



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 10:17 AM EDT

PDB ID : 4XLR
Title : Crystal structure of T.aquaticus transcription initiation complex with CarD containing bubble promoter and RNA
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-13
Resolution : 4.30 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

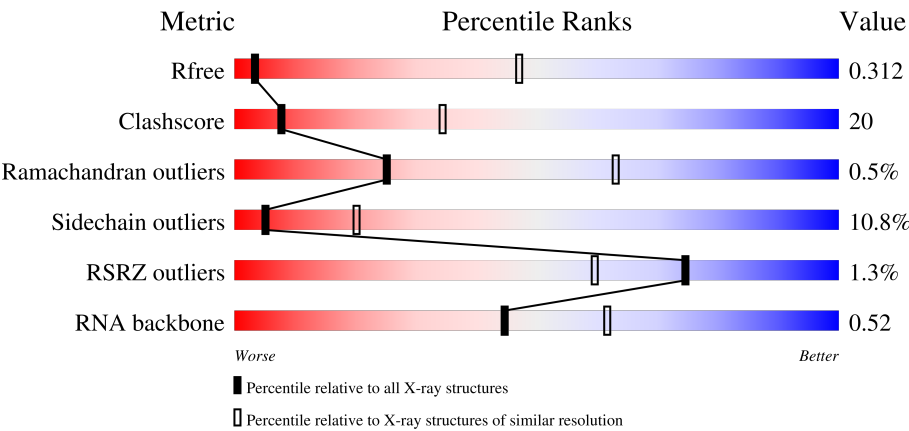
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	164625	1028 (4.72-3.86)
Clashscore	180529	1030 (4.70-3.90)
Ramachandran outliers	177936	1014 (4.76-3.84)
Sidechain outliers	177891	1022 (4.76-3.82)
RSRZ outliers	164620	1026 (4.72-3.86)
RNA backbone	3690	1156 (5.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	<div><div>%</div><div>37%31%•28%</div></div>
1	B	314	<div><div>%</div><div>42%26%•28%</div></div>
1	G	314	<div><div>%</div><div>37%31%•28%</div></div>
1	H	314	<div><div>%</div><div>42%26%•28%</div></div>

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	M	164	
6	N	164	
7	O	48	
7	R	48	
8	P	48	
8	S	48	
9	Q	4	
9	T	4	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 60854 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	23			
2	I	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	23			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a protein called CarD-like transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			
6	N	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			
7	R	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			

- Molecule 8 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			
8	S	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			

- Molecule 9 is a RNA chain called RNA (5'-R(P*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Q	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			
9	T	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Zn	0	0
			2	2		
10	J	2	Total	Zn	0	0
			2	2		

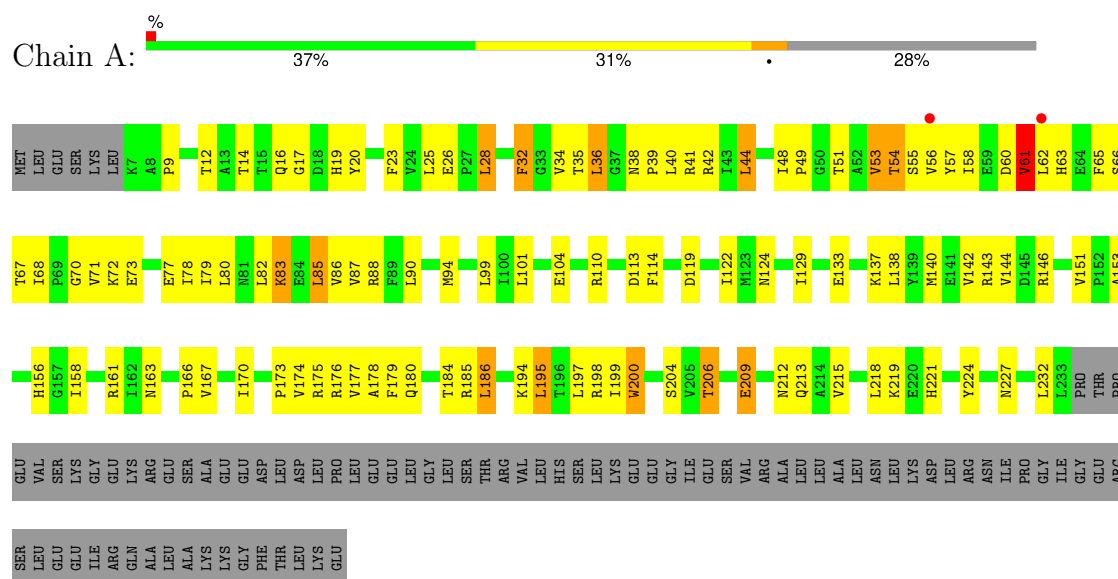
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Mg	0	0
			1	1		
11	J	1	Total	Mg	0	0
			1	1		

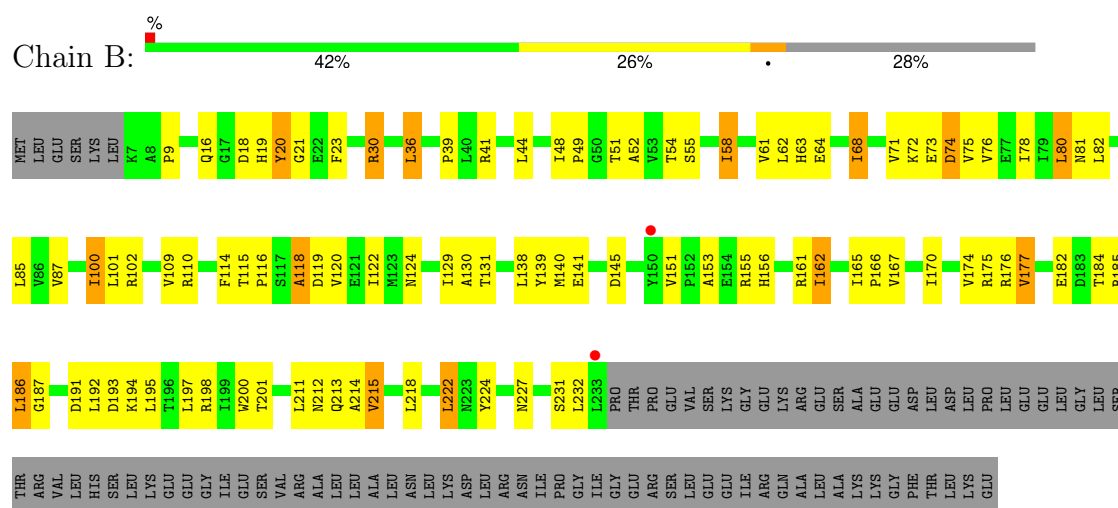
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase subunit alpha

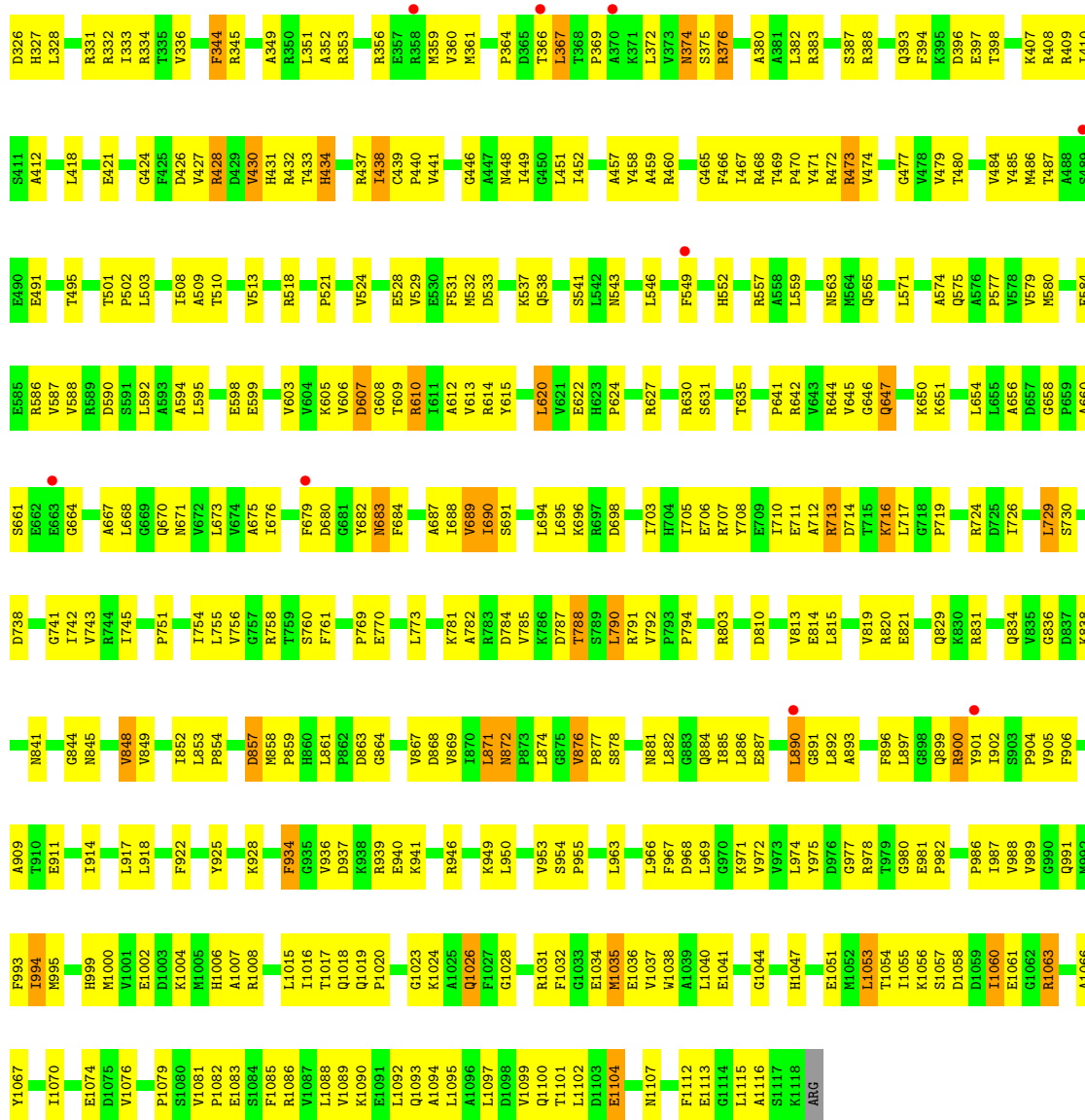


• Molecule 1: DNA-directed RNA polymerase subunit alpha

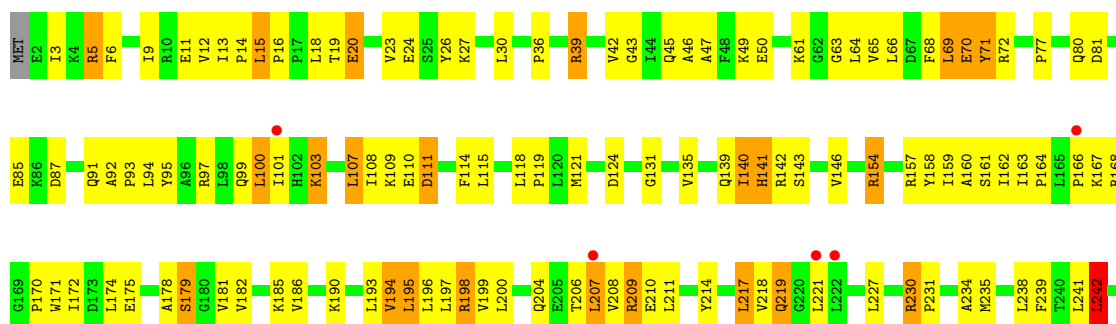


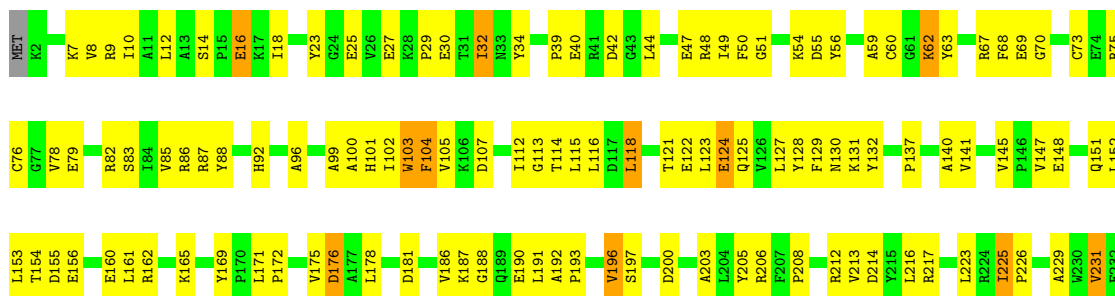
• Molecule 1: DNA-directed RNA polymerase subunit alpha



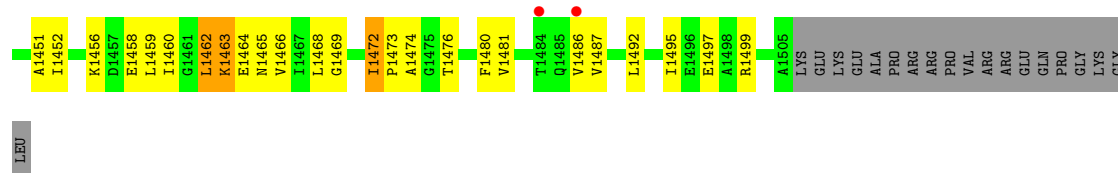


● Molecule 2: DNA-directed RNA polymerase subunit beta

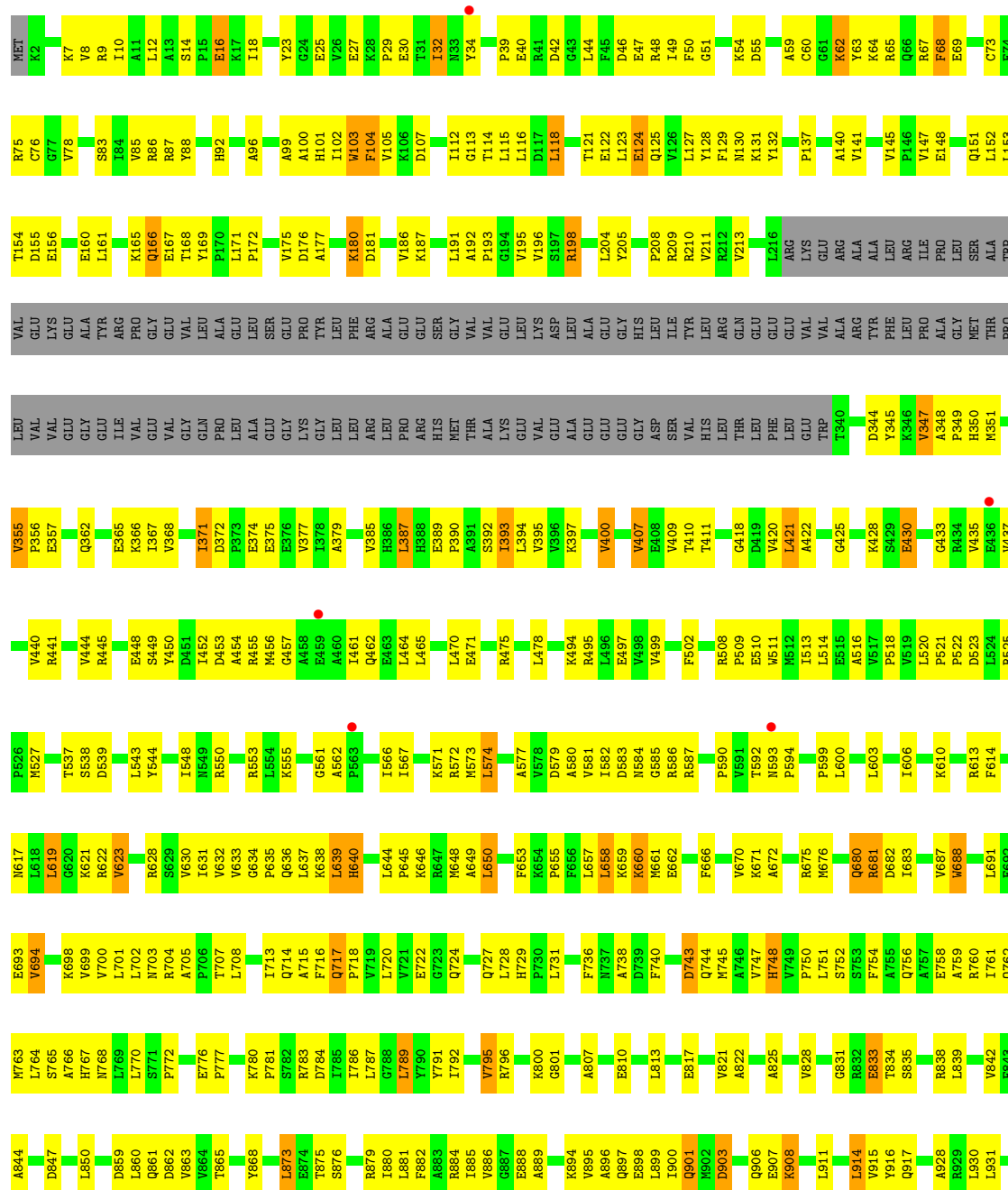


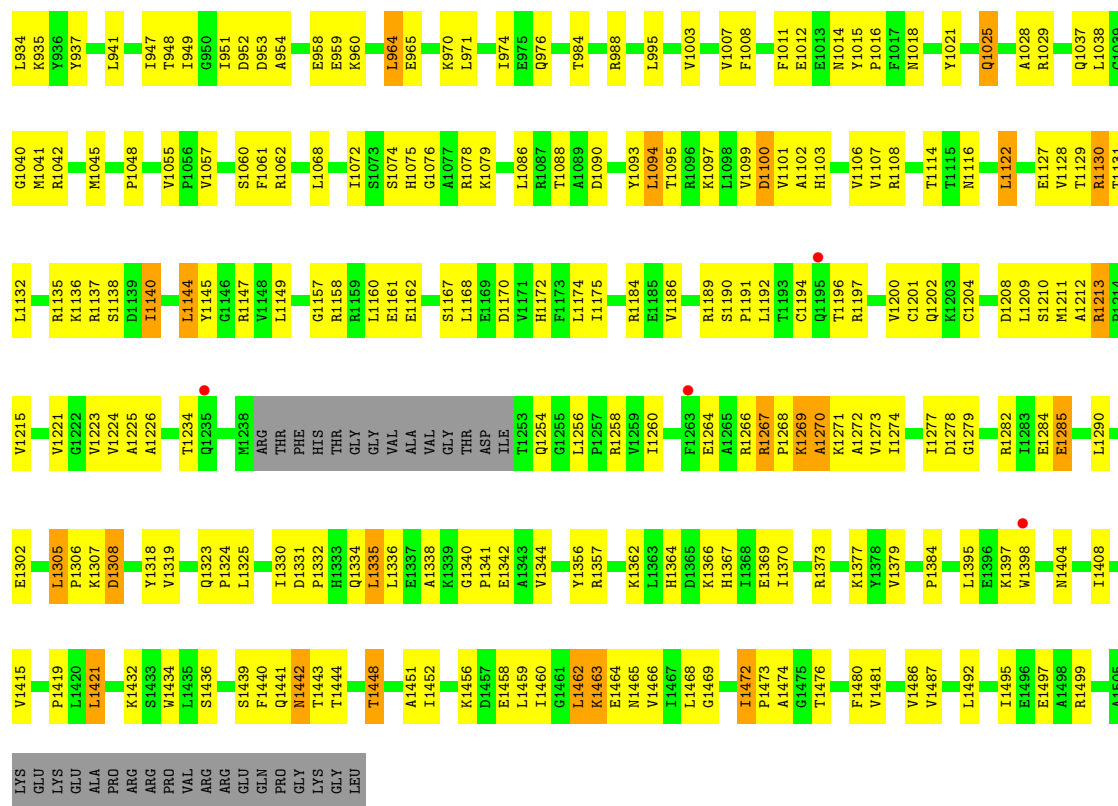


P1341	THR	E1161	S1073	E965	I880	K780	T707	L637	G561	L465	P373	Q302	K233
E1342	ASP	E1162	H1075	K970	F882	R780	L708	K638	A562	L470	E374	Q302	E234
V1344	ILE	L1168	A1077	L971	R883	R783	I713	L639	I566	E471	E375	P303	A235
Y1356	Q1254	E1169	R1078	Q973	R885	I786	W715	L644	I567	R475	A381	G307	V236
R1357	G1255	D1170	K1079	Q973	V886	I786	F716	K645	R568	R475	A381	G307	P238
	L1256	V1171	E975	E974	G887	L789	Q717	K646	N569	L478	V385	K308	
K1362	R1258	H1172	L1086	Q976	E888	Y790	P718	R647	K571	R489	H388	L311	L242
L1363	V1259	F1173	T1087	Q976	A889	Y790	W719	R648	R572	A490	H388	R312	A243
H1364	A1088	L1174	T1088	A977	E889	I792	L720	A649	M573		E389	L313	E244
D1365	I1175	A1089	A1089	T984	K894	I792	W721	L650	L574	R493	P390	P314	S246
K1366	F1283	R1366	D1090	T984	V895	W795	E722	F653	A577	R493	V395	R315	E247
H1367	E1284	R1184	Y1093	R988	A896	R796	Q724	K654	V578	K494	V395	H316	P248
E1368	A1285	E1185	Y1093	R988	Q897	Q723	Q724	K654	V578	R495	V396	M317	Y249
E1369	R1286	V1186	L1094	L995	E898	K800	Q801	P655	D579	L496	K397	T318	L250
I1370	T1095	L1095	T1095	L995	R899	Q801	Q727	F656	V581	W498	D406	A319	F251
	R1096	R1096	R1096	V1003	I900	Q801	Q727	F656	V581	W498	D406	A319	R252
R1373	S1190	K1289	K1097	V1003	Q901	Q801	Q727	L657	V581	W498	D406	A319	R252
A1270	P1191	L1191	L1098	V1007	Q902	E810	W729	L658	I582	V499	V407	V322	A253
K1377	K1271	L1192	D1100	F1008	D903	L813	L731	K660	N584	F502	V409	E323	E254
Y1378	A1272	V1107	D1100	F1008	D903	L813	L731	K660	N584	F502	V409	E323	E254
V1379	V1273	R1108	R1108	F1017	L914	A825	W743	E662	G585	M661	V409	E323	E254
	I1274	E1102	E1012	F1011	Q906	E817	W737	E662	R566	R508	G412	V331	S330
P1384	I1277	C1201	E1013	N1018	E907	W828	Q744	K671	R567	P509	D413	H332	G257
E1391	D1278	Q1202	N1014	Y1015	K908	A822	D739	A677	P590	E510	R414	L333	V258
G1392	G1279	V1106	V1106	Y1015	L911	A822	W739	A677	P590	E510	R414	L333	V258
		V1107	V1107	Y1015	L911	A822	W739	A677	P590	E510	R414	L333	V258
L1395	R1282	D1208	T1114	Q1025	L914	A825	D743	V670	T592	I513	P417	L335	L261
E1396	I1283	L1209	T1115	Q1025	L914	A825	D743	V670	T592	I513	P417	L335	L261
E1284	E1284	S1210	N1116	Q1025	L914	A825	D743	V670	T592	I513	P417	L335	L261
W1398	E1285	M1211	N1116	Q1025	L914	A825	D743	V670	T592	I513	P417	L335	L261
		A1212	L1122	Q1025	L914	A825	D743	V670	T592	I513	P417	L335	L261
M1404	L1290	R1213	L1122	Q1025	L914	A825	D743	V670	T592	I513	P417	L335	L261
		P1214	E1127	R1029	L931	L839	W750	Q680	I606	L520	E430	D344	L269
I1408	E1302	V1215	V1128	D932	L931	L839	W750	Q680	I606	L520	E430	D344	L269
V1415	L1305	V1215	V1128	D932	L931	L839	W750	Q680	I606	L520	E430	D344	L269
P1419	P1307	V1221	T1129	Q1037	A933	W842	S753	L683	R613	L524	R434	P349	E276
L1420	G1222	L1131	R1130	C1039	L934	R843	S753	L683	R613	L524	R434	P349	E276
D1308	V1223	L1132	L1132	G1040	K935	A844	A755	K684	F614	R525	V435	R350	E277
V1224	V1224	L1132	L1132	G1040	K935	A844	A755	K684	F614	R525	V435	R350	E277
A1225	A1225	L1132	L1132	G1040	K935	A844	A755	K684	F614	R525	V435	R350	E277
K1426	Y1318	R1135	R1135	R1042	Y937	D847	Q756	V687	N617	P526	L439	K351	E277
V1319	L1310	K1136	K1136	R1042	Y937	D847	Q756	V687	N617	P526	L439	K351	E277
A1321	E1320	R1137	R1137	M1045	L941	L850	A757	V688	L618	F535	V440	N352	V278
G1322	L1321	S1138	S1138	M1045	L941	L850	A757	V688	L618	F535	V440	N352	V278
Q1323	G1322	D1139	D1139	P1048	I947	D859	W760	A690	L619	F535	V440	N352	V278
P1324	Q1323	P1048	P1048	P1048	I947	D859	W760	A690	L619	F535	V440	N352	V278
L1325	L1325	V1055	V1055	V1055	I949	Q861	Q762	E692	K621	P526	L445	V355	A280
	ARG	V1056	V1056	V1056	I949	Q861	Q762	E692	K621	P526	L445	V355	A280
THR	THR	L1144	L1144	P1056	G950	D862	W764	L691	G620	T537	R445	V355	A280
PHE	PHE	Y1145	Y1145	V1057	G950	D862	W764	L691	G620	T537	R445	V355	A280
HIS	HIS	G1146	G1146	V1057	G950	D862	W764	L691	G620	T537	R445	V355	A280
THR	THR	R1147	R1147	S1060	A954	T865	W767	V700	R630	I548	M456	A363	V292
GLY	GLY	F1061	F1061	S1060	A954	T865	W767	V700	R630	I548	M456	A363	V292
L1441	L1441	L1062	L1062	F1061	E958	E874	L769	L701	I631	R550	G457	V367	E294
VAL	VAL	L1149	L1149	F1061	E958	E874	L769	L701	I631	R550	G457	V367	E294
L1336	L1336	ALA	ALA	L1068	K960	S876	P772	W705	P635	R553	M456	A363	E294
		R1158	R1158	L1068	K960	S876	P772	W705	P635	R553	M456	A363	E294
		L1159	L1159	L1068	K960	S876	P772	W705	P635	R553	M456	A363	E294
G1340	G1340	T1160	T1160	L1070	L964	R870	W776	R706	Q626	K555	E463	D372	E299

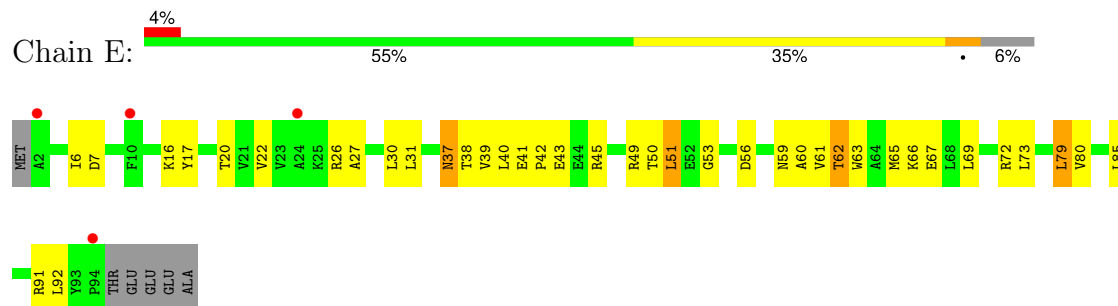


• Molecule 3: DNA-directed RNA polymerase subunit beta'

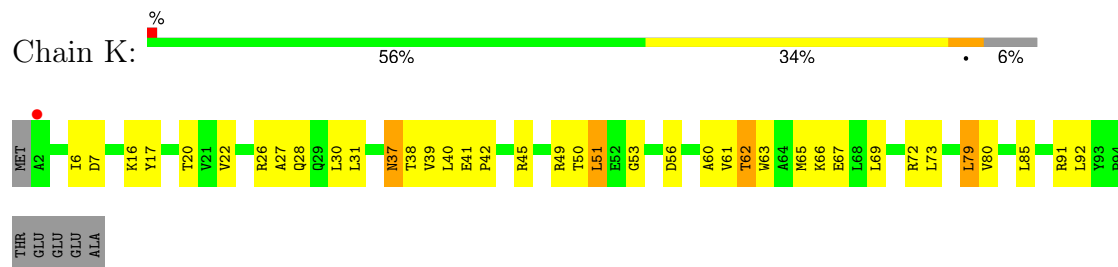




• Molecule 4: DNA-directed RNA polymerase subunit omega

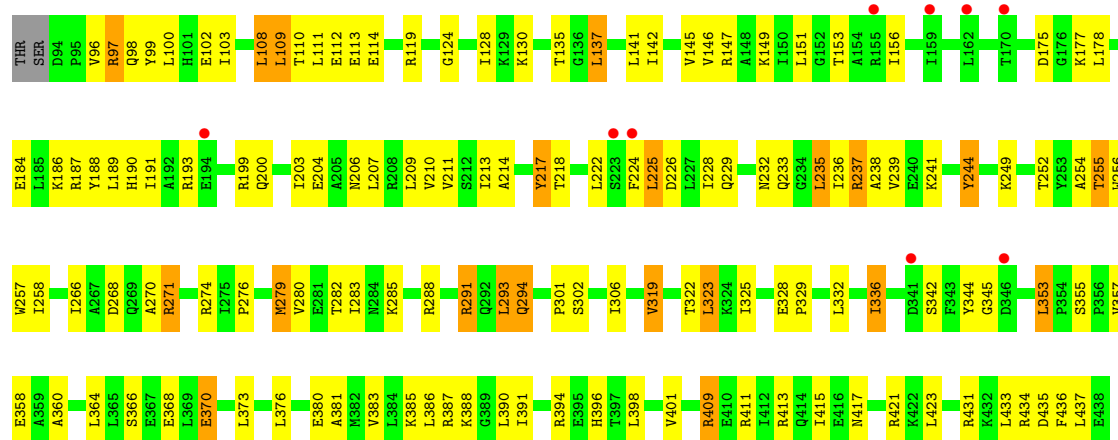


• Molecule 4: DNA-directed RNA polymerase subunit omega

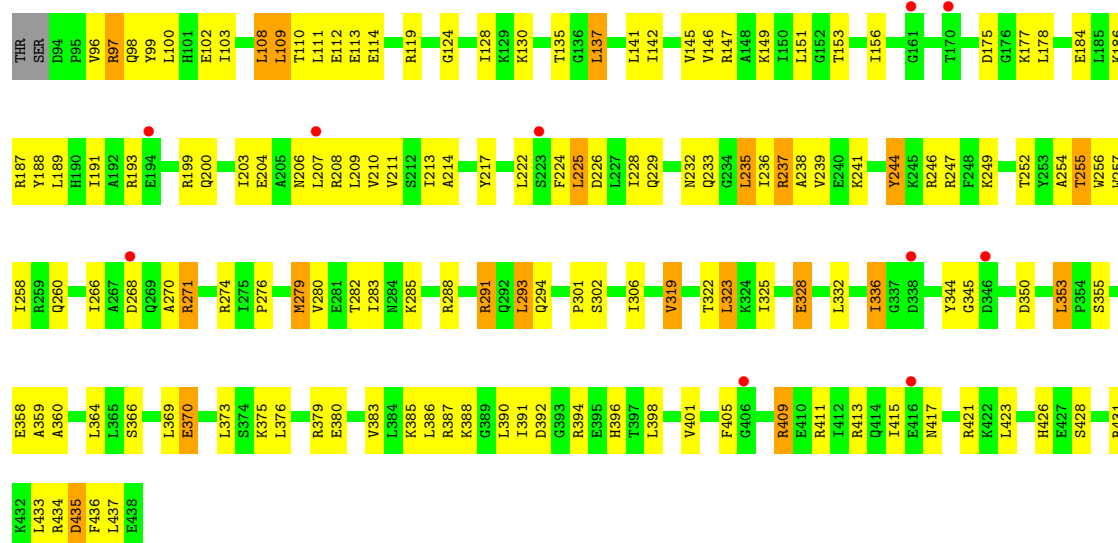


• Molecule 5: RNA polymerase sigma factor SigA

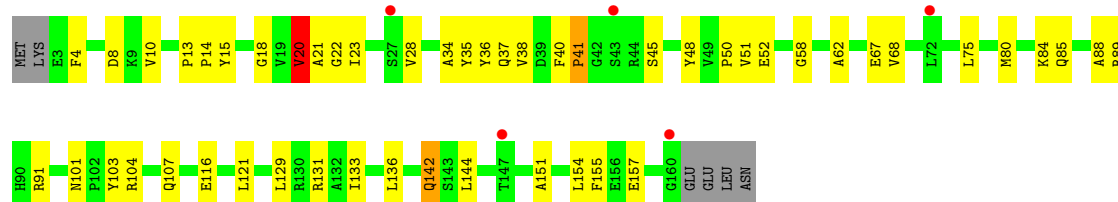




• Molecule 5: RNA polymerase sigma factor SigA

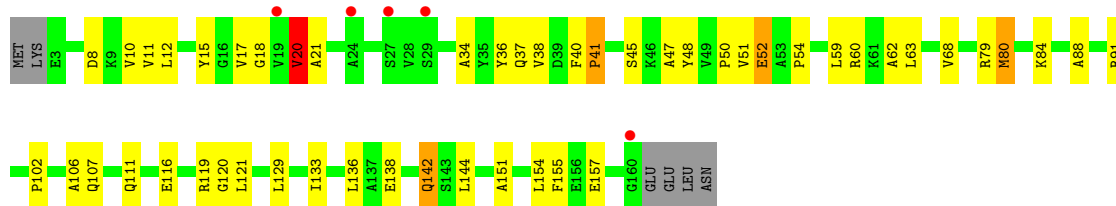


• Molecule 6: CarD-like transcriptional regulator



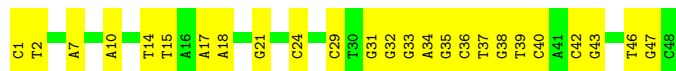
• Molecule 6: CarD-like transcriptional regulator





- Molecule 7: DNA (48-MER)

Chain O: 48% 52%



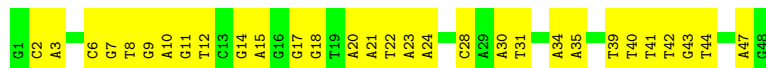
- Molecule 7: DNA (48-MER)

Chain R: 42% 58%



- Molecule 8: DNA (48-MER)

Chain P: 38% 63%



- Molecule 8: DNA (48-MER)

Chain S: 42% 54%



- Molecule 9: RNA (5'-R(P*UP*CP*GP*A)-3')

Chain Q: 25% 75%



- Molecule 9: RNA (5'-R(P*UP*CP*GP*A)-3')

Chain T: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	289.84Å 289.84Å 536.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 4.30 39.56 – 4.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.56-4.30) 94.6 (39.56-4.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.275 , 0.310 0.277 , 0.312	Depositor DCC
R_{free} test set	7337 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	165.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 165.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	60854	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.29	0/1804	0.52	0/2455
1	B	0.27	0/1804	0.49	0/2455
1	G	0.30	0/1804	0.52	0/2455
1	H	0.27	0/1804	0.49	0/2455
2	C	0.29	0/8929	0.51	1/12074 (0.0%)
2	I	0.29	0/8929	0.51	1/12074 (0.0%)
3	D	0.29	0/11963	0.50	0/16165
3	J	0.28	0/10959	0.49	0/14802
4	E	0.27	0/783	0.53	0/1054
4	K	0.27	0/783	0.53	0/1054
5	F	0.34	0/2829	0.54	0/3804
5	L	0.33	0/2829	0.54	0/3804
6	M	0.35	0/1267	0.55	0/1719
6	N	0.35	0/1267	0.55	0/1719
7	O	0.59	0/1109	0.92	0/1712
7	R	0.56	0/1109	0.92	0/1712
8	P	0.64	0/1106	0.88	0/1706
8	S	0.61	0/1106	0.90	2/1706 (0.1%)
9	Q	0.24	0/94	0.71	0/144
9	T	0.24	0/94	0.76	0/144
All	All	0.33	0/62372	0.55	4/85213 (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
2	C	0	2
2	I	0	2
3	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
6	M	0	2
6	N	0	2
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	23	DA	O5'-P-OP1	-6.61	99.75	105.70
2	C	242	LEU	CA-CB-CG	5.68	128.36	115.30
2	I	242	LEU	CA-CB-CG	5.57	128.10	115.30
8	S	22	DT	OP1-P-O3'	5.13	116.48	105.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	360	VAL	Peptide
2	C	71	TYR	Mainchain
3	D	1270	ALA	Peptide
2	I	360	VAL	Peptide
2	I	71	TYR	Mainchain
3	J	1270	ALA	Peptide
6	M	20	VAL	Mainchain,Peptide
6	N	20	VAL	Mainchain,Peptide

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	1770	0	1799	87	0
1	B	1770	0	1799	66	0
1	G	1770	0	1799	88	0
1	H	1770	0	1799	65	0
2	C	8762	0	8854	435	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	8762	0	8854	436	0
3	D	11761	0	11976	537	0
3	J	10779	0	10993	490	0
4	E	768	0	784	38	0
4	K	768	0	784	36	0
5	F	2787	0	2866	122	0
5	L	2787	0	2866	127	0
6	M	1239	0	1259	38	0
6	N	1239	0	1259	39	0
7	O	988	0	544	30	0
7	R	988	0	544	38	0
8	P	985	0	543	36	0
8	S	985	0	543	30	0
9	Q	85	0	43	1	0
9	T	85	0	43	2	0
10	D	2	0	0	0	0
10	J	2	0	0	0	0
11	D	1	0	0	0	0
11	J	1	0	0	0	0
All	All	60854	0	59951	2363	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 20.

All (2363) 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)
3:D:73:CYS:HB3	3:D:76:CYS:SG	1.97	1.04
3:J:73:CYS:HB3	3:J:76:CYS:SG	1.97	1.04
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.89
3:D:412:GLY:HA2	3:D:434:ARG:HD3	1.55	0.89
3:J:105:VAL:HA	3:J:112:ILE:HD11	1.55	0.88
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.38	0.86
3:D:208:PRO:HA	3:D:390:PRO:HA	1.56	0.85
1:G:42:ARG:HH12	2:I:857:ASP:HB3	1.38	0.85
3:J:210:ARG:HG2	3:J:389:GLU:HB3	1.58	0.85
2:I:679:PHE:H	2:I:683:ASN:HD21	1.25	0.85
2:C:858:MET:H	2:C:977:GLY:HA3	1.40	0.84
2:I:374:ASN:HD21	5:L:291:ARG:HE	1.22	0.84
2:I:858:MET:H	2:I:977:GLY:HA3	1.42	0.84
5:L:203:ILE:HG12	5:L:239:VAL:HG21	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:SER:HB3	1:G:143:ARG:HB2	1.61	0.83
2:C:679:PHE:H	2:C:683:ASN:HD21	1.26	0.82
2:C:374:ASN:HD21	5:F:291:ARG:HE	1.26	0.82
5:F:203:ILE:HG12	5:F:239:VAL:HG21	1.61	0.82
2:I:364:PRO:HA	2:I:367:LEU:HD12	1.61	0.82
2:C:364:PRO:HA	2:C:367:LEU:HD12	1.61	0.82
6:N:20:VAL:HA	6:N:38:VAL:HA	1.60	0.81
2:C:836:GLY:H	2:C:849:VAL:HB	1.44	0.81
3:D:954:ALA:O	3:D:1062:ARG:NH1	2.12	0.81
3:J:208:PRO:HB3	3:J:387:LEU:HD21	1.60	0.81
2:I:836:GLY:H	2:I:849:VAL:HB	1.45	0.80
1:A:55:SER:HB3	1:A:143:ARG:HB2	1.61	0.80
2:C:603:VAL:HB	2:C:646:GLY:HA2	1.63	0.80
2:I:292:ARG:HH11	2:I:292:ARG:H	1.29	0.80
2:I:603:VAL:HA	2:I:613:VAL:HG12	1.63	0.80
6:M:20:VAL:HA	6:M:38:VAL:HA	1.63	0.80
2:C:71:TYR:HA	2:C:95:TYR:O	1.81	0.80
2:C:712:ALA:HB3	2:C:821:GLU:H	1.47	0.80
2:C:603:VAL:HA	2:C:613:VAL:HG12	1.64	0.80
3:D:73:CYS:CB	3:D:76:CYS:SG	2.65	0.80
8:P:30:DA:H2"	8:P:31:DT:H5"	1.64	0.80
2:C:292:ARG:HH11	2:C:292:ARG:H	1.30	0.80
3:D:1103:HIS:HB2	3:D:1462:LEU:HD11	1.64	0.79
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.63	0.79
3:J:73:CYS:CB	3:J:76:CYS:SG	2.64	0.79
2:I:71:TYR:HA	2:I:95:TYR:O	1.83	0.79
3:J:954:ALA:O	3:J:1062:ARG:NH1	2.15	0.79
2:I:603:VAL:HB	2:I:646:GLY:HA2	1.63	0.79
2:I:1102:LEU:HB2	3:J:7:LYS:HB2	1.63	0.78
3:D:1189:ARG:NH2	3:D:1204:CYS:SG	2.55	0.78
7:R:7:DA:H61	8:S:42:DT:H3	1.30	0.78
3:D:130:ASN:HD22	5:F:98:GLN:HE22	1.31	0.78
3:J:1103:HIS:HB2	3:J:1462:LEU:HD11	1.66	0.78
2:I:63:GLY:HA3	2:I:103:LYS:HB2	1.67	0.77
2:C:374:ASN:HD21	5:F:291:ARG:NE	1.83	0.77
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.65	0.77
2:I:154:ARG:HD3	2:I:178:ALA:HB2	1.65	0.77
2:I:1063:ARG:HH22	5:L:353:LEU:HD11	1.49	0.77
2:I:712:ALA:HB3	2:I:821:GLU:H	1.48	0.77
3:D:953:ASP:O	3:D:1018:ASN:ND2	2.17	0.77
8:S:30:DA:H2"	8:S:31:DT:H5"	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:367:ILE:HG22	3:D:368:VAL:HG23	1.67	0.77
3:J:953:ASP:O	3:J:1018:ASN:ND2	2.16	0.77
2:C:63:GLY:HA3	2:C:103:LYS:HB2	1.67	0.77
3:J:951:ILE:O	3:J:1062:ARG:NH1	2.18	0.76
3:D:323:GLU:HB3	3:D:334:THR:H	1.49	0.76
2:C:154:ARG:HD3	2:C:178:ALA:HB2	1.66	0.76
5:F:218:THR:O	8:P:23:DA:N6	2.19	0.76
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.68	0.76
2:I:427:VAL:HG22	7:R:38:DG:H21	1.51	0.76
2:I:537:LYS:HZ3	2:I:905:VAL:H	1.32	0.76
3:J:48:ARG:HA	3:J:78:VAL:HG22	1.68	0.75
3:J:462:GLN:HB2	3:J:513:ILE:HG21	1.67	0.75
3:J:1189:ARG:NH2	3:J:1204:CYS:SG	2.56	0.75
3:D:423:ASP:HB3	3:D:426:LYS:HB3	1.69	0.75
3:J:130:ASN:HD22	5:L:98:GLN:HE22	1.31	0.75
3:D:951:ILE:O	3:D:1062:ARG:NH1	2.19	0.75
4:K:79:LEU:HG	4:K:80:VAL:HG22	1.69	0.75
3:D:48:ARG:HA	3:D:78:VAL:HG22	1.69	0.75
2:I:911:GLU:OE1	3:J:1062:ARG:NH2	2.20	0.75
1:G:53:VAL:HG23	1:G:144:VAL:HG22	1.69	0.74
3:J:715:ALA:HB3	3:J:764:LEU:HA	1.67	0.74
5:F:398:LEU:HB3	5:F:409:ARG:HB2	1.67	0.74
2:I:694:LEU:HD11	2:I:868:ASP:HB3	1.68	0.74
2:C:876:VAL:HG11	2:C:885:ILE:HD11	1.70	0.74
4:E:79:LEU:HG	4:E:80:VAL:HG22	1.69	0.74
2:I:167:LYS:HD3	7:R:35:DG:H5'	1.69	0.74
5:L:428:SER:HA	5:L:434:ARG:HH22	1.52	0.74
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.69	0.74
3:J:67:ARG:HD2	5:L:394:ARG:HD3	1.67	0.74
5:L:332:LEU:HD22	5:L:345:GLY:HA2	1.70	0.74
3:D:760:ARG:HH22	4:E:62:THR:HG23	1.50	0.74
2:I:876:VAL:HG11	2:I:885:ILE:HD11	1.70	0.74
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.69	0.74
1:A:53:VAL:HG23	1:A:144:VAL:HG22	1.68	0.74
3:D:188:GLY:N	3:D:197:SER:O	2.20	0.74
3:J:760:ARG:HH22	4:K:62:THR:HG23	1.51	0.74
3:D:214:ASP:HA	3:D:342:PRO:HA	1.69	0.74
2:I:3:ILE:HG23	2:I:900:ARG:HB2	1.70	0.73
2:I:108:ILE:HB	6:N:48:TYR:HB2	1.70	0.73
3:D:792:ILE:HG21	3:D:941:LEU:HD22	1.70	0.73
3:J:786:ILE:HD13	3:J:908:LYS:HG2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1254:GLN:HB2	3:J:1258:ARG:HB2	1.70	0.73
5:L:398:LEU:HB3	5:L:409:ARG:HB2	1.69	0.73
3:J:1379:VAL:HG12	3:J:1419:PRO:HA	1.71	0.73
2:C:3:ILE:HG23	2:C:900:ARG:HB2	1.71	0.73
3:J:792:ILE:HG21	3:J:941:LEU:HD22	1.71	0.72
5:L:235:LEU:HB2	5:L:258:ILE:HD11	1.70	0.72
2:C:427:VAL:HG22	7:O:38:DG:H21	1.55	0.72
3:D:786:ILE:HD13	3:D:908:LYS:HG2	1.69	0.72
3:J:670:VAL:HB	5:L:364:LEU:HD11	1.70	0.72
5:F:235:LEU:HB2	5:F:258:ILE:HD11	1.70	0.72
2:C:911:GLU:OE1	3:D:1062:ARG:NH2	2.23	0.71
2:I:72:ARG:HB2	2:I:95:TYR:HB2	1.71	0.71
2:I:1019:GLN:HG3	3:J:617:ASN:HD22	1.54	0.71
2:C:366:THR:HA	6:M:14:PRO:HG3	1.72	0.71
3:J:18:ILE:HG12	3:J:518:PRO:HG3	1.72	0.71
2:C:72:ARG:HB2	2:C:95:TYR:HB2	1.72	0.71
1:A:179:PHE:HB3	1:A:197:LEU:HD12	1.73	0.71
3:D:1436:SER:HB2	3:D:1464:GLU:HG2	1.72	0.71
2:C:971:LYS:HB2	2:C:986:PRO:HB2	1.72	0.71
3:D:917:GLN:HE22	3:D:1168:LEU:HD11	1.57	0.70
3:D:1254:GLN:HB2	3:D:1258:ARG:HB2	1.71	0.70
3:D:1135:ARG:HH21	3:D:1357:ARG:HH12	1.39	0.70
2:I:14:PRO:HB3	2:I:586:ARG:HH22	1.57	0.70
2:C:537:LYS:HZ3	2:C:905:VAL:H	1.37	0.70
3:D:226:PRO:HA	3:D:330:SER:HA	1.73	0.70
1:A:175:ARG:N	1:A:200:TRP:O	2.25	0.70
1:G:175:ARG:N	1:G:200:TRP:O	2.24	0.70
2:I:214:TYR:HB2	2:I:217:LEU:HD11	1.74	0.70
3:D:165:LYS:HB3	3:D:397:LYS:HE2	1.72	0.70
5:F:293:LEU:HD11	5:F:306:ILE:HD13	1.74	0.70
2:C:217:LEU:HD13	2:C:311:PHE:HD2	1.57	0.69
3:D:1472:ILE:HG13	3:D:1474:ALA:H	1.56	0.69
2:I:971:LYS:HB2	2:I:986:PRO:HB2	1.72	0.69
1:B:175:ARG:HB3	3:D:847:ASP:HB3	1.73	0.69
2:C:214:TYR:HB2	2:C:217:LEU:HD11	1.74	0.69
2:C:472:ARG:HD3	2:C:479:VAL:HG13	1.74	0.69
2:I:230:ARG:HH21	2:I:231:PRO:HD2	1.57	0.69
3:D:18:ILE:HG12	3:D:518:PRO:HG3	1.74	0.69
1:H:175:ARG:HB3	3:J:847:ASP:HB3	1.74	0.69
3:J:1135:ARG:HH21	3:J:1357:ARG:HH12	1.40	0.69
2:I:472:ARG:HD3	2:I:479:VAL:HG13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:293:LEU:HD11	5:L:306:ILE:HD13	1.74	0.69
1:A:34:VAL:HG11	2:C:981:GLU:HG2	1.74	0.69
2:C:230:ARG:HH21	2:C:231:PRO:HD2	1.57	0.69
3:D:628:ARG:NH2	3:D:744:GLN:OE1	2.24	0.69
1:G:179:PHE:HB3	1:G:197:LEU:HD12	1.74	0.69
3:J:658:LEU:HD22	3:J:670:VAL:HG13	1.74	0.69
2:C:872:ASN:HD21	2:C:874:LEU:HG	1.57	0.69
5:F:411:ARG:HD3	7:O:1:DC:H2'	1.75	0.69
2:I:324:ASP:HB3	2:I:327:HIS:HB2	1.75	0.69
2:I:484:VAL:HG21	2:I:531:PHE:HE1	1.57	0.69
2:I:872:ASN:HD21	2:I:874:LEU:HG	1.58	0.69
3:J:1472:ILE:HG13	3:J:1474:ALA:H	1.57	0.69
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.74	0.69
2:C:484:VAL:HG21	2:C:531:PHE:HE1	1.56	0.69
3:D:835:SER:HB3	3:D:838:ARG:HG3	1.75	0.69
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.74	0.69
3:D:704:ARG:HG2	3:D:738:ALA:HB2	1.75	0.69
2:I:304:LEU:HB3	2:I:305:PRO:HD3	1.75	0.69
3:J:917:GLN:HE22	3:J:1168:LEU:HD11	1.57	0.69
3:D:9:ARG:HG3	3:D:1456:LYS:HB3	1.75	0.68
1:A:41:ARG:HG3	1:A:177:VAL:HB	1.76	0.68
3:J:1122:LEU:HD23	3:J:1140:ILE:HG21	1.75	0.68
6:M:88:ALA:HA	6:M:91:ARG:HD2	1.76	0.68
5:F:288:ARG:NH1	8:P:24:DA:OP1	2.26	0.68
1:G:34:VAL:HG11	2:I:981:GLU:HG2	1.74	0.68
1:G:41:ARG:HG3	1:G:177:VAL:HB	1.75	0.68
3:J:356:PRO:HB3	3:J:441:ARG:HA	1.75	0.68
3:J:628:ARG:NH2	3:J:744:GLN:OE1	2.25	0.68
3:J:835:SER:HB3	3:J:838:ARG:HG3	1.75	0.68
7:O:7:DA:H61	8:P:42:DT:H3	1.39	0.68
2:C:1063:ARG:HH22	5:F:353:LEU:HD11	1.59	0.68
3:J:704:ARG:HG2	3:J:738:ALA:HB2	1.75	0.68
2:C:264:PRO:HG2	2:C:265:LYS:HE2	1.75	0.68
3:D:1122:LEU:HD23	3:D:1140:ILE:HG21	1.75	0.68
2:I:502:PRO:HB2	2:I:509:ALA:HB3	1.74	0.68
3:J:572:ARG:NH1	5:L:98:GLN:HE21	1.92	0.68
5:L:124:GLY:HA2	5:L:191:ILE:HG22	1.76	0.68
7:R:2:DT:H3	8:S:47:DA:H2	1.40	0.68
2:C:6:PHE:HE1	2:C:901:TYR:HD1	1.42	0.68
3:D:743:ASP:HA	9:Q:4:A:H4'	1.75	0.68
2:I:217:LEU:HD13	2:I:311:PHE:HD2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:ILE:HB	6:M:48:TYR:HB2	1.76	0.67
2:C:902:ILE:HG22	2:C:904:PRO:HD3	1.75	0.67
2:I:711:GLU:O	2:I:758:ARG:NH1	2.27	0.67
2:I:6:PHE:HE1	2:I:901:TYR:HD1	1.42	0.67
2:C:328:LEU:HD22	2:C:437:ARG:HD2	1.75	0.67
2:C:711:GLU:O	2:C:758:ARG:NH1	2.27	0.67
5:F:103:ILE:HG21	5:F:211:VAL:HG21	1.76	0.67
3:J:67:ARG:HG3	5:L:392:ASP:HB2	1.77	0.67
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.59	0.67
2:C:14:PRO:HB3	2:C:586:ARG:HH22	1.58	0.67
3:D:102:ILE:HD11	3:D:587:ARG:HG3	1.77	0.67
2:I:12:VAL:HG11	2:I:472:ARG:HH12	1.59	0.67
3:J:9:ARG:HG3	3:J:1456:LYS:HB3	1.77	0.67
3:J:12:LEU:HD11	3:J:1452:ILE:HA	1.77	0.67
2:C:487:THR:O	2:C:491:GLU:N	2.28	0.66
3:D:572:ARG:NH1	5:F:98:GLN:HE21	1.92	0.66
2:I:902:ILE:HG22	2:I:904:PRO:HD3	1.75	0.66
2:I:487:THR:O	2:I:491:GLU:N	2.28	0.66
3:J:743:ASP:HA	9:T:4:A:HA4'	1.77	0.66
2:I:211:LEU:HD11	2:I:221:LEU:HB3	1.78	0.66
2:I:770:GLU:HG2	5:L:366:SER:HA	1.76	0.66
7:R:10:DA:H2	8:S:39:DT:H3	1.43	0.66
2:C:770:GLU:HG2	5:F:366:SER:HA	1.76	0.66
5:F:383:VAL:HG13	5:F:401:VAL:HG11	1.78	0.66
2:C:12:VAL:HG11	2:C:472:ARG:HH12	1.60	0.66
3:D:543:LEU:HG	3:D:600:LEU:HD23	1.78	0.66
5:F:124:GLY:HA2	5:F:191:ILE:HG22	1.76	0.66
2:I:328:LEU:HD22	2:I:437:ARG:HD2	1.76	0.66
2:I:468:ARG:HB3	2:I:485:TYR:O	1.96	0.66
2:I:1008:ARG:HH11	2:I:1028:GLY:HA2	1.59	0.66
3:D:191:LEU:HD11	3:D:197:SER:HB2	1.76	0.66
3:D:349:PRO:HB3	5:F:112:GLU:HG2	1.77	0.66
2:I:264:PRO:HG2	2:I:265:LYS:HE2	1.76	0.66
3:D:12:LEU:HD11	3:D:1452:ILE:HA	1.78	0.66
5:F:332:LEU:HD22	5:F:345:GLY:HA2	1.75	0.66
2:I:859:PRO:HB2	2:I:974:LEU:HD23	1.76	0.66
6:M:21:ALA:O	6:M:37:GLN:HB3	1.96	0.66
1:B:176:ARG:HD2	3:D:884:ARG:HH22	1.61	0.66
3:D:178:LEU:HD21	3:D:190:GLU:HB3	1.78	0.66
4:E:30:LEU:HA	4:E:37:ASN:HD21	1.60	0.66
2:I:100:LEU:HB2	2:I:369:PRO:HD3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.77	0.66
3:J:543:LEU:HG	3:J:600:LEU:HD23	1.76	0.66
1:H:55:SER:HB2	1:H:166:PRO:HA	1.78	0.65
2:I:199:VAL:HA	2:I:231:PRO:HB3	1.77	0.65
2:I:595:LEU:HB2	2:I:656:ALA:HB3	1.76	0.65
5:L:103:ILE:HG21	5:L:211:VAL:HG21	1.77	0.65
2:C:100:LEU:HB2	2:C:369:PRO:HD3	1.77	0.65
2:C:630:ARG:HA	2:C:705:ILE:HD13	1.77	0.65
3:D:1331:ASP:HB3	3:D:1334:GLN:HB2	1.78	0.65
2:I:1095:LEU:HD11	3:J:603:LEU:HB3	1.77	0.65
3:J:102:ILE:HD11	3:J:587:ARG:HG3	1.77	0.65
2:C:468:ARG:HB3	2:C:485:TYR:O	1.96	0.65
5:F:222:LEU:HB3	5:F:226:ASP:HB3	1.78	0.65
7:R:39:DT:H2''	7:R:40:DC:H5'	1.77	0.65
2:C:859:PRO:HB2	2:C:974:LEU:HD23	1.78	0.65
3:D:561:GLY:HA3	5:F:147:ARG:HD3	1.77	0.65
2:I:458:TYR:HB3	2:I:470:PRO:HG2	1.78	0.65
4:K:30:LEU:HA	4:K:37:ASN:HD21	1.61	0.65
1:B:55:SER:HB2	1:B:166:PRO:HA	1.78	0.65
3:D:973:GLN:HG2	3:J:831:GLY:HA2	1.78	0.65
3:J:1331:ASP:HB3	3:J:1334:GLN:HB2	1.79	0.65
8:P:17:DG:H2''	8:P:18:DG:O4'	1.97	0.65
7:O:39:DT:H2''	7:O:40:DC:H5'	1.77	0.65
2:C:211:LEU:HD11	2:C:221:LEU:HB3	1.77	0.65
3:J:411:THR:HG22	3:J:437:VAL:H	1.62	0.65
3:D:1088:THR:HG22	3:D:1234:THR:HG23	1.78	0.65
2:I:158:TYR:HB2	2:I:314:THR:HG22	1.79	0.65
1:A:53:VAL:HG22	1:A:54:THR:H	1.61	0.65
2:C:595:LEU:HB2	2:C:656:ALA:HB3	1.78	0.65
3:D:759:ALA:HA	3:D:763:MET:HB3	1.78	0.65
2:I:751:PRO:HD2	3:J:681:ARG:HD2	1.78	0.64
1:H:176:ARG:HD2	3:J:884:ARG:HH22	1.62	0.64
5:L:222:LEU:HB3	5:L:226:ASP:HB3	1.78	0.64
2:C:143:SER:H	2:C:331:ARG:HA	1.63	0.64
3:J:561:GLY:HA3	5:L:147:ARG:HD3	1.79	0.64
7:R:46:DT:H3	8:S:3:DA:H61	1.45	0.64
2:C:374:ASN:ND2	5:F:291:ARG:HE	1.94	0.64
2:I:36:PRO:HB2	2:I:70:GLU:HG2	1.79	0.64
1:A:73:GLU:HB3	1:A:77:GLU:HB3	1.80	0.64
3:D:1138:SER:HB3	3:D:1362:LYS:HD3	1.80	0.64
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.80	0.64
3:D:32:ILE:HG22	3:D:39:PRO:HA	1.80	0.64
2:I:374:ASN:HD21	5:L:291:ARG:NE	1.95	0.64
1:A:219:LYS:HB2	1:B:222:LEU:HD22	1.79	0.64
2:I:874:LEU:HD13	3:J:783:ARG:HB3	1.80	0.64
2:I:966:LEU:HD11	2:I:986:PRO:HG3	1.80	0.64
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.80	0.64
3:J:1486:VAL:HG11	4:K:22:VAL:HG13	1.80	0.64
5:L:383:VAL:HG13	5:L:401:VAL:HG11	1.79	0.64
2:C:157:ARG:HH22	2:C:314:THR:HB	1.62	0.63
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.79	0.63
3:J:759:ALA:HA	3:J:763:MET:HB3	1.78	0.63
3:D:229:ALA:HA	3:D:245:LEU:H	1.63	0.63
6:N:18:GLY:HA2	6:N:41:PRO:HD3	1.78	0.63
8:S:14:DG:H1	9:T:2:C:H42	1.46	0.63
2:C:458:TYR:HB3	2:C:470:PRO:HG2	1.78	0.63
1:G:219:LYS:HB2	1:H:222:LEU:HD22	1.79	0.63
3:J:168:THR:HA	3:J:394:LEU:HG	1.81	0.63
1:B:184:THR:HG23	1:B:192:LEU:HB2	1.81	0.63
3:D:637:LEU:O	3:D:935:LYS:NZ	2.32	0.63
3:D:1459:LEU:HD21	3:D:1468:LEU:HG	1.80	0.63
1:G:53:VAL:HG22	1:G:54:THR:H	1.63	0.63
2:I:42:VAL:HA	2:I:46:ALA:HB2	1.81	0.63
2:I:914:ILE:HA	2:I:917:LEU:HD12	1.81	0.63
3:D:1432:LYS:HG3	3:D:1460:ILE:HD11	1.81	0.63
3:J:1138:SER:HB3	3:J:1362:LYS:HD3	1.80	0.63
3:D:1038:LEU:O	3:D:1060:SER:OG	2.17	0.63
1:G:73:GLU:HB3	1:G:77:GLU:HB3	1.79	0.63
3:J:192:ALA:HB1	3:J:193:PRO:HD2	1.81	0.63
2:C:158:TYR:HB2	2:C:314:THR:HG22	1.80	0.63
4:E:41:GLU:HB3	4:E:42:PRO:HD2	1.81	0.63
2:I:157:ARG:HH22	2:I:314:THR:HB	1.63	0.63
3:J:1432:LYS:HG3	3:J:1460:ILE:HD11	1.80	0.63
5:L:409:ARG:NH2	7:R:5:DA:H61	1.95	0.63
3:D:291:LEU:HD23	3:D:303:PRO:HB2	1.80	0.63
1:H:184:THR:HG23	1:H:192:LEU:HB2	1.81	0.63
2:I:437:ARG:NH1	2:I:467:ILE:O	2.32	0.63
7:O:47:DG:N2	8:P:2:DC:N3	2.46	0.63
3:D:675:ARG:HH12	5:F:437:LEU:HG	1.64	0.63
2:I:675:ALA:HA	2:I:989:VAL:HG12	1.81	0.63
1:B:186:LEU:HD13	4:E:51:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1064:ASN:HD22	5:L:359:ALA:HB2	1.64	0.62
3:J:1038:LEU:O	3:J:1060:SER:OG	2.17	0.62
5:L:431:ARG:HG3	5:L:434:ARG:HE	1.64	0.62
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.81	0.62
2:C:1034:GLU:HG2	3:D:619:LEU:HB3	1.82	0.62
3:D:658:LEU:HD22	3:D:670:VAL:HG13	1.81	0.62
3:D:1323:GLN:HG2	3:D:1324:PRO:HD2	1.81	0.62
2:I:245:GLY:HA2	5:L:97:ARG:HD2	1.81	0.62
6:N:20:VAL:HA	6:N:38:VAL:CA	2.29	0.62
3:J:1323:GLN:HG2	3:J:1324:PRO:HD2	1.81	0.62
3:D:264:LEU:HG	3:D:316:HIS:HE2	1.63	0.62
2:I:876:VAL:HG13	2:I:884:GLN:HE21	1.65	0.62
3:J:1088:THR:HG22	3:J:1234:THR:HG23	1.80	0.62
2:C:914:ILE:HA	2:C:917:LEU:HD12	1.81	0.62
2:C:1055:ILE:HD11	2:C:1079:PRO:HD3	1.82	0.62
3:J:32:ILE:HG22	3:J:39:PRO:HA	1.81	0.62
3:J:1201:CYS:SG	3:J:1204:CYS:HB2	2.40	0.62
2:C:118:LEU:HD12	2:C:119:PRO:HD2	1.82	0.62
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.81	0.62
3:D:30:GLU:HB2	5:F:274:ARG:HB2	1.82	0.62
3:J:680:GLN:O	3:J:682:ASP:N	2.29	0.62
4:K:41:GLU:HB3	4:K:42:PRO:HD2	1.81	0.62
3:D:1201:CYS:SG	3:D:1204:CYS:HB2	2.39	0.62
3:J:125:GLN:NE2	3:J:130:ASN:OD1	2.33	0.62
3:J:462:GLN:HA	3:J:513:ILE:HG13	1.82	0.62
2:C:876:VAL:HG13	2:C:884:GLN:HE21	1.65	0.62
1:H:186:LEU:HD13	4:K:51:LEU:HD13	1.80	0.62
2:I:124:ASP:O	2:I:407:LYS:NZ	2.31	0.61
2:I:143:SER:H	2:I:331:ARG:HA	1.64	0.61
2:C:164:PRO:HB3	2:C:269:LEU:HG	1.82	0.61
2:C:437:ARG:NH1	2:C:467:ILE:O	2.33	0.61
7:R:11:DG:N2	8:S:38:DC:O2	2.32	0.61
1:A:14:THR:HG1	1:B:231:SER:HG	1.46	0.61
3:D:8:VAL:HG21	3:D:1468:LEU:HD21	1.82	0.61
3:J:30:GLU:HB2	5:L:274:ARG:HB2	1.80	0.61
2:C:1060:ILE:HG13	2:C:1061:GLU:H	1.65	0.61
3:J:700:VAL:HG22	3:J:718:PRO:HG3	1.82	0.61
3:J:1436:SER:HB2	3:J:1464:GLU:HG2	1.82	0.61
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.81	0.61
3:J:1106:VAL:HB	3:J:1108:ARG:HH22	1.66	0.61
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1100:GLN:HB2	3:J:9:ARG:HB3	1.82	0.61
2:C:966:LEU:HD11	2:C:986:PRO:HG3	1.82	0.61
3:D:417:PRO:HA	3:D:430:GLU:HA	1.82	0.61
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.35	0.61
6:N:21:ALA:O	6:N:37:GLN:HB3	2.00	0.61
3:D:700:VAL:HG22	3:D:718:PRO:HG3	1.82	0.61
1:G:175:ARG:HB3	1:G:200:TRP:HB3	1.83	0.61
2:I:15:LEU:HD21	2:I:457:ALA:HB1	1.83	0.61
2:C:197:LEU:HD23	2:C:200:LEU:HD23	1.81	0.61
3:J:770:LEU:HB2	3:J:1210:SER:HA	1.83	0.61
3:J:1384:PRO:HA	3:J:1415:VAL:HG13	1.83	0.61
3:J:1459:LEU:HD21	3:J:1468:LEU:HG	1.83	0.61
2:I:383:ARG:HH21	2:I:388:ARG:NH2	1.99	0.61
2:C:15:LEU:HD21	2:C:457:ALA:HB1	1.83	0.60
2:C:383:ARG:HH21	2:C:388:ARG:NH2	1.99	0.60
3:D:125:GLN:NE2	3:D:130:ASN:OD1	2.33	0.60
2:I:1060:ILE:HG13	2:I:1061:GLU:H	1.65	0.60
3:J:191:LEU:HB2	3:J:195:VAL:HG11	1.81	0.60
3:J:1465:ASN:O	3:J:1468:LEU:N	2.34	0.60
3:D:101:HIS:NE2	3:D:582:ILE:HG21	2.17	0.60
2:I:139:GLN:HB3	2:I:334:ARG:HB2	1.83	0.60
3:J:1149:LEU:HB3	3:J:1162:GLU:HA	1.83	0.60
1:A:175:ARG:HB3	1:A:200:TRP:HB3	1.84	0.60
3:D:462:GLN:HA	3:D:513:ILE:HG13	1.82	0.60
3:D:699:VAL:HG13	3:D:760:ARG:HD3	1.83	0.60
3:J:100:ALA:HA	3:J:513:ILE:HA	1.83	0.60
3:J:637:LEU:O	3:J:935:LYS:NZ	2.34	0.60
4:K:37:ASN:N	4:K:37:ASN:OD1	2.34	0.60
2:C:994:ILE:HG22	2:C:995:MET:H	1.65	0.60
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.84	0.60
3:D:1106:VAL:HB	3:D:1108:ARG:HH22	1.66	0.60
3:D:1149:LEU:HB3	3:D:1162:GLU:HA	1.83	0.60
4:E:37:ASN:OD1	4:E:37:ASN:N	2.34	0.60
1:A:40:LEU:O	1:A:44:LEU:HB2	2.02	0.60
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.82	0.60
2:I:276:LYS:HD3	2:I:466:PHE:HZ	1.67	0.60
3:D:162:ARG:HG2	3:D:414:ARG:HH22	1.67	0.60
3:D:960:LYS:O	3:D:964:LEU:HB3	2.02	0.60
2:I:714:ASP:HA	2:I:719:PRO:HA	1.84	0.60
3:D:100:ALA:HA	3:D:513:ILE:HA	1.84	0.60
2:I:549:PHE:HZ	2:I:890:LEU:HD12	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:729:HIS:HE1	3:J:731:LEU:HD23	1.66	0.60
3:D:213:VAL:HG22	3:D:385:VAL:HG12	1.82	0.60
3:D:1465:ASN:O	3:D:1468:LEU:N	2.34	0.60
3:J:433:GLY:HA2	3:J:449:SER:H	1.67	0.60
3:J:644:LEU:HD12	3:J:645:PRO:HD2	1.83	0.60
7:O:32:DG:H2'	7:O:33:DG:C8	2.37	0.60
1:A:32:PHE:O	1:A:35:THR:OG1	2.16	0.59
2:C:139:GLN:HB3	2:C:334:ARG:HB2	1.82	0.59
4:K:67:GLU:HB3	4:K:73:LEU:HD11	1.84	0.59
6:M:18:GLY:HA2	6:M:41:PRO:HD3	1.84	0.59
2:C:532:MET:HG2	2:C:533:ASP:H	1.68	0.59
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.83	0.59
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.84	0.59
1:G:215:VAL:HG13	1:H:222:LEU:HD23	1.84	0.59
1:H:18:ASP:O	1:H:201:THR:OG1	2.11	0.59
2:I:994:ILE:HG22	2:I:995:MET:H	1.66	0.59
3:J:699:VAL:HG13	3:J:760:ARG:HD3	1.83	0.59
4:E:38:THR:HG21	4:E:63:TRP:HZ3	1.67	0.59
1:G:14:THR:OG1	1:H:231:SER:OG	2.20	0.59
2:I:197:LEU:HD23	2:I:200:LEU:HD23	1.83	0.59
3:J:729:HIS:CE1	3:J:731:LEU:HD23	2.37	0.59
3:J:960:LYS:O	3:J:964:LEU:HB3	2.01	0.59
5:L:210:VAL:HA	5:L:213:ILE:HD12	1.85	0.59
2:C:15:LEU:HD13	2:C:16:PRO:HD2	1.84	0.59
2:C:182:VAL:HG21	2:C:193:LEU:HD12	1.85	0.59
2:C:238:LEU:HD23	2:C:241:LEU:HD12	1.84	0.59
2:C:575:GLN:HB3	2:C:670:GLN:HG3	1.84	0.59
2:C:1100:GLN:HB2	3:D:9:ARG:HB3	1.82	0.59
3:D:729:HIS:HE1	3:D:731:LEU:HD23	1.66	0.59
2:I:163:ILE:HD13	2:I:171:TRP:CD1	2.37	0.59
2:I:193:LEU:HD21	2:I:307:LEU:HD11	1.84	0.59
3:J:421:LEU:H	3:J:428:LYS:HA	1.67	0.59
3:J:127:LEU:HG	3:J:461:ILE:HG13	1.85	0.59
3:J:1197:ARG:HE	3:J:1398:TRP:HB3	1.66	0.59
6:N:106:ALA:HA	6:N:136:LEU:HD11	1.85	0.59
1:A:215:VAL:HG13	1:B:222:LEU:HD23	1.84	0.59
2:C:886:LEU:HD21	3:D:951:ILE:HD13	1.84	0.59
2:C:1019:GLN:HG3	3:D:617:ASN:HD22	1.67	0.59
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.84	0.59
1:G:40:LEU:O	1:G:44:LEU:HB2	2.02	0.59
2:I:238:LEU:HD23	2:I:241:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:575:GLN:HB3	2:I:670:GLN:HG3	1.83	0.59
3:J:101:HIS:NE2	3:J:582:ILE:HG21	2.17	0.59
2:C:714:ASP:HA	2:C:719:PRO:HA	1.85	0.59
2:I:754:ILE:HG12	2:I:791:ARG:HD3	1.85	0.59
2:I:886:LEU:HD21	3:J:951:ILE:HD13	1.85	0.59
6:N:88:ALA:HA	6:N:91:ARG:HD2	1.84	0.59
2:C:261:LEU:HB3	2:C:290:LEU:HD12	1.85	0.59
3:D:181:ASP:HB3	3:D:357:GLU:HG2	1.85	0.59
2:I:1034:GLU:HG2	3:J:619:LEU:HB3	1.85	0.59
3:J:186:VAL:HG12	3:J:187:LYS:H	1.67	0.59
2:I:118:LEU:HD12	2:I:119:PRO:HD2	1.84	0.58
2:I:1056:LYS:HE2	3:J:751:LEU:HG	1.84	0.58
3:J:355:VAL:HG12	3:J:356:PRO:HD2	1.85	0.58
4:K:38:THR:HG21	4:K:63:TRP:HZ3	1.68	0.58
2:C:14:PRO:HB3	2:C:586:ARG:NH2	2.18	0.58
3:D:977:ALA:HB2	3:J:831:GLY:HA3	1.85	0.58
3:D:1201:CYS:SG	3:D:1204:CYS:CB	2.91	0.58
1:B:18:ASP:O	1:B:201:THR:OG1	2.11	0.58
2:C:163:ILE:HD13	2:C:171:TRP:CD1	2.37	0.58
3:D:729:HIS:CE1	3:D:731:LEU:HD23	2.37	0.58
2:I:164:PRO:HB3	2:I:269:LEU:HG	1.83	0.58
7:O:10:DA:H2	8:P:39:DT:H3	1.51	0.58
2:I:532:MET:HG2	2:I:533:ASP:H	1.68	0.58
3:D:1197:ARG:HE	3:D:1398:TRP:HB3	1.66	0.58
3:J:1336:LEU:HD22	3:J:1421:LEU:HB3	1.86	0.58
5:L:364:LEU:HD22	5:L:436:PHE:HZ	1.68	0.58
1:A:53:VAL:HA	1:A:144:VAL:HG13	1.85	0.58
3:D:245:LEU:HD11	3:D:249:TYR:HB3	1.85	0.58
3:D:1045:MET:HE2	3:D:1057:VAL:HG11	1.86	0.58
2:I:15:LEU:HD13	2:I:16:PRO:HD2	1.84	0.58
2:I:182:VAL:HG21	2:I:193:LEU:HD12	1.86	0.58
2:I:261:LEU:HB3	2:I:290:LEU:HD12	1.85	0.58
2:I:1082:PRO:HG3	3:J:1469:GLY:HA3	1.86	0.58
4:K:91:ARG:HH21	4:K:92:LEU:HG	1.68	0.58
6:M:151:ALA:HA	6:M:154:LEU:HD12	1.86	0.58
7:O:32:DG:H2''	7:O:33:DG:H5'	1.86	0.58
2:C:239:PHE:HA	2:C:242:LEU:HD12	1.85	0.58
3:D:127:LEU:HG	3:D:461:ILE:HG13	1.85	0.58
4:E:67:GLU:HB3	4:E:73:LEU:HD11	1.84	0.58
3:J:1201:CYS:SG	3:J:1204:CYS:CB	2.91	0.58
6:M:20:VAL:HA	6:M:38:VAL:CA	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:549:PHE:HZ	2:C:890:LEU:HD12	1.68	0.58
2:C:773:LEU:HD13	5:F:388:LYS:HG3	1.86	0.58
5:F:210:VAL:HA	5:F:213:ILE:HD12	1.85	0.58
5:L:417:ASN:HD22	5:L:421:ARG:HH12	1.52	0.58
2:C:432:ARG:HH12	2:C:518:ARG:HH21	1.52	0.58
3:D:1336:LEU:HD22	3:D:1421:LEU:HB3	1.86	0.58
2:I:14:PRO:HB3	2:I:586:ARG:NH2	2.17	0.58
3:J:371:ILE:HD12	5:L:247:ARG:HE	1.68	0.58
6:M:116:GLU:HB2	6:M:121:LEU:HD22	1.84	0.58
7:O:2:DT:H3	8:P:47:DA:H2	1.52	0.58
2:C:754:ILE:HG12	2:C:791:ARG:HD3	1.86	0.58
2:C:1047:HIS:O	2:C:1051:GLU:HG2	2.04	0.58
5:F:252:THR:HA	7:O:29:DC:H5	1.69	0.58
2:I:949:LYS:HD2	3:J:796:ARG:HH11	1.69	0.58
2:C:1057:SER:HB3	3:D:623:VAL:HG13	1.86	0.57
2:I:239:PHE:HA	2:I:242:LEU:HD12	1.85	0.57
2:I:1017:THR:HG21	3:J:617:ASN:ND2	2.18	0.57
3:J:1045:MET:HE2	3:J:1057:VAL:HG11	1.86	0.57
5:L:151:LEU:HD23	5:L:156:ILE:HD12	1.86	0.57
1:A:36:LEU:HB2	1:A:195:LEU:HD12	1.86	0.57
2:C:86:LYS:HE2	2:C:814:GLU:H	1.68	0.57
3:D:672:ALA:O	3:D:676:MET:HB2	2.04	0.57
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.44	0.57
3:D:520:LEU:HB3	3:D:525:ARG:HD3	1.86	0.57
3:D:527:MET:HG3	3:D:537:THR:HB	1.86	0.57
5:F:100:LEU:HD13	7:O:31:DG:H21	1.69	0.57
3:D:44:LEU:HB3	3:D:525:ARG:HH22	1.70	0.57
1:G:53:VAL:HA	1:G:144:VAL:HG13	1.87	0.57
1:A:224:TYR:CE1	1:B:9:PRO:HG2	2.39	0.57
3:D:1462:LEU:HD12	3:D:1463:LYS:H	1.69	0.57
3:J:527:MET:HG3	3:J:537:THR:HB	1.87	0.57
3:J:661:MET:HG2	3:J:666:PHE:CZ	2.39	0.57
1:B:72:LYS:HG3	1:B:131:THR:HB	1.86	0.57
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.85	0.57
4:E:91:ARG:HH21	4:E:92:LEU:HG	1.69	0.57
3:J:60:CYS:SG	3:J:76:CYS:HB3	2.45	0.57
2:C:167:LYS:HD3	7:O:35:DG:H5'	1.86	0.57
2:I:1057:SER:HB3	3:J:623:VAL:HG13	1.87	0.57
3:J:1097:LYS:HE2	3:J:1440:PHE:HZ	1.69	0.57
2:C:690:ILE:HD11	2:C:849:VAL:HG22	1.87	0.57
1:H:72:LYS:HG3	1:H:131:THR:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:773:LEU:HD13	5:L:388:LYS:HG3	1.85	0.57
2:C:163:ILE:HD13	2:C:171:TRP:HD1	1.69	0.57
2:C:949:LYS:HD2	3:D:796:ARG:HH11	1.69	0.57
3:D:229:ALA:HB1	3:D:243:ALA:HB1	1.86	0.57
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.87	0.57
2:I:285:LEU:HD23	2:I:286:SER:H	1.70	0.57
2:I:660:ALA:HB1	2:I:667:ALA:O	2.05	0.57
3:J:141:VAL:HG12	3:J:450:TYR:HE2	1.69	0.57
3:J:1462:LEU:HD12	3:J:1463:LYS:H	1.69	0.57
2:C:193:LEU:HD21	2:C:307:LEU:HD11	1.86	0.57
1:G:178:ALA:HB2	2:I:864:GLY:HA3	1.87	0.57
3:J:1045:MET:HB2	3:J:1072:ILE:HG22	1.86	0.57
2:C:93:PRO:HB3	2:C:114:PHE:HE1	1.69	0.56
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.87	0.56
5:F:252:THR:HA	7:O:29:DC:C5	2.40	0.56
2:I:432:ARG:HH12	2:I:518:ARG:HH21	1.53	0.56
3:J:672:ALA:O	3:J:676:MET:HB2	2.04	0.56
3:J:703:ASN:HB2	3:J:713:ILE:HG12	1.87	0.56
3:J:828:VAL:HA	3:J:833:GLU:HA	1.87	0.56
1:A:153:ALA:HB1	1:A:166:PRO:HB2	1.86	0.56
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.88	0.56
1:G:36:LEU:HB2	1:G:195:LEU:HD12	1.86	0.56
1:G:224:TYR:CE1	1:H:9:PRO:HG2	2.40	0.56
2:I:93:PRO:HB3	2:I:114:PHE:HE1	1.70	0.56
2:I:194:VAL:HA	2:I:197:LEU:HD12	1.87	0.56
1:A:67:THR:HG21	2:C:627:ARG:HG3	1.87	0.56
2:C:71:TYR:HA	2:C:95:TYR:C	2.26	0.56
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.87	0.56
2:C:376:ARG:HH22	5:F:294:GLN:HG3	1.70	0.56
3:D:886:VAL:HG11	3:D:900:ILE:HD11	1.86	0.56
3:D:1045:MET:HB2	3:D:1072:ILE:HG22	1.86	0.56
4:E:38:THR:HG21	4:E:63:TRP:CZ3	2.40	0.56
5:F:151:LEU:HD23	5:F:156:ILE:HD12	1.87	0.56
2:I:26:TYR:HB2	2:I:336:VAL:HB	1.87	0.56
2:I:69:LEU:HB2	2:I:97:ARG:O	2.05	0.56
2:I:163:ILE:HD13	2:I:171:TRP:HD1	1.69	0.56
3:J:349:PRO:HB3	5:L:112:GLU:HG2	1.85	0.56
3:J:613:ARG:HD3	3:J:617:ASN:OD1	2.05	0.56
3:J:628:ARG:HH12	8:S:14:DG:H2"	1.69	0.56
3:J:886:VAL:HG11	3:J:900:ILE:HD11	1.86	0.56
3:J:901:GLN:HG2	3:J:906:GLN:HE22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1042:ARG:HE	3:J:1061:PHE:HE2	1.53	0.56
3:J:1377:LYS:O	3:J:1397:LYS:N	2.38	0.56
1:A:62:LEU:HD13	2:C:745:ILE:HG21	1.88	0.56
2:I:853:LEU:HD12	2:I:854:PRO:HD2	1.86	0.56
3:J:86:ARG:O	3:J:521:PRO:HB3	2.06	0.56
5:L:252:THR:HA	7:R:29:DC:C5	2.41	0.56
7:R:47:DG:N2	8:S:2:DC:N3	2.54	0.56
2:C:437:ARG:HB3	2:C:467:ILE:HG21	1.88	0.56
2:I:606:VAL:HG23	2:I:645:VAL:HA	1.87	0.56
2:I:690:ILE:HD11	2:I:849:VAL:HG22	1.87	0.56
3:J:916:TYR:HE2	3:J:1168:LEU:HD22	1.71	0.56
3:J:1068:LEU:H	3:J:1068:LEU:HD12	1.70	0.56
3:D:1042:ARG:HE	3:D:1061:PHE:HE2	1.54	0.56
2:C:473:ARG:O	2:C:480:THR:OG1	2.17	0.56
2:C:606:VAL:HG23	2:C:645:VAL:HA	1.87	0.56
2:C:1066:ALA:HA	2:C:1076:VAL:HG12	1.87	0.56
3:D:439:LEU:HD22	3:D:439:LEU:H	1.70	0.56
1:G:67:THR:HG21	2:I:627:ARG:HG3	1.87	0.56
2:I:458:TYR:HD1	2:I:538:GLN:HB3	1.70	0.56
3:J:208:PRO:HA	3:J:390:PRO:HA	1.88	0.56
2:C:146:VAL:HG21	2:C:281:LEU:HD11	1.88	0.56
2:C:374:ASN:ND2	2:C:375:SER:H	2.04	0.56
3:D:613:ARG:HD3	3:D:617:ASN:OD1	2.06	0.56
5:F:417:ASN:HD22	5:F:421:ARG:HH12	1.53	0.56
1:G:32:PHE:O	1:G:35:THR:OG1	2.18	0.56
1:G:153:ALA:HB1	1:G:166:PRO:HB2	1.87	0.56
2:I:473:ARG:O	2:I:480:THR:OG1	2.19	0.56
2:I:1047:HIS:O	2:I:1051:GLU:HG2	2.05	0.56
3:J:470:LEU:HD22	3:J:499:VAL:HG13	1.88	0.56
3:J:572:ARG:HH12	5:L:98:GLN:HE21	1.54	0.56
5:L:252:THR:HG23	7:R:29:DC:H41	1.71	0.56
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.86	0.56
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.88	0.56
2:C:660:ALA:HB1	2:C:667:ALA:O	2.05	0.56
3:D:317:MET:HB3	3:D:337:LEU:HD21	1.86	0.56
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.88	0.56
2:I:146:VAL:HG21	2:I:281:LEU:HD11	1.88	0.56
3:J:44:LEU:HB3	3:J:525:ARG:HH22	1.71	0.56
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.71	0.56
3:D:638:LYS:HG2	3:D:639:LEU:H	1.70	0.56
2:I:71:TYR:HA	2:I:95:TYR:C	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:99:TYR:HA	5:L:102:GLU:HB2	1.88	0.56
2:C:245:GLY:HA2	5:F:97:ARG:HD2	1.88	0.55
2:C:328:LEU:HD21	2:C:438:ILE:HD11	1.88	0.55
2:C:605:LYS:HG2	2:C:612:ALA:HB3	1.88	0.55
2:C:853:LEU:HD12	2:C:854:PRO:HD2	1.87	0.55
3:D:203:ALA:HB2	3:D:395:VAL:HB	1.87	0.55
3:D:470:LEU:HD22	3:D:499:VAL:HG13	1.88	0.55
3:D:828:VAL:HA	3:D:833:GLU:HA	1.88	0.55
3:D:901:GLN:HG2	3:D:906:GLN:HE22	1.70	0.55
2:I:1066:ALA:HA	2:I:1076:VAL:HG12	1.88	0.55
3:J:171:LEU:HD12	3:J:393:ILE:HD11	1.88	0.55
3:J:758:GLU:HG2	3:J:1476:THR:HG21	1.87	0.55
2:C:69:LEU:HB2	2:C:97:ARG:O	2.06	0.55
2:C:428:ARG:HH11	2:C:451:LEU:HD21	1.71	0.55
3:D:234:GLU:HA	3:D:322:VAL:HB	1.88	0.55
3:D:453:ASP:OD2	3:D:455:ARG:NE	2.37	0.55
2:I:23:VAL:HA	2:I:121:MET:SD	2.47	0.55
3:J:407:VAL:HA	3:J:422:ALA:HB1	1.87	0.55
3:J:800:LYS:HB3	3:J:822:ALA:HB2	1.87	0.55
6:N:151:ALA:HA	6:N:154:LEU:HD12	1.88	0.55
2:C:124:ASP:O	2:C:407:LYS:NZ	2.38	0.55
3:D:1458:GLU:HB2	3:D:1460:ILE:HG23	1.89	0.55
3:J:1272:ALA:HB3	3:J:1330:ILE:HD13	1.88	0.55
2:C:26:TYR:HB2	2:C:336:VAL:HB	1.88	0.55
3:D:758:GLU:HG2	3:D:1476:THR:HG21	1.88	0.55
3:D:1444:THR:O	3:D:1448:THR:OG1	2.24	0.55
2:I:328:LEU:H	2:I:328:LEU:HD12	1.72	0.55
3:J:371:ILE:HG23	3:J:372:ASP:H	1.72	0.55
3:J:520:LEU:HB3	3:J:525:ARG:HD3	1.87	0.55
3:J:1404:ASN:O	3:J:1408:ILE:HG12	2.06	0.55
4:K:38:THR:HG21	4:K:63:TRP:CZ3	2.41	0.55
2:C:278:GLU:HG3	2:C:284:GLY:HA2	1.89	0.55
2:C:458:TYR:HD1	2:C:538:GLN:HB3	1.69	0.55
3:D:421:LEU:H	3:D:421:LEU:HD12	1.71	0.55
5:F:99:TYR:HA	5:F:102:GLU:HB2	1.88	0.55
2:I:344:PHE:HA	2:I:382:LEU:HD21	1.89	0.55
3:J:140:ALA:HB1	3:J:161:LEU:HD21	1.88	0.55
2:C:71:TYR:HD1	2:C:94:LEU:HD11	1.71	0.55
2:C:172:ILE:HA	2:C:186:VAL:HG22	1.89	0.55
5:F:235:LEU:HD12	5:F:254:ALA:HB1	1.89	0.55
2:I:428:ARG:HH11	2:I:451:LEU:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:897:LEU:HB3	2:I:899:GLN:HE21	1.72	0.55
3:J:633:VAL:HG13	3:J:635:PRO:HD3	1.87	0.55
3:J:699:VAL:HA	3:J:718:PRO:HD3	1.89	0.55
2:I:439:CYS:HB2	2:I:541:SER:HB3	1.88	0.55
3:J:176:ASP:OD1	3:J:177:ALA:N	2.40	0.55
3:J:1444:THR:O	3:J:1448:THR:OG1	2.25	0.55
5:L:235:LEU:HD12	5:L:254:ALA:HB1	1.88	0.55
7:R:46:DT:H2"	7:R:47:DG:C8	2.41	0.55
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.71	0.55
2:I:259:GLY:HA2	2:I:263:ASP:HB2	1.89	0.55
2:I:605:LYS:HG2	2:I:612:ALA:HB3	1.89	0.55
3:J:130:ASN:HD22	5:L:98:GLN:NE2	2.04	0.55
3:J:1011:PHE:HD1	3:J:1021:TYR:HB2	1.71	0.55
2:C:328:LEU:H	2:C:328:LEU:HD12	1.72	0.55
2:C:344:PHE:HA	2:C:382:LEU:HD21	1.89	0.55
3:D:792:ILE:HG12	3:D:941:LEU:HD13	1.88	0.55
3:D:1404:ASN:O	3:D:1408:ILE:HG12	2.07	0.55
3:J:1273:VAL:HG23	3:J:1325:LEU:HB2	1.89	0.55
3:D:258:VAL:HG22	3:D:273:ARG:HG2	1.88	0.55
3:D:976:GLN:HG2	3:J:807:ALA:HB1	1.87	0.55
3:D:1377:LYS:O	3:D:1397:LYS:N	2.37	0.55
2:I:546:LEU:HB2	2:I:565:GLN:HE22	1.72	0.55
2:I:571:LEU:HB2	2:I:574:ALA:HB2	1.89	0.55
2:C:988:VAL:H	3:D:948:THR:HG21	1.73	0.54
2:C:1067:TYR:CZ	5:F:357:VAL:HG12	2.41	0.54
3:D:1042:ARG:HD3	3:D:1045:MET:HE3	1.89	0.54
3:D:1068:LEU:H	3:D:1068:LEU:HD12	1.71	0.54
2:I:328:LEU:HD21	2:I:438:ILE:HD11	1.88	0.54
2:I:584:GLU:HA	2:I:587:VAL:HB	1.89	0.54
3:J:792:ILE:HG12	3:J:941:LEU:HD13	1.89	0.54
2:C:50:GLU:HG2	2:C:265:LYS:HZ2	1.73	0.54
2:C:607:ASP:OD2	2:C:610:ARG:NH1	2.40	0.54
3:D:680:GLN:C	3:D:682:ASP:H	2.10	0.54
3:D:1011:PHE:HD1	3:D:1021:TYR:HB2	1.72	0.54
5:F:302:SER:O	5:F:306:ILE:HG22	2.08	0.54
1:G:221:HIS:HA	1:G:224:TYR:CD1	2.42	0.54
3:J:453:ASP:OD2	3:J:455:ARG:NE	2.38	0.54
2:C:584:GLU:HA	2:C:587:VAL:HB	1.89	0.54
3:D:535:PHE:O	5:F:329:PRO:HA	2.06	0.54
3:D:634:GLY:O	3:D:637:LEU:N	2.40	0.54
3:D:1290:LEU:HD12	3:D:1307:LYS:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:ILE:HA	1:H:81:ASN:HD22	1.72	0.54
2:I:195:LEU:HD12	2:I:198:ARG:HH11	1.71	0.54
3:J:418:GLY:H	3:J:430:GLU:HA	1.72	0.54
7:R:14:DT:H1'	7:R:15:DT:H5''	1.89	0.54
1:A:184:THR:HB	1:A:194:LYS:HB3	1.90	0.54
3:D:1209:LEU:O	3:D:1212:ALA:N	2.36	0.54
3:D:1272:ALA:HB3	3:D:1330:ILE:HD13	1.88	0.54
1:G:44:LEU:O	1:G:174:VAL:HG11	2.06	0.54
3:J:8:VAL:HG23	3:J:1459:LEU:HD11	1.89	0.54
3:J:573:MET:SD	5:L:229:GLN:HG3	2.47	0.54
5:L:204:GLU:O	5:L:207:LEU:HB3	2.07	0.54
3:D:8:VAL:HG23	3:D:1459:LEU:HD11	1.89	0.54
3:D:29:PRO:HB3	3:D:548:ILE:HB	1.90	0.54
3:D:573:MET:SD	5:F:229:GLN:HG3	2.47	0.54
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.08	0.54
3:D:1472:ILE:HD12	3:D:1473:PRO:HD2	1.90	0.54
2:I:278:GLU:HG3	2:I:284:GLY:HA2	1.89	0.54
2:I:437:ARG:HB3	2:I:467:ILE:HG21	1.89	0.54
3:J:1093:TYR:HD1	8:S:10:DA:H5''	1.71	0.54
7:O:43:DG:H1	8:P:6:DC:H42	1.55	0.54
3:D:916:TYR:HE2	3:D:1168:LEU:HD22	1.72	0.54
2:I:71:TYR:HD1	2:I:94:LEU:HD11	1.71	0.54
2:I:172:ILE:HA	2:I:186:VAL:HG22	1.88	0.54
3:J:147:VAL:HG21	3:J:153:LEU:HD21	1.89	0.54
2:C:969:LEU:HG	3:D:952:ASP:HB2	1.90	0.54
3:D:140:ALA:HB1	3:D:161:LEU:HD21	1.89	0.54
3:D:414:ARG:HG3	3:D:451:ASP:HB2	1.89	0.54
3:D:572:ARG:HH12	5:F:98:GLN:HE21	1.54	0.54
3:D:699:VAL:HA	3:D:718:PRO:HD3	1.89	0.54
3:D:1048:PRO:HD3	3:D:1075:HIS:HB3	1.90	0.54
1:G:38:ASN:HB2	2:I:980:GLY:HA3	1.90	0.54
3:J:704:ARG:NE	3:J:705:ALA:O	2.41	0.54
3:J:1202:GLN:NE2	3:J:1215:VAL:O	2.32	0.54
5:L:100:LEU:HD13	7:R:31:DG:H21	1.73	0.54
1:A:38:ASN:HB2	2:C:980:GLY:HA3	1.90	0.54
1:B:58:ILE:HB	1:B:61:VAL:HB	1.90	0.54
2:C:276:LYS:HD3	2:C:466:PHE:HZ	1.73	0.54
2:C:283:VAL:HG11	2:C:305:PRO:HG3	1.90	0.54
1:G:184:THR:HB	1:G:194:LYS:HB3	1.90	0.54
2:I:1035:MET:HG3	3:J:707:THR:HB	1.89	0.54
3:J:101:HIS:HB3	3:J:104:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:881:LEU:O	3:J:885:ILE:HG13	2.08	0.54
3:J:1290:LEU:HD12	3:J:1307:LYS:HG2	1.89	0.54
1:A:44:LEU:O	1:A:174:VAL:HG11	2.07	0.54
1:B:151:VAL:HG13	1:B:155:ARG:HB2	1.89	0.54
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	1.89	0.54
5:F:204:GLU:O	5:F:207:LEU:HB3	2.06	0.54
1:H:58:ILE:HB	1:H:61:VAL:HB	1.90	0.54
2:I:936:VAL:HB	2:I:941:LYS:HE2	1.90	0.54
3:J:8:VAL:HG21	3:J:1468:LEU:HD21	1.89	0.54
2:C:195:LEU:HD12	2:C:198:ARG:HH11	1.73	0.54
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.88	0.54
1:G:35:THR:HG22	1:H:39:PRO:HA	1.89	0.54
2:I:47:ALA:HA	2:I:345:ARG:HG2	1.90	0.54
2:I:111:ASP:HA	6:N:45:SER:HB2	1.89	0.54
3:J:610:LYS:NZ	8:S:10:DA:OP2	2.37	0.54
3:J:1042:ARG:HD3	3:J:1045:MET:HE3	1.90	0.54
2:C:285:LEU:HD23	2:C:286:SER:H	1.71	0.53
2:C:1023:GLY:HA2	8:P:15:DA:OP2	2.08	0.53
3:D:225:ILE:O	3:D:331:VAL:HG12	2.08	0.53
3:D:628:ARG:HH22	8:P:14:DG:H2"	1.73	0.53
3:D:977:ALA:HB2	3:J:831:GLY:N	2.24	0.53
3:D:1147:ARG:HH12	3:D:1190:SER:HA	1.73	0.53
1:H:151:VAL:HG13	1:H:155:ARG:HB2	1.90	0.53
4:K:27:ALA:HB1	4:K:60:ALA:HB1	1.90	0.53
2:C:829:GLN:HE21	2:C:831:ARG:HH21	1.57	0.53
3:D:147:VAL:HG21	3:D:153:LEU:HD21	1.90	0.53
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.89	0.53
3:D:245:LEU:HB2	3:D:311:LEU:HD21	1.90	0.53
3:D:810:GLU:HA	3:D:813:LEU:HD12	1.89	0.53
3:D:1202:GLN:NE2	3:D:1215:VAL:O	2.32	0.53
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.89	0.53
5:F:217:TYR:O	8:P:23:DA:N6	2.41	0.53
6:N:119:ARG:HG3	6:N:120:GLY:H	1.72	0.53
1:A:79:ILE:HA	1:A:82:LEU:HD12	1.90	0.53
3:D:407:VAL:HG22	3:D:409:VAL:H	1.73	0.53
2:I:142:ARG:HG3	2:I:331:ARG:HG2	1.89	0.53
3:J:211:VAL:HG12	3:J:345:TYR:HB2	1.89	0.53
3:J:1256:LEU:O	3:J:1260:ILE:HG13	2.08	0.53
3:J:1274:ILE:HD11	3:J:1334:GLN:HG2	1.90	0.53
2:C:1017:THR:HG21	3:D:617:ASN:ND2	2.24	0.53
2:C:1035:MET:HG3	3:D:707:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:110:THR:HG23	5:F:113:GLU:H	1.74	0.53
2:I:124:ASP:HA	2:I:592:LEU:HD12	1.90	0.53
2:I:988:VAL:HG22	3:J:948:THR:OG1	2.09	0.53
5:L:302:SER:O	5:L:306:ILE:HG22	2.07	0.53
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.90	0.53
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.07	0.53
3:D:223:LEU:HB2	3:D:251:PHE:HZ	1.74	0.53
2:I:742:ILE:HD12	2:I:803:ARG:HD2	1.91	0.53
3:J:357:GLU:HG2	3:J:387:LEU:HB2	1.91	0.53
2:C:47:ALA:HA	2:C:345:ARG:HG2	1.90	0.53
2:C:668:LEU:HB2	2:C:993:PHE:HZ	1.73	0.53
3:D:231:VAL:HB	3:D:243:ALA:H	1.73	0.53
3:D:371:ILE:HG23	3:D:372:ASP:H	1.73	0.53
2:I:502:PRO:HG3	2:I:510:THR:HG22	1.89	0.53
2:I:552:HIS:HB3	2:I:882:LEU:HB2	1.91	0.53
2:I:668:LEU:HB2	2:I:993:PHE:HZ	1.74	0.53
2:I:969:LEU:HG	3:J:952:ASP:HB2	1.90	0.53
1:A:221:HIS:HA	1:A:224:TYR:CD1	2.43	0.53
1:B:78:ILE:HA	1:B:81:ASN:HD22	1.72	0.53
2:C:878:SER:HB3	3:D:1029:ARG:HG3	1.91	0.53
3:D:801:GLY:HA2	3:D:821:VAL:HA	1.90	0.53
3:D:1269:LYS:HD3	3:D:1269:LYS:H	1.74	0.53
5:F:210:VAL:HG11	5:F:232:ASN:HA	1.91	0.53
1:G:58:ILE:HG22	1:G:60:ASP:H	1.74	0.53
2:I:1037:VAL:O	2:I:1041:GLU:HG3	2.09	0.53
3:J:638:LYS:HG2	3:J:639:LEU:H	1.72	0.53
3:J:1209:LEU:O	3:J:1212:ALA:N	2.37	0.53
3:D:101:HIS:HB3	3:D:104:PHE:CE2	2.44	0.53
2:I:374:ASN:ND2	2:I:375:SER:H	2.07	0.53
2:I:577:PRO:HG2	2:I:580:MET:HB3	1.90	0.53
2:I:607:ASP:OD2	2:I:610:ARG:NH1	2.41	0.53
3:J:421:LEU:HD21	3:J:444:VAL:HG11	1.90	0.53
1:B:68:ILE:HG23	1:B:71:VAL:HB	1.91	0.53
1:B:118:ALA:O	1:B:120:VAL:N	2.42	0.53
2:C:388:ARG:NH2	8:P:20:DA:O5'	2.42	0.53
2:C:552:HIS:HB3	2:C:882:LEU:HB2	1.90	0.53
2:C:859:PRO:HA	2:C:975:TYR:O	2.09	0.53
2:C:936:VAL:HB	2:C:941:LYS:HE2	1.91	0.53
3:D:881:LEU:O	3:D:885:ILE:HG13	2.09	0.53
2:I:374:ASN:ND2	5:L:291:ARG:HE	2.00	0.53
2:I:878:SER:HB3	3:J:1029:ARG:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:17:DG:H2''	8:S:18:DG:O4'	2.08	0.53
2:C:142:ARG:HG3	2:C:331:ARG:HG2	1.90	0.53
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.90	0.53
2:C:684:PHE:HE1	3:D:783:ARG:HB2	1.74	0.53
3:D:313:LEU:HG	3:D:314:PRO:HD2	1.91	0.53
2:I:352:ALA:HB1	2:I:356:ARG:NH1	2.23	0.53
2:I:971:LYS:HA	2:I:988:VAL:HA	1.91	0.53
3:J:49:ILE:HG13	3:J:50:PHE:H	1.72	0.53
3:J:99:ALA:HB2	3:J:574:LEU:HD21	1.91	0.53
3:J:577:ALA:O	3:J:581:VAL:HG23	2.09	0.53
3:J:810:GLU:HA	3:J:813:LEU:HD12	1.90	0.53
6:N:80:MET:HB3	6:N:107:GLN:HG2	1.90	0.53
2:C:23:VAL:HA	2:C:121:MET:SD	2.49	0.52
2:C:988:VAL:HG22	3:D:948:THR:OG1	2.08	0.52
2:C:988:VAL:HG21	3:D:949:ILE:O	2.09	0.52
3:D:49:ILE:HG13	3:D:50:PHE:H	1.73	0.52
3:D:704:ARG:NE	3:D:705:ALA:O	2.42	0.52
3:D:1145:TYR:O	3:D:1364:HIS:NE2	2.37	0.52
2:I:204:GLN:HB2	2:I:227:LEU:HD21	1.92	0.52
2:I:577:PRO:HA	2:I:671:ASN:HD21	1.74	0.52
2:I:1013:TYR:O	5:L:350:ASP:N	2.42	0.52
3:J:801:GLY:HA2	3:J:821:VAL:HA	1.90	0.52
3:J:1145:TYR:O	3:J:1364:HIS:NE2	2.37	0.52
6:N:20:VAL:CA	6:N:38:VAL:HA	2.35	0.52
8:S:22:DT:H2''	8:S:23:DA:C8	2.44	0.52
2:C:577:PRO:HG2	2:C:580:MET:HB3	1.90	0.52
3:D:99:ALA:HB2	3:D:574:LEU:HD21	1.92	0.52
3:D:1060:SER:OG	3:D:1061:PHE:N	2.42	0.52
2:I:87:ASP:HA	2:I:131:GLY:HA3	1.92	0.52
3:J:180:LYS:HA	3:J:205:TYR:CZ	2.45	0.52
5:L:398:LEU:HD21	5:L:413:ARG:HB2	1.91	0.52
8:P:8:DT:H1'	8:P:9:DG:H5''	1.89	0.52
2:C:742:ILE:HD12	2:C:803:ARG:HD2	1.91	0.52
1:H:118:ALA:O	1:H:120:VAL:N	2.43	0.52
3:J:29:PRO:HB3	3:J:548:ILE:HB	1.92	0.52
1:A:104:GLU:HG3	1:A:137:LYS:HG2	1.91	0.52
2:I:457:ALA:HB3	2:I:538:GLN:HA	1.92	0.52
2:I:644:ARG:HG2	2:I:647:GLN:HG2	1.92	0.52
2:I:988:VAL:H	3:J:948:THR:HG21	1.73	0.52
3:J:699:VAL:HG22	3:J:760:ARG:HG2	1.92	0.52
3:J:1060:SER:OG	3:J:1061:PHE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1273:VAL:HG21	3:J:1305:LEU:HD22	1.91	0.52
2:C:374:ASN:HD22	2:C:375:SER:H	1.58	0.52
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.92	0.52
2:C:694:LEU:O	2:C:698:ASP:N	2.42	0.52
2:C:971:LYS:HA	2:C:988:VAL:HA	1.91	0.52
3:D:10:ILE:HG23	3:D:1451:ALA:HA	1.92	0.52
3:D:577:ALA:O	3:D:581:VAL:HG23	2.09	0.52
5:L:210:VAL:HG11	5:L:232:ASN:HA	1.92	0.52
6:M:68:VAL:HG21	6:M:144:LEU:HD21	1.92	0.52
1:G:79:ILE:HA	1:G:82:LEU:HD12	1.92	0.52
1:G:104:GLU:HG3	1:G:137:LYS:HG2	1.90	0.52
1:H:68:ILE:HG23	1:H:71:VAL:HB	1.91	0.52
2:I:283:VAL:HG11	2:I:305:PRO:HG3	1.92	0.52
2:I:988:VAL:HG21	3:J:949:ILE:O	2.10	0.52
3:J:367:ILE:HD11	3:J:379:ALA:HB2	1.92	0.52
3:J:1269:LYS:HD3	3:J:1269:LYS:H	1.75	0.52
3:D:27:GLU:H	3:D:42:ASP:HB3	1.75	0.52
3:D:650:LEU:HD12	3:D:688:TRP:HZ3	1.74	0.52
5:F:398:LEU:HD21	5:F:413:ARG:HB2	1.90	0.52
2:C:352:ALA:HB1	2:C:356:ARG:NH1	2.24	0.52
3:D:977:ALA:HB2	3:J:831:GLY:CA	2.39	0.52
5:F:285:LYS:O	5:F:288:ARG:HB3	2.10	0.52
5:F:385:LYS:HA	5:F:390:LEU:HD12	1.91	0.52
2:I:332:ARG:HB2	2:I:465:GLY:HA3	1.91	0.52
3:J:1048:PRO:HD3	3:J:1075:HIS:HB3	1.90	0.52
3:J:1436:SER:O	3:J:1439:SER:OG	2.23	0.52
5:L:411:ARG:HD3	7:R:1:DC:C6	2.45	0.52
7:O:46:DT:H2''	7:O:47:DG:C8	2.44	0.52
3:D:1021:TYR:O	3:D:1025:GLN:HB2	2.10	0.52
1:G:16:GLN:HB3	1:G:20:TYR:O	2.10	0.52
1:G:42:ARG:NH1	2:I:978:ARG:HA	2.25	0.52
2:I:431:HIS:H	2:I:434:HIS:CE1	2.28	0.52
2:I:448:ASN:HA	2:I:451:LEU:HD23	1.92	0.52
2:I:694:LEU:O	2:I:698:ASP:N	2.43	0.52
2:C:292:ARG:H	2:C:292:ARG:NH1	2.04	0.52
2:C:448:ASN:HA	2:C:451:LEU:HD23	1.92	0.52
3:D:86:ARG:O	3:D:521:PRO:HB3	2.10	0.52
3:D:1426:LYS:HE3	7:O:43:DG:H5''	1.91	0.52
2:I:859:PRO:HA	2:I:975:TYR:O	2.09	0.52
2:I:974:LEU:HD13	2:I:987:ILE:HB	1.92	0.52
1:A:35:THR:HG22	1:B:39:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:GLN:HB2	2:C:227:LEU:HD21	1.92	0.51
2:C:966:LEU:HD21	2:C:986:PRO:HB3	1.92	0.51
3:D:699:VAL:HG22	3:D:760:ARG:HG2	1.92	0.51
3:J:96:ALA:HB2	3:J:555:LYS:HG2	1.92	0.51
8:S:34:DA:H1'	8:S:35:DA:H5'	1.92	0.51
1:B:161:ARG:HG2	1:B:162:ILE:H	1.76	0.51
2:C:27:LYS:HA	2:C:30:LEU:HD22	1.92	0.51
2:C:644:ARG:HG2	2:C:647:GLN:HG2	1.92	0.51
3:D:1273:VAL:HG21	3:D:1305:LEU:HD22	1.91	0.51
5:F:130:LYS:HD3	5:F:188:TYR:CZ	2.45	0.51
2:I:376:ARG:HD2	5:L:291:ARG:CZ	2.40	0.51
3:J:1147:ARG:HH12	3:J:1190:SER:HA	1.74	0.51
5:L:336:ILE:HB	8:S:17:DG:H21	1.75	0.51
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.93	0.51
4:E:26:ARG:HH22	4:E:37:ASN:HB2	1.76	0.51
1:G:9:PRO:HB2	1:G:25:LEU:HD21	1.91	0.51
3:J:27:GLU:H	3:J:42:ASP:HB3	1.75	0.51
3:J:650:LEU:HD12	3:J:688:TRP:HZ3	1.76	0.51
4:K:26:ARG:HH22	4:K:37:ASN:HB2	1.76	0.51
5:L:130:LYS:HD3	5:L:188:TYR:CZ	2.45	0.51
6:N:62:ALA:HB1	6:N:142:GLN:HE22	1.75	0.51
3:D:260:GLU:HA	3:D:294:GLU:HG3	1.92	0.51
2:I:65:VAL:HG13	2:I:101:ILE:HB	1.92	0.51
2:I:557:ARG:O	2:I:844:GLY:HA3	2.10	0.51
2:I:684:PHE:HE1	3:J:783:ARG:HB2	1.76	0.51
3:J:175:VAL:HG11	3:J:193:PRO:HG3	1.92	0.51
3:J:640:HIS:O	3:J:717:GLN:HB2	2.09	0.51
3:J:1458:GLU:HB2	3:J:1460:ILE:HG23	1.92	0.51
5:L:206:ASN:HB3	5:L:235:LEU:HD11	1.92	0.51
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.26	0.51
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.92	0.51
3:D:675:ARG:HH22	5:F:437:LEU:HG	1.76	0.51
3:D:1100:ASP:CG	3:D:1440:PHE:HB2	2.31	0.51
5:F:186:LYS:O	5:F:189:LEU:HB3	2.10	0.51
5:F:387:ARG:HD3	5:F:398:LEU:HD12	1.93	0.51
3:J:628:ARG:NH1	8:S:14:DG:H2''	2.26	0.51
3:J:1021:TYR:O	3:J:1025:GLN:HB2	2.11	0.51
5:L:285:LYS:O	5:L:288:ARG:HB3	2.10	0.51
5:L:387:ARG:HD3	5:L:398:LEU:HD12	1.93	0.51
6:M:62:ALA:HB1	6:M:142:GLN:HE22	1.76	0.51
1:A:218:LEU:HB3	1:B:222:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ALA:HA	1:B:156:HIS:CE1	2.46	0.51
2:C:332:ARG:HB2	2:C:465:GLY:HA3	1.93	0.51
3:D:465:LEU:HD22	3:D:509:PRO:HB2	1.93	0.51
3:D:592:THR:HG22	3:D:599:PRO:HA	1.93	0.51
5:L:110:THR:HG23	5:L:113:GLU:H	1.75	0.51
6:N:37:GLN:HA	6:N:47:ALA:O	2.10	0.51
1:A:16:GLN:HB3	1:A:20:TYR:O	2.10	0.51
1:A:32:PHE:O	1:A:36:LEU:HG	2.11	0.51
1:B:184:THR:OG1	1:B:185:ARG:N	2.44	0.51
2:C:65:VAL:HG13	2:C:101:ILE:HB	1.92	0.51
2:C:124:ASP:HA	2:C:592:LEU:HD12	1.92	0.51
3:D:493:ARG:HD3	3:D:1392:GLY:O	2.11	0.51
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.93	0.51
5:F:413:ARG:HD2	8:P:44:DT:H72	1.92	0.51
1:H:48:ILE:HA	1:H:213:GLN:HE22	1.76	0.51
3:J:137:PRO:HA	3:J:452:ILE:HG13	1.92	0.51
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.75	0.51
3:D:67:ARG:HD2	5:F:394:ARG:HD3	1.92	0.51
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.92	0.51
1:G:63:HIS:HE2	2:I:801:VAL:HG13	1.76	0.51
3:J:367:ILE:HG22	3:J:368:VAL:HG23	1.91	0.51
5:L:252:THR:O	5:L:255:THR:OG1	2.26	0.51
7:O:46:DT:H3	8:P:3:DA:H61	1.58	0.51
1:B:177:VAL:HG12	1:B:197:LEU:HD11	1.92	0.51
2:C:471:TYR:N	2:C:484:VAL:O	2.37	0.51
2:C:974:LEU:HD13	2:C:987:ILE:HB	1.92	0.51
3:D:680:GLN:O	3:D:682:ASP:N	2.31	0.51
3:D:1442:ASN:N	8:P:9:DG:OP1	2.42	0.51
5:F:199:ARG:O	5:F:203:ILE:HG13	2.11	0.51
2:I:292:ARG:H	2:I:292:ARG:NH1	2.04	0.51
2:I:966:LEU:HD21	2:I:986:PRO:HB3	1.92	0.51
3:J:1472:ILE:HD12	3:J:1473:PRO:HD2	1.92	0.51
6:M:20:VAL:CA	6:M:38:VAL:HA	2.36	0.51
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.26	0.51
3:D:1274:ILE:HD11	3:D:1334:GLN:HG2	1.92	0.51
1:G:218:LEU:HB3	1:H:222:LEU:HD21	1.93	0.51
1:H:153:ALA:HA	1:H:156:HIS:CE1	2.46	0.51
3:J:1003:VAL:O	3:J:1007:VAL:HG23	2.11	0.51
5:L:385:LYS:HA	5:L:390:LEU:HD12	1.93	0.51
1:B:198:ARG:NH1	3:D:937:TYR:OH	2.42	0.50
2:C:431:HIS:H	2:C:434:HIS:CE1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.92	0.50
3:D:188:GLY:HA2	3:D:196:VAL:HG23	1.93	0.50
1:H:184:THR:OG1	1:H:185:ARG:N	2.44	0.50
2:I:1032:PHE:HZ	2:I:1040:LEU:HD13	1.76	0.50
3:J:592:THR:HG22	3:J:599:PRO:HA	1.92	0.50
3:J:1279:GLY:H	3:J:1319:VAL:HG23	1.75	0.50
5:L:214:ALA:HB3	5:L:228:ILE:HG13	1.91	0.50
1:G:232:LEU:HD23	1:H:16:GLN:HG3	1.93	0.50
2:I:27:LYS:HA	2:I:30:LEU:HD22	1.93	0.50
3:J:121:THR:HA	3:J:124:GLU:HB3	1.93	0.50
3:J:636:GLN:HG2	3:J:637:LEU:HD12	1.93	0.50
3:J:680:GLN:C	3:J:682:ASP:H	2.12	0.50
3:J:699:VAL:HG12	3:J:717:GLN:HG2	1.92	0.50
3:J:1042:ARG:HB3	3:J:1057:VAL:HG21	1.93	0.50
1:A:151:VAL:HG22	1:A:156:HIS:HD2	1.77	0.50
2:C:688:ILE:HG22	2:C:689:VAL:H	1.76	0.50
3:D:272:LEU:O	3:D:279:VAL:N	2.42	0.50
3:D:636:GLN:HG2	3:D:637:LEU:HD12	1.94	0.50
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.11	0.50
2:I:18:LEU:HD12	2:I:408:ARG:NE	2.26	0.50
2:I:758:ARG:HB3	2:I:788:THR:HB	1.93	0.50
1:A:232:LEU:HD23	1:B:16:GLN:HG3	1.92	0.50
3:D:1042:ARG:HB3	3:D:1057:VAL:HG21	1.94	0.50
3:J:420:VAL:HG21	3:J:425:GLY:HA2	1.94	0.50
3:J:634:GLY:O	3:J:637:LEU:N	2.41	0.50
2:C:758:ARG:HB3	2:C:788:THR:HB	1.93	0.50
3:D:121:THR:HA	3:D:124:GLU:HB3	1.94	0.50
3:D:791:TYR:CD1	3:D:947:ILE:HD11	2.46	0.50
1:G:32:PHE:O	1:G:36:LEU:HG	2.12	0.50
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.93	0.50
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.94	0.50
2:C:18:LEU:HD12	2:C:408:ARG:NE	2.26	0.50
2:C:690:ILE:HG22	2:C:691:SER:H	1.76	0.50
2:C:1082:PRO:HG3	3:D:1469:GLY:HA3	1.94	0.50
3:D:537:THR:O	5:F:332:LEU:N	2.43	0.50
3:D:628:ARG:HB2	3:D:745:MET:O	2.12	0.50
3:D:645:PRO:HB2	3:D:648:MET:HB3	1.93	0.50
3:D:1279:GLY:H	3:D:1319:VAL:HG23	1.76	0.50
5:F:206:ASN:HB3	5:F:235:LEU:HD11	1.92	0.50
2:I:110:GLU:O	6:N:45:SER:HB2	2.12	0.50
2:I:743:VAL:HG11	2:I:755:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:937:ASP:HB3	2:I:940:GLU:HG3	1.92	0.50
3:J:10:ILE:HG23	3:J:1451:ALA:HA	1.94	0.50
3:J:660:LYS:HD3	3:J:693:GLU:HB3	1.93	0.50
5:L:319:VAL:O	5:L:323:LEU:HB2	2.11	0.50
7:O:34:DA:H2''	7:O:35:DG:O4'	2.12	0.50
1:B:48:ILE:HA	1:B:213:GLN:HE22	1.76	0.50
2:C:714:ASP:OD1	2:C:820:ARG:HB2	2.12	0.50
2:C:1032:PHE:HZ	2:C:1040:LEU:HD13	1.76	0.50
3:D:714:GLN:HB2	3:D:736:PHE:HZ	1.76	0.50
1:G:68:ILE:HG21	1:G:138:LEU:HD13	1.93	0.50
2:I:162:ILE:HB	2:I:172:ILE:HB	1.94	0.50
3:J:1037:GLN:HB3	3:J:1042:ARG:HG3	1.93	0.50
3:J:1201:CYS:SG	3:J:1204:CYS:N	2.84	0.50
4:K:40:LEU:HD21	4:K:67:GLU:HA	1.93	0.50
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.47	0.50
1:A:68:ILE:HG21	1:A:138:LEU:HD13	1.93	0.50
1:B:185:ARG:NH1	1:B:187:GLY:O	2.45	0.50
3:D:413:ASP:O	3:D:435:VAL:HG22	2.11	0.50
1:H:80:LEU:HD11	3:J:842:VAL:HG12	1.94	0.50
2:I:1060:ILE:HG23	2:I:1083:GLU:HB2	1.93	0.50
3:J:87:ARG:HG2	3:J:523:ASP:HB3	1.94	0.50
3:J:750:PRO:HG2	3:J:756:GLN:NE2	2.26	0.50
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.93	0.50
3:D:1018:ASN:HB3	3:D:1021:TYR:HB3	1.94	0.50
3:D:1436:SER:O	3:D:1439:SER:OG	2.24	0.50
5:F:206:ASN:O	5:F:210:VAL:HG23	2.12	0.50
2:I:766:GLU:OE2	3:J:64:LYS:HB3	2.12	0.50
3:J:137:PRO:HG3	3:J:148:GLU:HA	1.93	0.50
3:J:1285:GLU:HB3	3:J:1290:LEU:HG	1.94	0.50
6:N:12:LEU:HD13	6:N:59:LEU:HD13	1.93	0.50
6:N:12:LEU:HB3	6:N:40:PHE:HE1	1.76	0.50
2:C:841:ASN:HD21	2:C:845:ASN:HB3	1.77	0.49
3:D:137:PRO:HG3	3:D:148:GLU:HA	1.93	0.49
3:D:1037:GLN:HB3	3:D:1042:ARG:HG3	1.93	0.49
2:I:750:LYS:HD3	3:J:681:ARG:HG3	1.93	0.49
3:J:465:LEU:HD22	3:J:509:PRO:HB2	1.92	0.49
3:J:1462:LEU:HD12	3:J:1463:LYS:N	2.26	0.49
1:A:101:LEU:HB3	1:A:140:MET:HB3	1.94	0.49
2:C:1031:ARG:HB3	3:D:622:ARG:HD3	1.93	0.49
3:D:1462:LEU:HD12	3:D:1463:LYS:N	2.26	0.49
1:G:151:VAL:HG22	1:G:156:HIS:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:ARG:NH1	3:J:937:TYR:OH	2.41	0.49
2:I:167:LYS:HD3	7:R:35:DG:C5'	2.42	0.49
2:I:369:PRO:HA	2:I:372:LEU:HB3	1.94	0.49
3:J:789:LEU:O	3:J:792:ILE:HG13	2.13	0.49
5:L:186:LYS:O	5:L:189:LEU:HB3	2.11	0.49
2:C:162:ILE:HB	2:C:172:ILE:HB	1.93	0.49
2:C:557:ARG:O	2:C:844:GLY:HA3	2.12	0.49
3:D:1094:LEU:HD21	3:D:1260:ILE:HG12	1.93	0.49
1:H:161:ARG:HG2	1:H:162:ILE:H	1.77	0.49
3:J:461:ILE:HG22	3:J:465:LEU:HD12	1.95	0.49
3:J:1099:VAL:HG22	3:J:1226:ALA:HB1	1.94	0.49
3:J:1264:GLU:HB3	3:J:1266:ARG:HG3	1.93	0.49
3:J:1448:THR:O	3:J:1452:ILE:HG12	2.12	0.49
6:N:18:GLY:HA3	6:N:40:PHE:HA	1.94	0.49
8:S:19:DT:OP1	8:S:19:DT:H4'	2.12	0.49
1:A:70:GLY:HA2	1:A:133:GLU:HG2	1.94	0.49
2:C:94:LEU:HD23	2:C:115:LEU:HD12	1.93	0.49
3:D:900:ILE:HG12	3:D:914:LEU:HD11	1.94	0.49
5:F:214:ALA:HB3	5:F:228:ILE:HG13	1.93	0.49
1:H:185:ARG:NH1	1:H:187:GLY:O	2.45	0.49
3:J:348:ALA:HB1	3:J:350:HIS:ND1	2.28	0.49
3:J:1094:LEU:HD21	3:J:1260:ILE:HG12	1.94	0.49
5:L:199:ARG:O	5:L:203:ILE:HG13	2.12	0.49
8:S:8:DT:H1'	8:S:9:DG:H5''	1.93	0.49
2:C:1115:LEU:HD13	3:D:88:TYR:CG	2.48	0.49
1:G:39:PRO:HG3	1:H:39:PRO:HG3	1.93	0.49
1:G:63:HIS:CE1	1:G:65:PHE:HB2	2.47	0.49
1:G:218:LEU:HD23	1:H:222:LEU:HD21	1.93	0.49
1:H:177:VAL:HG12	1:H:197:LEU:HD11	1.94	0.49
6:M:101:ASN:HD22	6:M:104:ARG:H	1.57	0.49
1:A:88:ARG:HB2	1:A:204:SER:HA	1.94	0.49
2:C:170:PRO:HB3	7:O:36:DC:H42	1.76	0.49
2:C:610:ARG:HA	2:C:624:PRO:HA	1.94	0.49
2:C:743:VAL:HG11	2:C:755:LEU:HD22	1.94	0.49
2:C:874:LEU:O	2:C:877:PRO:HD2	2.12	0.49
3:D:562:ALA:HB3	3:D:567:ILE:HD11	1.94	0.49
5:F:319:VAL:O	5:F:323:LEU:HB2	2.12	0.49
1:H:78:ILE:O	1:H:82:LEU:HG	2.12	0.49
2:I:217:LEU:HD13	2:I:311:PHE:CD2	2.43	0.49
2:I:231:PRO:O	2:I:235:MET:HB2	2.13	0.49
2:I:1075:ASP:OD1	4:K:28:GLN:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:791:TYR:CD1	3:J:947:ILE:HD11	2.47	0.49
5:L:254:ALA:O	5:L:258:ILE:HG12	2.13	0.49
1:A:90:LEU:HB2	1:A:119:ASP:HA	1.94	0.49
2:C:387:SER:HB2	2:C:388:ARG:HH11	1.77	0.49
3:D:347:VAL:HG23	3:D:368:VAL:HG11	1.94	0.49
3:D:1099:VAL:HG22	3:D:1226:ALA:HB1	1.94	0.49
2:I:207:LEU:HD21	2:I:221:LEU:O	2.13	0.49
2:I:714:ASP:OD1	2:I:820:ARG:HB2	2.13	0.49
2:I:874:LEU:O	2:I:877:PRO:HD2	2.13	0.49
2:I:1053:LEU:HG	3:J:621:LYS:HD3	1.94	0.49
5:L:224:PHE:HZ	7:R:33:DG:H5'	1.76	0.49
1:A:58:ILE:HG22	1:A:60:ASP:H	1.76	0.49
1:A:133:GLU:OE1	2:C:606:VAL:N	2.46	0.49
5:F:224:PHE:HE1	7:O:32:DG:H21	1.59	0.49
5:F:235:LEU:O	5:F:239:VAL:HG23	2.13	0.49
1:G:70:GLY:HA2	1:G:133:GLU:HG2	1.94	0.49
1:G:101:LEU:HB3	1:G:140:MET:HB3	1.94	0.49
2:I:437:ARG:HA	2:I:459:ALA:HB2	1.95	0.49
2:I:688:ILE:HG22	2:I:689:VAL:H	1.77	0.49
3:J:907:GLU:O	3:J:911:LEU:HG	2.13	0.49
3:J:1225:ALA:HB2	3:J:1370:ILE:HD12	1.94	0.49
5:L:280:VAL:HA	5:L:283:ILE:HD12	1.95	0.49
2:C:369:PRO:HA	2:C:372:LEU:HB3	1.94	0.49
2:C:684:PHE:CE1	3:D:783:ARG:HB2	2.47	0.49
3:D:489:ARG:HD3	3:D:1391:GLU:OE2	2.12	0.49
3:D:660:LYS:HD3	3:D:693:GLU:HB3	1.93	0.49
3:D:761:ILE:HD13	4:E:20:THR:HA	1.95	0.49
3:D:1225:ALA:HB2	3:D:1370:ILE:HD12	1.95	0.49
2:I:387:SER:HB2	2:I:388:ARG:HH11	1.77	0.49
2:I:690:ILE:HG22	2:I:691:SER:H	1.77	0.49
2:I:742:ILE:HG22	2:I:756:VAL:HG13	1.95	0.49
3:J:628:ARG:HB2	3:J:745:MET:O	2.12	0.49
3:J:761:ILE:HD13	4:K:20:THR:HA	1.94	0.49
3:J:1011:PHE:CD1	3:J:1021:TYR:HB2	2.48	0.49
2:C:434:HIS:CD2	2:C:438:ILE:HD13	2.48	0.49
2:C:437:ARG:HA	2:C:459:ALA:HB2	1.95	0.49
2:C:1060:ILE:HG23	2:C:1083:GLU:HB2	1.94	0.49
3:D:671:LYS:HG3	5:F:436:PHE:CE2	2.47	0.49
1:G:57:TYR:HD1	1:G:163:ASN:O	1.96	0.49
1:G:133:GLU:OE1	2:I:606:VAL:N	2.46	0.49
2:I:610:ARG:HA	2:I:624:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:129:PHE:O	3:J:572:ARG:NH2	2.46	0.49
3:D:130:ASN:HD22	5:F:98:GLN:NE2	2.04	0.48
3:D:423:ASP:HB2	3:D:427:VAL:HG12	1.93	0.48
3:D:1495:ILE:HD12	4:E:85:LEU:HA	1.94	0.48
2:I:135:VAL:HG21	2:I:407:LYS:HG2	1.95	0.48
3:J:645:PRO:HB2	3:J:648:MET:HB3	1.94	0.48
3:J:1018:ASN:HB3	3:J:1021:TYR:HB3	1.93	0.48
4:K:61:VAL:O	4:K:65:MET:HG2	2.12	0.48
6:M:34:ALA:HB3	6:M:51:VAL:HG21	1.94	0.48
1:A:9:PRO:HB2	1:A:25:LEU:HD21	1.94	0.48
1:B:78:ILE:O	1:B:82:LEU:HG	2.12	0.48
2:C:231:PRO:O	2:C:235:MET:HB2	2.13	0.48
3:D:129:PHE:O	3:D:572:ARG:NH2	2.46	0.48
3:D:706:PRO:HG3	8:P:11:DG:N2	2.27	0.48
3:D:789:LEU:O	3:D:792:ILE:HG13	2.13	0.48
4:E:61:VAL:O	4:E:65:MET:HG2	2.11	0.48
1:G:218:LEU:HG	1:H:222:LEU:HD11	1.95	0.48
2:I:434:HIS:CD2	2:I:438:ILE:HD13	2.48	0.48
2:I:471:TYR:N	2:I:484:VAL:O	2.37	0.48
3:J:1495:ILE:HD12	4:K:85:LEU:HA	1.94	0.48
4:K:26:ARG:HH12	4:K:37:ASN:HD22	1.60	0.48
1:A:72:LYS:HG3	2:C:606:VAL:HG11	1.96	0.48
2:C:571:LEU:HD23	2:C:668:LEU:O	2.14	0.48
5:F:280:VAL:HA	5:F:283:ILE:HD12	1.95	0.48
1:G:72:LYS:HG3	2:I:606:VAL:HG11	1.96	0.48
2:I:280:LYS:HD3	2:I:323:ASP:OD2	2.13	0.48
2:I:352:ALA:HB1	2:I:356:ARG:HH12	1.78	0.48
2:I:607:ASP:O	2:I:609:THR:N	2.47	0.48
2:I:1097:LEU:HB3	3:J:10:ILE:HD11	1.95	0.48
3:J:900:ILE:HG12	3:J:914:LEU:HD11	1.94	0.48
3:J:970:LYS:O	3:J:974:ILE:HG13	2.14	0.48
3:J:1462:LEU:O	3:J:1466:VAL:HG23	2.13	0.48
2:C:437:ARG:HH11	2:C:467:ILE:HG22	1.79	0.48
2:C:607:ASP:O	2:C:609:THR:N	2.46	0.48
3:D:203:ALA:HA	3:D:395:VAL:HA	1.95	0.48
3:D:238:PRO:HB3	3:D:315:ARG:O	2.13	0.48
3:D:1448:THR:O	3:D:1452:ILE:HG12	2.13	0.48
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.14	0.48
5:F:142:ILE:O	5:F:146:VAL:HG23	2.13	0.48
2:I:1115:LEU:HD13	3:J:88:TYR:CG	2.47	0.48
3:J:14:SER:HB3	3:J:511:TRP:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:357:GLU:HG2	3:J:387:LEU:CB	2.43	0.48
3:J:822:ALA:HB3	3:J:825:ALA:HB2	1.96	0.48
1:A:173:PRO:HB3	1:A:204:SER:HB2	1.96	0.48
1:A:176:ARG:HG3	1:A:200:TRP:CE3	2.49	0.48
2:C:110:GLU:O	6:M:45:SER:HB2	2.14	0.48
2:C:280:LYS:HD3	2:C:323:ASP:OD2	2.13	0.48
2:C:397:GLU:HB3	2:C:631:SER:HB2	1.94	0.48
2:C:742:ILE:HG22	2:C:756:VAL:HG13	1.96	0.48
3:D:699:VAL:HB	3:D:716:PHE:O	2.13	0.48
3:D:1285:GLU:HB3	3:D:1290:LEU:HG	1.94	0.48
3:D:1440:PHE:CE1	3:D:1441:GLN:HG2	2.49	0.48
3:D:1487:VAL:HG21	3:D:1492:LEU:HD23	1.95	0.48
2:I:94:LEU:HD23	2:I:115:LEU:HD12	1.94	0.48
2:I:397:GLU:HB3	2:I:631:SER:HB2	1.95	0.48
2:I:706:GLU:HB3	2:I:708:TYR:HE1	1.78	0.48
3:J:1442:ASN:N	8:S:9:DG:OP1	2.45	0.48
5:L:235:LEU:O	5:L:239:VAL:HG23	2.13	0.48
3:D:253:ALA:HB2	3:D:304:LEU:HG	1.95	0.48
3:D:255:GLU:OE2	3:D:256:SER:N	2.45	0.48
3:D:761:ILE:O	3:D:767:HIS:ND1	2.47	0.48
3:D:1201:CYS:SG	3:D:1204:CYS:N	2.85	0.48
3:D:1476:THR:HA	4:E:17:TYR:HB3	1.95	0.48
4:E:39:VAL:HB	4:E:72:ARG:HD2	1.95	0.48
2:I:684:PHE:CE1	3:J:783:ARG:HB2	2.48	0.48
3:J:714:GLN:HB3	3:J:765:SER:HB3	1.96	0.48
3:J:714:GLN:HB2	3:J:736:PHE:HZ	1.78	0.48
3:D:714:GLN:HB3	3:D:765:SER:HB3	1.96	0.48
3:D:764:LEU:HB3	3:D:767:HIS:CD2	2.49	0.48
5:F:199:ARG:HE	5:F:200:GLN:NE2	2.12	0.48
2:I:706:GLU:HB3	2:I:708:TYR:CE1	2.49	0.48
2:I:1035:MET:HA	2:I:1038:TRP:CE3	2.49	0.48
2:I:1094:ALA:HB2	3:J:520:LEU:HD13	1.96	0.48
6:N:91:ARG:NH1	7:R:27:DT:OP1	2.46	0.48
7:R:32:DG:H2'	7:R:33:DG:C8	2.48	0.48
2:C:706:GLU:HB3	2:C:708:TYR:HE1	1.79	0.48
3:D:907:GLU:O	3:D:911:LEU:HG	2.14	0.48
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.14	0.48
1:G:173:PRO:HB3	1:G:204:SER:HB2	1.96	0.48
2:I:374:ASN:HD22	2:I:375:SER:H	1.61	0.48
2:I:857:ASP:OD1	2:I:857:ASP:N	2.42	0.48
2:I:1008:ARG:NH2	2:I:1020:PRO:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:900:ILE:HA	3:J:914:LEU:HD21	1.96	0.48
3:J:1487:VAL:HG21	3:J:1492:LEU:HD23	1.94	0.48
8:P:34:DA:H1'	8:P:35:DA:H5'	1.96	0.48
1:B:156:HIS:O	1:B:156:HIS:ND1	2.47	0.48
2:C:658:GLY:H	2:C:661:SER:HB3	1.79	0.48
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.48	0.48
3:D:263:ASP:HB3	3:D:268:HIS:CD2	2.49	0.48
3:D:461:ILE:HG22	3:D:465:LEU:HD12	1.95	0.48
5:F:398:LEU:HD13	8:P:43:DG:OP2	2.13	0.48
1:G:88:ARG:HB2	1:G:204:SER:HA	1.94	0.48
2:I:299:LYS:HG3	2:I:300:ASP:H	1.79	0.48
4:K:39:VAL:HB	4:K:72:ARG:HD2	1.95	0.48
2:C:409:ARG:HG2	2:C:452:ILE:HG22	1.96	0.48
2:C:430:VAL:HG12	2:C:434:HIS:CD2	2.49	0.48
2:C:892:LEU:HD23	2:C:918:LEU:HD11	1.96	0.48
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.49	0.48
3:D:87:ARG:HG2	3:D:523:ASP:HB3	1.94	0.48
2:I:658:GLY:H	2:I:661:SER:HB3	1.77	0.48
3:J:622:ARG:HH12	8:S:14:DG:H5'	1.79	0.48
3:J:1364:HIS:CE1	3:J:1366:LYS:HG3	2.48	0.48
7:O:14:DT:H1'	7:O:15:DT:H5''	1.96	0.48
2:C:430:VAL:HG12	2:C:434:HIS:HD2	1.79	0.47
3:D:900:ILE:HA	3:D:914:LEU:HD21	1.97	0.47
3:D:1341:PRO:O	3:D:1344:VAL:HB	2.14	0.47
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.49	0.47
1:G:90:LEU:HB2	1:G:119:ASP:HA	1.96	0.47
2:I:430:VAL:HG12	2:I:434:HIS:CD2	2.49	0.47
3:J:63:TYR:HE2	3:J:73:CYS:HA	1.79	0.47
3:J:131:LYS:HG2	3:J:153:LEU:O	2.14	0.47
3:J:761:ILE:O	3:J:767:HIS:ND1	2.47	0.47
5:L:252:THR:HA	7:R:29:DC:H5	1.78	0.47
1:A:218:LEU:HG	1:B:222:LEU:HD11	1.96	0.47
1:B:186:LEU:HD22	4:E:51:LEU:HD22	1.96	0.47
2:C:49:LYS:NZ	2:C:50:GLU:HG3	2.29	0.47
2:C:726:ILE:HB	2:C:729:LEU:HB2	1.96	0.47
2:C:1053:LEU:HG	3:D:621:LYS:HD3	1.94	0.47
3:D:762:GLN:HB3	4:E:16:LYS:HE2	1.96	0.47
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.97	0.47
3:D:1144:LEU:HD21	3:D:1186:VAL:HG11	1.96	0.47
3:D:1264:GLU:HB3	3:D:1266:ARG:HG3	1.94	0.47
1:G:65:PHE:CE1	2:I:703:ILE:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:521:PRO:HG2	3:J:1055:VAL:HG21	1.96	0.47
2:I:892:LEU:HD23	2:I:918:LEU:HD11	1.95	0.47
2:I:1067:TYR:CE1	3:J:655:PRO:HG3	2.49	0.47
3:J:762:GLN:HB3	4:K:16:LYS:HE2	1.97	0.47
3:J:1476:THR:HA	4:K:17:TYR:HB3	1.96	0.47
5:L:137:LEU:HB3	5:L:141:LEU:HD23	1.96	0.47
5:L:206:ASN:O	5:L:210:VAL:HG23	2.13	0.47
1:A:26:GLU:HG3	1:A:186:LEU:HD12	1.96	0.47
2:C:508:ILE:HD11	2:C:529:VAL:HG11	1.96	0.47
2:C:1097:LEU:HB3	3:D:10:ILE:HD11	1.96	0.47
3:D:1097:LYS:HE2	3:D:1440:PHE:HZ	1.79	0.47
1:G:26:GLU:HG3	1:G:186:LEU:HD12	1.96	0.47
3:J:10:ILE:HB	3:J:1434:TRP:CH2	2.50	0.47
3:J:743:ASP:OD1	3:J:743:ASP:N	2.47	0.47
3:J:764:LEU:HB3	3:J:767:HIS:CD2	2.48	0.47
4:K:65:MET:O	4:K:69:LEU:HG	2.13	0.47
5:L:119:ARG:HA	5:L:244:TYR:CE1	2.49	0.47
6:M:75:LEU:HD11	6:M:136:LEU:HD13	1.96	0.47
1:A:17:GLY:HA3	1:A:19:HIS:CE1	2.49	0.47
1:A:198:ARG:HD2	2:C:934:PHE:CE1	2.49	0.47
2:C:18:LEU:HD12	2:C:408:ARG:HE	1.80	0.47
3:D:585:GLY:HA2	3:D:590:PRO:HG3	1.96	0.47
3:D:646:LYS:HA	3:D:720:LEU:HD22	1.96	0.47
3:D:1042:ARG:HD3	3:D:1045:MET:CE	2.45	0.47
2:I:430:VAL:HG12	2:I:434:HIS:HD2	1.79	0.47
2:I:437:ARG:HH11	2:I:467:ILE:HG22	1.80	0.47
2:I:971:LYS:HD2	2:I:986:PRO:HG2	1.96	0.47
2:I:1031:ARG:HB3	3:J:622:ARG:HD3	1.95	0.47
3:J:165:LYS:H	3:J:397:LYS:HE2	1.79	0.47
5:L:271:ARG:HG2	5:L:328:GLU:HB3	1.96	0.47
1:A:57:TYR:HD1	1:A:163:ASN:O	1.97	0.47
2:C:352:ALA:HB1	2:C:356:ARG:HH12	1.79	0.47
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.49	0.47
4:E:26:ARG:HH12	4:E:37:ASN:HD22	1.61	0.47
2:I:140:ILE:HG12	2:I:141:HIS:N	2.30	0.47
2:I:185:LYS:HD3	2:I:190:LYS:HB3	1.96	0.47
2:I:817:PRO:HB3	5:L:323:LEU:HB3	1.96	0.47
3:J:140:ALA:HA	3:J:450:TYR:CD2	2.50	0.47
2:C:682:TYR:HA	3:D:633:VAL:HG11	1.95	0.47
3:D:131:LYS:HG2	3:D:153:LEU:O	2.15	0.47
3:D:141:VAL:HG12	3:D:450:TYR:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:639:LEU:HD22	3:D:766:ALA:HA	1.97	0.47
1:H:186:LEU:HD22	4:K:51:LEU:HD22	1.97	0.47
2:I:1112:PHE:HB3	2:I:1115:LEU:HB2	1.97	0.47
3:J:630:VAL:HG22	3:J:631:ILE:H	1.79	0.47
8:P:9:DG:H2''	8:P:10:DA:H5'	1.97	0.47
2:C:1026:GLN:HE21	2:C:1026:GLN:HB2	1.50	0.47
3:D:273:ARG:HB3	3:D:278:VAL:HG12	1.95	0.47
3:D:471:GLU:O	3:D:475:ARG:HG2	2.15	0.47
3:D:630:VAL:HG22	3:D:631:ILE:H	1.79	0.47
3:D:772:PRO:O	3:D:1209:LEU:HD12	2.14	0.47
5:F:137:LEU:HB3	5:F:141:LEU:HD23	1.97	0.47
5:F:368:GLU:HB3	5:F:433:LEU:HD21	1.97	0.47
1:H:52:ALA:HB3	1:H:145:ASP:O	2.15	0.47
2:I:18:LEU:HD12	2:I:408:ARG:HE	1.80	0.47
2:I:36:PRO:CB	2:I:70:GLU:HG2	2.45	0.47
2:I:163:ILE:HD12	2:I:164:PRO:HD2	1.96	0.47
2:I:424:GLY:H	2:I:427:VAL:CG2	2.28	0.47
2:I:508:ILE:HD11	2:I:529:VAL:HG11	1.96	0.47
3:J:367:ILE:HB	3:J:377:VAL:HB	1.97	0.47
3:J:1341:PRO:O	3:J:1344:VAL:HB	2.15	0.47
6:M:136:LEU:HB3	6:M:155:PHE:CZ	2.50	0.47
6:N:68:VAL:HG21	6:N:144:LEU:HD21	1.96	0.47
1:A:53:VAL:HA	1:A:144:VAL:HA	1.97	0.47
2:C:135:VAL:HG21	2:C:407:LYS:HG2	1.95	0.47
2:C:398:THR:HA	2:C:635:THR:HG21	1.97	0.47
2:I:68:PHE:O	2:I:69:LEU:HD13	2.14	0.47
2:I:409:ARG:HG2	2:I:452:ILE:HG22	1.97	0.47
2:I:708:TYR:HE2	2:I:792:VAL:HG23	1.79	0.47
2:I:922:PHE:HB2	2:I:967:PHE:CD2	2.50	0.47
3:J:646:LYS:HA	3:J:720:LEU:HD22	1.96	0.47
3:J:1267:ARG:H	3:J:1267:ARG:NE	2.13	0.47
2:C:1112:PHE:HB3	2:C:1115:LEU:HB2	1.97	0.47
3:D:151:GLN:HG2	3:D:152:LEU:H	1.80	0.47
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.97	0.47
3:D:1089:ALA:O	8:P:11:DG:H5'	2.15	0.47
1:G:176:ARG:HG3	1:G:200:TRP:CE3	2.50	0.47
1:G:198:ARG:HD2	2:I:934:PHE:CE1	2.49	0.47
1:H:30:ARG:HB3	1:H:191:ASP:O	2.15	0.47
1:H:156:HIS:ND1	1:H:156:HIS:O	2.48	0.47
3:J:167:GLU:OE2	3:J:198:ARG:NH2	2.48	0.47
3:J:699:VAL:HB	3:J:716:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:PHE:O	2:C:69:LEU:HD13	2.15	0.47
2:C:207:LEU:HD21	2:C:221:LEU:O	2.15	0.47
3:D:83:SER:O	3:D:86:ARG:HB2	2.15	0.47
3:D:970:LYS:O	3:D:974:ILE:HG13	2.15	0.47
2:I:101:ILE:HG12	2:I:108:ILE:HG23	1.95	0.47
2:I:549:PHE:HE1	2:I:909:ALA:HB3	1.80	0.47
2:I:726:ILE:HB	2:I:729:LEU:HB2	1.96	0.47
3:J:112:ILE:HD12	3:J:113:GLY:N	2.29	0.47
3:J:538:SER:HA	5:L:332:LEU:HB2	1.97	0.47
3:J:1364:HIS:CD2	3:J:1366:LYS:HE2	2.49	0.47
6:N:34:ALA:HB3	6:N:51:VAL:HG21	1.96	0.47
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.50	0.46
3:D:10:ILE:HB	3:D:1434:TRP:CH2	2.50	0.46
3:D:339:TRP:HE1	3:D:341:GLU:HG3	1.79	0.46
3:D:628:ARG:NH2	8:P:14:DG:H2''	2.30	0.46
3:D:881:LEU:HG	3:D:885:ILE:HD11	1.96	0.46
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.49	0.46
5:F:276:PRO:O	5:F:280:VAL:HG23	2.15	0.46
5:F:342:SER:OG	8:P:17:DG:N2	2.48	0.46
5:F:386:LEU:HB3	5:F:396:HIS:HB2	1.98	0.46
1:G:94:MET:O	1:G:146:ARG:HD3	2.16	0.46
2:I:42:VAL:HG12	2:I:43:GLY:H	1.79	0.46
2:I:841:ASN:HD21	2:I:845:ASN:HB3	1.78	0.46
3:J:585:GLY:HA2	3:J:590:PRO:HG3	1.96	0.46
3:J:896:ALA:O	3:J:900:ILE:HG13	2.15	0.46
3:J:1042:ARG:HD3	3:J:1045:MET:CE	2.45	0.46
5:L:142:ILE:O	5:L:146:VAL:HG23	2.15	0.46
5:L:411:ARG:HD3	7:R:1:DC:H6	1.78	0.46
5:L:413:ARG:HE	8:S:44:DT:H2'	1.80	0.46
2:C:470:PRO:HG3	2:C:485:TYR:CZ	2.50	0.46
2:C:874:LEU:O	3:D:1029:ARG:HG2	2.15	0.46
2:C:893:ALA:HB2	2:C:918:LEU:HD22	1.97	0.46
2:C:1094:ALA:HB2	3:D:520:LEU:HD13	1.96	0.46
2:I:893:ALA:HB2	2:I:918:LEU:HD22	1.97	0.46
3:J:34:TYR:HD1	5:L:325:ILE:HG21	1.80	0.46
3:J:166:GLN:HE21	3:J:166:GLN:HB2	1.52	0.46
3:J:657:LEU:HB2	3:J:691:LEU:HD13	1.97	0.46
3:J:1144:LEU:HD21	3:J:1186:VAL:HG11	1.98	0.46
3:J:1440:PHE:CE1	3:J:1441:GLN:HG2	2.50	0.46
5:L:187:ARG:O	5:L:191:ILE:HG13	2.15	0.46
2:C:971:LYS:HD2	2:C:986:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:TYR:HD1	5:F:325:ILE:HG21	1.80	0.46
3:D:63:TYR:HE2	3:D:73:CYS:HA	1.80	0.46
5:F:254:ALA:O	5:F:258:ILE:HG12	2.15	0.46
1:G:9:PRO:HG3	1:H:224:TYR:CZ	2.50	0.46
1:G:133:GLU:OE1	2:I:607:ASP:HB2	2.15	0.46
3:J:881:LEU:HG	3:J:885:ILE:HD11	1.96	0.46
2:C:101:ILE:HG12	2:C:108:ILE:HG23	1.97	0.46
2:C:140:ILE:HG12	2:C:141:HIS:N	2.30	0.46
2:C:163:ILE:HD12	2:C:164:PRO:HD2	1.97	0.46
2:C:708:TYR:HE2	2:C:792:VAL:HG23	1.80	0.46
2:C:882:LEU:HD21	3:D:1038:LEU:HD22	1.97	0.46
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.30	0.46
3:D:169:TYR:CZ	3:D:197:SER:HA	2.50	0.46
3:D:229:ALA:HA	3:D:244:GLU:HB2	1.97	0.46
3:D:259:VAL:HG23	3:D:294:GLU:HA	1.98	0.46
3:D:363:ALA:HA	3:D:381:ALA:O	2.16	0.46
3:D:671:LYS:H	5:F:364:LEU:HD11	1.81	0.46
1:H:78:ILE:HD12	1:H:130:ALA:HB2	1.97	0.46
1:H:80:LEU:HD12	3:J:844:ALA:HB2	1.98	0.46
2:I:438:ILE:HD12	2:I:438:ILE:H	1.80	0.46
2:I:874:LEU:O	3:J:1029:ARG:HG2	2.14	0.46
3:J:772:PRO:O	3:J:1209:LEU:HD12	2.15	0.46
5:L:369:LEU:HD23	5:L:433:LEU:HD13	1.96	0.46
1:B:52:ALA:HB3	1:B:145:ASP:O	2.16	0.46
2:C:185:LYS:HD3	2:C:190:LYS:HB3	1.97	0.46
2:C:521:PRO:HG2	3:D:1055:VAL:HG21	1.98	0.46
3:D:729:HIS:CE1	3:D:935:LYS:HD3	2.50	0.46
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.97	0.46
1:H:74:ASP:O	1:H:78:ILE:HG12	2.15	0.46
2:I:107:LEU:HD12	6:N:50:PRO:HD2	1.98	0.46
3:J:562:ALA:HB3	3:J:567:ILE:HD11	1.96	0.46
3:J:606:ILE:HG22	3:J:613:ARG:HB2	1.98	0.46
5:L:199:ARG:HE	5:L:200:GLN:NE2	2.13	0.46
5:L:355:SER:HB3	5:L:358:GLU:HG3	1.97	0.46
5:L:360:ALA:O	5:L:364:LEU:HB2	2.16	0.46
2:C:42:VAL:HG12	2:C:43:GLY:H	1.79	0.46
2:C:418:LEU:HD11	7:O:38:DG:C4	2.50	0.46
2:C:472:ARG:HB3	2:C:532:MET:HB3	1.97	0.46
2:C:1083:GLU:HA	2:C:1086:ARG:HG3	1.98	0.46
3:D:1267:ARG:H	3:D:1267:ARG:NE	2.13	0.46
4:E:65:MET:O	4:E:69:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:149:LYS:HB3	5:F:193:ARG:HH12	1.81	0.46
1:G:83:LYS:HD3	1:G:83:LYS:H	1.81	0.46
2:I:49:LYS:NZ	2:I:50:GLU:HG3	2.29	0.46
2:I:571:LEU:HD23	2:I:668:LEU:O	2.15	0.46
2:I:607:ASP:O	2:I:610:ARG:N	2.49	0.46
5:L:411:ARG:HB2	7:R:1:DC:H2'	1.97	0.46
1:B:20:TYR:HD1	1:B:21:GLY:H	1.64	0.46
2:C:588:VAL:HG21	2:C:664:GLY:HA2	1.98	0.46
2:C:1104:GLU:H	2:C:1104:GLU:HG2	1.52	0.46
3:D:1011:PHE:CD1	3:D:1021:TYR:HB2	2.49	0.46
5:F:364:LEU:HD22	5:F:436:PHE:HZ	1.81	0.46
2:I:140:ILE:HG23	2:I:412:ALA:HA	1.98	0.46
3:J:440:VAL:HG13	3:J:441:ARG:HD2	1.98	0.46
3:J:580:ALA:O	3:J:584:ASN:HB2	2.16	0.46
3:J:639:LEU:HD22	3:J:766:ALA:HA	1.98	0.46
3:J:1192:LEU:HD23	3:J:1373:ARG:HB2	1.98	0.46
3:J:1282:ARG:NH1	3:J:1284:GLU:OE2	2.49	0.46
6:N:20:VAL:HG22	6:N:38:VAL:HG22	1.96	0.46
2:C:86:LYS:HE2	2:C:813:VAL:HA	1.97	0.46
2:C:1038:TRP:O	3:D:1223:VAL:HG11	2.16	0.46
3:D:233:LYS:HB3	3:D:236:TYR:CZ	2.51	0.46
3:D:263:ASP:HA	3:D:268:HIS:HA	1.97	0.46
3:D:539:ASP:HB3	3:D:600:LEU:HG	1.97	0.46
3:D:606:ILE:HG22	3:D:613:ARG:HB2	1.98	0.46
3:D:657:LEU:HB2	3:D:691:LEU:HD13	1.98	0.46
3:D:896:ALA:O	3:D:900:ILE:HG13	2.16	0.46
3:D:1192:LEU:HD23	3:D:1373:ARG:HB2	1.98	0.46
5:F:119:ARG:HA	5:F:244:TYR:CE1	2.50	0.46
1:G:17:GLY:HA3	1:G:19:HIS:CE1	2.50	0.46
2:I:163:ILE:HA	2:I:164:PRO:HD2	1.75	0.46
2:I:398:THR:HA	2:I:635:THR:HG21	1.97	0.46
2:I:682:TYR:HA	3:J:633:VAL:HG11	1.96	0.46
3:J:151:GLN:HG2	3:J:152:LEU:H	1.80	0.46
3:J:1095:THR:O	3:J:1099:VAL:HG23	2.15	0.46
1:B:64:GLU:HG3	1:B:165:ILE:HG21	1.98	0.46
2:C:332:ARG:HH11	2:C:334:ARG:HD2	1.81	0.46
2:C:438:ILE:HD12	2:C:438:ILE:H	1.81	0.46
5:F:431:ARG:HG3	5:F:434:ARG:CZ	2.46	0.46
2:I:472:ARG:HB3	2:I:532:MET:HB3	1.98	0.46
3:J:729:HIS:CE1	3:J:935:LYS:HD3	2.51	0.46
5:L:413:ARG:NH2	8:S:45:DC:OP2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:10:VAL:HB	6:N:60:ARG:O	2.16	0.46
7:R:34:DA:H2"	7:R:35:DG:O4'	2.16	0.46
2:C:15:LEU:HD11	2:C:457:ALA:O	2.16	0.46
2:C:424:GLY:H	2:C:427:VAL:CG2	2.29	0.46
2:C:607:ASP:O	2:C:610:ARG:N	2.49	0.46
2:C:620:LEU:H	2:C:620:LEU:HD12	1.81	0.46
2:C:1102:LEU:HD21	3:D:9:ARG:HB2	1.97	0.46
3:D:783:ARG:HD3	3:D:1028:ALA:O	2.16	0.46
3:D:834:THR:HG21	3:D:839:LEU:HD21	1.98	0.46
5:F:244:TYR:CD2	5:F:244:TYR:N	2.84	0.46
1:H:20:TYR:HD1	1:H:21:GLY:H	1.64	0.46
1:H:20:TYR:HD1	1:H:21:GLY:N	2.14	0.46
2:I:676:ILE:HA	2:I:871:LEU:O	2.16	0.46
5:L:276:PRO:O	5:L:280:VAL:HG23	2.16	0.46
5:L:386:LEU:HB3	5:L:396:HIS:HB2	1.98	0.46
8:P:6:DC:H2"	8:P:7:DG:H5'	1.98	0.46
1:A:133:GLU:OE1	2:C:607:ASP:HB2	2.15	0.45
1:A:185:ARG:HG2	1:A:185:ARG:O	2.16	0.45
2:C:409:ARG:NH2	2:C:563:ASN:OD1	2.49	0.45
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.98	0.45
2:I:1083:GLU:HA	2:I:1086:ARG:HG3	1.98	0.45
2:I:1102:LEU:HD21	3:J:9:ARG:HB2	1.97	0.45
3:J:862:ASP:O	3:J:876:SER:HA	2.16	0.45
3:J:889:ALA:HB1	3:J:930:LEU:HA	1.98	0.45
6:M:23:ILE:HA	6:M:35:TYR:O	2.16	0.45
2:C:954:SER:HA	2:C:955:PRO:HD3	1.85	0.45
3:D:112:ILE:HD12	3:D:113:GLY:N	2.30	0.45
3:D:156:GLU:O	3:D:160:GLU:HB2	2.16	0.45
3:D:406:ASP:HB3	3:D:407:VAL:H	1.50	0.45
3:D:1318:TYR:N	3:J:1157:GLY:O	2.49	0.45
5:F:252:THR:O	5:F:255:THR:OG1	2.25	0.45
1:G:53:VAL:HA	1:G:144:VAL:HA	1.97	0.45
1:H:138:LEU:HD22	1:H:139:TYR:N	2.31	0.45
2:I:167:LYS:HD2	2:I:167:LYS:O	2.15	0.45
2:I:620:LEU:H	2:I:620:LEU:HD12	1.80	0.45
2:C:204:GLN:HA	2:C:227:LEU:HD11	1.98	0.45
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.82	0.45
3:D:859:ASP:HB2	3:D:862:ASP:OD2	2.17	0.45
3:D:1040:GLY:O	3:D:1060:SER:HB2	2.16	0.45
2:I:109:LYS:HG2	6:N:15:TYR:OH	2.16	0.45
2:I:276:LYS:HD3	2:I:466:PHE:CZ	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:521:PRO:HA	3:J:522:PRO:HD3	1.77	0.45
3:J:539:ASP:HB3	3:J:600:LEU:HG	1.97	0.45
3:J:783:ARG:HD3	3:J:1028:ALA:O	2.15	0.45
3:J:1100:ASP:CG	3:J:1440:PHE:HB2	2.37	0.45
1:A:71:VAL:HG11	1:A:78:ILE:HD11	1.99	0.45
1:B:20:TYR:HD1	1:B:21:GLY:N	2.13	0.45
1:B:214:ALA:O	1:B:218:LEU:HD13	2.16	0.45
2:C:676:ILE:HA	2:C:871:LEU:O	2.15	0.45
2:C:1083:GLU:OE1	3:D:88:TYR:OH	2.34	0.45
3:D:743:ASP:N	3:D:743:ASP:OD1	2.48	0.45
3:D:1197:ARG:NE	3:D:1398:TRP:HB3	2.32	0.45
2:I:204:GLN:HA	2:I:227:LEU:HD11	1.96	0.45
2:I:769:PRO:HB3	5:L:390:LEU:HA	1.98	0.45
2:I:1086:ARG:HD2	2:I:1112:PHE:CD2	2.52	0.45
3:J:169:TYR:O	3:J:392:SER:OG	2.34	0.45
3:J:675:ARG:HH12	5:L:437:LEU:HB3	1.80	0.45
3:J:699:VAL:HG21	3:J:764:LEU:HD13	1.99	0.45
3:J:1269:LYS:HG2	3:J:1270:ALA:N	2.31	0.45
7:R:15:DT:H6	7:R:15:DT:H5'	1.81	0.45
1:A:9:PRO:HG3	1:B:224:TYR:CZ	2.51	0.45
1:B:30:ARG:HB3	1:B:191:ASP:O	2.16	0.45
1:B:138:LEU:HD22	1:B:139:TYR:N	2.32	0.45
2:C:167:LYS:HD2	2:C:167:LYS:O	2.17	0.45
2:C:729:LEU:HD13	2:C:730:SER:O	2.16	0.45
3:D:16:GLU:H	3:D:16:GLU:CD	2.20	0.45
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.99	0.45
3:D:1282:ARG:NH1	3:D:1284:GLU:OE2	2.49	0.45
2:I:332:ARG:HH11	2:I:334:ARG:HD2	1.81	0.45
2:I:470:PRO:HG3	2:I:485:TYR:CZ	2.51	0.45
2:I:588:VAL:HG21	2:I:664:GLY:HA2	1.98	0.45
2:I:939:ARG:HB3	2:I:982:PRO:HG3	1.97	0.45
2:I:1026:GLN:HE21	2:I:1026:GLN:HB2	1.51	0.45
3:J:859:ASP:HB2	3:J:862:ASP:OD2	2.17	0.45
3:J:1040:GLY:O	3:J:1060:SER:HB2	2.16	0.45
6:M:4:PHE:HE1	6:M:10:VAL:HG11	1.82	0.45
7:R:32:DG:H2''	7:R:33:DG:O4'	2.17	0.45
1:B:63:HIS:CD2	1:B:64:GLU:H	2.35	0.45
2:C:549:PHE:HE1	2:C:909:ALA:HB3	1.81	0.45
2:C:724:ARG:HD3	2:C:741:GLY:N	2.32	0.45
3:D:186:VAL:HG13	3:D:200:ASP:OD1	2.17	0.45
3:D:217:ARG:HH12	3:D:381:ALA:CB	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:ALA:O	3:D:584:ASN:HB2	2.16	0.45
3:D:699:VAL:HG21	3:D:764:LEU:HD13	1.99	0.45
3:D:973:GLN:CG	3:J:831:GLY:HA2	2.46	0.45
3:D:1072:ILE:O	3:D:1075:HIS:HB2	2.17	0.45
5:F:355:SER:HB3	5:F:358:GLU:HG3	1.99	0.45
2:I:15:LEU:HD11	2:I:457:ALA:O	2.16	0.45
2:I:521:PRO:HB2	3:J:1055:VAL:HG11	1.98	0.45
2:I:1089:VAL:HG13	2:I:1099:VAL:HG11	1.98	0.45
3:J:83:SER:O	3:J:86:ARG:HB2	2.17	0.45
3:J:704:ARG:HB2	3:J:745:MET:HG2	1.97	0.45
3:J:903:ASP:OD1	3:J:903:ASP:N	2.49	0.45
7:R:39:DT:C2'	7:R:40:DC:H5'	2.43	0.45
2:C:299:LYS:HG3	2:C:300:ASP:H	1.81	0.45
2:C:642:ARG:HD3	2:C:642:ARG:HA	1.55	0.45
2:C:751:PRO:HA	2:C:792:VAL:HG13	1.99	0.45
2:C:1089:VAL:O	2:C:1093:GLN:HG2	2.16	0.45
3:D:101:HIS:CE1	3:D:103:TRP:HB2	2.52	0.45
3:D:102:ILE:HB	3:D:579:ASP:HB3	1.99	0.45
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.52	0.45
5:F:96:VAL:HA	5:F:225:LEU:HD11	1.97	0.45
5:F:124:GLY:O	5:F:128:ILE:HG13	2.17	0.45
2:I:409:ARG:NH2	2:I:563:ASN:OD1	2.49	0.45
2:I:658:GLY:N	2:I:661:SER:HB3	2.32	0.45
3:J:118:LEU:HD12	3:J:123:LEU:HB2	1.99	0.45
3:J:351:MET:HE3	3:J:375:GLU:O	2.17	0.45
8:S:19:DT:H5'	8:S:20:DA:OP1	2.16	0.45
1:B:78:ILE:HD12	1:B:130:ALA:HB2	1.98	0.45
1:B:80:LEU:HD12	3:D:844:ALA:HB2	1.99	0.45
2:C:521:PRO:HB2	3:D:1055:VAL:HG11	1.99	0.45
2:C:905:VAL:HG12	2:C:906:PHE:CD2	2.52	0.45
2:C:1086:ARG:HD2	2:C:1112:PHE:CD2	2.52	0.45
3:D:862:ASP:O	3:D:876:SER:HA	2.16	0.45
2:I:882:LEU:HD21	3:J:1038:LEU:HD22	1.97	0.45
2:I:1083:GLU:OE1	3:J:88:TYR:OH	2.34	0.45
3:J:101:HIS:CE1	3:J:103:TRP:HB2	2.52	0.45
4:K:31:LEU:HG	4:K:60:ALA:HB2	1.98	0.45
5:L:96:VAL:HA	5:L:225:LEU:HD11	1.97	0.45
6:M:20:VAL:HG22	6:M:38:VAL:HG22	1.98	0.45
6:N:84:LYS:HE2	6:N:84:LYS:HB2	1.75	0.45
1:A:53:VAL:HG22	1:A:54:THR:N	2.29	0.45
1:A:158:ILE:HG13	1:A:166:PRO:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASP:O	1:B:78:ILE:HG12	2.17	0.45
2:C:217:LEU:HD13	2:C:311:PHE:CD2	2.43	0.45
3:D:880:ILE:H	3:D:880:ILE:HG12	1.42	0.45
3:D:1208:ASP:N	3:D:1213:ARG:O	2.47	0.45
3:D:1269:LYS:HG2	3:D:1270:ALA:N	2.32	0.45
1:H:211:LEU:O	1:H:215:VAL:HG13	2.16	0.45
2:I:211:LEU:HD22	2:I:218:VAL:HA	1.99	0.45
2:I:729:LEU:HD13	2:I:730:SER:O	2.16	0.45
3:J:123:LEU:HG	3:J:127:LEU:HD12	1.98	0.45
3:J:550:ARG:HG3	3:J:553:ARG:HH21	1.82	0.45
3:J:764:LEU:HD23	3:J:767:HIS:CD2	2.52	0.45
5:L:244:TYR:CD2	5:L:244:TYR:N	2.83	0.45
1:A:83:LYS:H	1:A:83:LYS:HD3	1.82	0.45
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.76	0.45
2:C:726:ILE:HG23	2:C:787:ASP:HB2	1.99	0.45
2:C:829:GLN:NE2	2:C:831:ARG:HH21	2.14	0.45
2:C:1054:THR:OG1	2:C:1079:PRO:HG3	2.17	0.45
3:D:245:LEU:HA	3:D:245:LEU:HD23	1.66	0.45
3:D:369:ALA:HA	3:D:376:GLU:HG2	1.99	0.45
2:I:160:ALA:HB2	2:I:310:LEU:HD13	1.99	0.45
2:I:368:THR:HB	6:N:15:TYR:HE2	1.82	0.45
3:J:102:ILE:HB	3:J:579:ASP:HB3	1.99	0.45
3:J:156:GLU:O	3:J:160:GLU:HB2	2.16	0.45
1:A:28:LEU:HD13	1:A:36:LEU:HD11	1.99	0.44
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.99	0.44
2:C:209:ARG:HG3	2:C:210:GLU:N	2.32	0.44
2:C:891:GLY:HA3	2:C:991:GLN:O	2.17	0.44
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.78	0.44
3:D:1340:GLY:O	3:D:1344:VAL:HG23	2.17	0.44
1:G:71:VAL:HG11	1:G:78:ILE:HD11	1.98	0.44
1:H:214:ALA:O	1:H:218:LEU:HD13	2.16	0.44
2:I:1102:LEU:HA	2:I:1107:ASN:O	2.17	0.44
3:J:16:GLU:CD	3:J:16:GLU:H	2.19	0.44
3:J:365:GLU:HG2	3:J:366:LYS:H	1.82	0.44
7:O:39:DT:C2'	7:O:40:DC:H5'	2.44	0.44
3:D:1170:ASP:O	3:D:1174:LEU:HG	2.18	0.44
5:F:187:ARG:O	5:F:191:ILE:HG13	2.16	0.44
1:G:56:VAL:HG22	1:G:142:VAL:HG12	1.99	0.44
1:H:63:HIS:CD2	1:H:64:GLU:H	2.35	0.44
1:H:73:GLU:HB2	1:H:78:ILE:HD11	1.99	0.44
2:I:111:ASP:HA	6:N:45:SER:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:446:GLY:O	2:I:449:ILE:HG13	2.18	0.44
2:I:1008:ARG:NH1	2:I:1028:GLY:HA2	2.31	0.44
2:I:1089:VAL:O	2:I:1093:GLN:HG2	2.16	0.44
5:L:336:ILE:HD11	5:L:344:TYR:HD2	1.82	0.44
6:M:18:GLY:HA3	6:M:40:PHE:HA	1.99	0.44
2:C:36:PRO:CB	2:C:70:GLU:HG2	2.46	0.44
2:C:327:HIS:O	2:C:331:ARG:HG3	2.17	0.44
2:C:838:LYS:HD3	2:C:999:HIS:HB2	1.99	0.44
3:D:248:PRO:HA	3:D:307:GLY:O	2.17	0.44
3:D:1221:VAL:HA	3:D:1224:VAL:HB	2.00	0.44
5:F:360:ALA:O	5:F:364:LEU:HB2	2.17	0.44
1:G:28:LEU:HD13	1:G:36:LEU:HD11	2.00	0.44
2:I:64:LEU:HD11	2:I:100:LEU:HD11	2.00	0.44
2:I:1066:ALA:O	2:I:1070:ILE:HD12	2.17	0.44
5:L:149:LYS:HB3	5:L:193:ARG:HH12	1.81	0.44
1:B:36:LEU:C	1:B:39:PRO:HD2	2.37	0.44
1:B:211:LEU:O	1:B:215:VAL:HG13	2.17	0.44
2:C:484:VAL:HG12	2:C:486:MET:H	1.82	0.44
2:C:1019:GLN:OE1	3:D:621:LYS:HE3	2.18	0.44
2:C:1035:MET:SD	8:P:12:DT:H4'	2.57	0.44
3:D:470:LEU:HD11	3:D:502:PHE:HB3	2.00	0.44
3:D:550:ARG:HG3	3:D:553:ARG:HH21	1.82	0.44
3:D:566:ILE:HG23	5:F:229:GLN:HE22	1.83	0.44
4:E:41:GLU:O	4:E:45:ARG:HG2	2.18	0.44
1:H:101:LEU:HD22	1:H:102:ARG:H	1.82	0.44
2:I:708:TYR:CE2	2:I:792:VAL:HG23	2.52	0.44
2:I:1038:TRP:O	3:J:1223:VAL:HG11	2.17	0.44
3:J:702:LEU:HG	3:J:747:VAL:HG22	1.99	0.44
3:J:1003:VAL:HG21	3:J:1041:MET:HB3	1.99	0.44
3:J:1170:ASP:O	3:J:1174:LEU:HG	2.17	0.44
6:N:17:VAL:HG13	6:N:138:GLU:HB3	1.98	0.44
1:A:133:GLU:OE1	2:C:605:LYS:HB2	2.17	0.44
1:B:87:VAL:HG12	1:B:122:ILE:HG12	2.00	0.44
2:C:658:GLY:N	2:C:661:SER:HB3	2.33	0.44
3:D:32:ILE:HA	3:D:40:GLU:HG2	2.00	0.44
3:D:894:LYS:H	3:D:894:LYS:HG2	1.53	0.44
3:D:1003:VAL:HG21	3:D:1041:MET:HB3	1.99	0.44
3:D:1190:SER:HB2	3:D:1369:GLU:OE1	2.18	0.44
3:D:1209:LEU:HD23	3:D:1209:LEU:HA	1.73	0.44
2:I:484:VAL:HG12	2:I:486:MET:H	1.83	0.44
2:I:946:ARG:HH12	3:J:860:LEU:HD13	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:59:ALA:HB2	3:J:78:VAL:HG21	1.98	0.44
3:J:205:TYR:CD2	3:J:387:LEU:HD22	2.53	0.44
3:J:566:ILE:HG23	5:L:229:GLN:HE22	1.82	0.44
3:J:1172:HIS:O	3:J:1175:ILE:HB	2.18	0.44
6:N:11:VAL:HG22	6:N:17:VAL:HG12	1.98	0.44
7:O:17:DA:H1'	7:O:18:DA:H5''	1.98	0.44
7:O:21:DG:N2	8:P:28:DC:O2	2.51	0.44
1:A:94:MET:O	1:A:146:ARG:HD3	2.17	0.44
2:C:683:ASN:HB2	2:C:872:ASN:HB3	1.99	0.44
3:D:314:PRO:HB2	3:D:317:MET:HG3	2.00	0.44
2:I:166:PRO:C	2:I:168:ARG:H	2.21	0.44
2:I:549:PHE:CE1	2:I:909:ALA:HB3	2.53	0.44
2:I:773:LEU:HD22	5:L:390:LEU:HD11	1.99	0.44
2:I:838:LYS:HD3	2:I:999:HIS:HB2	2.00	0.44
3:J:101:HIS:HB3	3:J:104:PHE:CZ	2.52	0.44
3:J:130:ASN:O	3:J:456:MET:HE1	2.18	0.44
3:J:1197:ARG:NE	3:J:1398:TRP:HB3	2.32	0.44
3:J:1495:ILE:HD13	4:K:80:VAL:HG21	1.99	0.44
5:L:252:THR:O	5:L:256:TRP:HD1	2.01	0.44
5:L:266:ILE:O	5:L:270:ALA:HB2	2.18	0.44
8:P:40:DT:H1'	8:P:41:DT:H5'	1.99	0.44
2:C:154:ARG:HB2	2:C:157:ARG:HB2	1.99	0.44
2:C:200:LEU:HD12	2:C:200:LEU:HA	1.82	0.44
3:D:353:VAL:HG22	3:D:355:VAL:H	1.82	0.44
3:D:1122:LEU:H	3:D:1122:LEU:HD12	1.82	0.44
3:J:465:LEU:HD12	3:J:513:ILE:HD11	1.99	0.44
3:J:471:GLU:O	3:J:475:ARG:HG2	2.17	0.44
3:J:911:LEU:O	3:J:915:VAL:HG23	2.17	0.44
6:M:84:LYS:HB2	6:M:84:LYS:HE2	1.79	0.44
2:C:650:LYS:HG2	2:C:651:LYS:H	1.82	0.44
2:C:708:TYR:CE2	2:C:792:VAL:HG23	2.53	0.44
3:D:130:ASN:O	3:D:456:MET:HE1	2.18	0.44
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.99	0.44
3:D:675:ARG:HH12	5:F:437:LEU:H	1.65	0.44
3:D:1093:TYR:HD1	8:P:10:DA:H5''	1.82	0.44
1:H:156:HIS:NE2	1:H:167:VAL:O	2.51	0.44
2:I:324:ASP:O	2:I:330:ASN:ND2	2.51	0.44
2:I:440:PRO:HB2	3:J:1074:SER:OG	2.18	0.44
2:I:724:ARG:HD3	2:I:741:GLY:N	2.33	0.44
3:J:834:THR:HG21	3:J:839:LEU:HD21	1.98	0.44
1:A:82:LEU:O	1:A:85:LEU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:ARG:N	2:C:95:TYR:O	2.49	0.44
2:C:166:PRO:C	2:C:168:ARG:H	2.22	0.44
2:C:716:LYS:H	2:C:716:LYS:HG2	1.59	0.44
2:C:1102:LEU:CD2	3:D:9:ARG:HB2	2.48	0.44
2:C:1116:ALA:HA	3:D:23:TYR:OH	2.18	0.44
3:D:895:VAL:O	3:D:898:GLU:HB3	2.18	0.44
3:D:1090:ASP:O	3:D:1093:TYR:HB3	2.18	0.44
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.99	0.44
5:F:336:ILE:HD11	5:F:344:TYR:HD2	1.81	0.44
1:G:133:GLU:OE1	2:I:605:LYS:HB2	2.18	0.44
1:G:209:GLU:HA	1:G:212:ASN:HB2	2.00	0.44
2:I:46:ALA:O	2:I:50:GLU:HB2	2.18	0.44
2:I:501:THR:O	2:I:503:LEU:HG	2.18	0.44
2:I:1019:GLN:OE1	3:J:621:LYS:HE3	2.18	0.44
5:L:375:LYS:HD2	5:L:426:HIS:ND1	2.32	0.44
2:C:211:LEU:HD22	2:C:218:VAL:HA	2.00	0.43
2:C:328:LEU:HD21	2:C:434:HIS:HA	2.00	0.43
2:C:446:GLY:O	2:C:449:ILE:HG13	2.17	0.43
2:C:673:LEU:H	2:C:673:LEU:HD12	1.83	0.43
2:C:1067:TYR:CE2	5:F:357:VAL:HA	2.53	0.43
3:D:171:LEU:HD21	3:D:175:VAL:O	2.17	0.43
3:D:622:ARG:NH1	8:P:14:DG:OP2	2.51	0.43
3:D:670:VAL:HB	5:F:364:LEU:HD11	2.00	0.43
2:I:72:ARG:N	2:I:95:TYR:O	2.49	0.43
2:I:230:ARG:NH2	2:I:231:PRO:HD2	2.28	0.43
2:I:874:LEU:HD22	3:J:1029:ARG:HB2	2.00	0.43
3:J:129:PHE:CE1	3:J:457:GLY:HA3	2.53	0.43
3:J:400:VAL:HG12	3:J:445:ARG:HG2	1.99	0.43
3:J:1267:ARG:HE	3:J:1267:ARG:HB2	1.63	0.43
1:A:206:THR:HG23	1:A:209:GLU:OE2	2.17	0.43
2:C:160:ALA:HB2	2:C:310:LEU:HD13	1.99	0.43
2:C:751:PRO:HD2	3:D:681:ARG:HD2	2.00	0.43
2:C:946:ARG:HH12	3:D:860:LEU:HD13	1.83	0.43
3:D:439:LEU:HD11	5:F:190:HIS:CB	2.48	0.43
3:D:762:GLN:CB	4:E:16:LYS:HE2	2.48	0.43
3:D:1172:HIS:O	3:D:1175:ILE:HB	2.18	0.43
3:D:1433:SER:HB3	3:D:1464:GLU:CD	2.39	0.43
5:F:266:ILE:O	5:F:270:ALA:HB2	2.18	0.43
2:I:3:ILE:HG13	2:I:900:ARG:HG3	2.00	0.43
2:I:19:THR:HG22	2:I:407:LYS:HZ1	1.82	0.43
2:I:892:LEU:HD13	2:I:989:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:905:VAL:HG12	2:I:906:PHE:CD2	2.53	0.43
2:I:1081:VAL:HG21	2:I:1086:ARG:CZ	2.48	0.43
3:J:1072:ILE:O	3:J:1075:HIS:HB2	2.18	0.43
3:J:1208:ASP:HB3	3:J:1211:MET:HB2	2.00	0.43
4:K:30:LEU:HD11	4:K:67:GLU:OE2	2.17	0.43
4:K:42:PRO:HA	4:K:45:ARG:HG3	1.99	0.43
5:L:124:GLY:O	5:L:128:ILE:HG13	2.18	0.43
1:A:179:PHE:HD1	1:A:195:LEU:HD21	1.84	0.43
2:C:683:ASN:C	2:C:687:ALA:HB3	2.39	0.43
2:C:769:PRO:HB3	5:F:390:LEU:HA	1.99	0.43
2:C:773:LEU:HD22	5:F:390:LEU:HD11	2.01	0.43
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	2.00	0.43
2:C:1066:ALA:O	2:C:1070:ILE:HD12	2.18	0.43
3:D:123:LEU:HG	3:D:127:LEU:HD12	1.99	0.43
3:D:716:PHE:CZ	3:D:728:LEU:HD11	2.54	0.43
3:D:1225:ALA:HA	3:D:1367:HIS:HB3	2.00	0.43
1:G:206:THR:HG23	1:G:209:GLU:OE2	2.19	0.43
1:H:87:VAL:HG12	1:H:122:ILE:HG12	2.00	0.43
2:I:327:HIS:O	2:I:331:ARG:HG3	2.17	0.43
2:I:351:LEU:HD11	2:I:374:ASN:H	1.84	0.43
2:I:376:ARG:O	2:I:380:ALA:HB3	2.19	0.43
3:J:675:ARG:HD3	5:L:435:ASP:OD2	2.18	0.43
3:J:1225:ALA:HA	3:J:1367:HIS:HB3	2.00	0.43
4:K:45:ARG:HD2	4:K:63:TRP:CH2	2.54	0.43
6:M:67:GLU:OE2	6:M:103:TYR:OH	2.36	0.43
1:A:63:HIS:CE1	1:A:66:SER:HB2	2.53	0.43
2:C:166:PRO:HA	7:O:37:DT:H71	2.01	0.43
2:C:440:PRO:HB2	3:D:1074:SER:OG	2.18	0.43
3:D:465:LEU:HD12	3:D:513:ILE:HD11	2.00	0.43
3:D:475:ARG:O	3:D:478:LEU:HB2	2.19	0.43
3:D:702:LEU:HG	3:D:747:VAL:HG22	1.99	0.43
3:D:1127:GLU:C	3:D:1129:THR:H	2.22	0.43
4:E:31:LEU:HG	4:E:60:ALA:HB2	2.00	0.43
4:E:42:PRO:HA	4:E:45:ARG:HG3	1.99	0.43
1:G:71:VAL:HG21	1:G:138:LEU:HD22	2.01	0.43
1:G:158:ILE:HG13	1:G:166:PRO:HG3	2.00	0.43
2:I:20:GLU:O	2:I:24:GLU:N	2.44	0.43
2:I:181:VAL:HG22	2:I:182:VAL:H	1.83	0.43
2:I:683:ASN:HB2	2:I:872:ASN:HB3	1.99	0.43
3:J:895:VAL:O	3:J:898:GLU:HB3	2.18	0.43
3:J:1090:ASP:O	3:J:1093:TYR:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1208:ASP:N	3:J:1213:ARG:O	2.47	0.43
1:B:101:LEU:HD22	1:B:102:ARG:N	2.33	0.43
2:C:219:GLN:H	2:C:219:GLN:HG3	1.60	0.43
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.31	0.43
2:C:1067:TYR:CE1	3:D:655:PRO:HG3	2.53	0.43
3:D:107:ASP:HA	3:D:586:ARG:HH21	1.84	0.43
3:D:1167:SER:H	3:D:1170:ASP:HB2	1.83	0.43
1:G:53:VAL:HG22	1:G:54:THR:N	2.31	0.43
1:G:63:HIS:CE1	1:G:66:SER:HB2	2.53	0.43
1:G:110:ARG:HA	1:G:129:ILE:HG12	2.00	0.43
2:I:427:VAL:HG22	7:R:38:DG:N2	2.26	0.43
2:I:650:LYS:HG2	2:I:651:LYS:H	1.83	0.43
2:I:781:LYS:HE2	2:I:782:ALA:O	2.19	0.43
2:I:1044:GLY:HA3	4:K:17:TYR:CE1	2.53	0.43
5:L:238:ALA:HB2	5:L:257:TRP:CG	2.54	0.43
8:P:24:DA:H3'	8:P:24:DA:P	2.58	0.43
1:B:174:VAL:HA	1:B:200:TRP:O	2.19	0.43
2:C:5:ARG:HB2	2:C:902:ILE:HB	2.01	0.43
2:C:140:ILE:HG23	2:C:412:ALA:HA	1.99	0.43
2:C:501:THR:O	2:C:503:LEU:HG	2.19	0.43
2:C:781:LYS:HE2	2:C:782:ALA:O	2.18	0.43
3:D:132:TYR:HB3	3:D:454:ALA:HB1	2.00	0.43
3:D:439:LEU:HD11	5:F:190:HIS:HB3	2.01	0.43
3:D:897:GLN:HE21	3:D:897:GLN:HB3	1.66	0.43
5:F:241:LYS:HE2	7:O:24:DC:H3'	1.99	0.43
1:G:58:ILE:HG22	1:G:60:ASP:N	2.33	0.43
1:H:64:GLU:HG3	1:H:165:ILE:HG21	1.98	0.43
1:H:101:LEU:HD22	1:H:102:ARG:N	2.32	0.43
2:I:754:ILE:HA	2:I:791:ARG:HA	2.01	0.43
2:I:1023:GLY:HA2	8:S:15:DA:P	2.58	0.43
2:I:1055:ILE:HD11	2:I:1079:PRO:HD3	2.01	0.43
3:J:44:LEU:HD21	3:J:544:TYR:HB3	2.01	0.43
3:J:362:GLN:HB2	3:J:365:GLU:HB2	2.00	0.43
3:J:561:GLY:HA2	5:L:151:LEU:HD22	2.00	0.43
3:J:762:GLN:CB	4:K:16:LYS:HE2	2.49	0.43
6:M:22:GLY:O	6:M:36:TYR:HA	2.19	0.43
2:C:46:ALA:O	2:C:50:GLU:HB2	2.18	0.43
2:C:760:SER:O	2:C:785:VAL:HA	2.19	0.43
3:D:372:ASP:HB3	3:D:374:GLU:HG3	2.00	0.43
3:D:475:ARG:HG2	3:D:475:ARG:H	1.67	0.43
3:D:930:LEU:O	3:D:934:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:999:HIS:CD2	2:I:1004:LYS:HE3	2.54	0.43
2:I:1102:LEU:CD2	3:J:9:ARG:HB2	2.49	0.43
3:J:508:ARG:HB2	3:J:511:TRP:CE2	2.53	0.43
6:M:80:MET:HB3	6:M:107:GLN:HG2	1.99	0.43
6:M:85:GLN:H	6:M:85:GLN:HG2	1.58	0.43
1:A:110:ARG:HA	1:A:129:ILE:HG12	2.00	0.43
2:C:276:LYS:HD3	2:C:466:PHE:CZ	2.54	0.43
2:C:537:LYS:HZ3	2:C:905:VAL:N	2.12	0.43
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.53	0.43
2:C:946:ARG:NH2	3:D:860:LEU:H	2.17	0.43
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.53	0.43
2:C:1102:LEU:HA	2:C:1107:ASN:O	2.17	0.43
3:D:51:GLY:HA3	3:D:85:VAL:HG23	2.00	0.43
3:D:54:LYS:HD3	3:D:55:ASP:N	2.34	0.43
3:D:129:PHE:CE1	3:D:457:GLY:HA3	2.54	0.43
3:D:646:LYS:HD2	3:D:722:GLU:OE1	2.18	0.43
3:D:911:LEU:O	3:D:915:VAL:HG23	2.18	0.43
3:D:1191:PRO:O	3:D:1373:ARG:HD3	2.19	0.43
2:I:751:PRO:HA	2:I:792:VAL:HG13	2.00	0.43
2:I:1007:ALA:HB2	3:J:648:MET:HG3	2.01	0.43
2:I:1016:ILE:HG13	2:I:1017:THR:H	1.83	0.43
3:J:537:THR:C	5:L:332:LEU:HG	2.39	0.43
4:K:41:GLU:O	4:K:45:ARG:HG2	2.18	0.43
6:M:18:GLY:CA	6:M:41:PRO:HD3	2.47	0.43
7:R:43:DG:H1	8:S:6:DC:H42	1.67	0.43
2:C:1018:GLN:HB2	2:C:1058:ASP:HB2	2.00	0.43
2:C:1081:VAL:HG21	2:C:1086:ARG:CZ	2.49	0.43
2:C:1092:LEU:HD22	2:C:1097:LEU:HD13	2.00	0.43
3:D:248:PRO:HG3	3:D:308:LYS:HD3	2.00	0.43
3:D:632:VAL:O	3:D:727:GLN:HA	2.19	0.43
1:G:179:PHE:HD1	1:G:195:LEU:HD21	1.83	0.43
2:I:64:LEU:HD22	2:I:359:MET:SD	2.59	0.43
2:I:208:VAL:HA	2:I:211:LEU:HB2	2.00	0.43
2:I:726:ILE:HG23	2:I:787:ASP:HB2	2.00	0.43
2:I:874:LEU:HD23	2:I:874:LEU:HA	1.91	0.43
2:I:1090:LYS:HA	2:I:1090:LYS:HD2	1.72	0.43
3:J:409:VAL:HG23	3:J:437:VAL:HG22	2.01	0.43
3:J:587:ARG:HE	3:J:587:ARG:HB3	1.62	0.43
5:L:137:LEU:HD11	5:L:178:LEU:HD11	2.00	0.43
2:C:351:LEU:HD11	2:C:374:ASN:H	1.84	0.43
2:C:874:LEU:HD22	3:D:1029:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:892:LEU:HD13	2:C:989:VAL:HG23	2.01	0.43
3:D:101:HIS:HB3	3:D:104:PHE:CZ	2.54	0.43
3:D:903:ASP:OD1	3:D:903:ASP:N	2.51	0.43
3:D:1480:PHE:CD2	3:D:1481:VAL:HG13	2.54	0.43
5:F:238:ALA:HB2	5:F:257:TRP:CG	2.54	0.43
1:H:36:LEU:C	1:H:39:PRO:HD2	2.38	0.43
1:H:109:VAL:HG12	1:H:129:ILE:HB	2.01	0.43
2:I:159:ILE:HG13	2:I:175:GLU:HA	2.01	0.43
2:I:328:LEU:HD21	2:I:434:HIS:HA	2.01	0.43
2:I:1081:VAL:HG21	2:I:1086:ARG:NE	2.34	0.43
2:I:1082:PRO:O	2:I:1083:GLU:HB3	2.19	0.43
3:J:583:ASP:OD1	3:J:586:ARG:HB2	2.18	0.43
3:J:671:LYS:HG3	5:L:436:PHE:CE2	2.54	0.43
3:J:1127:GLU:C	3:J:1129:THR:H	2.22	0.43
3:J:1167:SER:H	3:J:1170:ASP:HB2	1.84	0.43
3:J:1221:VAL:HA	3:J:1224:VAL:HB	2.01	0.43
6:N:36:TYR:HE2	6:N:54:PRO:HG3	1.83	0.43
6:N:52:GLU:H	6:N:52:GLU:HG2	1.52	0.43
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.19	0.42
2:C:109:LYS:HE2	6:M:40:PHE:CZ	2.53	0.42
2:C:376:ARG:O	2:C:380:ALA:HB3	2.19	0.42
2:C:1089:VAL:HG13	2:C:1099:VAL:HG11	2.00	0.42
3:D:698:LYS:HB3	3:D:756:GLN:NE2	2.34	0.42
3:D:1267:ARG:HE	3:D:1267:ARG:HB2	1.62	0.42
1:H:182:GLU:HG3	1:H:194:LYS:HB3	2.01	0.42
2:I:418:LEU:HD11	7:R:38:DG:C4	2.54	0.42
2:I:572:ILE:HD11	2:I:703:ILE:HD11	2.00	0.42
2:I:925:TYR:O	2:I:928:LYS:HB3	2.19	0.42
2:I:1038:TRP:CE3	3:J:1099:VAL:HG21	2.54	0.42
3:J:51:GLY:HA3	3:J:85:VAL:HG23	1.99	0.42
3:J:470:LEU:HD11	3:J:502:PHE:HB3	2.01	0.42
3:J:716:PHE:CZ	3:J:728:LEU:HD11	2.53	0.42
3:J:1093:TYR:CD1	8:S:10:DA:H5''	2.52	0.42
3:J:1122:LEU:H	3:J:1122:LEU:HD12	1.84	0.42
7:R:32:DG:H2''	7:R:33:DG:H5'	2.01	0.42
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.91	0.42
1:A:209:GLU:HA	1:A:212:ASN:HB2	2.02	0.42
2:C:64:LEU:HD11	2:C:100:LEU:HD11	2.01	0.42
2:C:159:ILE:HG13	2:C:175:GLU:HA	2.01	0.42
3:D:212:ARG:HG2	3:D:344:ASP:HB3	2.01	0.42
3:D:561:GLY:HA2	5:F:151:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:691:LEU:HA	3:D:694:VAL:HG23	2.01	0.42
5:F:279:MET:O	5:F:283:ILE:HG13	2.19	0.42
5:F:431:ARG:HG3	5:F:434:ARG:NE	2.34	0.42
1:G:23:PHE:HE2	1:G:199:ILE:HD12	1.85	0.42
1:G:185:ARG:O	1:G:185:ARG:HG2	2.18	0.42
2:I:549:PHE:HB3	2:I:552:HIS:CD2	2.54	0.42
2:I:760:SER:O	2:I:785:VAL:HA	2.20	0.42
2:I:946:ARG:NH2	3:J:860:LEU:H	2.17	0.42
2:I:1006:HIS:HB2	2:I:1024:LYS:HG3	2.00	0.42
2:I:1116:ALA:HA	3:J:23:TYR:OH	2.19	0.42
3:J:103:TRP:CH2	3:J:1444:THR:HA	2.54	0.42
3:J:107:ASP:HA	3:J:586:ARG:HH21	1.84	0.42
3:J:209:ARG:H	3:J:390:PRO:HA	1.83	0.42
3:J:1099:VAL:O	3:J:1103:HIS:HB3	2.19	0.42
1:B:101:LEU:HD22	1:B:102:ARG:H	1.84	0.42
2:C:477:GLY:HA2	2:C:508:ILE:HG13	2.02	0.42
2:C:1038:TRP:CE3	3:D:1099:VAL:HG21	2.54	0.42
3:D:583:ASP:OD1	3:D:586:ARG:HB2	2.18	0.42
3:D:706:PRO:HG3	8:P:11:DG:H21	1.83	0.42
5:F:137:LEU:HD11	5:F:178:LEU:HD11	2.00	0.42
2:I:647:GLN:HE21	2:I:647:GLN:HB2	1.52	0.42
2:I:1090:LYS:HD2	2:I:1093:GLN:HG3	2.01	0.42
3:J:68:PHE:CZ	5:L:394:ARG:HD2	2.54	0.42
3:J:752:SER:O	3:J:756:GLN:N	2.50	0.42
3:J:789:LEU:HD23	3:J:882:PHE:HE1	1.84	0.42
3:J:914:LEU:HD13	3:J:914:LEU:HA	1.84	0.42
3:J:1340:GLY:O	3:J:1344:VAL:HG23	2.18	0.42
5:L:108:LEU:O	5:L:109:LEU:HB3	2.19	0.42
5:L:199:ARG:HG3	5:L:239:VAL:HG11	2.02	0.42
8:S:40:DT:H1'	8:S:41:DT:H5'	2.02	0.42
1:A:54:THR:O	1:A:167:VAL:HG22	2.19	0.42
1:B:109:VAL:HG12	1:B:129:ILE:HB	2.01	0.42
1:B:176:ARG:HG2	1:B:177:VAL:N	2.34	0.42
2:C:16:PRO:HB2	2:C:460:ARG:NH2	2.34	0.42
2:C:111:ASP:HA	6:M:45:SER:HB2	2.00	0.42
2:C:208:VAL:HA	2:C:211:LEU:HB2	2.00	0.42
2:C:374:ASN:HD22	2:C:375:SER:N	2.17	0.42
2:C:614:ARG:HH21	2:C:620:LEU:HD23	1.84	0.42
2:C:881:ASN:OD1	2:C:884:GLN:NE2	2.52	0.42
2:C:1007:ALA:HB2	3:D:648:MET:HG3	2.02	0.42
2:C:1081:VAL:HG21	2:C:1086:ARG:NE	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:407:VAL:HG23	3:D:422:ALA:HB2	2.00	0.42
3:D:508:ARG:HB2	3:D:511:TRP:CE2	2.54	0.42
3:D:752:SER:O	3:D:756:GLN:N	2.49	0.42
3:D:795:VAL:HG13	3:D:879:ARG:NH2	2.34	0.42
3:D:970:LYS:O	3:D:973:GLN:HB3	2.20	0.42
3:D:1208:ASP:HB3	3:D:1211:MET:HB2	2.00	0.42
4:E:30:LEU:HD11	4:E:67:GLU:OE2	2.18	0.42
5:F:135:THR:HG21	5:F:177:LYS:HG2	2.01	0.42
1:G:36:LEU:HD12	1:G:195:LEU:HD12	2.01	0.42
1:G:54:THR:O	1:G:167:VAL:HG22	2.19	0.42
1:G:99:LEU:HB2	1:G:142:VAL:HG23	2.02	0.42
2:I:477:GLY:HA2	2:I:508:ILE:HG13	2.01	0.42
3:J:32:ILE:HA	3:J:40:GLU:HG2	2.01	0.42
3:J:132:TYR:HB3	3:J:454:ALA:HB1	2.00	0.42
3:J:141:VAL:HG12	3:J:450:TYR:CE2	2.52	0.42
3:J:475:ARG:O	3:J:478:LEU:HB2	2.19	0.42
3:J:658:LEU:HD21	3:J:670:VAL:O	2.20	0.42
3:J:691:LEU:HA	3:J:694:VAL:HG23	2.01	0.42
3:J:698:LYS:HB3	3:J:756:GLN:NE2	2.34	0.42
3:J:795:VAL:HG13	3:J:879:ARG:NH2	2.34	0.42
3:J:884:ARG:NE	3:J:888:GLU:OE2	2.52	0.42
3:J:1191:PRO:O	3:J:1373:ARG:HD3	2.20	0.42
5:L:135:THR:HG21	5:L:177:LYS:HG2	2.02	0.42
1:B:73:GLU:HB2	1:B:78:ILE:HD11	2.02	0.42
2:C:198:ARG:HG2	2:C:234:ALA:HB3	2.02	0.42
2:C:549:PHE:CE1	2:C:909:ALA:HB3	2.54	0.42
2:C:999:HIS:CD2	2:C:1004:LYS:HE3	2.54	0.42
2:C:1082:PRO:O	2:C:1083:GLU:HB3	2.18	0.42
3:D:44:LEU:HD21	3:D:544:TYR:HB3	2.01	0.42
3:D:118:LEU:HD12	3:D:123:LEU:HB2	2.01	0.42
3:D:638:LYS:C	3:D:729:HIS:HD2	2.22	0.42
3:D:720:LEU:HD23	3:D:720:LEU:HA	1.90	0.42
3:D:1114:THR:OG1	3:D:1116:ASN:ND2	2.48	0.42
5:F:380:GLU:HB2	5:F:415:ILE:HG23	2.02	0.42
2:I:77:PRO:HD3	2:I:92:ALA:HA	2.00	0.42
2:I:683:ASN:C	2:I:687:ALA:HB3	2.40	0.42
2:I:688:ILE:HG23	2:I:871:LEU:HD23	2.02	0.42
2:I:810:ASP:O	2:I:813:VAL:HG12	2.19	0.42
2:I:1092:LEU:HD22	2:I:1097:LEU:HD13	2.00	0.42
3:J:421:LEU:CD2	3:J:422:ALA:H	2.32	0.42
3:J:649:ALA:HB3	3:J:720:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1190:SER:HB2	3:J:1369:GLU:OE1	2.20	0.42
3:J:1480:PHE:CD2	3:J:1481:VAL:HG13	2.54	0.42
6:N:129:LEU:O	6:N:133:ILE:HG12	2.19	0.42
1:A:71:VAL:HG21	1:A:138:LEU:HD22	2.01	0.42
1:B:100:ILE:HG22	1:B:141:GLU:HB3	2.02	0.42
2:C:39:ARG:HD3	2:C:45:GLN:OE1	2.20	0.42
2:C:179:SER:OG	2:C:181:VAL:HG12	2.20	0.42
2:C:925:TYR:O	2:C:928:LYS:HB3	2.19	0.42
2:C:1017:THR:OG1	2:C:1019:GLN:HG2	2.20	0.42
2:C:1056:LYS:HG3	3:D:751:LEU:HD11	2.02	0.42
3:D:171:LEU:HD23	3:D:172:PRO:O	2.19	0.42
3:D:181:ASP:HB2	3:D:205:TYR:CE2	2.54	0.42
5:F:199:ARG:HG3	5:F:239:VAL:HG11	2.02	0.42
2:I:99:GLN:HB3	2:I:110:GLU:HG3	2.01	0.42
2:I:247:PRO:HA	2:I:248:PRO:HD3	1.76	0.42
2:I:891:GLY:HA3	2:I:991:GLN:O	2.19	0.42
3:J:167:GLU:HB3	3:J:395:VAL:HG12	2.01	0.42
3:J:553:ARG:NH2	5:L:226:ASP:OD1	2.47	0.42
3:J:632:VAL:O	3:J:727:GLN:HA	2.19	0.42
4:K:50:THR:HB	4:K:53:GLY:O	2.20	0.42
1:B:182:GLU:HG3	1:B:194:LYS:HB3	2.01	0.42
2:C:77:PRO:HD3	2:C:92:ALA:HA	2.01	0.42
2:C:181:VAL:HG22	2:C:182:VAL:H	1.84	0.42
2:C:524:VAL:HB	2:C:528:GLU:HG3	2.01	0.42
2:C:1031:ARG:HA	3:D:622:ARG:HA	2.02	0.42
3:D:176:ASP:OD2	3:D:388:HIS:HB3	2.19	0.42
3:D:610:LYS:NZ	8:P:10:DA:OP2	2.28	0.42
5:F:252:THR:O	5:F:256:TRP:HD1	2.03	0.42
1:G:180:GLN:HB3	2:I:934:PHE:CZ	2.54	0.42
2:I:441:VAL:O	2:I:559:LEU:HD12	2.20	0.42
2:I:524:VAL:HB	2:I:528:GLU:HG3	2.00	0.42
2:I:946:ARG:HH22	3:J:860:LEU:HD13	1.84	0.42
2:I:954:SER:HA	2:I:955:PRO:HD3	1.85	0.42
3:J:397:LYS:HE3	3:J:448:GLU:O	2.19	0.42
3:J:520:LEU:HD12	3:J:521:PRO:HD2	2.01	0.42
3:J:593:ASN:HA	3:J:594:PRO:HD3	1.91	0.42
3:J:1008:PHE:O	3:J:1012:GLU:HG3	2.20	0.42
3:J:1103:HIS:HE1	3:J:1464:GLU:HG3	1.84	0.42
1:A:180:GLN:HB3	2:C:934:PHE:CZ	2.55	0.42
2:C:122:THR:OG1	2:C:126:SER:O	2.35	0.42
3:D:514:LEU:HD11	3:D:516:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:914:LEU:HA	3:D:914:LEU:HD13	1.84	0.42
5:F:114:GLU:OE1	5:F:249:LYS:HD2	2.20	0.42
2:I:848:VAL:HG22	3:J:740:PHE:O	2.20	0.42
3:J:930:LEU:O	3:J:934:LEU:HD12	2.19	0.42
3:J:1268:PRO:HB2	3:J:1271:LYS:HB2	2.02	0.42
5:L:370:GLU:O	5:L:373:LEU:HB3	2.20	0.42
6:M:131:ARG:HD2	6:M:131:ARG:HA	1.89	0.42
1:B:76:VAL:O	1:B:80:LEU:HD22	2.20	0.42
2:C:99:GLN:HB3	2:C:110:GLU:HG3	2.00	0.42
2:C:109:LYS:HG2	6:M:15:TYR:OH	2.20	0.42
2:C:946:ARG:HH22	3:D:860:LEU:HD13	1.85	0.42
2:C:1056:LYS:HE3	2:C:1056:LYS:HB2	1.84	0.42
3:D:789:LEU:HD23	3:D:882:PHE:HE1	1.84	0.42
3:D:1462:LEU:H	3:D:1462:LEU:HG	1.71	0.42
4:E:45:ARG:HD2	4:E:63:TRP:CH2	2.55	0.42
1:H:58:ILE:HG23	1:H:140:MET:HB3	2.02	0.42
1:H:174:VAL:HA	1:H:200:TRP:O	2.19	0.42
2:I:179:SER:OG	2:I:181:VAL:HG12	2.20	0.42
2:I:1019:GLN:HE21	3:J:617:ASN:HB3	1.85	0.42
2:I:1031:ARG:HA	3:J:622:ARG:HA	2.02	0.42
3:J:720:LEU:HD23	3:J:720:LEU:HA	1.90	0.42
5:L:376:LEU:HD21	5:L:423:LEU:HG	2.02	0.42
8:S:24:DA:H3'	8:S:24:DA:OP1	2.20	0.42
1:A:58:ILE:HG22	1:A:60:ASP:N	2.34	0.42
2:C:72:ARG:CB	2:C:95:TYR:HB2	2.46	0.42
2:C:91:GLN:HA	2:C:119:PRO:HA	2.02	0.42
2:C:349:ALA:O	2:C:353:ARG:HG2	2.19	0.42
2:C:848:VAL:HG22	3:D:740:PHE:O	2.20	0.42
2:C:1090:LYS:HD2	2:C:1093:GLN:HG3	2.00	0.42
3:D:494:LYS:O	3:D:497:GLU:HB3	2.19	0.42
3:D:658:LEU:HD21	3:D:670:VAL:O	2.20	0.42
4:E:50:THR:HB	4:E:53:GLY:O	2.20	0.42
2:I:16:PRO:HB2	2:I:460:ARG:NH2	2.34	0.42
2:I:200:LEU:HD12	2:I:200:LEU:HA	1.83	0.42
2:I:552:HIS:ND1	3:J:1061:PHE:O	2.50	0.42
2:I:934:PHE:HD2	2:I:934:PHE:HA	1.62	0.42
3:J:62:LYS:HD2	3:J:75:ARG:HD2	2.02	0.42
3:J:161:LEU:HD12	3:J:161:LEU:HA	1.78	0.42
3:J:508:ARG:HB3	3:J:510:GLU:CD	2.40	0.42
3:J:623:VAL:HB	3:J:748:HIS:CE1	2.55	0.42
4:K:39:VAL:HG21	4:K:72:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:111:LEU:H	5:L:111:LEU:HD22	1.85	0.42
5:L:206:ASN:O	5:L:209:LEU:HB3	2.20	0.42
6:N:116:GLU:HB2	6:N:121:LEU:HD22	2.02	0.42
8:P:22:DT:H4'	8:P:23:DA:OP1	2.19	0.42
1:B:85:LEU:HD12	1:B:124:ASN:HB3	2.01	0.41
2:C:441:VAL:O	2:C:559:LEU:HD12	2.20	0.41
2:C:1115:LEU:HD23	3:D:85:VAL:HG12	2.01	0.41
3:D:585:GLY:CA	3:D:590:PRO:HG3	2.50	0.41
3:D:640:HIS:H	3:D:640:HIS:CD2	2.38	0.41
3:D:660:LYS:HD2	3:D:694:VAL:HG22	2.02	0.41
3:D:682:ASP:C	3:D:684:LYS:H	2.24	0.41
5:F:388:LYS:HD3	5:F:388:LYS:HA	1.73	0.41
2:I:39:ARG:HD3	2:I:45:GLN:OE1	2.20	0.41
2:I:91:GLN:HA	2:I:119:PRO:HA	2.02	0.41
2:I:1023:GLY:HA2	8:S:15:DA:OP2	2.20	0.41
3:J:103:TRP:CE2	3:J:1444:THR:HG23	2.55	0.41
3:J:1014:ASN:O	3:J:1016:PRO:HD3	2.20	0.41
3:J:1331:ASP:HA	3:J:1332:PRO:HD3	1.90	0.41
6:N:12:LEU:HD23	6:N:40:PHE:CZ	2.55	0.41
6:N:136:LEU:HB3	6:N:155:PHE:CZ	2.55	0.41
1:A:23:PHE:HE2	1:A:199:ILE:HD12	1.85	0.41
1:A:36:LEU:HD12	1:A:195:LEU:HD12	2.01	0.41
1:B:115:THR:HA	1:B:116:PRO:HD3	1.90	0.41
1:B:176:ARG:HD2	3:D:884:ARG:NH2	2.30	0.41
2:C:594:ALA:HB1	2:C:654:LEU:HD11	2.01	0.41
2:C:688:ILE:HG23	2:C:871:LEU:HD23	2.02	0.41
3:D:260:GLU:O	3:D:270:ILE:HA	2.20	0.41
3:D:313:LEU:HG	3:D:314:PRO:CD	2.50	0.41
3:D:659:LYS:O	3:D:662:GLU:HB3	2.20	0.41
3:D:884:ARG:NE	3:D:888:GLU:OE2	2.53	0.41
3:D:976:GLN:HG2	3:J:807:ALA:CB	2.50	0.41
3:D:1008:PHE:O	3:D:1012:GLU:HG3	2.20	0.41
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.20	0.41
3:D:1268:PRO:HB2	3:D:1271:LYS:HB2	2.03	0.41
1:H:176:ARG:HG3	3:J:850:LEU:HD22	2.02	0.41
2:I:5:ARG:HB2	2:I:902:ILE:HB	2.02	0.41
2:I:198:ARG:HG2	2:I:234:ALA:HB3	2.02	0.41
2:I:724:ARG:NE	2:I:739:GLU:O	2.51	0.41
2:I:751:PRO:HB2	2:I:794:PRO:HA	2.02	0.41
3:J:1194:CYS:SG	3:J:1196:THR:OG1	2.69	0.41
5:L:380:GLU:HB2	5:L:415:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:O	1:A:61:VAL:HB	2.20	0.41
2:C:3:ILE:HG13	2:C:900:ARG:HG3	2.02	0.41
2:C:108:ILE:HD11	6:M:28:VAL:HG21	2.02	0.41
3:D:103:TRP:CH2	3:D:1444:THR:HA	2.55	0.41
3:D:225:ILE:HG23	3:D:229:ALA:HB3	2.02	0.41
3:D:351:MET:HB3	3:D:368:VAL:HG12	2.02	0.41
2:I:325:ILE:HG23	2:I:326:ASP:H	1.84	0.41
2:I:376:ARG:H	2:I:376:ARG:HG2	1.58	0.41
2:I:599:GLU:HA	2:I:651:LYS:HB3	2.03	0.41
2:I:614:ARG:HH21	2:I:620:LEU:HD23	1.84	0.41
3:J:585:GLY:CA	3:J:590:PRO:HG3	2.50	0.41
3:J:653:PHE:HB2	3:J:691:LEU:HD11	2.02	0.41
3:J:1042:ARG:NE	3:J:1061:PHE:HE2	2.18	0.41
3:J:1209:LEU:HD23	3:J:1209:LEU:HA	1.72	0.41
4:K:66:LYS:HA	4:K:69:LEU:HB2	2.02	0.41
5:L:249:LYS:HG2	7:R:29:DC:OP2	2.19	0.41
1:B:48:ILE:HA	1:B:49:PRO:HD2	1.94	0.41
1:B:176:ARG:HG3	3:D:850:LEU:HD22	2.02	0.41
3:D:675:ARG:NH1	5:F:437:LEU:H	2.19	0.41
3:D:1306:PRO:HB2	3:D:1308:ASP:OD1	2.21	0.41
5:F:108:LEU:O	5:F:109:LEU:HB3	2.19	0.41
1:G:63:HIS:CE1	1:G:66:SER:H	2.38	0.41
2:I:209:ARG:HG3	2:I:210:GLU:N	2.33	0.41
2:I:513:VAL:O	2:I:524:VAL:HG22	2.20	0.41
2:I:881:ASN:OD1	2:I:884:GLN:NE2	2.53	0.41
3:J:213:VAL:HG13	3:J:385:VAL:HG12	2.02	0.41
3:J:638:LYS:C	3:J:729:HIS:HD2	2.22	0.41
3:J:660:LYS:HD2	3:J:694:VAL:HG22	2.01	0.41
1:B:156:HIS:NE2	1:B:167:VAL:O	2.52	0.41
2:C:107:LEU:HA	6:M:50:PRO:HD3	2.03	0.41
2:C:513:VAL:O	2:C:524:VAL:HG22	2.20	0.41
3:D:62:LYS:HD2	3:D:75:ARG:HD2	2.03	0.41
3:D:129:PHE:CE1	3:D:571:LYS:HE2	2.56	0.41
3:D:186:VAL:HG12	3:D:187:LYS:N	2.36	0.41
3:D:298:VAL:HB	3:D:302:GLN:HG2	2.03	0.41
3:D:618:LEU:HD13	3:D:618:LEU:HA	1.87	0.41
3:D:623:VAL:HB	3:D:748:HIS:CE1	2.55	0.41
3:D:984:THR:O	3:D:988:ARG:HB2	2.20	0.41
3:D:1076:GLY:O	3:D:1079:LYS:HB3	2.21	0.41
4:E:39:VAL:HG21	4:E:72:ARG:HB2	2.02	0.41
1:G:170:ILE:HG23	2:I:696:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:ILE:HG22	1:H:141:GLU:HB3	2.02	0.41
2:I:1002:GLU:HA	3:J:724:GLN:OE1	2.20	0.41
5:L:279:MET:O	5:L:283:ILE:HG13	2.20	0.41
7:R:19:DT:H1'	7:R:20:DT:H5'	2.03	0.41
1:A:63:HIS:CE1	1:A:66:SER:H	2.37	0.41
2:C:872:ASN:OD1	2:C:874:LEU:HB2	2.20	0.41
2:C:1002:GLU:HA	3:D:724:GLN:OE1	2.21	0.41
3:D:314:PRO:HG3	3:D:317:MET:HE3	2.02	0.41
3:D:508:ARG:HB3	3:D:510:GLU:CD	2.41	0.41
3:D:638:LYS:HA	3:D:932:ASP:OD1	2.20	0.41
3:D:649:ALA:HB3	3:D:720:LEU:HD21	2.02	0.41
3:D:669:ASN:HD22	5:F:364:LEU:HD21	1.85	0.41
3:D:873:LEU:HD22	3:D:875:THR:HG23	2.02	0.41
5:F:370:GLU:O	5:F:373:LEU:HB3	2.21	0.41
5:F:381:ALA:O	5:F:385:LYS:HG3	2.20	0.41
1:G:82:LEU:O	1:G:85:LEU:HB3	2.20	0.41
1:H:76:VAL:O	1:H:80:LEU:HD22	2.21	0.41
1:H:85:LEU:HD12	1:H:124:ASN:HB3	2.02	0.41
2:I:349:ALA:O	2:I:353:ARG:HG2	2.20	0.41
2:I:594:ALA:HB1	2:I:654:LEU:HD11	2.01	0.41
2:I:1022:GLY:HA3	3:J:622:ARG:CZ	2.50	0.41
3:J:781:PRO:O	3:J:908:LYS:NZ	2.50	0.41
3:J:886:VAL:HG12	3:J:896:ALA:HB1	2.03	0.41
5:L:141:LEU:O	5:L:145:VAL:HG23	2.21	0.41
6:N:79:ARG:HB3	6:N:111:GLN:OE1	2.20	0.41
1:A:36:LEU:O	1:A:39:PRO:HD2	2.20	0.41
1:B:212:ASN:O	1:B:215:VAL:HG22	2.21	0.41
2:C:64:LEU:HD22	2:C:359:MET:SD	2.60	0.41
2:C:140:ILE:HB	2:C:333:ILE:HD13	2.03	0.41
2:C:325:ILE:HG23	2:C:326:ASP:H	1.86	0.41
2:C:754:ILE:HA	2:C:791:ARG:HA	2.02	0.41
2:C:1085:PHE:O	2:C:1089:VAL:HG23	2.21	0.41
3:D:1014:ASN:O	3:D:1016:PRO:HD3	2.20	0.41
5:F:206:ASN:O	5:F:209:LEU:HB3	2.21	0.41
2:I:161:SER:HA	2:I:172:ILE:O	2.21	0.41
2:I:1017:THR:OG1	2:I:1019:GLN:HG2	2.20	0.41
2:I:1018:GLN:HB2	2:I:1058:ASP:HB2	2.01	0.41
2:I:1085:PHE:O	2:I:1089:VAL:HG23	2.20	0.41
3:J:129:PHE:CE1	3:J:571:LYS:HE2	2.55	0.41
3:J:171:LEU:HD23	3:J:172:PRO:O	2.21	0.41
3:J:646:LYS:HE3	3:J:688:TRP:HZ2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1335:LEU:HA	3:J:1338:ALA:HB3	2.03	0.41
5:L:233:GLN:HG3	5:L:236:ILE:HD12	2.03	0.41
6:M:13:PRO:HD2	6:M:58:GLY:O	2.20	0.41
6:M:21:ALA:N	6:M:37:GLN:O	2.54	0.41
6:M:129:LEU:O	6:M:133:ILE:HG12	2.21	0.41
6:M:142:GLN:HE21	6:M:142:GLN:HB3	1.66	0.41
2:C:230:ARG:NH2	2:C:231:PRO:HD2	2.29	0.41
2:C:598:GLU:HG2	2:C:615:TYR:CE2	2.56	0.41
2:C:1037:VAL:HG12	2:C:1041:GLU:OE2	2.20	0.41
3:D:354:ILE:HD11	3:D:369:ALA:HB2	2.02	0.41
3:D:430:GLU:O	3:D:431:ILE:HB	2.20	0.41
3:D:1278:ASP:OD2	3:D:1321:ALA:N	2.54	0.41
4:E:6:ILE:HG23	4:E:7:ASP:H	1.85	0.41
4:E:66:LYS:HA	4:E:69:LEU:HB2	2.02	0.41
1:G:150:TYR:HE1	1:G:168:ASP:HB3	1.86	0.41
2:I:66:LEU:HD11	2:I:372:LEU:HD23	2.03	0.41
2:I:872:ASN:OD1	2:I:874:LEU:HB2	2.21	0.41
3:J:181:ASP:HB3	3:J:357:GLU:HG3	2.02	0.41
3:J:494:LYS:O	3:J:497:GLU:HB3	2.19	0.41
3:J:514:LEU:HD11	3:J:516:ALA:O	2.21	0.41
3:J:659:LYS:O	3:J:662:GLU:HB3	2.20	0.41
3:J:894:LYS:H	3:J:894:LYS:HG2	1.54	0.41
3:J:1076:GLY:O	3:J:1079:LYS:HB3	2.21	0.41
5:L:208:ARG:HH21	7:R:31:DG:H8	1.69	0.41
1:A:122:ILE:HG13	1:A:124:ASN:H	1.86	0.41
2:C:206:THR:HG22	2:C:209:ARG:NH2	2.36	0.41
2:C:249:LYS:HE2	2:C:249:LYS:HB3	1.88	0.41
2:C:437:ARG:NH2	2:C:469:THR:HG22	2.36	0.41
2:C:751:PRO:HB2	2:C:794:PRO:HA	2.03	0.41
2:C:1035:MET:HG2	2:C:1036:GLU:N	2.36	0.41
2:C:1051:GLU:OE1	2:C:1055:ILE:HD12	2.21	0.41
3:D:7:LYS:HE3	3:D:1458:GLU:OE1	2.21	0.41
3:D:56:TYR:HE2	3:D:82:ARG:HE	1.69	0.41
3:D:103:TRP:CE2	3:D:1444:THR:HG23	2.56	0.41
3:D:122:GLU:HG2	3:D:152:LEU:HD21	2.03	0.41
3:D:206:ARG:HA	3:D:206:ARG:HD3	1.76	0.41
3:D:299:GLU:O	3:D:302:GLN:HB3	2.21	0.41
3:D:352:ASN:O	3:D:368:VAL:HG13	2.21	0.41
3:D:490:ALA:O	3:D:493:ARG:HB3	2.21	0.41
3:D:553:ARG:NH2	5:F:226:ASP:OD1	2.47	0.41
3:D:569:ASN:O	3:D:572:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:653:PHE:HB2	3:D:691:LEU:HD11	2.02	0.41
3:D:1072:ILE:H	3:D:1072:ILE:HG13	1.69	0.41
3:D:1130:ARG:CZ	3:D:1130:ARG:HB3	2.51	0.41
5:F:233:GLN:HG3	5:F:236:ILE:HD12	2.03	0.41
5:F:252:THR:HG23	7:O:29:DC:H41	1.86	0.41
5:F:376:LEU:HD21	5:F:423:LEU:HG	2.02	0.41
1:G:36:LEU:O	1:G:39:PRO:HD2	2.20	0.41
1:G:99:LEU:HD13	1:G:144:VAL:HG23	2.03	0.41
2:I:217:LEU:H	2:I:217:LEU:HG	1.58	0.41
2:I:537:LYS:HZ3	2:I:905:VAL:N	2.08	0.41
2:I:608:GLY:HA2	2:I:641:PRO:HG2	2.03	0.41
2:I:673:LEU:H	2:I:673:LEU:HD12	1.85	0.41
2:I:885:ILE:HG22	2:I:889:HIS:NE2	2.36	0.41
2:I:1082:PRO:CG	3:J:1469:GLY:HA3	2.50	0.41
2:I:1115:LEU:HD23	3:J:85:VAL:HG12	2.02	0.41
3:J:39:PRO:HB3	3:J:46:ASP:HA	2.03	0.41
3:J:54:LYS:HD3	3:J:55:ASP:N	2.35	0.41
3:J:770:LEU:HD23	3:J:777:PRO:HA	2.03	0.41
3:J:873:LEU:HD22	3:J:875:THR:HG23	2.01	0.41
3:J:984:THR:O	3:J:988:ARG:HB2	2.20	0.41
3:J:1101:VAL:HG13	3:J:1102:ALA:H	1.86	0.41
5:L:114:GLU:OE1	5:L:249:LYS:HD2	2.21	0.41
5:L:237:ARG:NH1	5:L:241:LYS:HD2	2.36	0.41
5:L:293:LEU:HD13	5:L:301:PRO:HG3	2.02	0.41
8:P:21:DA:H4'	8:P:22:DT:OP1	2.21	0.41
8:S:5:DC:H2'	8:S:6:DC:C5	2.56	0.41
2:C:6:PHE:HE1	2:C:901:TYR:CD1	2.30	0.41
2:C:552:HIS:ND1	3:D:1061:PHE:O	2.49	0.41
2:C:1044:GLY:O	3:D:1476:THR:HG23	2.21	0.41
3:D:114:THR:O	3:D:495:ARG:HG3	2.20	0.41
3:D:440:VAL:HG13	3:D:441:ARG:H	1.85	0.41
3:D:970:LYS:HG2	3:D:995:LEU:HD13	2.03	0.41
3:D:1101:VAL:HG13	3:D:1102:ALA:H	1.85	0.41
5:F:293:LEU:HD13	5:F:301:PRO:HG3	2.02	0.41
1:H:176:ARG:HD2	3:J:884:ARG:NH2	2.32	0.41
2:I:9:ILE:H	2:I:9:ILE:HG13	1.70	0.41
2:I:893:ALA:HB2	2:I:918:LEU:HD13	2.03	0.41
3:J:67:ARG:HH11	5:L:394:ARG:NH1	2.19	0.41
3:J:114:THR:O	3:J:495:ARG:HG3	2.21	0.41
3:J:122:GLU:HG2	3:J:152:LEU:HD21	2.03	0.41
3:J:646:LYS:HD2	3:J:722:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:970:LYS:HG2	3:J:995:LEU:HD13	2.03	0.41
3:J:1306:PRO:HB2	3:J:1308:ASP:OD1	2.20	0.41
5:L:246:ARG:HG3	7:R:26:DA:N1	2.35	0.41
8:P:42:DT:H2"	8:P:43:DG:C8	2.56	0.41
1:B:58:ILE:HG23	1:B:140:MET:HB3	2.03	0.40
2:C:32:ALA:HB1	2:C:73:ILE:HD13	2.03	0.40
2:C:66:LEU:HD22	2:C:98:LEU:HD12	2.03	0.40
2:C:537:LYS:NZ	2:C:905:VAL:H	2.13	0.40
2:C:599:GLU:HA	2:C:651:LYS:HB3	2.03	0.40
3:D:236:TYR:HB3	3:D:313:LEU:HD13	2.03	0.40
3:D:273:ARG:HE	3:D:278:VAL:HG12	1.86	0.40
1:H:212:ASN:O	1:H:215:VAL:HG22	2.22	0.40
2:I:1035:MET:HG2	2:I:1036:GLU:N	2.37	0.40
3:J:176:ASP:HA	3:J:389:GLU:HA	2.03	0.40
3:J:683:ILE:H	3:J:683:ILE:HG12	1.67	0.40
3:J:1130:ARG:CZ	3:J:1130:ARG:HB3	2.51	0.40
5:L:379:ARG:HG3	5:L:405:PHE:CE2	2.56	0.40
7:R:17:DA:H1'	7:R:18:DA:H5"	2.03	0.40
1:A:99:LEU:HB2	1:A:142:VAL:HG23	2.03	0.40
2:C:690:ILE:HB	2:C:852:ILE:HG23	2.03	0.40
3:D:118:LEU:HD13	3:D:122:GLU:OE2	2.21	0.40
3:D:276:GLU:HG2	3:D:277:GLU:H	1.86	0.40
3:D:689:ASP:O	3:D:692:GLU:HB2	2.20	0.40
3:D:691:LEU:O	3:D:695:ILE:HG13	2.20	0.40
3:D:1266:ARG:CD	7:O:42:DC:H5"	2.51	0.40
5:F:111:LEU:H	5:F:111:LEU:HD22	1.86	0.40
1:G:60:ASP:O	1:G:61:VAL:HB	2.21	0.40
2:I:109:LYS:HE2	6:N:40:PHE:CZ	2.57	0.40
2:I:170:PRO:HB3	7:R:36:DC:H42	1.86	0.40
2:I:598:GLU:HG2	2:I:615:TYR:CE2	2.57	0.40
2:I:769:PRO:HD3	3:J:65:ARG:HH12	1.86	0.40
2:I:950:LEU:HD23	2:I:950:LEU:H	1.86	0.40
2:I:972:VAL:HG12	2:I:973:VAL:H	1.86	0.40
3:J:1129:THR:C	3:J:1131:THR:H	2.25	0.40
5:L:257:TRP:O	5:L:260:GLN:HB3	2.22	0.40
5:L:260:GLN:HB2	7:R:25:DT:O4	2.22	0.40
5:L:388:LYS:HA	5:L:388:LYS:HD3	1.73	0.40
1:A:170:ILE:HG23	2:C:696:LYS:HD3	2.03	0.40
2:C:608:GLY:HA2	2:C:641:PRO:HG2	2.03	0.40
2:C:710:ILE:HB	2:C:790:LEU:HD13	2.03	0.40
2:C:810:ASP:O	2:C:813:VAL:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:70:GLY:HA2	3:D:79:GLU:HG3	2.03	0.40
3:D:116:LEU:HD21	3:D:465:LEU:HG	2.03	0.40
3:D:161:LEU:HA	3:D:161:LEU:HD12	1.78	0.40
3:D:646:LYS:HE3	3:D:688:TRP:HZ2	1.86	0.40
3:D:731:LEU:HD13	3:D:731:LEU:HA	1.93	0.40
1:H:176:ARG:HG2	1:H:177:VAL:N	2.36	0.40
2:I:724:ARG:O	2:I:734:LEU:HD11	2.21	0.40
3:J:124:GLU:HG3	3:J:125:GLN:N	2.37	0.40
3:J:213:VAL:HG22	3:J:385:VAL:HG12	2.03	0.40
3:J:537:THR:O	5:L:332:LEU:N	2.54	0.40
6:N:63:LEU:HD11	6:N:102:PRO:HB2	2.04	0.40
1:B:44:LEU:HA	1:B:48:ILE:HD13	2.04	0.40
2:C:17:PRO:HA	2:C:590:ASP:OD1	2.21	0.40
2:C:630:ARG:HE	2:C:707:ARG:HH11	1.70	0.40
3:D:247:GLU:O	3:D:249:TYR:N	2.51	0.40
3:D:786:ILE:H	3:D:786:ILE:HG13	1.70	0.40
4:E:27:ALA:HB1	4:E:60:ALA:CB	2.51	0.40
4:E:41:GLU:HB2	4:E:43:GLU:OE2	2.22	0.40
5:F:141:LEU:O	5:F:145:VAL:HG23	2.21	0.40
5:F:237:ARG:NH1	5:F:241:LYS:HD2	2.37	0.40
1:G:58:ILE:HG23	1:G:139:TYR:O	2.21	0.40
1:H:115:THR:HA	1:H:116:PRO:HD3	1.90	0.40
2:I:72:ARG:CB	2:I:95:TYR:HB2	2.44	0.40
2:I:219:GLN:H	2:I:219:GLN:HG3	1.60	0.40
2:I:391:LEU:CD2	2:I:415:PRO:HD2	2.50	0.40
3:J:116:LEU:HD21	3:J:465:LEU:HG	2.03	0.40
3:J:928:ALA:HA	3:J:931:LEU:HD12	2.03	0.40
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.91	0.40
2:C:64:LEU:HD13	2:C:359:MET:HB2	2.04	0.40
2:C:185:LYS:HG2	2:C:190:LYS:HA	2.04	0.40
2:C:291:VAL:HG13	2:C:303:PHE:HE1	1.87	0.40
2:C:713:ARG:HA	2:C:819:VAL:HA	2.03	0.40
3:D:318:THR:O	3:D:337:LEU:HG	2.22	0.40
3:D:626:SER:HB3	3:D:748:HIS:CE1	2.56	0.40
3:D:1135:ARG:O	3:D:1140:ILE:HD11	2.21	0.40
4:E:59:ASN:HD21	4:E:61:VAL:HG23	1.86	0.40
5:F:271:ARG:H	5:F:271:ARG:HE	1.69	0.40
1:G:122:ILE:HG13	1:G:124:ASN:H	1.86	0.40
1:H:44:LEU:HA	1:H:48:ILE:HD13	2.04	0.40
2:I:6:PHE:HE1	2:I:901:TYR:CD1	2.31	0.40
2:I:174:LEU:HD23	2:I:174:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:206:THR:HG22	2:I:209:ARG:NH2	2.36	0.40
2:I:669:GLY:HA3	2:I:994:ILE:O	2.22	0.40
2:I:713:ARG:HA	2:I:819:VAL:HA	2.03	0.40
3:J:209:ARG:HA	3:J:347:VAL:CG1	2.51	0.40
3:J:374:GLU:HG3	3:J:375:GLU:N	2.36	0.40
3:J:784:ASP:O	3:J:787:LEU:HB3	2.22	0.40
3:J:1107:VAL:HG23	3:J:1221:VAL:HG11	2.03	0.40
3:J:1114:THR:OG1	3:J:1116:ASN:ND2	2.47	0.40
3:J:1135:ARG:O	3:J:1140:ILE:HD11	2.21	0.40
4:K:6:ILE:HG23	4:K:7:ASP:H	1.87	0.40
6:M:75:LEU:HD23	6:M:75:LEU:HA	1.92	0.40
7:O:18:DA:H5'	7:O:18:DA:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	225/314 (72%)	191 (85%)	32 (14%)	2 (1%)	14	50
1	B	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	14	50
1	G	225/314 (72%)	190 (84%)	33 (15%)	2 (1%)	14	50
1	H	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	14	50
2	C	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	30	67
2	I	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	30	67
3	D	1486/1524 (98%)	1306 (88%)	171 (12%)	9 (1%)	22	59
3	J	1361/1524 (89%)	1200 (88%)	156 (12%)	5 (0%)	30	67
4	E	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
4	K	91/99 (92%)	82 (90%)	9 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	343/347 (99%)	301 (88%)	41 (12%)	1 (0%)	37	72
5	L	343/347 (99%)	300 (88%)	42 (12%)	1 (0%)	37	72
6	M	156/164 (95%)	143 (92%)	11 (7%)	2 (1%)	10	42
6	N	156/164 (95%)	142 (91%)	12 (8%)	2 (1%)	10	42
All	All	7157/7762 (92%)	6277 (88%)	844 (12%)	36 (0%)	25	63

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	681	ARG
3	D	683	ILE
3	D	1128	VAL
1	G	53	VAL
3	J	681	ARG
3	J	1128	VAL
2	C	738	ASP
3	D	431	ILE
3	D	666	PHE
2	I	738	ASP
6	M	20	VAL
6	N	20	VAL
2	C	61	LYS
2	I	61	LYS
1	B	118	ALA
1	B	119	ASP
2	C	607	ASP
3	D	680	GLN
1	H	118	ALA
2	I	607	ASP
3	J	680	GLN
5	F	391	ILE
1	H	119	ASP
3	J	868	TYR
5	L	391	ILE
1	A	61	VAL
2	C	1060	ILE
3	D	667	ALA
1	G	61	VAL
2	I	1060	ILE
6	M	41	PRO

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Mol	Chain	Res	Type
6	N	41	PRO
3	D	1277	ILE
3	J	1277	ILE
3	D	238	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	194/270 (72%)	171 (88%)	23 (12%)	4	18
1	B	194/270 (72%)	167 (86%)	27 (14%)	3	15
1	G	194/270 (72%)	171 (88%)	23 (12%)	4	18
1	H	194/270 (72%)	167 (86%)	27 (14%)	3	15
2	C	931/936 (100%)	820 (88%)	111 (12%)	4	18
2	I	931/936 (100%)	820 (88%)	111 (12%)	4	18
3	D	1252/1281 (98%)	1115 (89%)	137 (11%)	5	20
3	J	1150/1281 (90%)	1033 (90%)	117 (10%)	6	21
4	E	83/88 (94%)	77 (93%)	6 (7%)	12	32
4	K	83/88 (94%)	77 (93%)	6 (7%)	12	32
5	F	296/299 (99%)	267 (90%)	29 (10%)	6	22
5	L	296/299 (99%)	267 (90%)	29 (10%)	6	22
6	M	127/133 (96%)	122 (96%)	5 (4%)	27	50
6	N	127/133 (96%)	122 (96%)	5 (4%)	27	50
All	All	6052/6554 (92%)	5396 (89%)	656 (11%)	5	20

All (656) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	28	LEU
1	A	32	PHE

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	44	LEU
1	A	51	THR
1	A	54	THR
1	A	61	VAL
1	A	80	LEU
1	A	83	LYS
1	A	85	LEU
1	A	86	VAL
1	A	87	VAL
1	A	113	ASP
1	A	114	PHE
1	A	161	ARG
1	A	186	LEU
1	A	195	LEU
1	A	200	TRP
1	A	206	THR
1	A	209	GLU
1	A	213	GLN
1	A	227	ASN
1	B	19	HIS
1	B	20	TYR
1	B	23	PHE
1	B	30	ARG
1	B	36	LEU
1	B	41	ARG
1	B	51	THR
1	B	54	THR
1	B	58	ILE
1	B	62	LEU
1	B	68	ILE
1	B	74	ASP
1	B	75	VAL
1	B	80	LEU
1	B	100	ILE
1	B	110	ARG
1	B	114	PHE
1	B	162	ILE
1	B	170	ILE
1	B	177	VAL
1	B	186	LEU
1	B	193	ASP

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Mol	Chain	Res	Type
1	B	195	LEU
1	B	215	VAL
1	B	222	LEU
1	B	227	ASN
1	B	232	LEU
2	C	5	ARG
2	C	11	GLU
2	C	13	ILE
2	C	15	LEU
2	C	20	GLU
2	C	39	ARG
2	C	69	LEU
2	C	70	GLU
2	C	80	GLN
2	C	81	ASP
2	C	85	GLU
2	C	100	LEU
2	C	103	LYS
2	C	107	LEU
2	C	111	ASP
2	C	140	ILE
2	C	141	HIS
2	C	154	ARG
2	C	179	SER
2	C	194	VAL
2	C	195	LEU
2	C	196	LEU
2	C	198	ARG
2	C	207	LEU
2	C	209	ARG
2	C	217	LEU
2	C	219	GLN
2	C	230	ARG
2	C	242	LEU
2	C	246	ASP
2	C	261	LEU
2	C	274	ARG
2	C	285	LEU
2	C	292	ARG
2	C	297	GLU
2	C	304	LEU
2	C	317	VAL

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Mol	Chain	Res	Type
2	C	322	VAL
2	C	325	ILE
2	C	344	PHE
2	C	361	MET
2	C	367	LEU
2	C	374	ASN
2	C	376	ARG
2	C	393	GLN
2	C	394	PHE
2	C	396	ASP
2	C	410	ILE
2	C	421	GLU
2	C	426	ASP
2	C	428	ARG
2	C	430	VAL
2	C	433	THR
2	C	434	HIS
2	C	438	ILE
2	C	473	ARG
2	C	474	VAL
2	C	495	THR
2	C	543	ASN
2	C	579	VAL
2	C	610	ARG
2	C	620	LEU
2	C	622	GLU
2	C	647	GLN
2	C	680	ASP
2	C	683	ASN
2	C	689	VAL
2	C	690	ILE
2	C	695	LEU
2	C	703	ILE
2	C	713	ARG
2	C	716	LYS
2	C	717	LEU
2	C	729	LEU
2	C	761	PHE
2	C	784	ASP
2	C	788	THR
2	C	790	LEU
2	C	815	LEU

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Mol	Chain	Res	Type
2	C	834	GLN
2	C	848	VAL
2	C	857	ASP
2	C	861	LEU
2	C	863	ASP
2	C	867	VAL
2	C	869	VAL
2	C	871	LEU
2	C	872	ASN
2	C	876	VAL
2	C	887	GLU
2	C	890	LEU
2	C	896	PHE
2	C	900	ARG
2	C	934	PHE
2	C	950	LEU
2	C	953	VAL
2	C	963	LEU
2	C	968	ASP
2	C	972	VAL
2	C	994	ILE
2	C	1000	MET
2	C	1015	LEU
2	C	1026	GLN
2	C	1035	MET
2	C	1053	LEU
2	C	1063	ARG
2	C	1074	GLU
2	C	1088	LEU
2	C	1101	THR
2	C	1104	GLU
2	C	1113	GLU
3	D	16	GLU
3	D	25	GLU
3	D	32	ILE
3	D	47	GLU
3	D	62	LYS
3	D	68	PHE
3	D	69	GLU
3	D	92	HIS
3	D	103	TRP
3	D	104	PHE

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Mol	Chain	Res	Type
3	D	115	LEU
3	D	118	LEU
3	D	124	GLU
3	D	128	TYR
3	D	145	VAL
3	D	154	THR
3	D	155	ASP
3	D	176	ASP
3	D	196	VAL
3	D	216	LEU
3	D	225	ILE
3	D	231	VAL
3	D	233	LYS
3	D	242	LEU
3	D	245	LEU
3	D	246	SER
3	D	251	PHE
3	D	255	GLU
3	D	261	LEU
3	D	266	GLU
3	D	273	ARG
3	D	281	ARG
3	D	289	THR
3	D	292	VAL
3	D	296	GLU
3	D	311	LEU
3	D	313	LEU
3	D	316	HIS
3	D	333	LEU
3	D	335	LEU
3	D	338	GLU
3	D	344	ASP
3	D	350	HIS
3	D	352	ASN
3	D	362	GLN
3	D	374	GLU
3	D	389	GLU
3	D	406	ASP
3	D	421	LEU
3	D	423	ASP
3	D	430	GLU
3	D	439	LEU

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Mol	Chain	Res	Type
3	D	445	ARG
3	D	464	LEU
3	D	497	GLU
3	D	574	LEU
3	D	614	PHE
3	D	619	LEU
3	D	623	VAL
3	D	639	LEU
3	D	640	HIS
3	D	650	LEU
3	D	658	LEU
3	D	660	LYS
3	D	687	VAL
3	D	688	TRP
3	D	694	VAL
3	D	701	LEU
3	D	708	LEU
3	D	717	GLN
3	D	743	ASP
3	D	748	HIS
3	D	754	PHE
3	D	768	ASN
3	D	776	GLU
3	D	780	LYS
3	D	789	LEU
3	D	795	VAL
3	D	817	GLU
3	D	833	GLU
3	D	861	GLN
3	D	863	VAL
3	D	865	THR
3	D	873	LEU
3	D	880	ILE
3	D	897	GLN
3	D	899	LEU
3	D	901	GLN
3	D	903	ASP
3	D	908	LYS
3	D	914	LEU
3	D	958	GLU
3	D	959	GLU
3	D	964	LEU

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Mol	Chain	Res	Type
3	D	965	GLU
3	D	971	LEU
3	D	976	GLN
3	D	1015	TYR
3	D	1025	GLN
3	D	1078	ARG
3	D	1086	LEU
3	D	1094	LEU
3	D	1100	ASP
3	D	1122	LEU
3	D	1130	ARG
3	D	1132	LEU
3	D	1136	LYS
3	D	1137	ARG
3	D	1140	ILE
3	D	1144	LEU
3	D	1158	ARG
3	D	1160	LEU
3	D	1161	GLU
3	D	1184	ARG
3	D	1200	VAL
3	D	1213	ARG
3	D	1267	ARG
3	D	1269	LYS
3	D	1278	ASP
3	D	1285	GLU
3	D	1302	GLU
3	D	1305	LEU
3	D	1308	ASP
3	D	1318	TYR
3	D	1335	LEU
3	D	1342	GLU
3	D	1356	TYR
3	D	1395	LEU
3	D	1421	LEU
3	D	1442	ASN
3	D	1443	THR
3	D	1448	THR
3	D	1462	LEU
3	D	1463	LYS
3	D	1472	ILE
3	D	1497	GLU

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Mol	Chain	Res	Type
3	D	1499	ARG
4	E	37	ASN
4	E	49	ARG
4	E	51	LEU
4	E	56	ASP
4	E	62	THR
4	E	79	LEU
5	F	97	ARG
5	F	108	LEU
5	F	109	LEU
5	F	137	LEU
5	F	153	THR
5	F	175	ASP
5	F	184	GLU
5	F	217	TYR
5	F	225	LEU
5	F	235	LEU
5	F	237	ARG
5	F	244	TYR
5	F	255	THR
5	F	268	ASP
5	F	271	ARG
5	F	279	MET
5	F	282	THR
5	F	291	ARG
5	F	293	LEU
5	F	294	GLN
5	F	319	VAL
5	F	322	THR
5	F	323	LEU
5	F	328	GLU
5	F	336	ILE
5	F	353	LEU
5	F	370	GLU
5	F	409	ARG
5	F	435	ASP
1	G	12	THR
1	G	28	LEU
1	G	32	PHE
1	G	36	LEU
1	G	44	LEU
1	G	51	THR

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Mol	Chain	Res	Type
1	G	54	THR
1	G	61	VAL
1	G	80	LEU
1	G	83	LYS
1	G	85	LEU
1	G	86	VAL
1	G	87	VAL
1	G	113	ASP
1	G	114	PHE
1	G	161	ARG
1	G	186	LEU
1	G	195	LEU
1	G	200	TRP
1	G	206	THR
1	G	209	GLU
1	G	213	GLN
1	G	227	ASN
1	H	19	HIS
1	H	20	TYR
1	H	23	PHE
1	H	30	ARG
1	H	36	LEU
1	H	41	ARG
1	H	51	THR
1	H	54	THR
1	H	58	ILE
1	H	62	LEU
1	H	68	ILE
1	H	74	ASP
1	H	75	VAL
1	H	80	LEU
1	H	100	ILE
1	H	110	ARG
1	H	114	PHE
1	H	162	ILE
1	H	170	ILE
1	H	177	VAL
1	H	186	LEU
1	H	193	ASP
1	H	195	LEU
1	H	215	VAL
1	H	222	LEU

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Mol	Chain	Res	Type
1	H	227	ASN
1	H	232	LEU
2	I	5	ARG
2	I	11	GLU
2	I	13	ILE
2	I	15	LEU
2	I	20	GLU
2	I	39	ARG
2	I	69	LEU
2	I	70	GLU
2	I	80	GLN
2	I	81	ASP
2	I	85	GLU
2	I	100	LEU
2	I	103	LYS
2	I	107	LEU
2	I	111	ASP
2	I	140	ILE
2	I	141	HIS
2	I	154	ARG
2	I	179	SER
2	I	194	VAL
2	I	195	LEU
2	I	196	LEU
2	I	198	ARG
2	I	207	LEU
2	I	209	ARG
2	I	217	LEU
2	I	219	GLN
2	I	230	ARG
2	I	242	LEU
2	I	246	ASP
2	I	261	LEU
2	I	274	ARG
2	I	285	LEU
2	I	292	ARG
2	I	297	GLU
2	I	304	LEU
2	I	317	VAL
2	I	322	VAL
2	I	344	PHE
2	I	361	MET

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Mol	Chain	Res	Type
2	I	367	LEU
2	I	374	ASN
2	I	376	ARG
2	I	393	GLN
2	I	394	PHE
2	I	396	ASP
2	I	410	ILE
2	I	421	GLU
2	I	426	ASP
2	I	428	ARG
2	I	430	VAL
2	I	433	THR
2	I	434	HIS
2	I	438	ILE
2	I	473	ARG
2	I	474	VAL
2	I	495	THR
2	I	516	ARG
2	I	543	ASN
2	I	579	VAL
2	I	610	ARG
2	I	620	LEU
2	I	622	GLU
2	I	647	GLN
2	I	680	ASP
2	I	683	ASN
2	I	689	VAL
2	I	690	ILE
2	I	695	LEU
2	I	703	ILE
2	I	713	ARG
2	I	716	LYS
2	I	717	LEU
2	I	729	LEU
2	I	761	PHE
2	I	784	ASP
2	I	788	THR
2	I	790	LEU
2	I	815	LEU
2	I	834	GLN
2	I	848	VAL
2	I	857	ASP

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Mol	Chain	Res	Type
2	I	861	LEU
2	I	863	ASP
2	I	867	VAL
2	I	869	VAL
2	I	871	LEU
2	I	872	ASN
2	I	876	VAL
2	I	887	GLU
2	I	890	LEU
2	I	896	PHE
2	I	900	ARG
2	I	934	PHE
2	I	950	LEU
2	I	953	VAL
2	I	963	LEU
2	I	968	ASP
2	I	972	VAL
2	I	994	ILE
2	I	1000	MET
2	I	1015	LEU
2	I	1026	GLN
2	I	1035	MET
2	I	1053	LEU
2	I	1063	ARG
2	I	1074	GLU
2	I	1088	LEU
2	I	1101	THR
2	I	1104	GLU
2	I	1113	GLU
3	J	16	GLU
3	J	25	GLU
3	J	32	ILE
3	J	47	GLU
3	J	62	LYS
3	J	68	PHE
3	J	69	GLU
3	J	92	HIS
3	J	103	TRP
3	J	104	PHE
3	J	115	LEU
3	J	118	LEU
3	J	124	GLU

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Mol	Chain	Res	Type
3	J	128	TYR
3	J	145	VAL
3	J	154	THR
3	J	155	ASP
3	J	166	GLN
3	J	180	LYS
3	J	196	VAL
3	J	198	ARG
3	J	204	LEU
3	J	344	ASP
3	J	347	VAL
3	J	355	VAL
3	J	371	ILE
3	J	387	LEU
3	J	393	ILE
3	J	400	VAL
3	J	407	VAL
3	J	410	THR
3	J	421	LEU
3	J	430	GLU
3	J	435	VAL
3	J	464	LEU
3	J	574	LEU
3	J	614	PHE
3	J	619	LEU
3	J	623	VAL
3	J	639	LEU
3	J	640	HIS
3	J	650	LEU
3	J	658	LEU
3	J	660	LYS
3	J	687	VAL
3	J	688	TRP
3	J	694	VAL
3	J	701	LEU
3	J	708	LEU
3	J	717	GLN
3	J	743	ASP
3	J	748	HIS
3	J	754	PHE
3	J	768	ASN
3	J	776	GLU

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Mol	Chain	Res	Type
3	J	780	LYS
3	J	789	LEU
3	J	795	VAL
3	J	817	GLU
3	J	833	GLU
3	J	861	GLN
3	J	863	VAL
3	J	865	THR
3	J	873	LEU
3	J	880	ILE
3	J	897	GLN
3	J	899	LEU
3	J	901	GLN
3	J	903	ASP
3	J	908	LYS
3	J	914	LEU
3	J	958	GLU
3	J	959	GLU
3	J	964	LEU
3	J	965	GLU
3	J	971	LEU
3	J	976	GLN
3	J	1015	TYR
3	J	1025	GLN
3	J	1078	ARG
3	J	1086	LEU
3	J	1094	LEU
3	J	1100	ASP
3	J	1122	LEU
3	J	1130	ARG
3	J	1132	LEU
3	J	1136	LYS
3	J	1137	ARG
3	J	1140	ILE
3	J	1144	LEU
3	J	1158	ARG
3	J	1160	LEU
3	J	1161	GLU
3	J	1184	ARG
3	J	1200	VAL
3	J	1213	ARG
3	J	1267	ARG

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Mol	Chain	Res	Type
3	J	1269	LYS
3	J	1278	ASP
3	J	1285	GLU
3	J	1302	GLU
3	J	1305	LEU
3	J	1308	ASP
3	J	1318	TYR
3	J	1335	LEU
3	J	1342	GLU
3	J	1356	TYR
3	J	1395	LEU
3	J	1421	LEU
3	J	1442	ASN
3	J	1443	THR
3	J	1448	THR
3	J	1462	LEU
3	J	1463	LYS
3	J	1472	ILE
3	J	1497	GLU
3	J	1499	ARG
4	K	37	ASN
4	K	49	ARG
4	K	51	LEU
4	K	56	ASP
4	K	62	THR
4	K	79	LEU
5	L	97	ARG
5	L	108	LEU
5	L	109	LEU
5	L	137	LEU
5	L	153	THR
5	L	175	ASP
5	L	184	GLU
5	L	217	TYR
5	L	225	LEU
5	L	235	LEU
5	L	237	ARG
5	L	244	TYR
5	L	255	THR
5	L	268	ASP
5	L	271	ARG
5	L	279	MET

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Mol	Chain	Res	Type
5	L	282	THR
5	L	291	ARG
5	L	293	LEU
5	L	294	GLN
5	L	319	VAL
5	L	322	THR
5	L	323	LEU
5	L	328	GLU
5	L	336	ILE
5	L	353	LEU
5	L	370	GLU
5	L	409	ARG
5	L	435	ASP
6	M	8	ASP
6	M	52	GLU
6	M	89	ARG
6	M	142	GLN
6	M	157	GLU
6	N	8	ASP
6	N	52	GLU
6	N	80	MET
6	N	142	GLN
6	N	157	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	213	GLN
1	B	63	HIS
1	B	81	ASN
1	B	213	GLN
2	C	80	GLN
2	C	99	GLN
2	C	187	ASN
2	C	374	ASN
2	C	434	HIS
2	C	498	GLN
2	C	538	GLN
2	C	565	GLN
2	C	647	GLN
2	C	683	ASN

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Mol	Chain	Res	Type
2	C	765	GLN
2	C	829	GLN
2	C	899	GLN
2	C	930	GLN
2	C	1026	GLN
2	C	1050	GLN
2	C	1093	GLN
2	C	1107	ASN
3	D	268	HIS
3	D	352	ASN
3	D	640	HIS
3	D	703	ASN
3	D	727	GLN
3	D	756	GLN
3	D	762	GLN
3	D	794	GLN
3	D	855	HIS
3	D	861	GLN
3	D	897	GLN
3	D	917	GLN
3	D	976	GLN
3	D	991	GLN
3	D	1195	GLN
3	D	1353	GLN
3	D	1374	GLN
3	D	1442	ASN
4	E	29	GLN
5	F	98	GLN
5	F	200	GLN
5	F	229	GLN
5	F	233	GLN
5	F	263	ASN
5	F	269	GLN
5	F	284	ASN
5	F	294	GLN
5	F	295	GLN
5	F	417	ASN
1	G	16	GLN
1	G	213	GLN
1	H	63	HIS
1	H	81	ASN
1	H	213	GLN

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Mol	Chain	Res	Type
2	I	80	GLN
2	I	99	GLN
2	I	187	ASN
2	I	374	ASN
2	I	434	HIS
2	I	498	GLN
2	I	565	GLN
2	I	647	GLN
2	I	683	ASN
2	I	765	GLN
2	I	899	GLN
2	I	930	GLN
2	I	999	HIS
2	I	1026	GLN
2	I	1050	GLN
2	I	1093	GLN
2	I	1107	ASN
3	J	166	GLN
3	J	362	GLN
3	J	703	ASN
3	J	727	GLN
3	J	756	GLN
3	J	762	GLN
3	J	794	GLN
3	J	855	HIS
3	J	861	GLN
3	J	897	GLN
3	J	906	GLN
3	J	917	GLN
3	J	976	GLN
3	J	991	GLN
3	J	1103	HIS
3	J	1195	GLN
3	J	1353	GLN
3	J	1374	GLN
3	J	1442	ASN
4	K	28	GLN
4	K	29	GLN
5	L	98	GLN
5	L	200	GLN
5	L	229	GLN
5	L	233	GLN

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Mol	Chain	Res	Type
5	L	263	ASN
5	L	269	GLN
5	L	294	GLN
5	L	295	GLN
5	L	417	ASN
6	M	55	HIS
6	M	101	ASN
6	M	142	GLN
6	N	101	ASN
6	N	142	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	Q	3/4 (75%)	2 (66%)	0
9	T	3/4 (75%)	0	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	Q	2	C
9	Q	3	G

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/314 (72%)	0.10	2 (0%) 81 66	144, 176, 208, 241	0
1	B	227/314 (72%)	0.03	2 (0%) 81 66	143, 164, 196, 228	0
1	G	227/314 (72%)	0.16	2 (0%) 81 66	148, 188, 218, 252	0
1	H	227/314 (72%)	0.04	0 100 100	145, 175, 207, 241	0
2	C	1117/1119 (99%)	0.17	16 (1%) 73 58	144, 172, 211, 253	0
2	I	1117/1119 (99%)	0.17	17 (1%) 71 56	144, 182, 221, 270	0
3	D	1490/1524 (97%)	0.13	13 (0%) 81 66	117, 162, 195, 251	0
3	J	1367/1524 (89%)	0.13	9 (0%) 84 70	120, 171, 204, 250	0
4	E	93/99 (93%)	0.37	4 (4%) 40 32	144, 165, 194, 217	0
4	K	93/99 (93%)	0.28	1 (1%) 77 62	144, 179, 206, 228	0
5	F	345/347 (99%)	0.17	9 (2%) 57 42	144, 179, 222, 245	0
5	L	345/347 (99%)	0.30	10 (2%) 54 40	145, 186, 225, 258	0
6	M	158/164 (96%)	0.35	5 (3%) 50 38	159, 207, 235, 243	0
6	N	158/164 (96%)	0.46	5 (3%) 50 38	171, 215, 240, 267	0
7	O	48/48 (100%)	0.27	0 100 100	157, 217, 256, 270	0
7	R	48/48 (100%)	0.19	0 100 100	163, 207, 251, 276	0
8	P	48/48 (100%)	0.33	0 100 100	161, 219, 260, 270	0
8	S	48/48 (100%)	0.36	0 100 100	161, 212, 250, 261	0
9	Q	4/4 (100%)	-0.18	0 100 100	175, 177, 186, 189	0
9	T	4/4 (100%)	-0.53	0 100 100	165, 183, 184, 196	0
All	All	7391/7962 (92%)	0.17	95 (1%) 74 59	117, 174, 219, 276	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	159	ILE	3.6
2	I	445	GLU	3.6
6	M	43	SER	3.5
6	N	160	GLY	3.4
2	I	207	LEU	3.4
5	L	223	SER	3.3
2	C	306	THR	3.3
2	I	101	ILE	3.2
5	F	223	SER	3.2
2	I	221	LEU	3.1
3	D	1097	LYS	3.0
3	J	436	GLU	3.0
4	E	24	ALA	3.0
5	F	194	GLU	2.9
2	I	306	THR	2.9
6	N	19	VAL	2.9
2	I	1080	SER	2.9
5	F	341	ASP	2.8
4	E	94	PRO	2.8
3	D	1486	VAL	2.7
2	I	628	TYR	2.7
2	C	489	SER	2.7
2	C	549	PHE	2.7
1	G	13	ALA	2.7
2	C	358	ARG	2.7
3	D	513	ILE	2.6
5	L	346	ASP	2.6
5	L	338	ASP	2.6
3	J	1195	GLN	2.6
2	C	679	PHE	2.6
2	C	201	GLY	2.6
2	I	166	PRO	2.6
4	K	2	ALA	2.5
2	I	570	PRO	2.5
1	G	170	ILE	2.5
6	M	72	LEU	2.5
5	F	170	THR	2.5
6	N	27	SER	2.5
2	I	319	GLY	2.4
2	C	58	ASP	2.4
2	C	246	ASP	2.4
5	F	162	LEU	2.4
5	L	207	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	E	2	ALA	2.4
3	D	538	SER	2.4
3	D	1263	PHE	2.4
6	M	147	THR	2.4
5	L	170	THR	2.4
5	F	346	ASP	2.4
1	B	150	TYR	2.3
2	C	890	LEU	2.3
5	F	155	ARG	2.3
2	I	222	LEU	2.3
3	J	593	ASN	2.3
5	L	161	GLY	2.3
2	C	663	GLU	2.3
5	L	406	GLY	2.3
3	D	919	PHE	2.3
3	J	563	PRO	2.3
2	C	123	GLU	2.3
5	L	194	GLU	2.2
3	J	1263	PHE	2.2
3	J	459	GLU	2.2
5	L	416	GLU	2.2
6	M	160	GLY	2.2
2	I	1026	GLN	2.2
3	J	34	TYR	2.2
1	A	62	LEU	2.2
2	I	567	GLN	2.2
2	I	246	ASP	2.2
3	D	1484	THR	2.1
5	L	268	ASP	2.1
1	A	56	VAL	2.1
2	I	296	GLY	2.1
6	M	27	SER	2.1
2	I	254	LEU	2.1
3	D	287	GLY	2.1
3	D	1144	LEU	2.1
6	N	29	SER	2.1
2	C	366	THR	2.1
3	J	1398	TRP	2.1
6	N	24	ALA	2.1
2	C	370	ALA	2.1
3	J	1235	GLN	2.1
5	F	224	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	194	VAL	2.0
3	D	648	MET	2.0
3	D	666	PHE	2.0
4	E	10	PHE	2.0
2	I	272	ALA	2.0
2	C	901	TYR	2.0
3	D	916	TYR	2.0
1	B	233	LEU	2.0
2	C	62	GLY	2.0
3	D	1062	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	MG	D	2003	1/1	0.83	0.08	283,283,283,283	0
11	MG	J	2003	1/1	0.92	0.06	270,270,270,270	0
10	ZN	J	2001	1/1	0.98	0.09	277,277,277,277	0
10	ZN	D	2002	1/1	0.99	0.07	237,237,237,237	0
10	ZN	J	2002	1/1	0.99	0.03	157,157,157,157	0
10	ZN	D	2001	1/1	1.00	0.06	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.