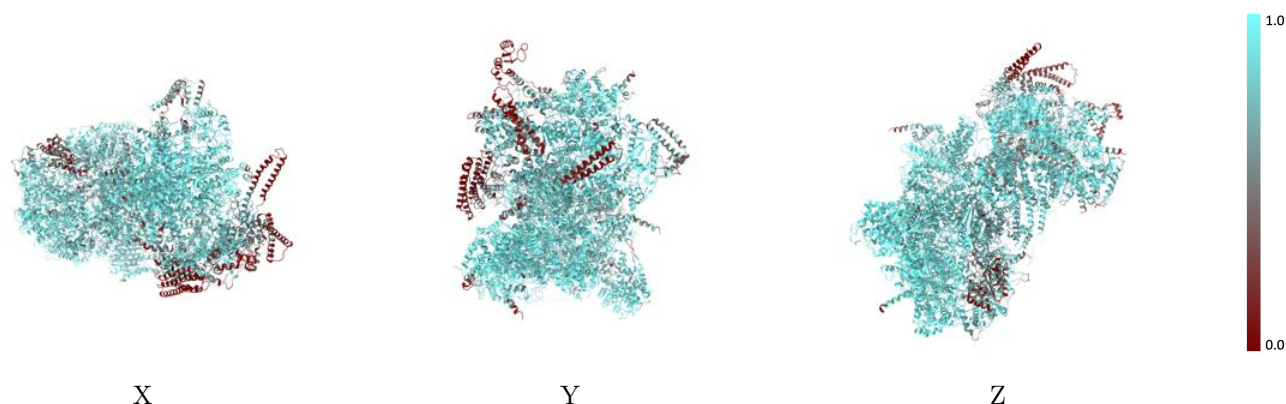
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



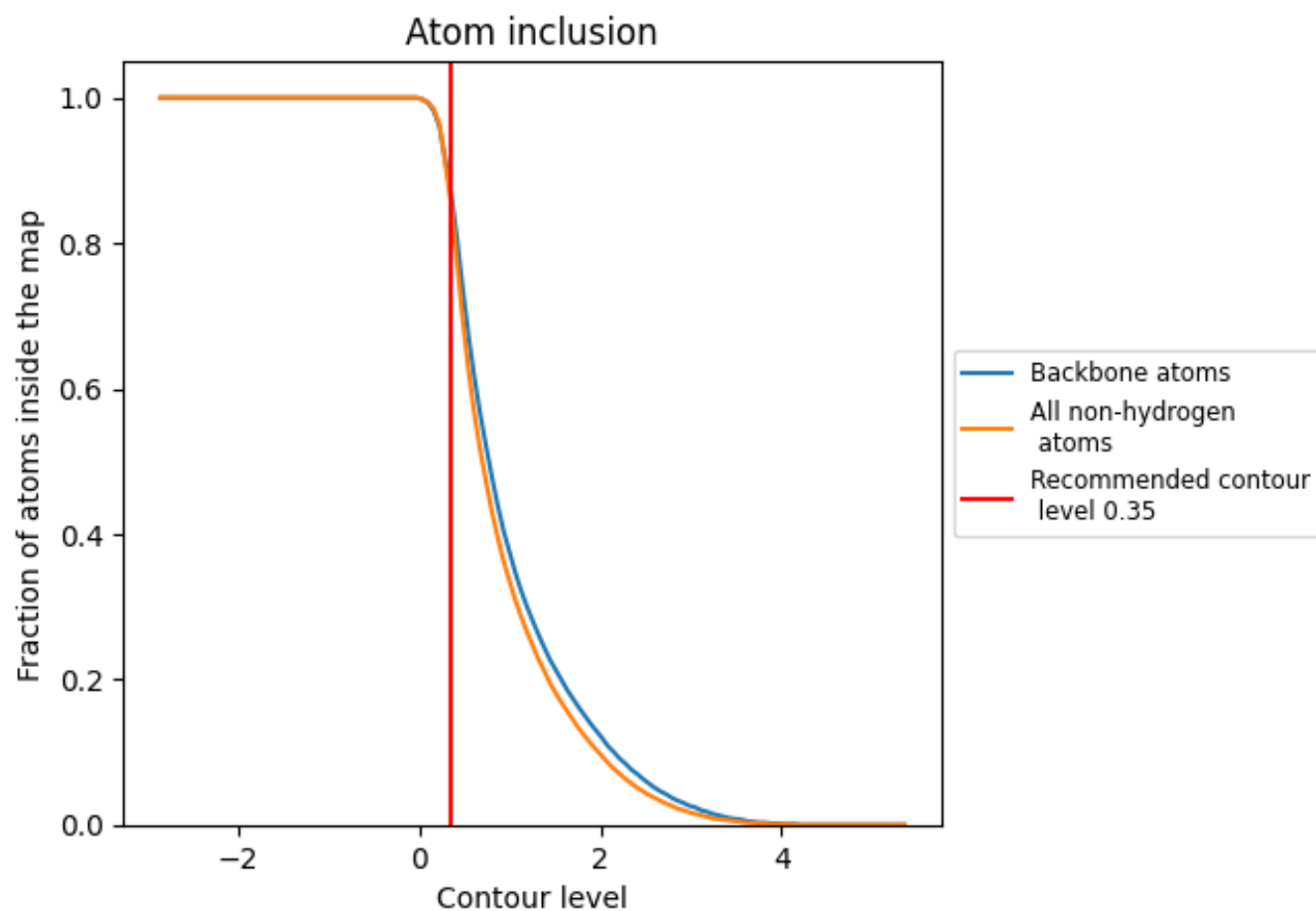
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.4600
A	 0.9350	 0.5320
B	 0.8990	 0.4820
C	 0.9030	 0.4870
D	 0.9160	 0.4980
E	 0.8460	 0.4370
F	 0.8860	 0.4840
G	 0.8990	 0.4840
H	 0.9360	 0.5300
I	 0.9650	 0.5610
J	 0.9310	 0.4850
K	 0.9640	 0.5580
L	 0.9000	 0.5080
M	 0.8810	 0.4540
N	 0.8800	 0.4740
O	 0.3620	 0.2090
P	 0.5780	 0.2660
Q	 0.5040	 0.2680
R	 0.9010	 0.4550
S	 0.7480	 0.3570
T	 0.6910	 0.2940
U	 0.6940	 0.2890
V	 0.8380	 0.2160

