Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 06:57 PM JST

PDB ID	:	8H9S / pdb_00008h9s
EMDB ID	:	EMD-34580
Title	:	Human ATP synthase state 1 (combined)
Authors	:	Lai, Y.; Zhang, Y.; Liu, F.; Gao, Y.; Gong, H.; Rao, Z.
Deposited on	:	2022-10-25
Resolution	:	2.53 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

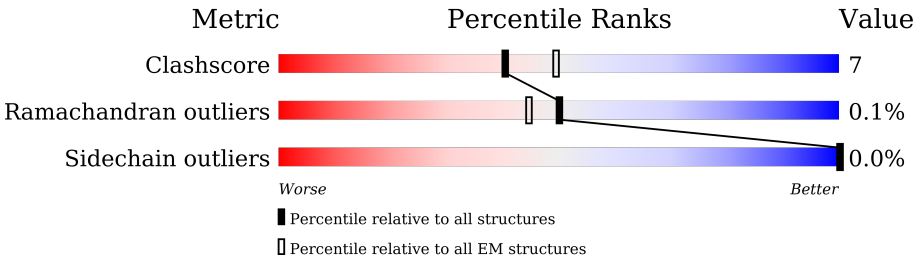
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	K	214	70% 23% 7%
2	L	108	13% 45% 17% 38%
3	M	160	76% 22%
4	A	510	86% 13%
4	B	510	80% 13% 6%
4	C	510	80% 15% 5%
5	D	482	80% 17%
5	E	482	78% 17% 5%

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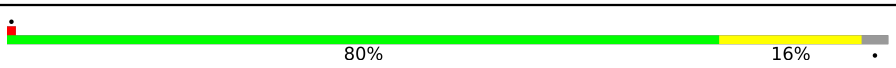
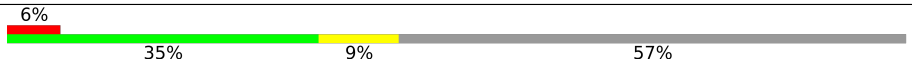
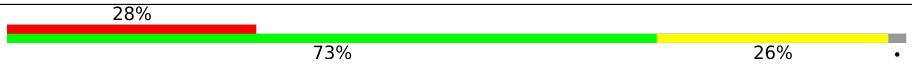
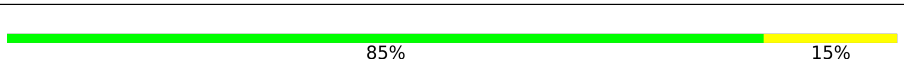
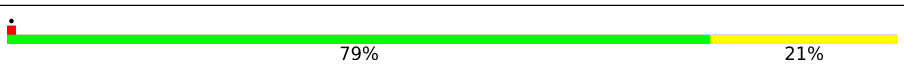
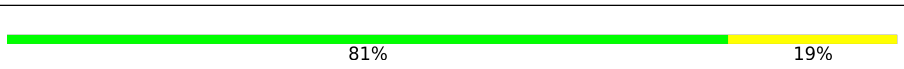
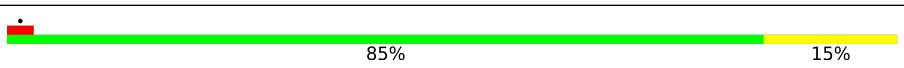
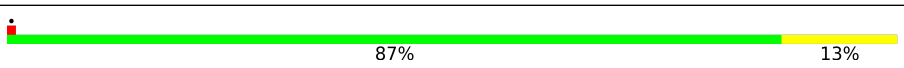
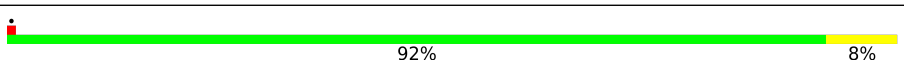
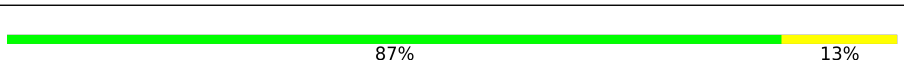
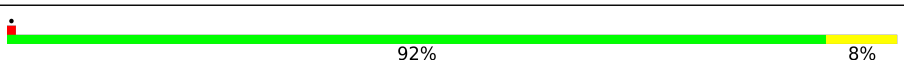
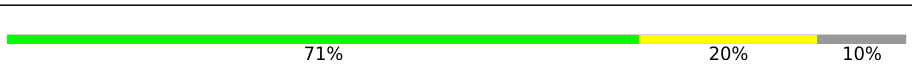
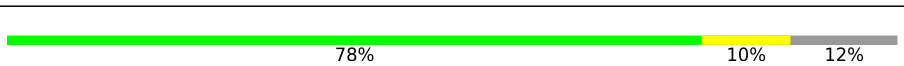
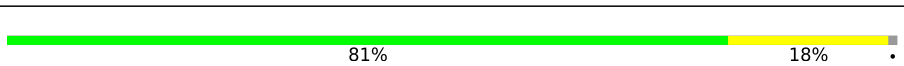
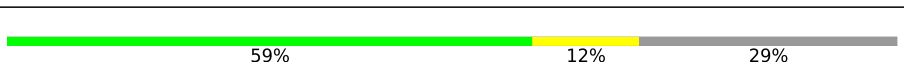
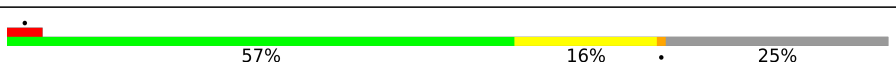
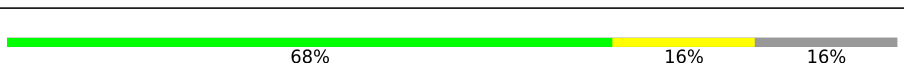
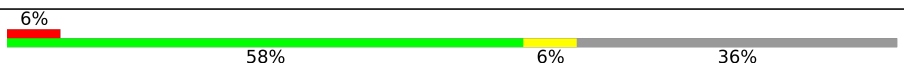
Mol	Chain	Length	Quality of chain
5	F	482	
6	G	273	
7	J	81	
8	O	190	
9	1	75	
9	2	75	
9	3	75	
9	4	75	
9	5	75	
9	6	75	
9	7	75	
9	8	75	
10	H	146	
11	I	51	
12	N	226	
13	P	58	
14	Q	68	
15	R	93	
16	S	102	
17	T	69	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 38930 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	198	Total	C	N	O	S	0	0
			1573	1013	270	285	5		

- Molecule 2 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	67	Total	C	N	O	S	0	0
			549	350	91	106	2		

- Molecule 3 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	156	Total	C	N	O	S	0	0
			1259	813	199	243	4		

- Molecule 4 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	503	Total	C	N	O	S	0	0
			3830	2410	675	732	13		
4	B	477	Total	C	N	O	S	0	0
			3639	2290	645	692	12		
4	C	487	Total	C	N	O	S	0	0
			3714	2338	656	707	13		

- Molecule 5 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	456	Total	C	N	O	S	0	0
			3458	2192	588	666	12		
5	F	466	Total	C	N	O	S	0	0
			3529	2238	598	680	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	470	Total	C	N	O	S	0	0
			3562	2257	604	688	13		

- Molecule 6 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	271	Total	C	N	O	S	0	0
			2103	1329	359	406	9		

- Molecule 7 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	35	Total	C	N	O	0	0
			270	163	54	53		

- Molecule 8 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	187	Total	C	N	O	S	0	0
			1437	909	252	270	6		

- Molecule 9 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
9	2	75	Total	C	N	O	S	1	0
			542	358	86	94	4		
9	3	75	Total	C	N	O	S	1	0
			542	358	86	94	4		
9	4	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
9	5	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
9	6	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
9	7	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
9	8	75	Total	C	N	O	S	0	0
			534	353	83	94	4		

- Molecule 10 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	132	Total	C	N	O	S	0	0
			975	614	164	195	2		

- Molecule 11 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	45	Total	C	N	O	S	0	0
			354	225	64	64	1		

- Molecule 12 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	223	Total	C	N	O	S	0	0
			1718	1145	273	289	11		

- Molecule 13 is a protein called ATP synthase subunit ATP5MJ, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	41	Total	C	N	O	S	0	0
			344	234	53	54	3		

- Molecule 14 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	51	Total	C	N	O	S	0	0
			422	281	67	68	6		

- Molecule 15 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	78	Total	C	N	O	S	0	0
			655	435	110	107	3		

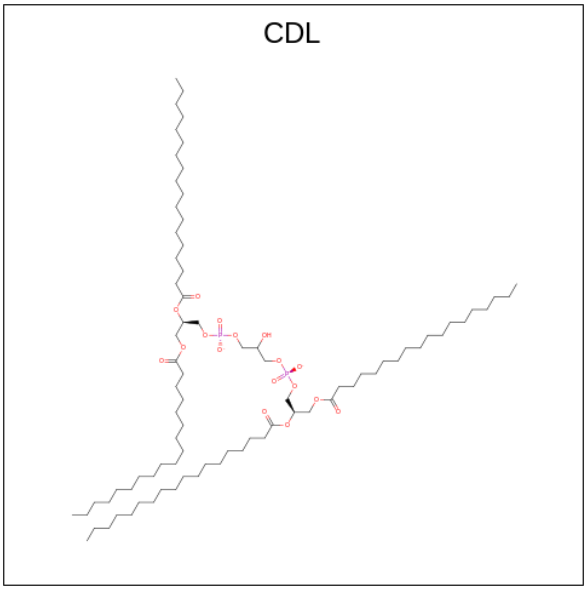
- Molecule 16 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	77	Total	C	N	O	S	0	0
			605	401	96	107	1		

- Molecule 17 is a protein called ATP synthase subunit e, mitochondrial.

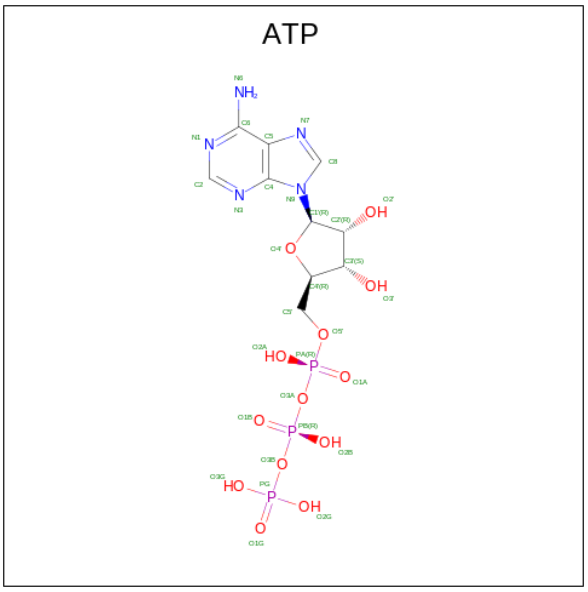
Mol	Chain	Residues	Atoms				AltConf	Trace
17	T	44	Total	C	N	O	0	0
			346	224	63	59		

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
18	K	1	Total	C	O	P	0
			72	53	17	2	
18	R	1	Total	C	O	P	0
			49	30	17	2	

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

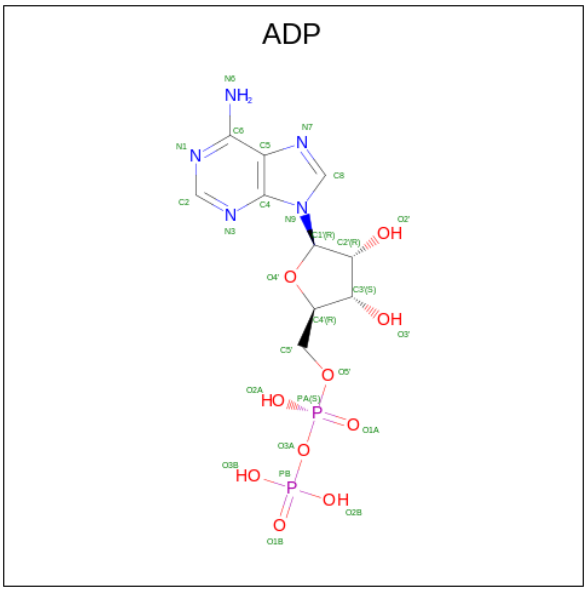


Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

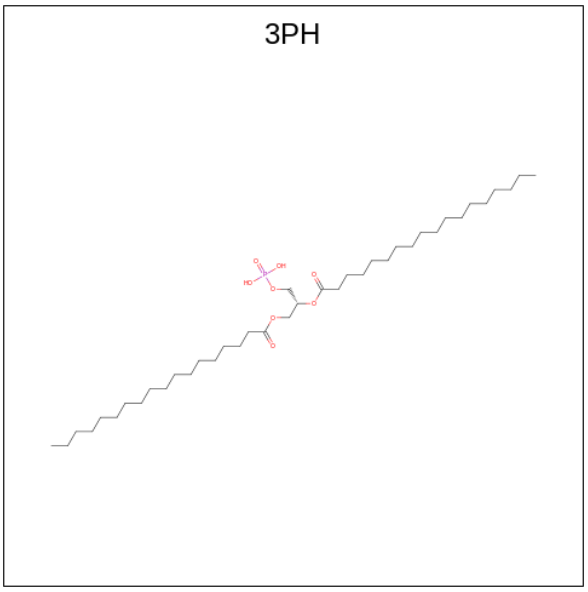
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Mg	0
			1	1	
20	B	1	Total	Mg	0
			1	1	
20	C	1	Total	Mg	0
			1	1	
20	F	1	Total	Mg	0
			1	1	
20	D	1	Total	Mg	0
			1	1	

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
21	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 22 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



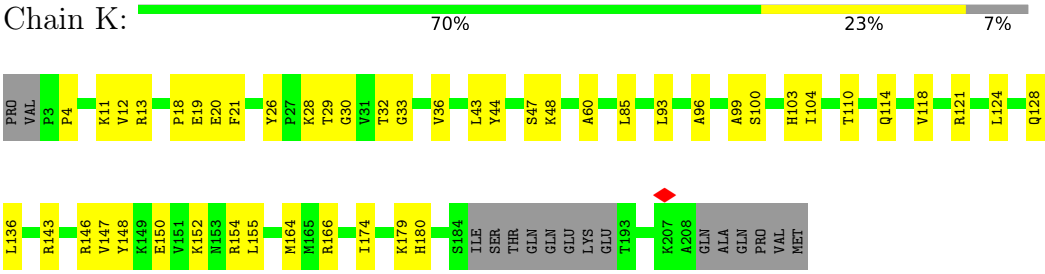
Mol	Chain	Residues	Atoms				AltConf
22	Q	1	Total	C	O	P	0
			27	18	8	1	

3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

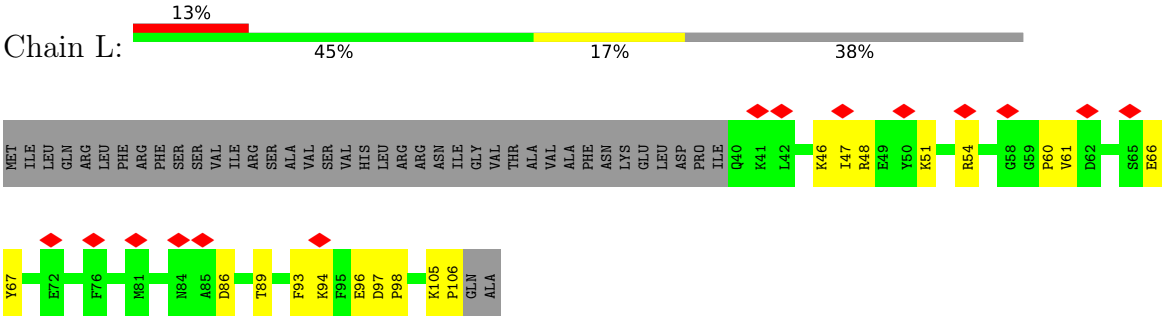
• Molecule 1: ATP synthase F(0) complex subunit B1, mitochondrial

Chain K:



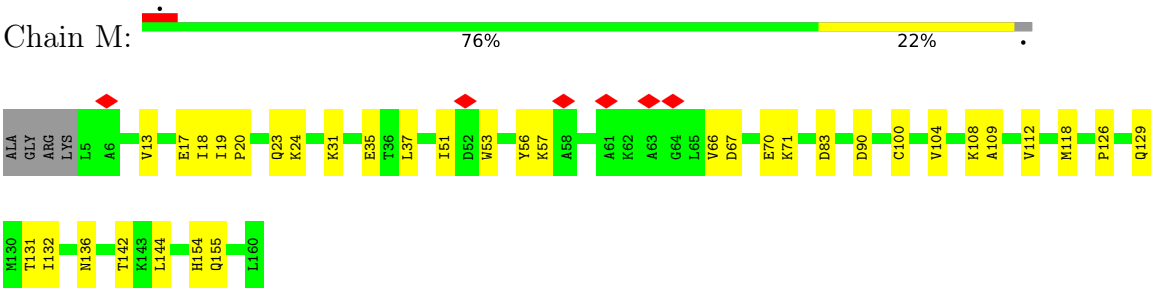
• Molecule 2: ATP synthase-coupling factor 6, mitochondrial

Chain L:



• Molecule 3: ATP synthase subunit d, mitochondrial

Chain M:

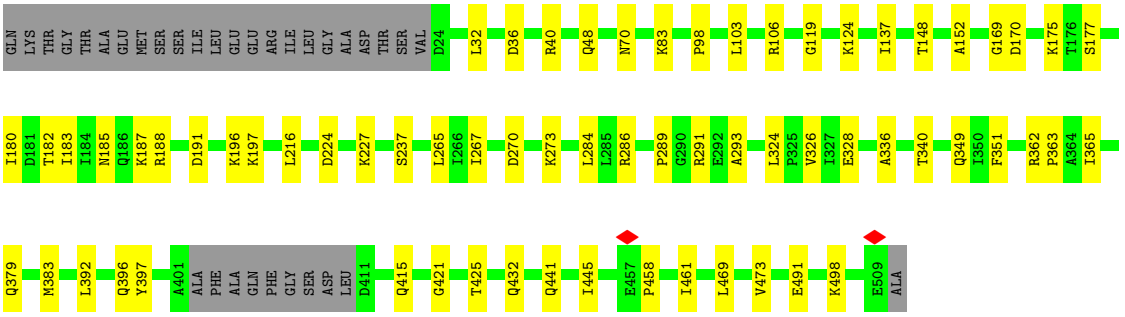


• Molecule 4: ATP synthase subunit alpha, mitochondrial

Chain A:

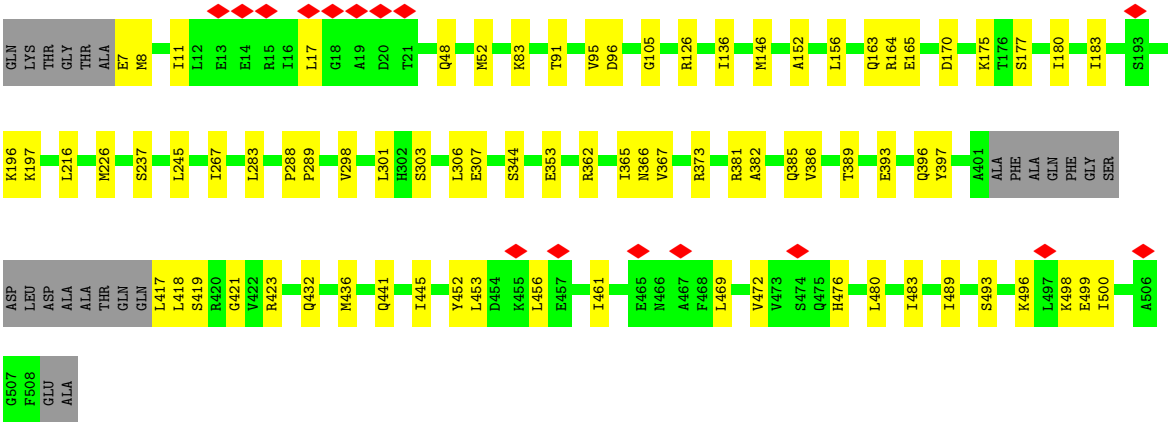
• Molecule 4: ATP synthase subunit alpha, mitochondrial

Chain B:



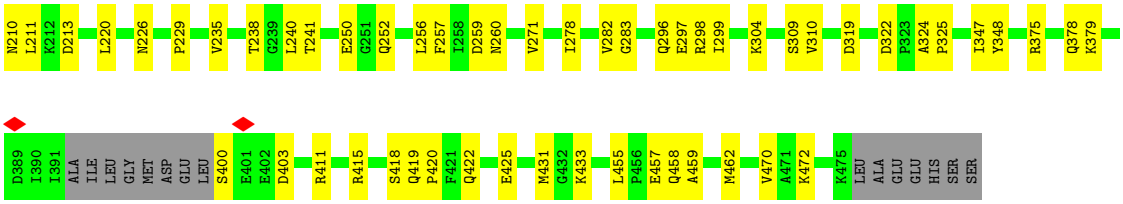
• Molecule 4: ATP synthase subunit alpha, mitochondrial

Chain C:

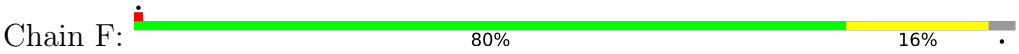


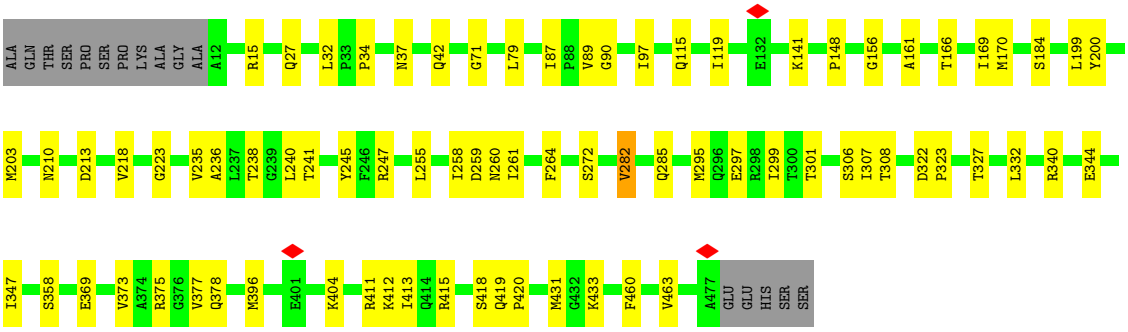
• Molecule 5: ATP synthase subunit beta, mitochondrial

Chain E:

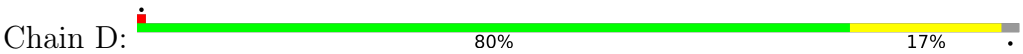


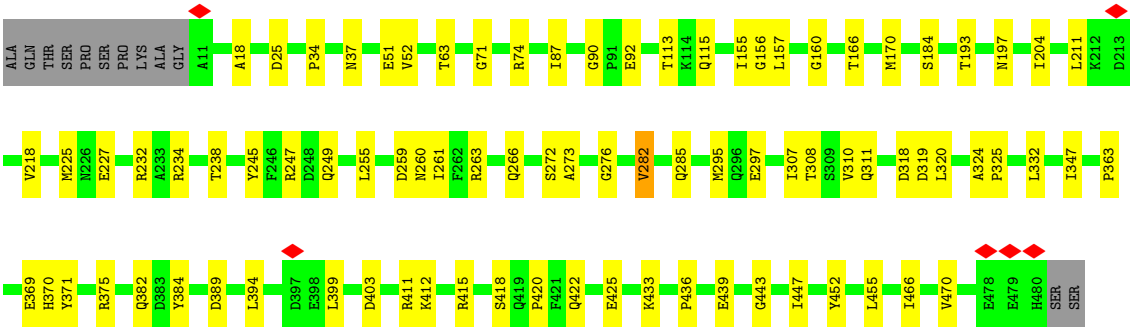
• Molecule 5: ATP synthase subunit beta, mitochondrial



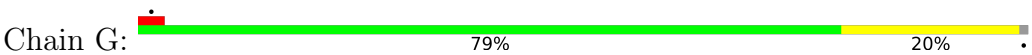


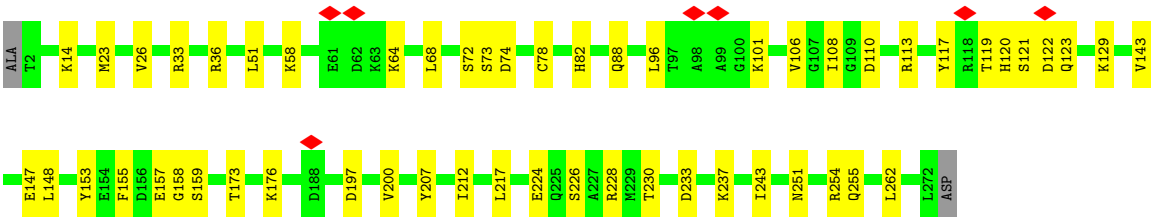
• Molecule 5: ATP synthase subunit beta, mitochondrial



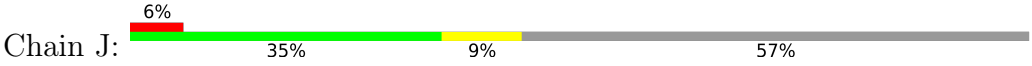


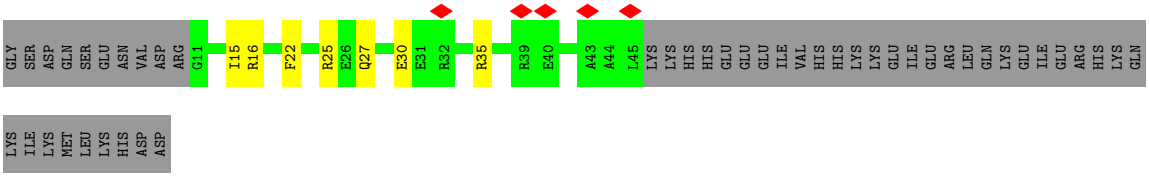
• Molecule 6: ATP synthase subunit gamma, mitochondrial





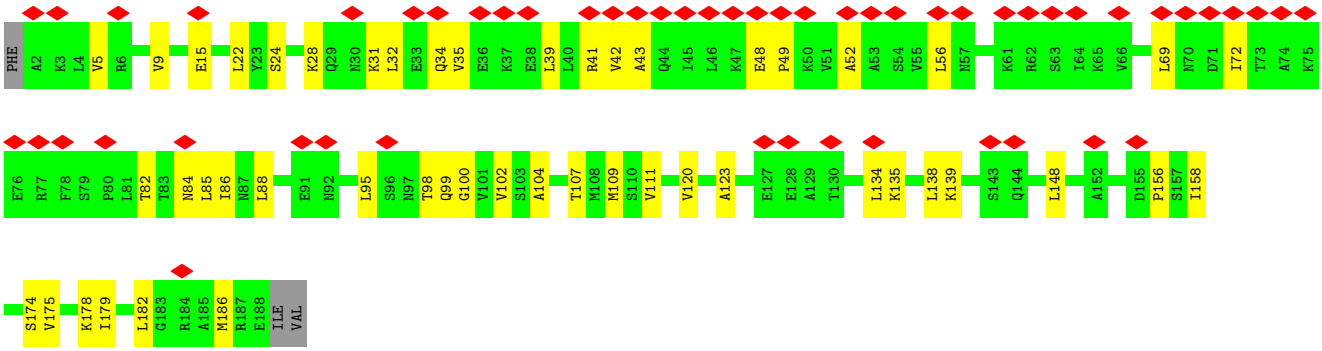
• Molecule 7: ATPase inhibitor, mitochondrial





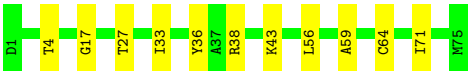
• Molecule 8: ATP synthase subunit O, mitochondrial

Chain O:



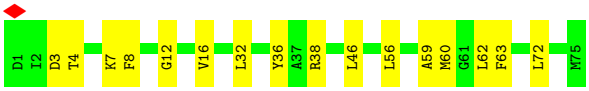
• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 1:



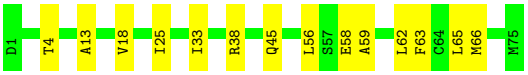
• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 2:



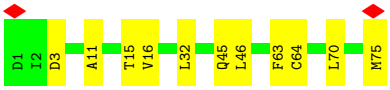
• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 3:



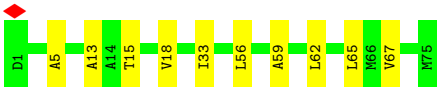
• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 4:



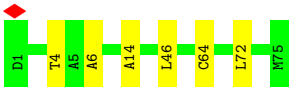
• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 5:



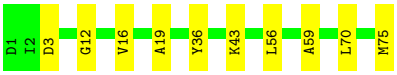
• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 6:



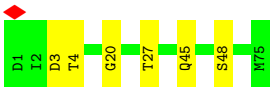
• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 7:



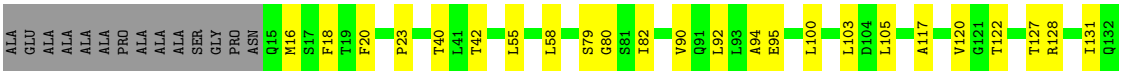
• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

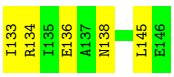
Chain 8:



• Molecule 10: ATP synthase subunit delta, mitochondrial

Chain H:



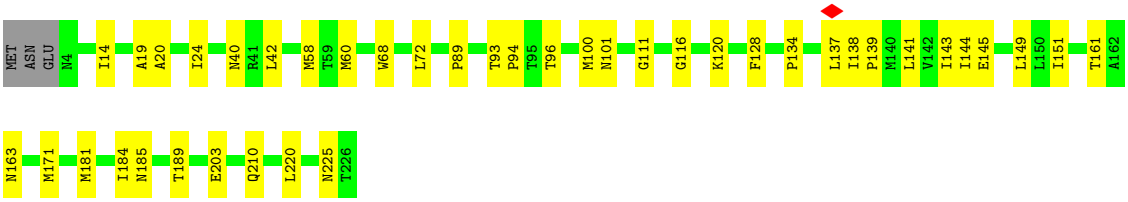


• Molecule 11: ATP synthase subunit epsilon, mitochondrial

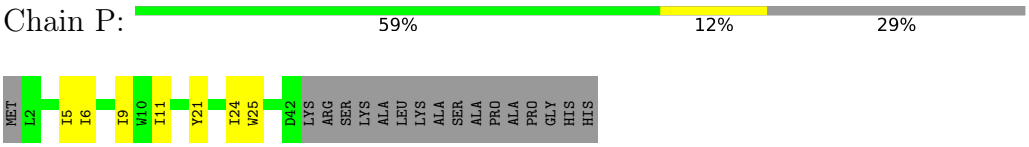
Chain I:

• Molecule 12: ATP synthase subunit a

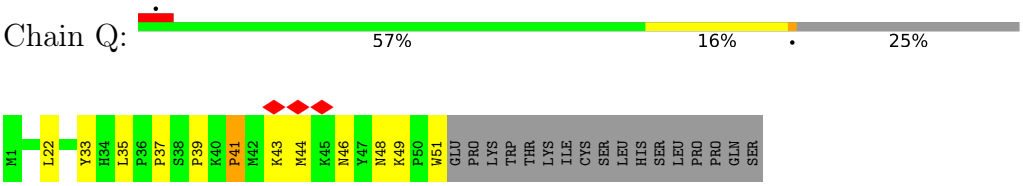
Chain N:



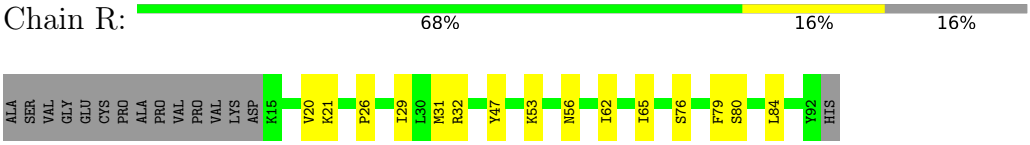
• Molecule 13: ATP synthase subunit ATP5MJ, mitochondrial



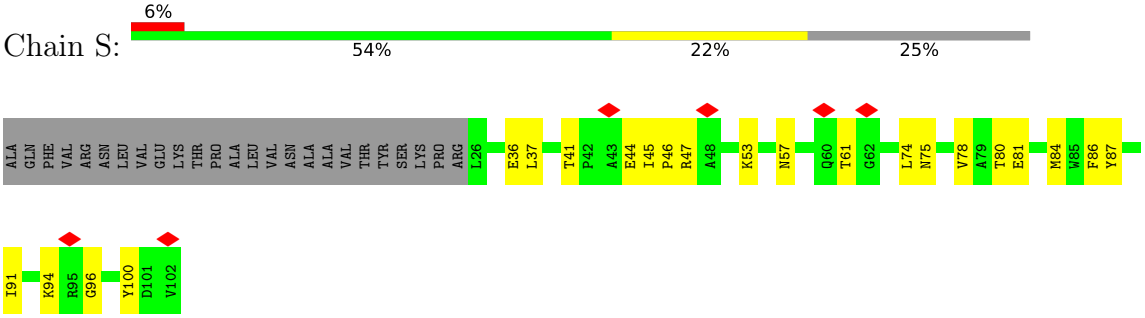
• Molecule 14: ATP synthase protein 8



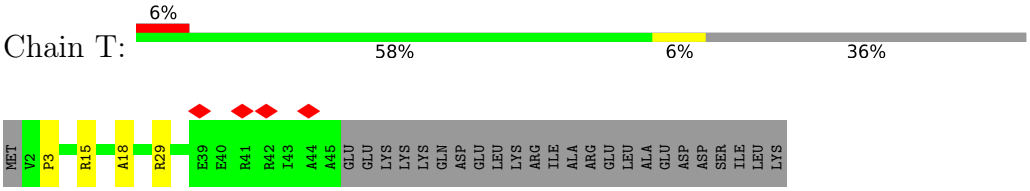
• Molecule 15: ATP synthase subunit f, mitochondrial



• Molecule 16: ATP synthase subunit g, mitochondrial



• Molecule 17: ATP synthase subunit e, mitochondrial



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68388	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	40.374	Depositor
Minimum map value	-24.867	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.095	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PH, ATP, MG, ADP

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	K	0.23	0/1605	0.35	0/2169
2	L	0.16	0/560	0.40	0/748
3	M	0.20	0/1291	0.33	0/1755
4	A	0.21	0/3880	0.33	0/5233
4	B	0.22	0/3687	0.33	0/4973
4	C	0.21	0/3762	0.34	0/5073
5	D	0.23	0/3621	0.36	0/4911
5	E	0.25	0/3515	0.37	0/4766
5	F	0.26	0/3587	0.36	0/4865
6	G	0.21	0/2129	0.32	0/2860
7	J	0.15	0/272	0.35	0/359
8	O	0.14	0/1453	0.35	0/1958
9	1	0.27	0/543	0.55	1/732 (0.1%)
9	2	0.24	0/554	0.38	0/746
9	3	0.25	0/554	0.35	0/746
9	4	0.23	0/543	0.32	0/732
9	5	0.23	0/543	0.34	0/732
9	6	0.25	0/543	0.35	0/732
9	7	0.25	0/543	0.35	0/732
9	8	0.24	0/543	0.35	0/732
10	H	0.29	0/987	0.43	0/1344
11	I	0.25	0/359	0.36	0/482
12	N	0.28	0/1755	0.38	0/2403
13	P	0.24	0/354	0.35	0/478
14	Q	0.46	0/437	0.63	1/598 (0.2%)
15	R	0.25	0/674	0.43	0/902
16	S	0.18	0/619	0.35	0/841
17	T	0.19	0/354	0.37	0/480
All	All	0.23	0/39267	0.36	2/53082 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	71	ILE	N-CA-C	-11.65	102.64	113.71
14	Q	41	PRO	N-CA-C	-5.79	107.11	114.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	K	1573	0	1552	52	0
2	L	549	0	533	15	0
3	M	1259	0	1238	31	0
4	A	3830	0	3928	42	0
4	B	3639	0	3741	43	0
4	C	3714	0	3825	51	0
5	D	3562	0	3609	53	0
5	E	3458	0	3508	50	0
5	F	3529	0	3584	53	0
6	G	2103	0	2174	38	0
7	J	270	0	257	5	0
8	O	1437	0	1536	30	0
9	1	534	0	553	8	0
9	2	542	0	566	15	0
9	3	542	0	566	15	0
9	4	534	0	553	11	0
9	5	534	0	553	9	0
9	6	534	0	553	6	0
9	7	534	0	553	9	0
9	8	534	0	553	5	0
10	H	975	0	979	17	0
11	I	354	0	364	5	0
12	N	1718	0	1879	27	0
13	P	344	0	361	6	0
14	Q	422	0	450	18	0
15	R	655	0	666	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	S	605	0	631	17	0
17	T	346	0	355	4	0
18	K	72	0	91	5	0
18	R	49	0	42	3	0
19	A	31	0	12	0	0
19	B	31	0	12	0	0
19	C	31	0	12	0	0
20	A	1	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	D	1	0	0	0	0
20	F	1	0	0	0	0
21	D	27	0	12	1	0
21	F	27	0	12	0	0
22	Q	27	0	27	1	0
All	All	38930	0	39840	538	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 7.

All (538) 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)
1:K:103:HIS:HB2	14:Q:41:PRO:HA	1.52	0.92
10:H:40:THR:HG22	10:H:42:THR:H	1.36	0.87
9:2:38[A]:ARG:HH11	9:3:38[A]:ARG:HH22	1.28	0.80
12:N:116:GLY:HA3	12:N:225:ASN:HD22	1.48	0.79
4:A:95:VAL:HG11	4:A:245:LEU:HD21	1.70	0.74
5:F:170:MET:HE1	5:F:199:LEU:HD13	1.70	0.72
9:6:72:LEU:HD21	9:7:75:MET:HE1	1.74	0.70
4:A:185:ASN:OD1	4:A:188:ARG:NH1	2.23	0.70
4:B:291:ARG:NH1	5:F:322:ASP:OD1	2.25	0.70
8:O:9:VAL:HB	8:O:111:VAL:HG11	1.74	0.69
8:O:39:LEU:HD12	8:O:102:VAL:HG22	1.73	0.69
6:G:78:CYS:SG	6:G:228:ARG:NH2	2.66	0.69
5:E:375:ARG:NH1	5:E:378:GLN:OE1	2.27	0.68
4:B:185:ASN:OD1	4:B:188:ARG:NH1	2.25	0.68
4:A:307:GLU:HG3	5:E:226:ASN:HB3	1.76	0.67
18:K:301:CDL:HB62	15:R:62:ILE:HB	1.77	0.67
1:K:104:ILE:HG13	3:M:118:MET:HE2	1.78	0.66
2:L:54:ARG:HA	4:C:8:MET:HE1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:121:ARG:NH1	3:M:18:ILE:O	2.29	0.66
12:N:184:ILE:HG22	12:N:185:ASN:H	1.60	0.66
16:S:86:PHE:HB2	17:T:18:ALA:HB1	1.77	0.66
5:E:348:TYR:HB2	5:E:462:MET:HE1	1.77	0.66
1:K:143:ARG:NH2	2:L:96:GLU:O	2.27	0.65
3:M:131:THR:HG22	3:M:132:ILE:H	1.61	0.65
4:A:407:GLY:HA2	4:A:410:LEU:HD12	1.78	0.65
5:D:422:GLN:NE2	5:D:425:GLU:OE1	2.29	0.65
6:G:106:VAL:HG21	6:G:148:LEU:HD21	1.79	0.64
8:O:15:GLU:HG2	8:O:100:GLY:HA3	1.78	0.64
12:N:134:PRO:HG2	12:N:137:LEU:HD12	1.80	0.63
6:G:119:THR:HG23	6:G:120:HIS:HD2	1.63	0.63
12:N:68:TRP:CH2	13:P:24:ILE:HD11	2.33	0.63
1:K:148:TYR:HE1	3:M:51:ILE:HG12	1.62	0.63
4:C:381:ARG:HG3	4:C:385:GLN:HE21	1.63	0.63
3:M:53:TRP:O	3:M:57:LYS:N	2.31	0.62
1:K:174:ILE:HG12	8:O:186:MET:HE2	1.82	0.62
5:E:198:ASP:O	5:E:202:GLU:HG3	1.99	0.62
5:D:227:GLU:O	5:D:232:ARG:NH1	2.33	0.62
4:C:373:ARG:NH2	21:D:501:ADP:O3B	2.33	0.62
8:O:138:LEU:HB3	8:O:148:LEU:HD21	1.81	0.61
1:K:154:ARG:NH1	2:L:89:THR:O	2.33	0.61
1:K:166:ARG:NH2	4:C:7:GLU:OE1	2.33	0.61
1:K:11:LYS:HB3	1:K:19:GLU:HG3	1.81	0.61
5:D:411:ARG:O	5:D:415:ARG:HG2	2.00	0.61
12:N:58:MET:HE3	12:N:72:LEU:HD12	1.80	0.61
1:K:93:LEU:HD23	14:Q:37:PRO:HG3	1.82	0.61
4:C:177:SER:OG	4:C:432:GLN:NE2	2.34	0.61
5:E:411:ARG:NE	5:E:457:GLU:OE2	2.24	0.61
4:B:83:LYS:HD3	5:E:34:PRO:HG3	1.83	0.61
5:F:301:THR:HG23	5:F:306:SER:HA	1.82	0.60
5:E:319:ASP:OD2	6:G:255:GLN:NE2	2.31	0.60
4:B:187:LYS:HE2	4:B:224:ASP:HB3	1.83	0.60
5:E:15:ARG:NH1	5:E:27:GLN:OE1	2.35	0.60
5:D:347:ILE:HG23	5:D:418:SER:HB3	1.83	0.60
5:F:87:ILE:HD13	5:F:238:THR:HG23	1.84	0.60
6:G:33:ARG:HG2	6:G:36:ARG:HH21	1.66	0.59
5:F:375:ARG:NH1	5:F:378:GLN:OE1	2.35	0.59
5:D:92:GLU:HB2	5:D:113:THR:HG22	1.85	0.59
5:D:412:LYS:NZ	5:D:455:LEU:O	2.31	0.59
8:O:82:THR:O	8:O:86:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:13:GLU:HG3	8:O:24:SER:HB3	1.82	0.59
5:F:411:ARG:O	5:F:415:ARG:HG2	2.01	0.59
5:D:255:LEU:HD23	5:D:308:THR:HB	1.84	0.59
4:A:440:GLU:HB3	4:A:469:LEU:HD11	1.84	0.59
5:D:155:ILE:HD12	5:D:310:VAL:HG22	1.85	0.59
4:A:12:LEU:HD22	8:O:88:LEU:HD21	1.83	0.59
5:E:210:ASN:ND2	5:E:213:ASP:OD2	2.36	0.59
9:4:15:THR:HG21	9:5:67:VAL:HG11	1.85	0.59
1:K:103:HIS:HD1	14:Q:41:PRO:C	2.11	0.59
9:3:65:LEU:HD11	9:4:63:PHE:HB3	1.85	0.58
8:O:158:ILE:HB	8:O:174:SER:HB2	1.85	0.58
9:1:56:LEU:O	9:1:59:ALA:HB3	2.04	0.58
4:B:187:LYS:NZ	4:B:191:ASP:OD2	2.36	0.58
1:K:96:ALA:HA	14:Q:39:PRO:HG3	1.85	0.58
4:C:362:ARG:HH12	5:F:375:ARG:HE	1.51	0.58
4:C:288:PRO:HB2	5:D:273:ALA:HB1	1.86	0.58
14:Q:49:LYS:O	14:Q:51:TRP:N	2.36	0.58
3:M:53:TRP:NE1	3:M:70:GLU:OE1	2.37	0.57
5:D:115:GLN:NE2	5:D:245:TYR:OH	2.37	0.57
9:2:60:MET:O	9:2:63:PHE:HB2	2.03	0.57
5:F:419:GLN:NE2	5:F:433:LYS:O	2.37	0.57
5:E:98:MET:HE3	5:E:102:GLY:HA2	1.86	0.57
5:E:419:GLN:NE2	5:E:433:LYS:O	2.35	0.57
4:B:106:ARG:NH2	4:B:119:GLY:O	2.36	0.57
5:F:258:ILE:HG21	5:F:261:ILE:HD13	1.87	0.57
4:C:353:GLU:OE2	4:C:366:ASN:ND2	2.38	0.57
14:Q:48:ASN:ND2	14:Q:51:TRP:O	2.38	0.57
5:F:199:LEU:HD11	5:F:203:MET:HE3	1.86	0.56
4:C:453:LEU:HD13	4:C:456:LEU:HD12	1.86	0.56
5:D:412:LYS:NZ	5:D:452:TYR:O	2.38	0.56
4:A:286:ARG:NH2	5:D:276:GLY:O	2.39	0.56
1:K:152:LYS:HE3	3:M:51:ILE:HG13	1.88	0.56
12:N:171:MET:HE2	12:N:203:GLU:HG3	1.86	0.56
5:D:34:PRO:HD2	5:D:37:ASN:ND2	2.21	0.56
10:H:16:MET:HE3	10:H:90:VAL:HG21	1.88	0.56
5:E:411:ARG:O	5:E:415:ARG:HG2	2.06	0.56
1:K:146:ARG:O	1:K:150:GLU:HG2	2.06	0.55
5:E:240:LEU:HD21	5:E:298:ARG:HB2	1.86	0.55
5:D:394:LEU:HD21	6:G:23:MET:HG3	1.88	0.55
4:C:496:LYS:O	4:C:500:ILE:HG13	2.05	0.55
1:K:147:VAL:HG23	2:L:93:PHE:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:250:GLU:OE1	5:E:252:GLN:NE2	2.40	0.55
4:A:15:ARG:O	8:O:84:ASN:ND2	2.39	0.55
4:C:170:ASP:O	4:C:175:LYS:NZ	2.40	0.55
4:C:417:LEU:HG	4:C:418:LEU:H	1.72	0.55
12:N:42:LEU:HD13	15:R:65:ILE:HD11	1.89	0.55
4:A:52:MET:HG2	4:A:95:VAL:HG22	1.89	0.54
4:A:186:GLN:O	4:A:190:ASN:ND2	2.35	0.54
4:B:36:ASP:HB3	4:B:284:LEU:HB3	1.89	0.54
8:O:69:LEU:HA	8:O:72:ILE:HG22	1.88	0.54
8:O:175:VAL:O	8:O:179:ILE:HG13	2.07	0.54
3:M:144:LEU:HD12	14:Q:35:LEU:HD13	1.90	0.54
18:K:301:CDL:HA62	18:K:301:CDL:C11	2.38	0.54
9:4:11:ALA:O	9:4:15:THR:HG23	2.07	0.54
18:K:301:CDL:HA62	18:K:301:CDL:H112	1.89	0.54
2:L:97:ASP:OD1	2:L:98:PRO:HD2	2.08	0.54
12:N:128:PHE:HA	12:N:145:GLU:HG2	1.89	0.54
5:D:204:ILE:HD13	5:D:211:LEU:HD11	1.89	0.54
5:F:34:PRO:HD2	5:F:37:ASN:ND2	2.23	0.54
1:K:43:LEU:O	1:K:47:SER:HB3	2.08	0.53
1:K:103:HIS:CB	14:Q:41:PRO:HA	2.31	0.53
3:M:126:PRO:HG2	3:M:129:GLN:OE1	2.09	0.53
5:F:415:ARG:O	5:F:418:SER:OG	2.26	0.53
18:R:101:CDL:HB32	18:R:101:CDL:HB22	1.91	0.53
5:F:15:ARG:NH1	5:F:27:GLN:OE1	2.41	0.53
5:F:161:ALA:O	5:F:340:ARG:NH2	2.38	0.53
13:P:9:ILE:HG23	14:Q:22:LEU:HD11	1.91	0.53
1:K:100:SER:O	1:K:104:ILE:HG12	2.09	0.53
5:F:236:ALA:O	5:F:240:LEU:HG	2.09	0.53
10:H:134:ARG:O	10:H:138:ASN:ND2	2.40	0.53
5:E:322:ASP:HB3	5:E:325:PRO:HD2	1.91	0.53
5:F:240:LEU:HD22	5:F:299:ILE:HG12	1.91	0.53
6:G:143:VAL:O	6:G:147:GLU:HG2	2.08	0.53
16:S:81:GLU:OE2	17:T:15:ARG:NH2	2.39	0.53
9:5:33:ILE:HG23	9:6:46:LEU:HD22	1.90	0.53
5:E:283:GLY:CA	6:G:262:LEU:HD11	2.39	0.53
5:F:255:LEU:HD23	5:F:308:THR:HB	1.90	0.53
4:B:289:PRO:HB2	4:B:293:ALA:HA	1.90	0.53
1:K:110:THR:O	1:K:114:GLN:HG2	2.09	0.52
1:K:134:MET:HE3	3:M:37:LEU:HB2	1.91	0.52
4:A:163:GLN:NE2	4:A:165:GLU:OE2	2.42	0.52
4:A:244:TYR:HE1	4:A:301:LEU:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:ILE:HG21	5:E:238:THR:HG23	1.92	0.52
3:M:67:ASP:OD1	3:M:71:LYS:HE2	2.09	0.52
4:A:237:SER:HB3	5:D:297:GLU:HG3	1.91	0.52
2:L:105:LYS:NZ	2:L:106:PRO:O	2.39	0.52
4:B:421:GLY:O	4:B:425:THR:HG23	2.09	0.52
4:C:303:SER:HB2	5:D:225:MET:HB3	1.91	0.52
8:O:43:ALA:HB1	8:O:99:GLN:HE22	1.74	0.52
9:7:56:LEU:O	9:7:59:ALA:HB3	2.10	0.52
4:C:423:ARG:HD2	4:C:461:ILE:HD11	1.91	0.52
13:P:21:TYR:O	13:P:25:TRP:HD1	1.92	0.52
4:B:170:ASP:O	4:B:175:LYS:NZ	2.42	0.52
1:K:154:ARG:NH1	2:L:86:ASP:O	2.43	0.52
5:D:184:SER:HB3	5:D:218:VAL:HG22	1.91	0.52
4:C:83:LYS:NZ	5:F:32:LEU:O	2.44	0.51
6:G:147:GLU:HG3	11:I:45:ILE:HG12	1.92	0.51
4:A:140:ILE:HG12	4:A:143:ARG:HH21	1.75	0.51
4:A:180:ILE:HD11	4:A:216:LEU:HD11	1.91	0.51
4:C:493:SER:HA	4:C:496:LYS:HG3	1.93	0.51
4:A:190:ASN:HA	4:A:198:LYS:HG2	1.92	0.51
5:F:184:SER:HB3	5:F:218:VAL:HG22	1.92	0.51
9:3:56:LEU:O	9:3:59:ALA:HB3	2.10	0.51
5:E:229:PRO:HB2	5:E:271:VAL:HG23	1.92	0.51
1:K:36:VAL:HG11	16:S:37:LEU:HD21	1.92	0.51
16:S:45:ILE:HG23	16:S:46:PRO:HD3	1.92	0.51
16:S:74:LEU:O	16:S:78:VAL:HG23	2.10	0.51
4:C:95:VAL:HG11	4:C:245:LEU:HD21	1.92	0.51
5:F:369:GLU:O	5:F:373:VAL:HG23	2.10	0.51
15:R:20:VAL:O	15:R:21:LYS:HB2	2.10	0.51
9:8:3:ASP:OD1	9:8:4:THR:N	2.44	0.51
3:M:155:GLN:NE2	14:Q:33:TYR:O	2.34	0.51
5:D:247:ARG:HD3	5:D:307:ILE:HG13	1.91	0.51
4:C:180:ILE:HD11	4:C:216:LEU:HD11	1.92	0.51
5:F:141:LYS:NZ	5:F:463:VAL:O	2.43	0.51
5:F:87:ILE:HD11	5:F:241:THR:HB	1.92	0.50
4:A:397:TYR:CG	4:A:421:GLY:HA3	2.46	0.50
4:B:237:SER:HB3	5:E:297:GLU:HG3	1.93	0.50
4:B:349:GLN:HG3	4:B:351:PHE:CE2	2.47	0.50
6:G:117:TYR:O	6:G:121:SER:OG	2.22	0.50
16:S:41:THR:OG1	16:S:44:GLU:OE1	2.28	0.50
4:A:426:GLU:HG2	4:A:461:ILE:HB	1.93	0.50
5:F:347:ILE:HG23	5:F:418:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:39:LEU:HA	8:O:42:VAL:HG12	1.93	0.50
9:2:4:THR:HA	9:2:7:LYS:HE3	1.93	0.50
10:H:103:LEU:HB2	10:H:145:LEU:HD21	1.94	0.50
4:C:396:GLN:OE1	7:J:35:ARG:NH2	2.31	0.50
5:E:52:VAL:HA	5:E:63:THR:HG22	1.94	0.49
1:K:118:VAL:HG13	3:M:100:CYS:HB3	1.94	0.49
4:C:344:SER:HB2	5:D:263:ARG:HH22	1.76	0.49
5:D:52:VAL:HA	5:D:63:THR:HG22	1.95	0.49
5:E:18:ALA:HB3	5:E:25:ASP:HB2	1.94	0.49
5:D:272:SER:OG	5:D:285:GLN:HB3	2.12	0.49
8:O:120:VAL:HG11	8:O:134:LEU:HD21	1.95	0.49
9:1:27:THR:HG21	9:8:27:THR:HA	1.94	0.49
1:K:20:GLU:OE1	15:R:53:LYS:NZ	2.45	0.49
12:N:163:ASN:HD22	12:N:210:GLN:CD	2.20	0.49
4:A:359:LYS:HG3	5:D:382:GLN:HG2	1.95	0.49
5:E:400:SER:HB2	5:E:403:ASP:OD1	2.13	0.49
4:B:441:GLN:O	4:B:445:ILE:HG12	2.13	0.49
5:D:87:ILE:HD13	5:D:238:THR:HG23	1.95	0.49
9:3:25:ILE:HD11	9:3:58:GLU:HB2	1.95	0.49
16:S:57:ASN:O	16:S:61:THR:HG22	2.13	0.49
4:B:196:LYS:HD3	4:B:197:LYS:HG3	1.94	0.49
8:O:32:LEU:HD13	8:O:109:MET:HE1	1.94	0.49
9:8:45:GLN:O	9:8:48:SER:HB3	2.12	0.49
5:D:90:GLY:HA2	5:D:245:TYR:CE1	2.48	0.49
9:2:38[A]:ARG:NH1	9:3:38[A]:ARG:HH22	2.06	0.49
4:B:224:ASP:OD2	4:B:227:LYS:NZ	2.34	0.48
8:O:123:ALA:HA	8:O:156:PRO:HA	1.95	0.48
4:B:148:THR:HA	4:B:182:THR:HG23	1.95	0.48
16:S:87:TYR:O	16:S:91:ILE:HG23	2.13	0.48
6:G:110:ASP:OD1	6:G:113:ARG:NH2	2.46	0.48
9:2:56:LEU:O	9:2:59:ALA:HB3	2.13	0.48
9:3:62:LEU:HD13	12:N:163:ASN:HA	1.94	0.48
1:K:13:ARG:HD2	1:K:19:GLU:CD	2.39	0.48
4:A:404:ALA:C	4:A:406:PHE:H	2.21	0.48
8:O:178:LYS:O	8:O:182:LEU:HG	2.14	0.48
12:N:14:ILE:HG22	12:N:19:ALA:HB2	1.95	0.48
2:L:66:GLU:HG3	2:L:67:TYR:H	1.78	0.48
5:D:369:GLU:HG2	5:D:370:HIS:N	2.28	0.48
4:C:163:GLN:NE2	4:C:165:GLU:OE2	2.45	0.48
4:C:436:MET:HE3	4:C:469:LEU:HD11	1.95	0.48
12:N:40:ASN:HD22	15:R:56:ASN:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:111:GLY:HA3	13:P:24:ILE:HD13	1.94	0.48
5:E:201:HIS:O	5:E:205:GLU:HG2	2.14	0.48
13:P:6:ILE:O	13:P:11:ILE:HG13	2.14	0.48
16:S:91:ILE:HA	16:S:94:LYS:HE2	1.95	0.48
4:C:389:THR:O	4:C:393:GLU:HG3	2.14	0.48
12:N:101:ASN:ND2	12:N:161:THR:OG1	2.30	0.48
1:K:4:PRO:HB3	3:M:129:GLN:HE21	1.78	0.48
1:K:21:PHE:HB2	18:R:101:CDL:H312	1.95	0.48
2:L:47:ILE:O	2:L:51:LYS:HG2	2.13	0.48
4:C:283:LEU:HD21	4:C:289:PRO:HB3	1.95	0.48
4:C:496:LYS:O	4:C:499:GLU:HG3	2.14	0.48
5:D:157:LEU:N	5:D:311:GLN:O	2.45	0.48
9:3:4:THR:OG1	9:4:3:ASP:OD1	2.32	0.48
5:F:223:GLY:N	5:F:235:VAL:HG21	2.28	0.48
1:K:28:LYS:HE3	16:S:75:ASN:HD21	1.79	0.47
4:B:180:ILE:HD11	4:B:216:LEU:HD11	1.95	0.47
9:4:45:GLN:OE1	9:4:45:GLN:N	2.44	0.47
12:N:60:MET:HE1	12:N:220:LEU:HD23	1.95	0.47
12:N:141:LEU:HA	12:N:144:ILE:HD12	1.96	0.47
3:M:56:TYR:HB3	3:M:66:VAL:HG21	1.96	0.47
8:O:22:LEU:HD13	8:O:85:LEU:HD22	1.95	0.47
1:K:44:TYR:CE1	1:K:48:LYS:HG3	2.49	0.47
5:E:420:PRO:HG2	5:E:433:LYS:HG2	1.97	0.47
10:H:58:LEU:HD12	10:H:79:SER:O	2.13	0.47
15:R:80:SER:O	15:R:84:LEU:HG	2.14	0.47
1:K:12:VAL:HA	1:K:18:PRO:HA	1.96	0.47
1:K:28:LYS:HE3	16:S:75:ASN:ND2	2.30	0.47
4:C:472:VAL:HG12	4:C:480:LEU:HD11	1.95	0.47
5:D:282:VAL:O	5:D:282:VAL:HG12	2.15	0.47
16:S:100:TYR:CE2	17:T:29:ARG:HD3	2.49	0.47
4:B:270:ASP:OD1	4:B:273:LYS:HG3	2.14	0.47
5:D:166:THR:HG22	5:D:170:MET:HE2	1.96	0.47
6:G:73:SER:OG	6:G:224:GLU:OE2	2.26	0.47
7:J:22:PHE:HA	7:J:25:ARG:HG2	1.97	0.47
4:C:183:ILE:HD11	4:C:267:ILE:HD13	1.97	0.47
9:1:4:THR:OG1	9:2:3:ASP:OD1	2.33	0.47
4:A:423:ARG:NH2	4:A:456:LEU:O	2.45	0.47
4:C:164:ARG:NH1	4:C:306:LEU:O	2.44	0.47
5:F:240:LEU:CD2	5:F:299:ILE:HG12	2.45	0.47
6:G:226:SER:O	6:G:230:THR:HG23	2.14	0.47
1:K:11:LYS:HA	1:K:11:LYS:HD3	1.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:ALA:HB3	14:Q:39:PRO:CG	2.45	0.47
5:F:340:ARG:O	5:F:344:GLU:HG2	2.14	0.47
4:A:196:LYS:HA	4:A:196:LYS:HD2	1.63	0.46
4:C:298:VAL:O	4:C:301:LEU:HB3	2.15	0.46
5:F:420:PRO:HG2	5:F:433:LYS:HG2	1.97	0.46
10:H:127:THR:O	10:H:131:ILE:HG12	2.15	0.46
4:C:483:ILE:HD12	4:C:489:ILE:HG22	1.97	0.46
5:D:259:ASP:HA	5:D:260:ASN:HA	1.70	0.46
9:3:18:VAL:HB	9:4:64:CYS:SG	2.55	0.46
3:M:131:THR:HG22	3:M:132:ILE:N	2.29	0.46
4:A:265:LEU:HD11	4:A:324:LEU:HG	1.97	0.46
9:1:38:ARG:HD3	9:2:38[B]:ARG:HH11	1.80	0.46
3:M:53:TRP:HB3	3:M:57:LYS:HE3	1.98	0.46
4:C:452:TYR:OH	4:C:498:LYS:HG3	2.14	0.46
14:Q:49:LYS:H	14:Q:49:LYS:HD3	1.81	0.46
1:K:136:LEU:HD11	3:M:83:ASP:HA	1.98	0.46
2:L:60:PRO:HB2	2:L:61:VAL:HG23	1.98	0.46
4:A:140:ILE:HG22	4:A:311:LYS:HG3	1.97	0.46
9:3:62:LEU:HD23	9:3:65:LEU:HD12	1.98	0.46
4:C:362:ARG:HH12	5:F:375:ARG:NE	2.13	0.46
4:A:210:ARG:HG3	4:A:235:THR:HG21	1.98	0.46
5:E:189:VAL:HG22	5:E:235:VAL:HG13	1.97	0.46
6:G:113:ARG:O	6:G:117:TYR:HB2	2.16	0.46
3:M:144:LEU:HD12	14:Q:35:LEU:CD1	2.46	0.45
4:B:392:LEU:O	4:B:396:GLN:HG3	2.16	0.45
5:E:283:GLY:HA2	6:G:262:LEU:HD11	1.98	0.45
5:D:87:ILE:HG21	5:D:238:THR:HG23	1.98	0.45
4:C:11:ILE:HB	8:O:186:MET:HE3	1.99	0.45
5:E:154:LYS:HE3	5:E:299:ILE:HB	1.98	0.45
1:K:29:THR:OG1	1:K:33:GLY:HA3	2.17	0.45
6:G:176:LYS:HB3	6:G:212:ILE:HD11	1.98	0.45
22:Q:101:3PH:H351	15:R:47:TYR:HB2	1.98	0.45
1:K:147:VAL:HG23	2:L:93:PHE:CE2	2.52	0.45
4:C:105:GLY:HA2	4:C:226:MET:O	2.16	0.45
5:D:324:ALA:HB3	5:D:325:PRO:HD3	1.97	0.45
4:B:491:GLU:OE1	4:B:491:GLU:N	2.48	0.45
5:F:90:GLY:HA2	5:F:245:TYR:CE2	2.51	0.45
9:3:63:PHE:O	9:3:66:MET:HB3	2.16	0.45
4:B:469:LEU:O	4:B:473:VAL:HG23	2.17	0.45
5:F:89:VAL:HG23	5:F:115:GLN:HG2	1.99	0.45
5:D:436:PRO:HD2	5:D:439:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:23:PRO:HD3	10:H:94:ALA:O	2.17	0.45
12:N:94:PRO:HB2	12:N:100:MET:SD	2.57	0.45
12:N:120:LYS:HG3	12:N:120:LYS:O	2.17	0.45
3:M:19:ILE:HG22	3:M:24:LYS:HD2	1.98	0.45
4:B:98:PRO:O	4:B:103:LEU:HD11	2.17	0.45
6:G:129:LYS:HE2	11:I:46:VAL:HG22	1.99	0.45
4:A:445:ILE:O	4:A:449:VAL:HG22	2.17	0.45
12:N:93:THR:HB	12:N:96:THR:HG23	1.99	0.45
1:K:155:LEU:HB3	3:M:56:TYR:CE1	2.52	0.45
5:F:156:GLY:HA3	5:F:332:LEU:HD13	1.99	0.45
5:D:363:PRO:HD3	5:D:371:TYR:CD2	2.51	0.45
8:O:5:VAL:HG23	8:O:28:LYS:HE3	1.99	0.45
16:S:80:THR:O	16:S:84:MET:HG2	2.17	0.45
18:K:301:CDL:OB7	18:K:301:CDL:H531	2.17	0.45
4:B:265:LEU:HD11	4:B:324:LEU:HG	1.99	0.45
4:B:379:GLN:NE2	4:B:383:MET:HG3	2.32	0.45
4:B:397:TYR:CG	4:B:421:GLY:HA3	2.52	0.45
4:C:156:LEU:HD13	4:C:367:VAL:HG11	1.99	0.45
5:D:384:TYR:OH	7:J:30:GLU:OE1	2.34	0.45
9:7:36:TYR:CE1	9:7:43:LYS:HB2	2.52	0.45
3:M:13:VAL:O	3:M:17:GLU:HG3	2.17	0.44
9:2:16:VAL:HG22	9:3:13:ALA:O	2.17	0.44
5:E:283:GLY:HA2	6:G:262:LEU:CD1	2.47	0.44
6:G:74:ASP:OD1	6:G:110:ASP:N	2.38	0.44
9:2:36:TYR:CZ	9:3:45:GLN:HG2	2.52	0.44
9:2:38[A]:ARG:HE	9:3:38[A]:ARG:NH2	2.14	0.44
15:R:26:PRO:O	15:R:29:ILE:HB	2.18	0.44
1:K:26:TYR:OH	17:T:3:PRO:O	2.26	0.44
5:F:323:PRO:O	5:F:327:THR:OG1	2.28	0.44
11:I:32:LYS:O	11:I:36:GLU:HG2	2.17	0.44
1:K:32:THR:O	1:K:36:VAL:HG13	2.18	0.44
1:K:155:LEU:HD23	1:K:155:LEU:HA	1.82	0.44
6:G:113:ARG:NH1	11:I:46:VAL:HG11	2.33	0.44
6:G:197:ASP:H	6:G:200:VAL:HG12	1.82	0.44
4:B:48:GLN:HB3	5:F:71:GLY:HA2	1.99	0.44
5:F:375:ARG:HD3	5:F:375:ARG:HA	1.84	0.44
5:D:51:GLU:CD	5:D:234:ARG:HE	2.25	0.44
5:D:245:TYR:CD2	5:D:249:GLN:HG3	2.53	0.44
6:G:88:GLN:HG3	6:G:173:THR:HG21	1.98	0.44
4:C:96:ASP:OD2	4:C:126:ARG:NE	2.43	0.44
5:D:399:LEU:HB3	5:D:403:ASP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:466:ILE:O	5:D:470:VAL:HG23	2.18	0.44
9:1:33:ILE:HG21	9:2:32:LEU:HA	1.99	0.44
9:4:75:MET:SD	9:4:75:MET:N	2.91	0.44
3:M:104:VAL:O	3:M:108:LYS:HG3	2.18	0.44
4:A:183:ILE:HD11	4:A:267:ILE:HD13	1.99	0.44
4:C:307:GLU:OE2	5:D:193:THR:OG1	2.27	0.44
5:D:263:ARG:HH11	5:D:266:GLN:HE22	1.64	0.44
5:D:443:GLY:O	5:D:447:ILE:HG13	2.18	0.44
9:5:5:ALA:HB1	9:6:6:ALA:HB2	1.98	0.44
12:N:139:PRO:O	12:N:143:ILE:HD12	2.18	0.44
4:A:239:ALA:HB1	4:A:241:PRO:HD2	1.98	0.44
5:E:459:ALA:HA	5:E:472:LYS:HD3	1.99	0.44
6:G:51:LEU:HD21	10:H:55:LEU:HD22	1.98	0.43
6:G:64:LYS:HD2	6:G:64:LYS:HA	1.83	0.43
9:5:18:VAL:HB	9:6:64:CYS:SG	2.58	0.43
9:7:19:ALA:HA	9:8:20:GLY:HA3	2.00	0.43
1:K:129:ARG:NH1	3:M:90:ASP:OD2	2.46	0.43
3:M:136:ASN:ND2	3:M:142:THR:O	2.52	0.43
4:A:74:VAL:HB	4:A:241:PRO:HG3	2.00	0.43
5:E:204:ILE:HD13	5:E:211:LEU:HD11	2.00	0.43
1:K:103:HIS:HE1	14:Q:43:LYS:H	1.65	0.43
4:C:382:ALA:O	4:C:386:VAL:HG22	2.17	0.43
4:C:419:SER:O	4:C:423:ARG:HD3	2.18	0.43
4:C:441:GLN:O	4:C:445:ILE:HG13	2.17	0.43
5:D:74:ARG:HG3	5:D:74:ARG:HH11	1.84	0.43
4:B:137:ILE:HD13	4:B:137:ILE:HA	1.88	0.43
5:E:458:GLN:O	5:E:472:LYS:NZ	2.42	0.43
10:H:105:LEU:HA	10:H:145:LEU:HD13	2.01	0.43
4:B:336:ALA:O	4:B:340:THR:OG1	2.23	0.43
5:E:259:ASP:HA	5:E:260:ASN:HA	1.76	0.43
5:F:272:SER:HB2	5:F:285:GLN:HB3	2.01	0.43
5:D:375:ARG:HA	5:D:375:ARG:HD3	1.84	0.43
6:G:233:ASP:OD1	6:G:237:LYS:NZ	2.42	0.43
8:O:104:ALA:O	8:O:107:THR:HG22	2.19	0.43
4:C:52:MET:O	4:C:91:THR:OG1	2.23	0.43
5:E:186:PHE:HB3	5:E:220:LEU:HD23	2.01	0.43
5:F:166:THR:O	5:F:170:MET:HG2	2.19	0.43
4:B:415:GLN:O	4:B:415:GLN:NE2	2.52	0.43
5:D:261:ILE:HD11	5:D:295:MET:HE1	2.00	0.43
6:G:122:ASP:OD1	6:G:123:GLN:N	2.52	0.43
6:G:251:ASN:HA	6:G:254:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:31:LYS:HG2	8:O:34:GLN:HB3	2.01	0.43
8:O:95:LEU:O	8:O:98:THR:OG1	2.23	0.43
4:A:152:ALA:HB3	4:A:365:ILE:HD12	2.00	0.43
10:H:122:THR:O	10:H:128:ARG:NH2	2.51	0.43
1:K:60:ALA:HA	12:N:89:PRO:HG3	2.01	0.42
5:E:56:LEU:HD11	5:E:62:ARG:HB2	2.01	0.42
5:D:18:ALA:HB3	5:D:25:ASP:HB2	2.01	0.42
2:L:46:LYS:HE3	4:C:17:LEU:N	2.35	0.42
3:M:144:LEU:HD23	3:M:154:HIS:HB2	2.01	0.42
5:E:100:VAL:HG13	5:E:101:ILE:HG23	2.00	0.42
5:E:324:ALA:HB3	5:E:325:PRO:HD3	1.99	0.42
10:H:18:PHE:CZ	10:H:20:PHE:HB2	2.53	0.42
1:K:164:MET:HE3	1:K:164:MET:HB3	1.91	0.42
18:K:301:CDL:H832	18:K:301:CDL:H801	1.85	0.42
4:B:177:SER:OG	4:B:432:GLN:NE2	2.49	0.42
4:C:397:TYR:CG	4:C:421:GLY:HA3	2.54	0.42
5:E:87:ILE:HD13	5:E:238:THR:HG23	2.00	0.42
6:G:108:ILE:HG21	6:G:217:LEU:HD21	2.01	0.42
9:1:17:GLY:HA3	9:1:64:CYS:SG	2.59	0.42
9:7:36:TYR:CE2	9:8:45:GLN:HG2	2.55	0.42
9:7:70:LEU:HG	9:7:75:MET:HE2	2.00	0.42
4:B:32:LEU:N	4:B:40:ARG:O	2.50	0.42
5:E:256:LEU:O	5:E:309:SER:HA	2.19	0.42
5:E:347:ILE:HG23	5:E:418:SER:OG	2.20	0.42
9:3:33:ILE:HG23	9:4:46:LEU:HD22	2.00	0.42
16:S:44:GLU:HB3	16:S:47:ARG:HH21	1.85	0.42
5:F:431:MET:HE2	5:F:431:MET:HB3	1.87	0.42
5:D:156:GLY:HA3	5:D:332:LEU:HD13	2.02	0.42
7:J:16:ARG:NH1	7:J:27:GLN:HG3	2.34	0.42
10:H:133:ILE:O	10:H:136:GLU:HG3	2.19	0.42
12:N:20:ALA:O	12:N:24:ILE:HG13	2.19	0.42
14:Q:43:LYS:HA	14:Q:43:LYS:HD2	1.82	0.42
3:M:109:ALA:O	3:M:112:VAL:HG12	2.19	0.42
4:B:458:PRO:HA	4:B:461:ILE:HG12	2.02	0.42
4:B:469:LEU:HD23	4:B:469:LEU:HA	1.91	0.42
5:E:304:LYS:HE3	5:E:304:LYS:HB3	1.81	0.42
5:E:422:GLN:HA	5:E:425:GLU:HG3	2.00	0.42
5:F:148:PRO:O	5:F:358:SER:OG	2.32	0.42
8:O:41:ARG:HD2	8:O:41:ARG:HA	1.94	0.42
9:4:16:VAL:HG22	9:5:13:ALA:O	2.20	0.42
9:7:12:GLY:O	9:7:16:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:261:ILE:O	5:F:264:PHE:HB3	2.19	0.42
8:O:48:GLU:HG2	8:O:49:PRO:HD2	2.02	0.42
13:P:5:ILE:HG23	13:P:6:ILE:H	1.85	0.42
5:F:119:ILE:HA	5:F:241:THR:OG1	2.20	0.42
5:F:377:VAL:HG13	5:F:413:ILE:HG21	2.02	0.42
6:G:153:TYR:CE2	6:G:155:PHE:HB3	2.54	0.42
9:5:62:LEU:HD23	9:5:62:LEU:HA	1.91	0.42
10:H:100:LEU:HD23	10:H:100:LEU:HA	1.91	0.42
4:C:196:LYS:HE2	4:C:196:LYS:HB2	1.83	0.41
9:5:15:THR:HG23	9:6:14:ALA:HA	2.02	0.41
6:G:157:GLU:HG3	6:G:158:GLY:N	2.35	0.41
9:1:36:TYR:CE1	9:1:43:LYS:HB2	2.55	0.41
12:N:181:MET:O	12:N:189:THR:OG1	2.37	0.41
14:Q:44:MET:HG3	14:Q:46:ASN:HB2	2.01	0.41
4:B:40:ARG:HH11	4:B:70:ASN:HD21	1.68	0.41
4:C:146:MET:HE3	4:C:146:MET:HB3	1.98	0.41
5:E:56:LEU:HD12	5:E:60:THR:HG22	2.02	0.41
5:E:431:MET:HE2	5:E:433:LYS:NZ	2.35	0.41
5:F:166:THR:HA	5:F:169:ILE:HG22	2.02	0.41
5:D:319:ASP:O	5:D:320:LEU:HB2	2.20	0.41
5:D:420:PRO:HG2	5:D:433:LYS:HG2	2.02	0.41
9:1:33:ILE:HG23	9:2:46:LEU:HD22	2.02	0.41
10:H:82:ILE:HD13	10:H:92:LEU:HD13	2.02	0.41
14:Q:39:PRO:O	14:Q:41:PRO:HD3	2.19	0.41
1:K:30:GLY:HA3	16:S:36:GLU:OE2	2.20	0.41
3:M:31:LYS:O	3:M:35:GLU:HG2	2.20	0.41
5:F:115:GLN:NE2	5:F:245:TYR:OH	2.54	0.41
8:O:31:LYS:O	8:O:35:VAL:HG22	2.20	0.41
9:2:62:LEU:HD13	12:N:151:ILE:HG21	2.01	0.41
9:5:65:LEU:HD23	9:5:65:LEU:HA	1.89	0.41
4:A:54:GLU:OE2	4:A:60:LYS:NZ	2.38	0.41
4:B:286:ARG:HA	5:E:278:ILE:HD12	2.02	0.41
4:C:136:ILE:O	5:D:197:ASN:ND2	2.51	0.41
6:G:72:SER:HB2	6:G:82:HIS:ND1	2.35	0.41
9:2:12:GLY:O	9:2:16:VAL:HG23	2.20	0.41
1:K:180:HIS:HD2	2:L:48:ARG:HH22	1.67	0.41
4:A:469:LEU:HD12	4:A:469:LEU:HA	1.88	0.41
4:B:169:GLY:O	4:B:328:GLU:HA	2.20	0.41
5:F:210:ASN:ND2	5:F:213:ASP:OD1	2.53	0.41
9:6:4:THR:OG1	9:7:3:ASP:OD1	2.38	0.41
16:S:53:LYS:HD3	16:S:53:LYS:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:4:PRO:HB3	3:M:129:GLN:NE2	2.36	0.41
1:K:124:LEU:O	1:K:128:GLN:HG3	2.19	0.41
4:B:183:ILE:HD11	4:B:267:ILE:HD13	2.03	0.41
5:D:389:ASP:HB3	7:J:15:ILE:HD12	2.03	0.41
6:G:58:LYS:HA	6:G:58:LYS:HD3	1.83	0.41
12:N:138:ILE:N	12:N:139:PRO:HD2	2.36	0.41
1:K:85:LEU:HD23	1:K:85:LEU:HA	1.95	0.41
4:B:152:ALA:HB3	4:B:365:ILE:HD12	2.02	0.41
5:E:134:GLU:HG3	5:E:151:LYS:HD2	2.02	0.41
5:F:247:ARG:HD3	5:F:307:ILE:HG13	2.03	0.41
5:F:261:ILE:HD12	5:F:261:ILE:HA	1.93	0.41
5:F:412:LYS:HD3	5:F:460:PHE:CE2	2.56	0.41
6:G:68:LEU:HD12	6:G:159:SER:HB2	2.03	0.41
9:5:56:LEU:O	9:5:59:ALA:HB3	2.21	0.41
15:R:31:MET:HE2	15:R:32:ARG:HH21	1.86	0.41
1:K:124:LEU:HD13	3:M:19:ILE:HD11	2.02	0.41
1:K:179:LYS:C	1:K:179:LYS:HD2	2.46	0.41
2:L:94:LYS:NZ	2:L:96:GLU:OE2	2.52	0.41
3:M:20:PRO:HD2	3:M:23:GLN:HE21	1.86	0.41
4:A:283:LEU:HD11	4:A:293:ALA:HB1	2.03	0.41
4:A:283:LEU:HD21	4:A:289:PRO:HB3	2.03	0.41
4:A:441:GLN:O	4:A:445:ILE:HG12	2.21	0.41
4:B:363:PRO:HB2	4:B:365:ILE:HG13	2.03	0.41
4:B:498:LYS:HB2	4:B:498:LYS:HE3	1.84	0.41
4:C:237:SER:HB3	5:F:297:GLU:HG3	2.02	0.41
5:F:42:GLN:CD	5:F:79:LEU:HD13	2.46	0.41
5:F:97:ILE:HD11	5:F:200:TYR:CD2	2.56	0.41
5:D:160:GLY:HA3	5:D:318:ASP:OD1	2.21	0.41
8:O:31:LYS:HB2	8:O:31:LYS:HE2	1.81	0.41
8:O:135:LYS:O	8:O:139:LYS:HG2	2.20	0.41
9:3:33:ILE:HG21	9:4:32:LEU:HA	2.02	0.41
9:4:70:LEU:HD23	9:4:70:LEU:HA	1.91	0.41
10:H:117:ALA:O	10:H:120:VAL:HG22	2.21	0.41
12:N:40:ASN:ND2	15:R:56:ASN:HA	2.36	0.41
16:S:94:LYS:HE3	16:S:96:GLY:O	2.20	0.41
5:E:455:LEU:HD21	5:E:470:VAL:HG12	2.03	0.41
6:G:207:TYR:CZ	10:H:80:GLY:HA2	2.56	0.41
14:Q:49:LYS:HD3	14:Q:49:LYS:N	2.36	0.41
15:R:76:SER:HA	15:R:79:PHE:CE1	2.56	0.41
4:A:270:ASP:HB2	4:A:326:VAL:O	2.21	0.40
4:A:406:PHE:HB3	6:G:26:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:124:LYS:N	4:B:124:LYS:HD2	2.36	0.40
6:G:14:LYS:HA	6:G:243:ILE:HD11	2.03	0.40
12:N:128:PHE:CE1	12:N:149:LEU:HD13	2.56	0.40
4:A:5:THR:HG22	4:A:32:LEU:HD13	2.03	0.40
4:A:497:LEU:O	4:A:501:VAL:HG12	2.21	0.40
5:E:119:ILE:HA	5:E:241:THR:OG1	2.21	0.40
5:E:257:PHE:HA	5:E:310:VAL:O	2.22	0.40
5:E:379:LYS:HE2	5:E:379:LYS:HB3	1.84	0.40
1:K:180:HIS:HD2	2:L:48:ARG:NH2	2.20	0.40
4:A:498:LYS:O	4:A:502:THR:HG22	2.20	0.40
4:C:48:GLN:HB3	5:D:71:GLY:HA2	2.03	0.40
4:C:152:ALA:HB3	4:C:365:ILE:HD12	2.04	0.40
5:F:396:MET:HE3	5:F:404:LYS:HG2	2.02	0.40
6:G:96:LEU:HD22	6:G:101:LYS:HD3	2.04	0.40
8:O:52:ALA:O	8:O:56:LEU:HB2	2.21	0.40
10:H:95:GLU:OE1	11:I:16:SER:OG	2.33	0.40
15:R:53:LYS:HD3	18:R:101:CDL:HB31	2.02	0.40
4:B:362:ARG:HA	4:B:363:PRO:C	2.47	0.40
4:C:197:LYS:HE2	4:C:197:LYS:HB3	1.92	0.40
5:E:154:LYS:HE2	5:E:296:GLN:HB3	2.03	0.40
5:F:259:ASP:HA	5:F:260:ASN:HA	1.72	0.40
5:F:295:MET:HE3	5:F:295:MET:HB3	1.79	0.40
9:7:56:LEU:HD23	9:7:56:LEU:HA	1.91	0.40
4:A:479:LEU:HD22	4:A:496:LYS:HG3	2.04	0.40
4:B:270:ASP:HB2	4:B:326:VAL:O	2.22	0.40
4:C:476:HIS:CG	4:C:500:ILE:HD13	2.57	0.40
6:G:148:LEU:HD23	6:G:148:LEU:HA	1.84	0.40
9:2:8:PHE:HD1	9:2:72:LEU:HD11	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	194/214 (91%)	189 (97%)	5 (3%)	0	100	100
2	L	65/108 (60%)	57 (88%)	8 (12%)	0	100	100
3	M	154/160 (96%)	147 (96%)	7 (4%)	0	100	100
4	A	499/510 (98%)	492 (99%)	7 (1%)	0	100	100
4	B	473/510 (93%)	464 (98%)	9 (2%)	0	100	100
4	C	483/510 (95%)	476 (99%)	7 (1%)	0	100	100
5	D	468/482 (97%)	445 (95%)	22 (5%)	1 (0%)	44	62
5	E	452/482 (94%)	439 (97%)	12 (3%)	1 (0%)	44	62
5	F	464/482 (96%)	450 (97%)	13 (3%)	1 (0%)	44	62
6	G	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
7	J	33/81 (41%)	33 (100%)	0	0	100	100
8	O	185/190 (97%)	180 (97%)	5 (3%)	0	100	100
9	1	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
9	2	74/75 (99%)	71 (96%)	3 (4%)	0	100	100
9	3	74/75 (99%)	72 (97%)	2 (3%)	0	100	100
9	4	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
9	5	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
9	6	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
9	7	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
9	8	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
10	H	130/146 (89%)	128 (98%)	2 (2%)	0	100	100
11	I	43/51 (84%)	43 (100%)	0	0	100	100
12	N	221/226 (98%)	207 (94%)	14 (6%)	0	100	100
13	P	39/58 (67%)	38 (97%)	1 (3%)	0	100	100
14	Q	49/68 (72%)	44 (90%)	5 (10%)	0	100	100
15	R	76/93 (82%)	73 (96%)	3 (4%)	0	100	100
16	S	75/102 (74%)	73 (97%)	2 (3%)	0	100	100
17	T	42/69 (61%)	40 (95%)	2 (5%)	0	100	100
All	All	5000/5415 (92%)	4851 (97%)	146 (3%)	3 (0%)	50	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	282	VAL
5	D	282	VAL
5	F	282	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	160/187 (86%)	160 (100%)	0	100	100
2	L	60/98 (61%)	60 (100%)	0	100	100
3	M	135/139 (97%)	135 (100%)	0	100	100
4	A	407/412 (99%)	407 (100%)	0	100	100
4	B	387/412 (94%)	387 (100%)	0	100	100
4	C	397/412 (96%)	397 (100%)	0	100	100
5	D	379/388 (98%)	379 (100%)	0	100	100
5	E	369/388 (95%)	369 (100%)	0	100	100
5	F	376/388 (97%)	375 (100%)	1 (0%)	91	96
6	G	228/229 (100%)	228 (100%)	0	100	100
7	J	23/68 (34%)	23 (100%)	0	100	100
8	O	162/165 (98%)	162 (100%)	0	100	100
9	1	51/51 (100%)	51 (100%)	0	100	100
9	2	52/51 (102%)	52 (100%)	0	100	100
9	3	52/51 (102%)	52 (100%)	0	100	100
9	4	51/51 (100%)	51 (100%)	0	100	100
9	5	51/51 (100%)	51 (100%)	0	100	100
9	6	51/51 (100%)	51 (100%)	0	100	100
9	7	51/51 (100%)	51 (100%)	0	100	100
9	8	51/51 (100%)	51 (100%)	0	100	100
10	H	103/108 (95%)	103 (100%)	0	100	100
11	I	36/42 (86%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	N	196/199 (98%)	196 (100%)	0	100	100
13	P	36/48 (75%)	36 (100%)	0	100	100
14	Q	51/68 (75%)	51 (100%)	0	100	100
15	R	69/82 (84%)	69 (100%)	0	100	100
16	S	64/85 (75%)	64 (100%)	0	100	100
17	T	34/58 (59%)	34 (100%)	0	100	100
All	All	4082/4384 (93%)	4081 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	282	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	23	GLN
1	K	88	GLN
1	K	114	GLN
1	K	115	GLN
1	K	183	GLN
3	M	23	GLN
3	M	136	ASN
4	A	396	GLN
4	A	432	GLN
4	A	503	ASN
4	B	70	ASN
4	B	415	GLN
4	B	432	GLN
4	B	476	HIS
4	B	503	ASN
4	C	208	GLN
4	C	215	GLN
4	C	432	GLN
4	C	503	ASN
5	E	197	ASN
5	E	224	GLN
5	E	382	GLN
5	E	445	GLN

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Mol	Chain	Res	Type
5	F	54	GLN
5	F	180	HIS
5	F	210	ASN
5	F	249	GLN
5	F	331	HIS
5	F	364	ASN
5	F	422	GLN
5	D	54	GLN
5	D	115	GLN
5	D	180	HIS
5	D	266	GLN
5	D	446	GLN
6	G	163	ASN
6	G	182	ASN
8	O	99	GLN
10	H	32	ASN
11	I	7	GLN
12	N	46	GLN
12	N	47	GLN
12	N	61	HIS
12	N	101	ASN
12	N	123	ASN
12	N	163	ASN
12	N	225	ASN
15	R	44	GLN
16	S	75	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	ATP	C	601	20	26,33,33	2.23	6 (23%)	31,52,52	1.62	7 (22%)
22	3PH	Q	101	-	26,26,47	1.14	4 (15%)	30,31,52	1.32	2 (6%)
21	ADP	D	501	20	24,29,29	2.37	8 (33%)	29,45,45	1.50	5 (17%)
21	ADP	F	501	20	24,29,29	2.36	8 (33%)	29,45,45	1.50	5 (17%)
18	CDL	R	101	-	48,48,99	0.41	0	54,60,111	0.45	0
19	ATP	A	601	20	26,33,33	2.25	6 (23%)	31,52,52	1.59	7 (22%)
18	CDL	K	301	-	71,71,99	0.38	0	77,83,111	0.51	1 (1%)
19	ATP	B	601	20	26,33,33	2.24	6 (23%)	31,52,52	1.67	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ATP	C	601	20	-	6/18/38/38	0/3/3/3
22	3PH	Q	101	-	-	10/28/28/49	-
21	ADP	D	501	20	-	6/12/32/32	0/3/3/3
21	ADP	F	501	20	-	7/12/32/32	0/3/3/3
18	CDL	R	101	-	-	21/59/59/110	-
19	ATP	A	601	20	-	3/18/38/38	0/3/3/3
18	CDL	K	301	-	-	42/82/82/110	-
19	ATP	B	601	20	-	2/18/38/38	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	601	ATP	O4'-C1'	7.75	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	601	ATP	O4'-C1'	7.74	1.51	1.41
19	C	601	ATP	O4'-C1'	7.67	1.51	1.41
21	D	501	ADP	O4'-C1'	6.69	1.50	1.41
21	F	501	ADP	O4'-C1'	6.49	1.50	1.41
21	D	501	ADP	C6-N6	4.50	1.50	1.34
21	F	501	ADP	C6-N6	4.49	1.50	1.34
19	A	601	ATP	C2'-C1'	-4.42	1.47	1.53
19	B	601	ATP	C2'-C1'	-4.30	1.47	1.53
21	F	501	ADP	C2'-C1'	-4.26	1.47	1.53
19	C	601	ATP	C2'-C1'	-4.25	1.47	1.53
21	D	501	ADP	C2'-C1'	-4.16	1.47	1.53
21	D	501	ADP	O4'-C4'	3.52	1.52	1.45
21	F	501	ADP	O4'-C4'	3.44	1.52	1.45
19	B	601	ATP	C6-N6	3.42	1.46	1.34
19	C	601	ATP	C6-N6	3.39	1.46	1.34
19	A	601	ATP	C6-N6	3.34	1.46	1.34
19	A	601	ATP	C2'-C3'	-3.12	1.44	1.53
19	C	601	ATP	C2'-C3'	-3.11	1.44	1.53
19	B	601	ATP	C2'-C3'	-3.09	1.44	1.53
21	F	501	ADP	C2'-C3'	-2.86	1.45	1.53
21	D	501	ADP	C2'-C3'	-2.74	1.45	1.53
21	F	501	ADP	C3'-C4'	-2.62	1.46	1.53
22	Q	101	3PH	O21-C2	-2.59	1.40	1.46
19	A	601	ATP	O4'-C4'	2.52	1.50	1.45
21	D	501	ADP	C3'-C4'	-2.50	1.46	1.53
19	C	601	ATP	O4'-C4'	2.40	1.50	1.45
22	Q	101	3PH	O31-C31	2.32	1.40	1.33
19	B	601	ATP	O4'-C4'	2.29	1.50	1.45
22	Q	101	3PH	O31-C3	-2.25	1.40	1.45
19	C	601	ATP	C4-N3	-2.22	1.32	1.35
19	A	601	ATP	C4-N3	-2.20	1.32	1.35
19	B	601	ATP	C4-N3	-2.19	1.32	1.35
21	F	501	ADP	PA-O5'	2.13	1.67	1.59
21	D	501	ADP	PA-O5'	2.11	1.67	1.59
22	Q	101	3PH	O21-C21	2.10	1.40	1.34
21	F	501	ADP	C6-C5	-2.06	1.35	1.43
21	D	501	ADP	C6-C5	-2.02	1.35	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Q	101	3PH	O21-C21-C22	4.45	121.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	601	ATP	C3'-C2'-C1'	4.41	107.62	100.98
21	F	501	ADP	N3-C2-N1	-4.22	122.08	128.68
19	C	601	ATP	N3-C2-N1	-4.06	122.33	128.68
19	B	601	ATP	N3-C2-N1	-4.04	122.36	128.68
21	D	501	ADP	N3-C2-N1	-3.98	122.45	128.68
19	A	601	ATP	N3-C2-N1	-3.96	122.49	128.68
19	C	601	ATP	C3'-C2'-C1'	3.92	106.89	100.98
19	C	601	ATP	C4-C5-N7	-3.86	105.38	109.40
19	B	601	ATP	C4-C5-N7	-3.83	105.41	109.40
19	A	601	ATP	C4-C5-N7	-3.78	105.46	109.40
21	D	501	ADP	C4-C5-N7	-3.71	105.53	109.40
21	F	501	ADP	C4-C5-N7	-3.65	105.60	109.40
21	D	501	ADP	C3'-C2'-C1'	3.28	105.91	100.98
19	A	601	ATP	C3'-C2'-C1'	3.24	105.86	100.98
21	F	501	ADP	C3'-C2'-C1'	3.07	105.60	100.98
19	B	601	ATP	PB-O3B-PG	-2.88	122.94	132.83
22	Q	101	3PH	O31-C31-C32	2.67	120.28	111.91
19	A	601	ATP	PB-O3B-PG	-2.66	123.70	132.83
21	D	501	ADP	PA-O3A-PB	-2.59	123.94	132.83
21	F	501	ADP	C1'-N9-C4	-2.56	122.15	126.64
19	A	601	ATP	C2'-C3'-C4'	2.40	107.31	102.64
18	K	301	CDL	OA6-CA5-C11	2.39	116.66	111.50
19	A	601	ATP	C1'-N9-C4	-2.38	122.46	126.64
19	C	601	ATP	PB-O3B-PG	-2.36	124.72	132.83
19	B	601	ATP	C1'-N9-C4	-2.30	122.59	126.64
21	F	501	ADP	PA-O3A-PB	-2.27	125.05	132.83
19	C	601	ATP	PA-O3A-PB	-2.26	125.06	132.83
19	B	601	ATP	C2'-C3'-C4'	2.24	106.99	102.64
21	D	501	ADP	C1'-N9-C4	-2.24	122.71	126.64
19	C	601	ATP	C1'-N9-C4	-2.19	122.79	126.64
19	A	601	ATP	PA-O3A-PB	-2.18	125.33	132.83
19	C	601	ATP	C2'-C3'-C4'	2.17	106.85	102.64

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	K	301	CDL	CA2-OA2-PA1-OA3
18	K	301	CDL	CA3-OA5-PA1-OA4
18	K	301	CDL	C11-CA5-OA6-CA4
18	K	301	CDL	CB2-OB2-PB2-OB3
18	K	301	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
18	K	301	CDL	CB2-OB2-PB2-OB5
18	K	301	CDL	CB3-OB5-PB2-OB3
18	R	101	CDL	O1-C1-CB2-OB2
18	R	101	CDL	CA2-OA2-PA1-OA4
18	R	101	CDL	C11-CA5-OA6-CA4
19	C	601	ATP	PB-O3B-PG-O2G
21	F	501	ADP	PA-O3A-PB-O3B
21	F	501	ADP	C5'-O5'-PA-O3A
21	D	501	ADP	C5'-O5'-PA-O3A
18	K	301	CDL	OA9-CA7-OA8-CA6
18	K	301	CDL	OA7-CA5-OA6-CA4
18	R	101	CDL	OA7-CA5-OA6-CA4
18	R	101	CDL	OA9-CA7-OA8-CA6
18	K	301	CDL	C31-CA7-OA8-CA6
18	R	101	CDL	C31-CA7-OA8-CA6
19	C	601	ATP	O4'-C4'-C5'-O5'
18	K	301	CDL	CA2-C1-CB2-OB2
18	K	301	CDL	OA5-CA3-CA4-OA6
22	Q	101	3PH	O11-C1-C2-O21
18	K	301	CDL	O1-C1-CB2-OB2
18	K	301	CDL	CB7-C71-C72-C73
21	D	501	ADP	C3'-C4'-C5'-O5'
18	R	101	CDL	CB7-C71-C72-C73
18	K	301	CDL	CA3-OA5-PA1-OA2
18	K	301	CDL	CB3-OB5-PB2-OB2
18	R	101	CDL	CA2-C1-CB2-OB2
22	Q	101	3PH	C32-C31-O31-C3
18	K	301	CDL	CA6-CA4-OA6-CA5
18	K	301	CDL	C54-C55-C56-C57
18	K	301	CDL	C82-C83-C84-C85
18	K	301	CDL	C31-C32-C33-C34
22	Q	101	3PH	O32-C31-O31-C3
18	K	301	CDL	C52-C53-C54-C55
18	K	301	CDL	C75-C76-C77-C78
18	K	301	CDL	C77-C78-C79-C80
21	D	501	ADP	O4'-C4'-C5'-O5'
18	K	301	CDL	C51-CB5-OB6-CB4
18	K	301	CDL	C58-C59-C60-C61
18	K	301	CDL	C71-C72-C73-C74
18	K	301	CDL	OB7-CB5-OB6-CB4
18	R	101	CDL	CA3-CA4-CA6-OA8
18	R	101	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
22	Q	101	3PH	C1-C2-C3-O31
22	Q	101	3PH	C34-C35-C36-C37
19	C	601	ATP	C3'-C4'-C5'-O5'
18	K	301	CDL	CA5-C11-C12-C13
18	K	301	CDL	C73-C74-C75-C76
18	R	101	CDL	CA3-CA4-OA6-CA5
18	R	101	CDL	C72-C73-C74-C75
18	K	301	CDL	CB5-C51-C52-C53
18	K	301	CDL	OA5-CA3-CA4-CA6
22	Q	101	3PH	O11-C1-C2-C3
18	K	301	CDL	CB3-CB4-CB6-OB8
18	R	101	CDL	OB5-CB3-CB4-OB6
18	R	101	CDL	CB5-C51-C52-C53
18	K	301	CDL	C32-C33-C34-C35
18	R	101	CDL	C51-C52-C53-C54
18	R	101	CDL	OB5-CB3-CB4-CB6
18	K	301	CDL	CA2-OA2-PA1-OA5
18	K	301	CDL	CB3-OB5-PB2-OB4
21	F	501	ADP	C5'-O5'-PA-O1A
21	F	501	ADP	C5'-O5'-PA-O2A
21	D	501	ADP	C5'-O5'-PA-O1A
21	D	501	ADP	C5'-O5'-PA-O2A
18	K	301	CDL	C71-CB7-OB8-CB6
18	K	301	CDL	OB6-CB4-CB6-OB8
18	R	101	CDL	OA6-CA4-CA6-OA8
18	R	101	CDL	OB6-CB4-CB6-OB8
22	Q	101	3PH	O21-C2-C3-O31
18	K	301	CDL	OB9-CB7-OB8-CB6
18	K	301	CDL	C79-C80-C81-C82
19	C	601	ATP	PB-O3A-PA-O1A
22	Q	101	3PH	C23-C24-C25-C26
18	K	301	CDL	C12-C13-C14-C15
18	R	101	CDL	CA5-C11-C12-C13
18	K	301	CDL	CB2-C1-CA2-OA2
19	A	601	ATP	PB-O3A-PA-O2A
21	F	501	ADP	C3'-C4'-C5'-O5'
18	R	101	CDL	CA4-CA3-OA5-PA1
19	A	601	ATP	PB-O3B-PG-O1G
21	F	501	ADP	PA-O3A-PB-O1B
22	Q	101	3PH	O21-C21-C22-C23
21	F	501	ADP	O4'-C4'-C5'-O5'
21	D	501	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
18	K	301	CDL	OA6-CA4-CA6-OA8
19	B	601	ATP	C5'-O5'-PA-O3A
19	C	601	ATP	PB-O3A-PA-O2A
22	Q	101	3PH	O22-C21-C22-C23
18	R	101	CDL	CA2-OA2-PA1-OA3
19	A	601	ATP	C5'-O5'-PA-O1A
19	B	601	ATP	C5'-O5'-PA-O2A
19	C	601	ATP	C5'-O5'-PA-O1A

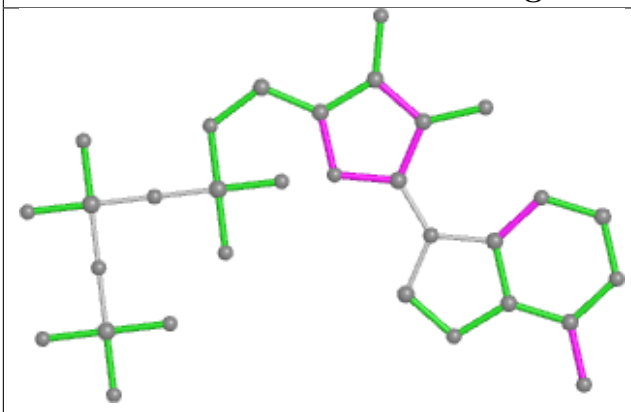
There are no ring outliers.

4 monomers are involved in 10 short contacts:

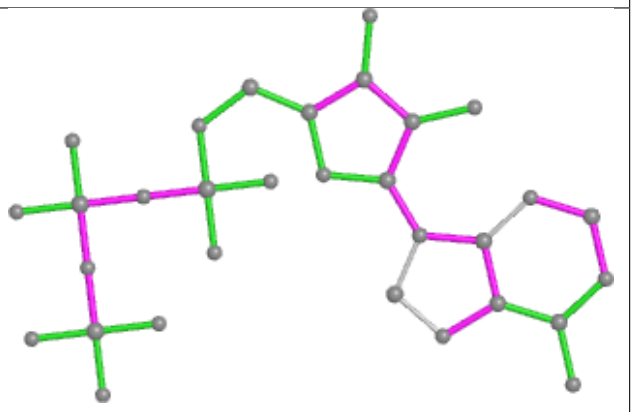
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Q	101	3PH	1	0
21	D	501	ADP	1	0
18	R	101	CDL	3	0
18	K	301	CDL	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

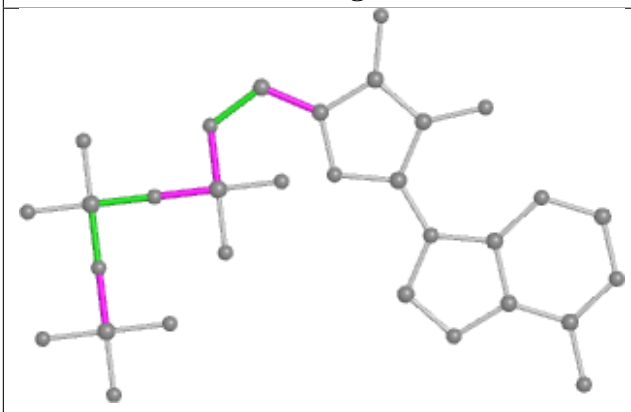
Ligand ATP C 601



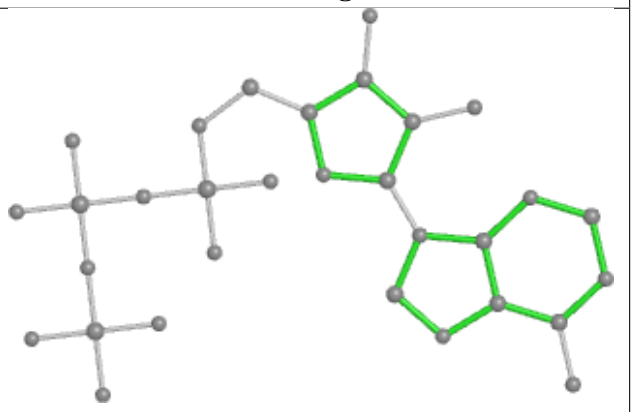
Bond lengths



Bond angles

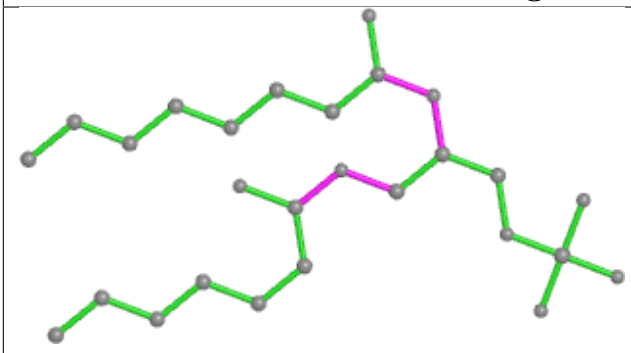


Torsions

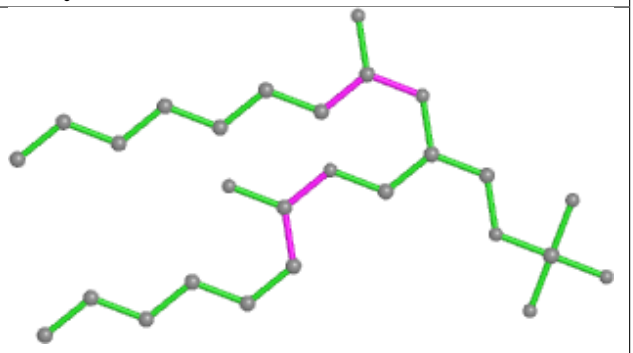


Rings

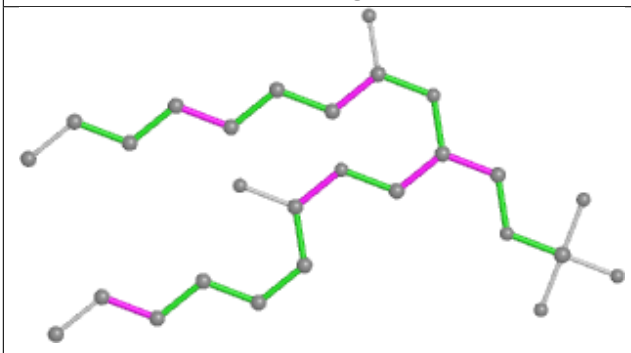
Ligand 3PH Q 101



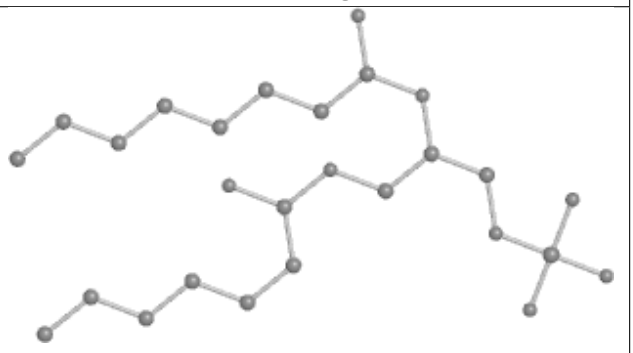
Bond lengths



Bond angles

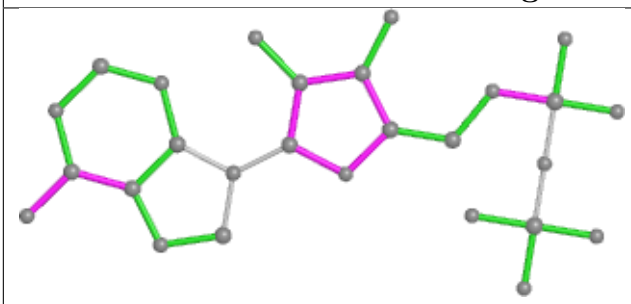


Torsions

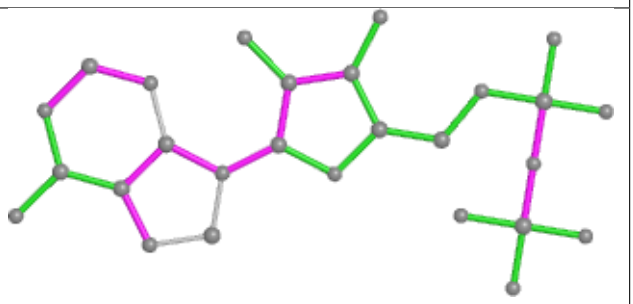


Rings

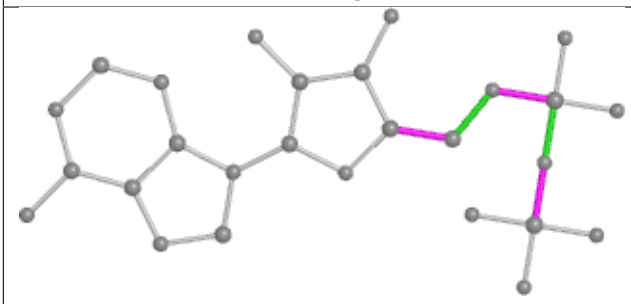
Ligand ADP D 501



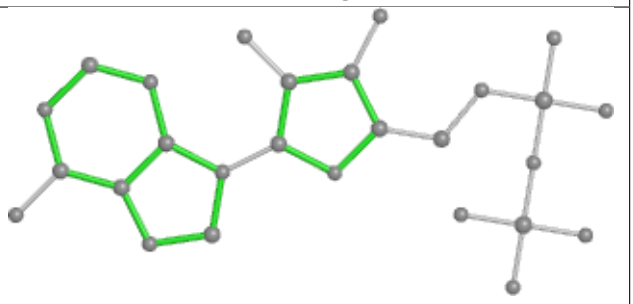
Bond lengths



Bond angles

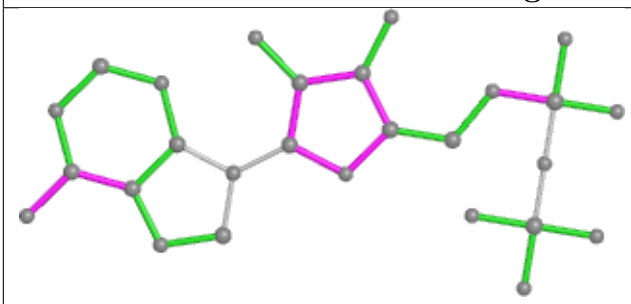


Torsions

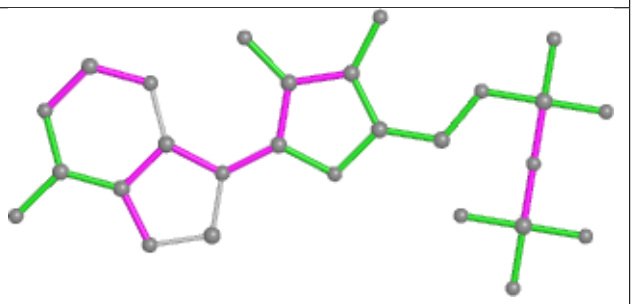


Rings

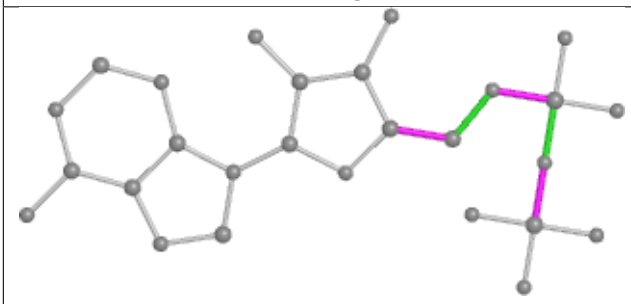
Ligand ADP F 501



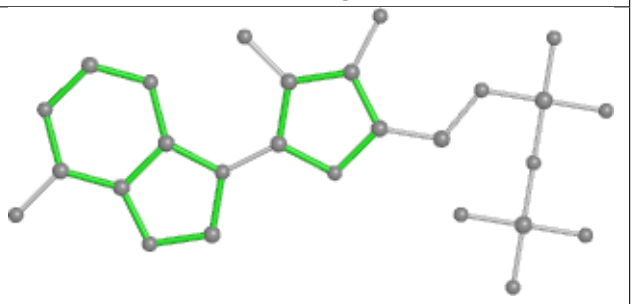
Bond lengths



Bond angles

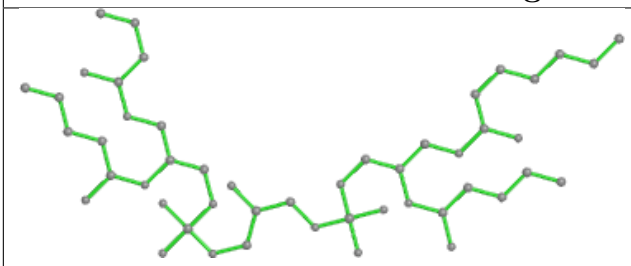


Torsions

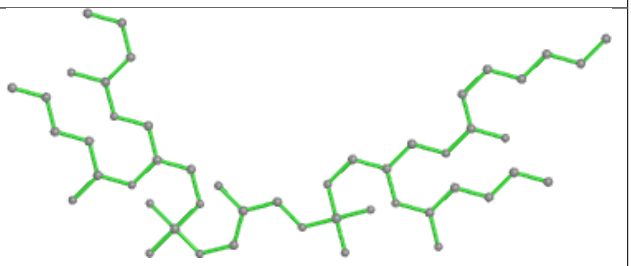


Rings

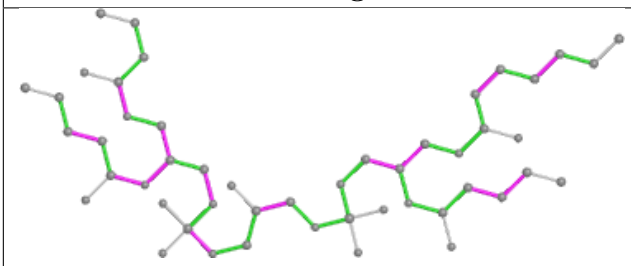
Ligand CDL R 101



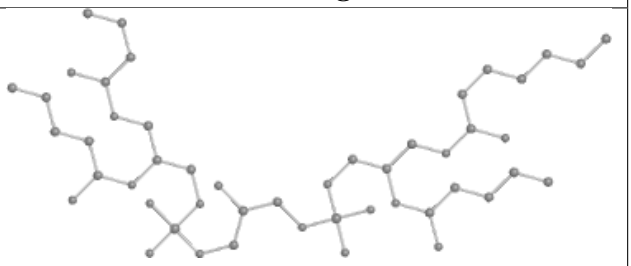
Bond lengths



Bond angles

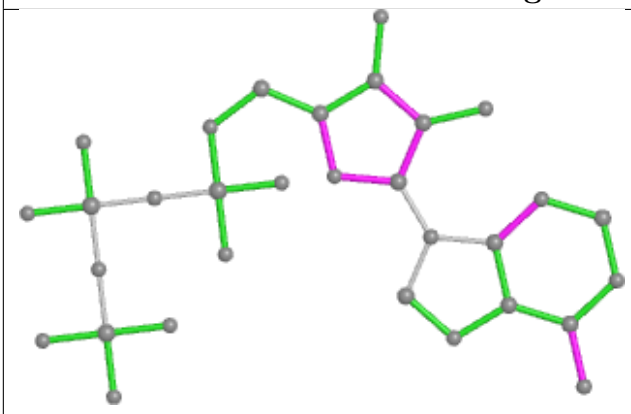


Torsions

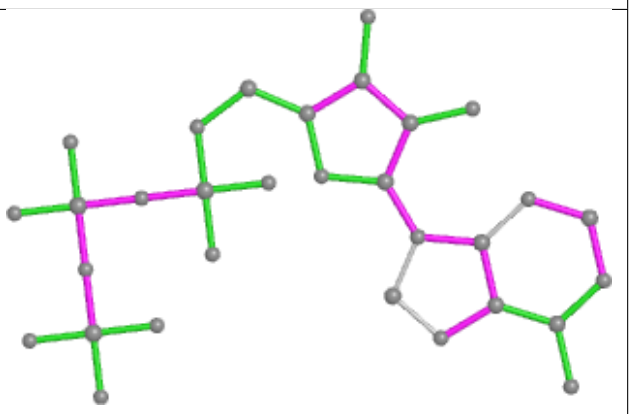


Rings

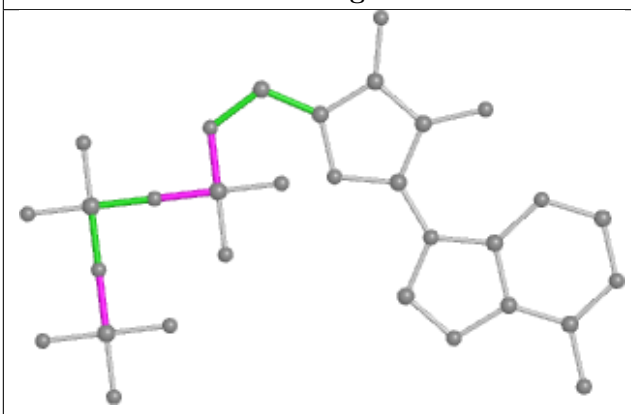
Ligand ATP A 601



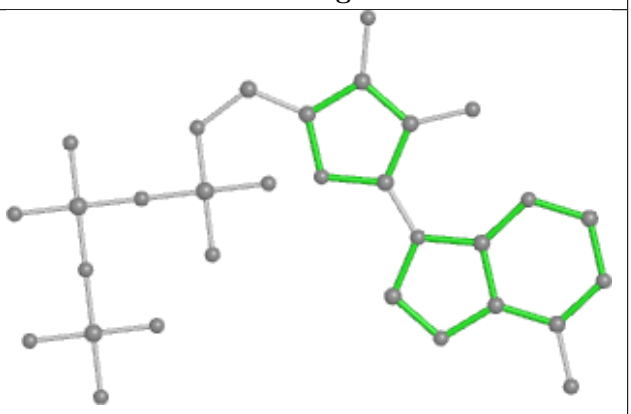
Bond lengths



Bond angles

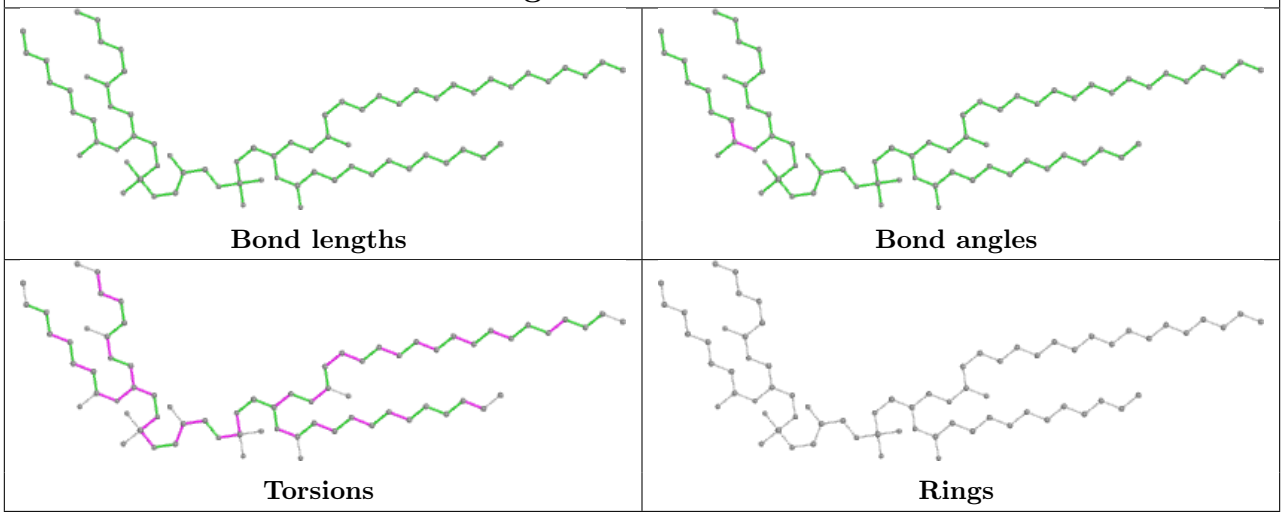


Torsions

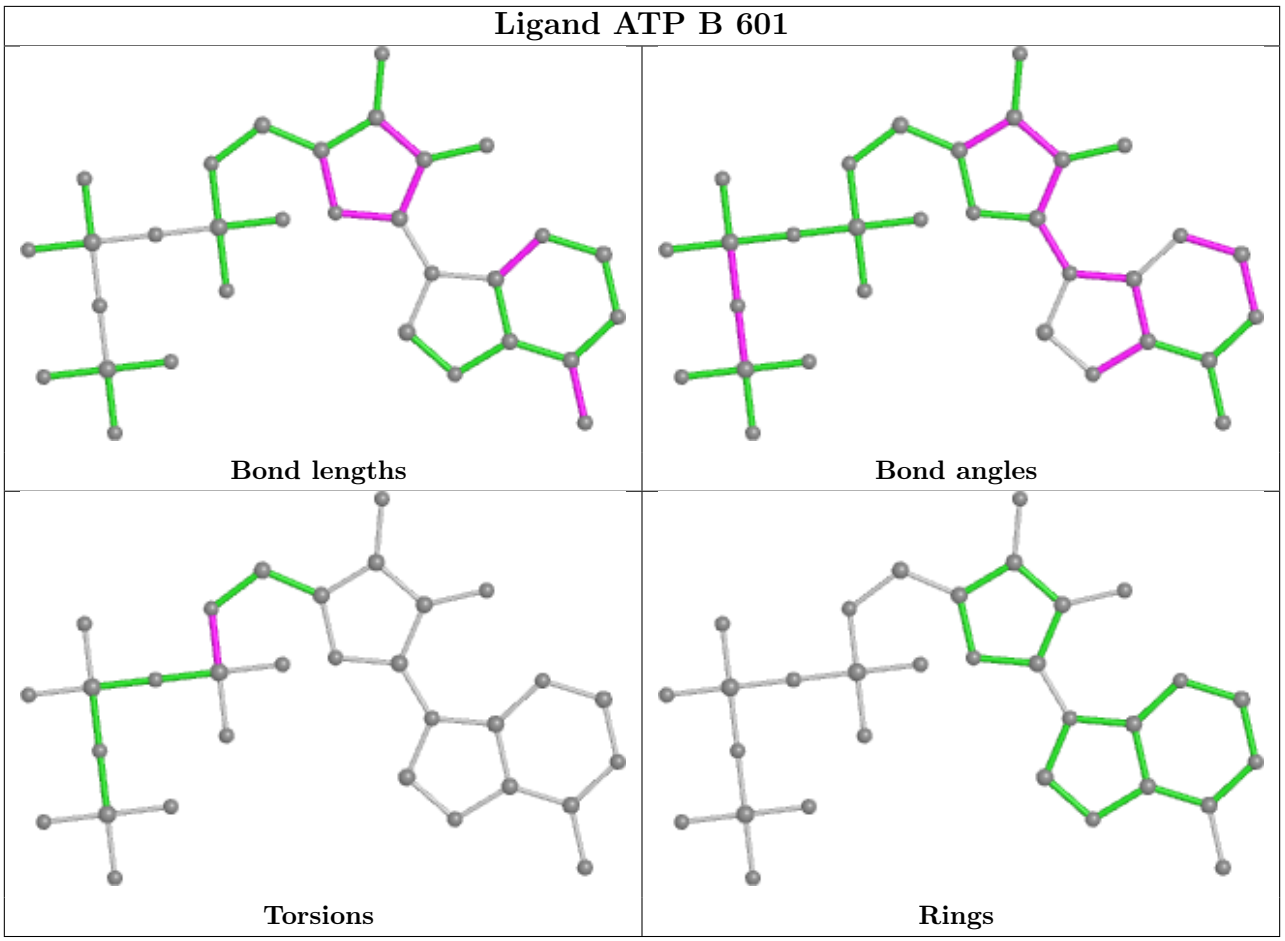


Rings

Ligand CDL K 301



Ligand ATP B 601



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.

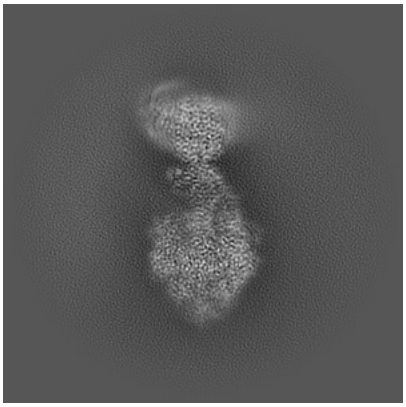
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34580. These allow visual inspection of the internal detail of the map and identification of artifacts.

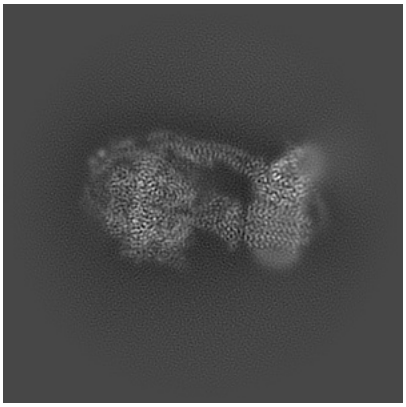
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

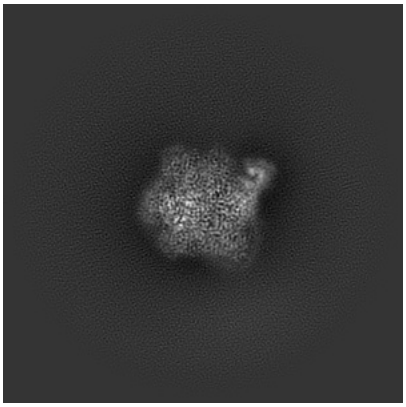
6.1.1 Primary map



X



Y

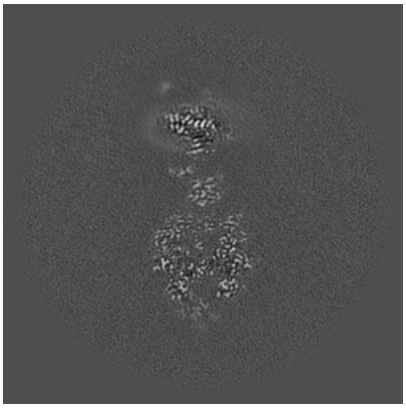


Z

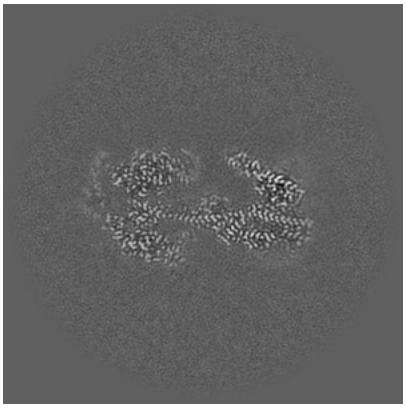
The images above show the map projected in three orthogonal directions.

6.2 Central slices

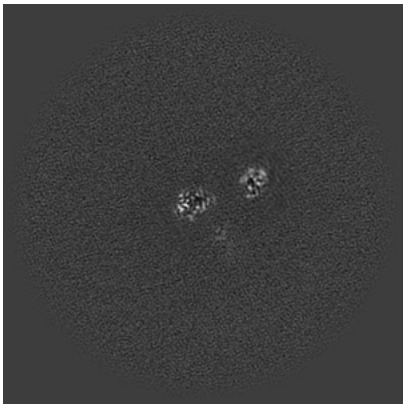
6.2.1 Primary map



X Index: 256



Y Index: 256

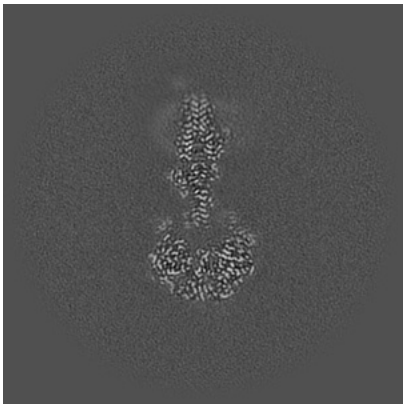


Z Index: 256

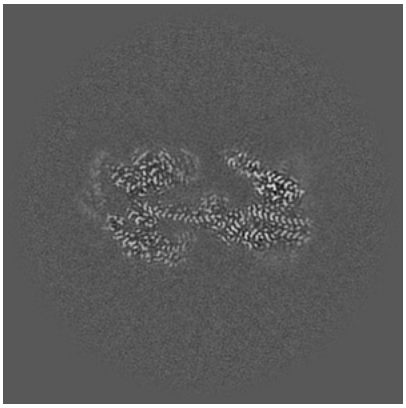
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

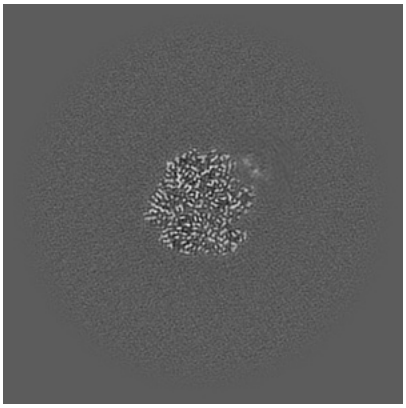
6.3.1 Primary map



X Index: 234



Y Index: 257

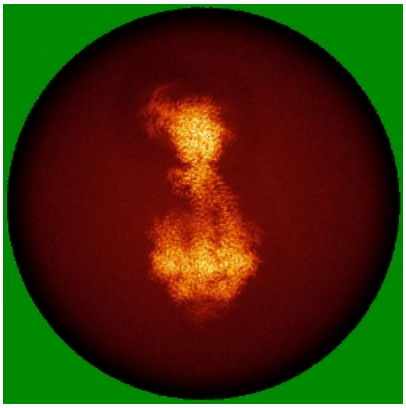


Z Index: 176

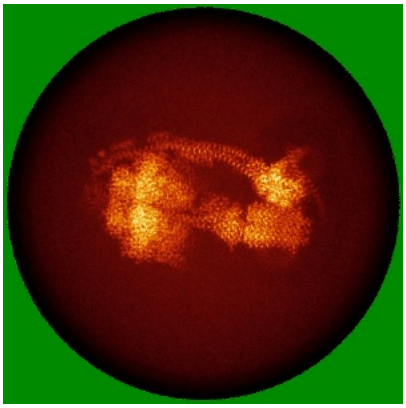
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

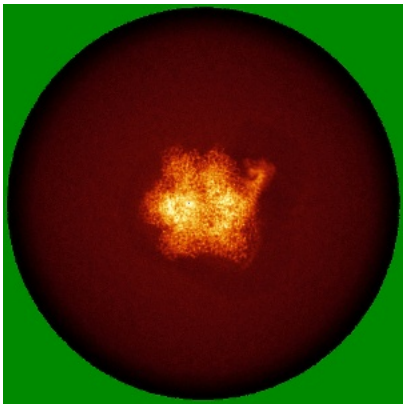
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

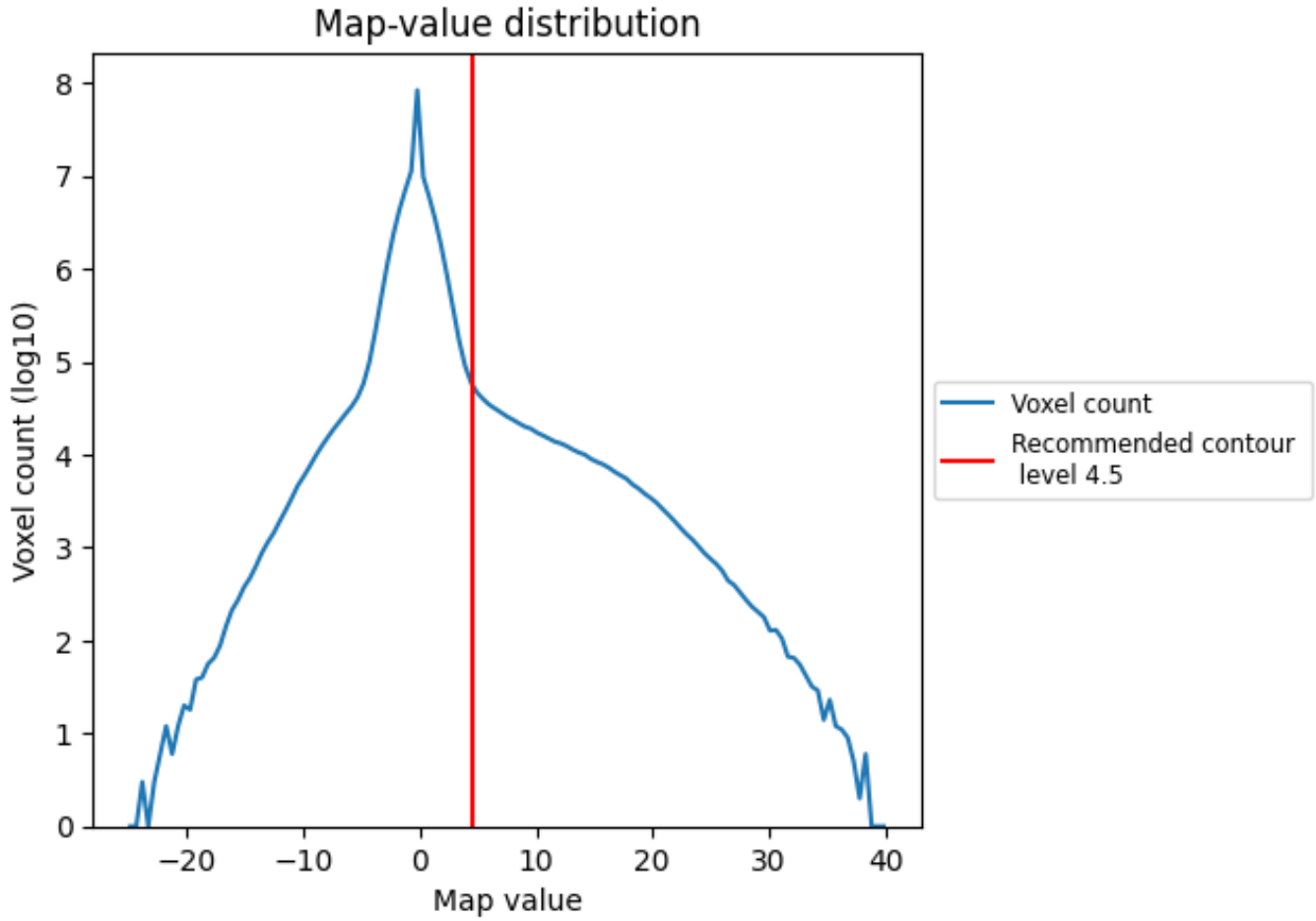
6.6 Mask visualisation (i)

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

7 Map analysis

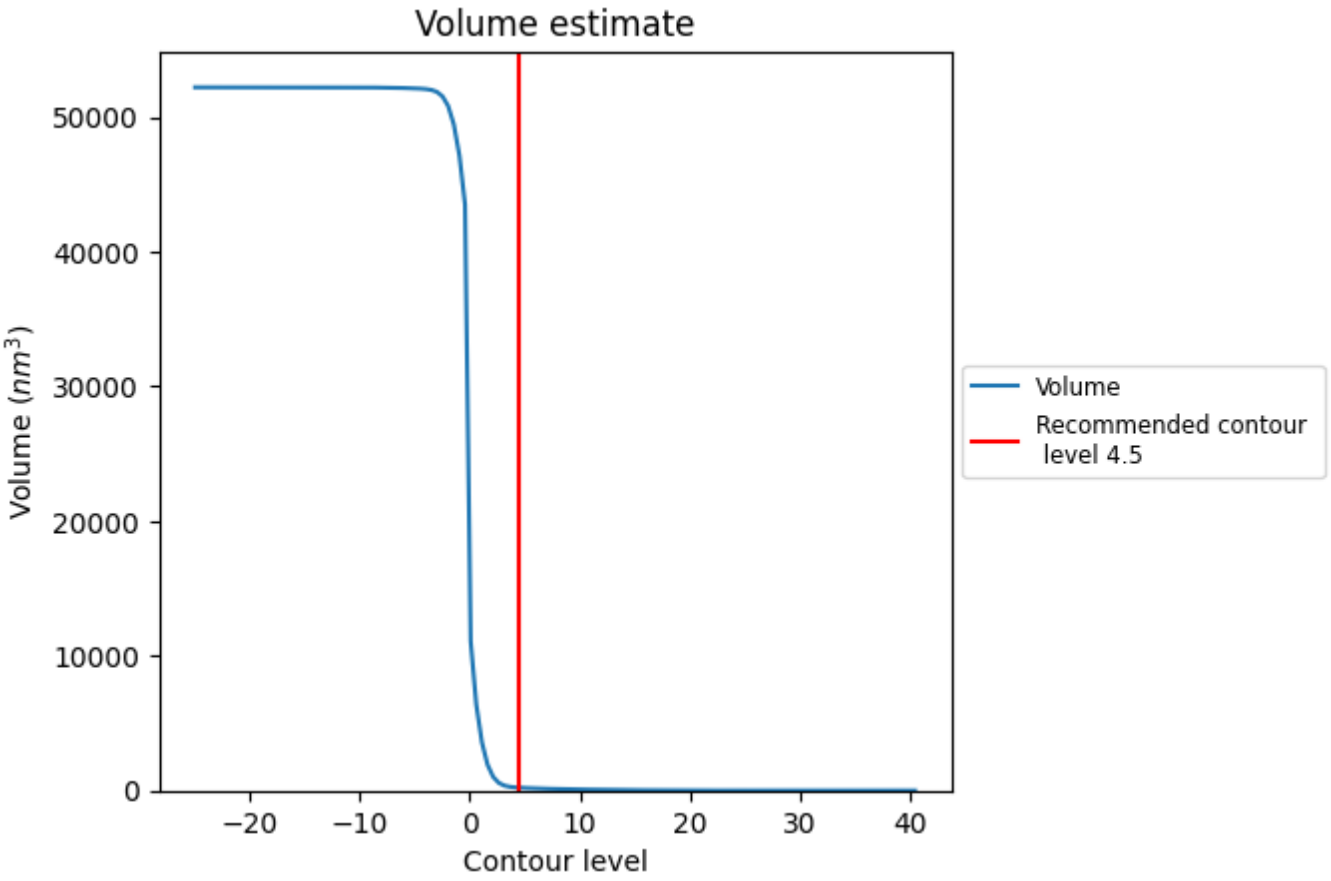
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

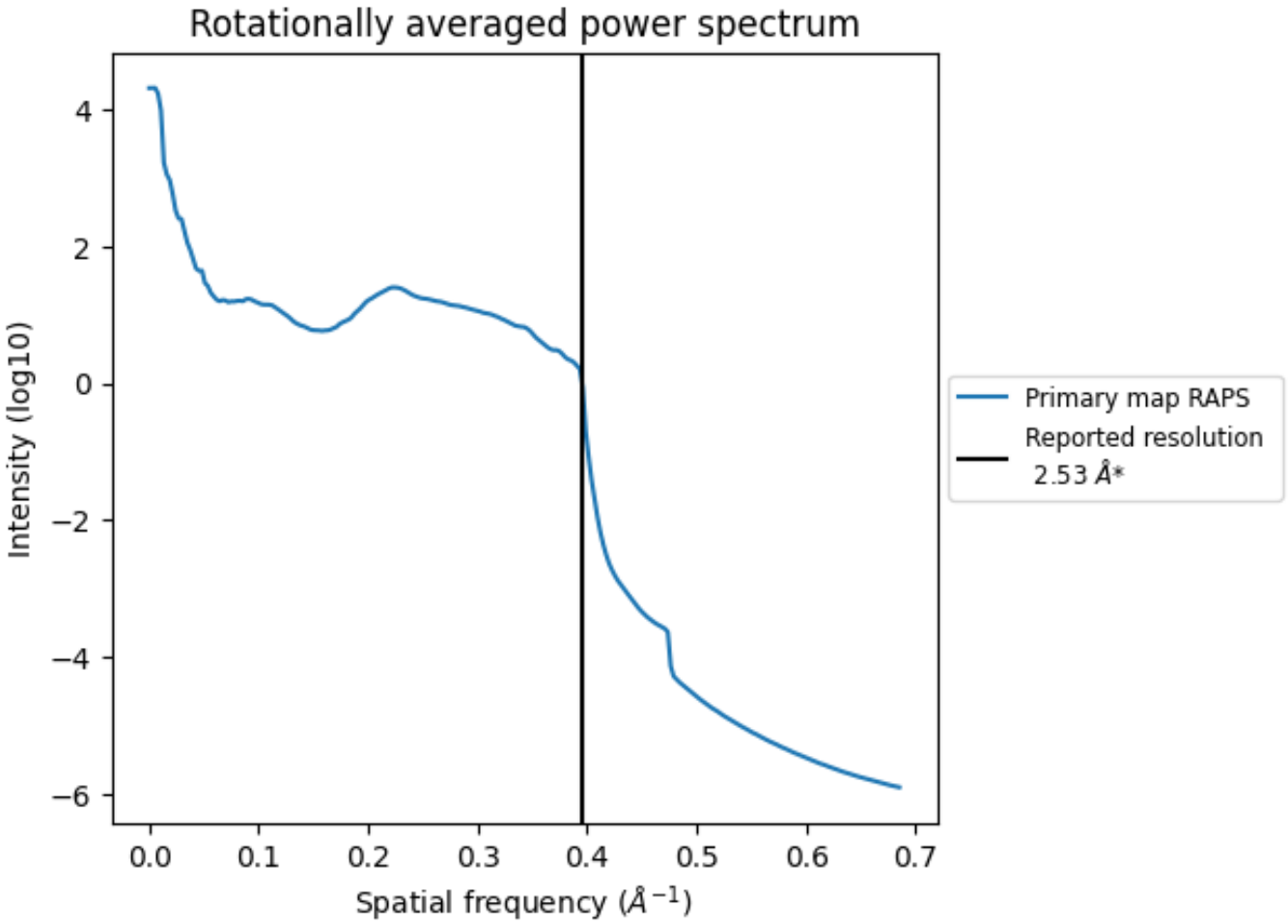
7.2 Volume estimate



The volume at the recommended contour level is 214 nm^3; this corresponds to an approximate mass of 194 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.395 Å^{-1}

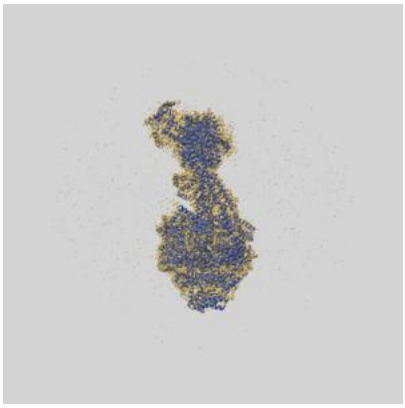
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

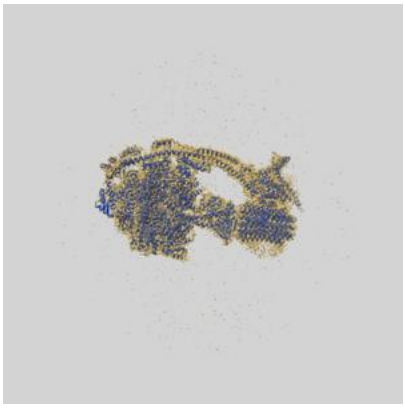
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34580 and PDB model 8H9S. Per-residue inclusion information can be found in section 3 on page 10.

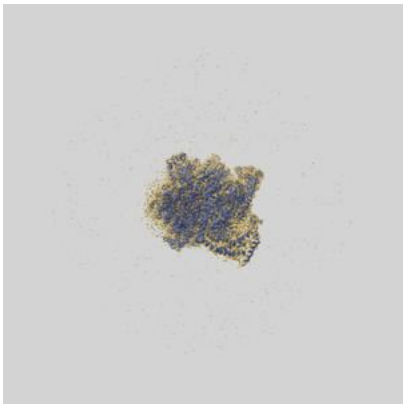
9.1 Map-model overlay



X



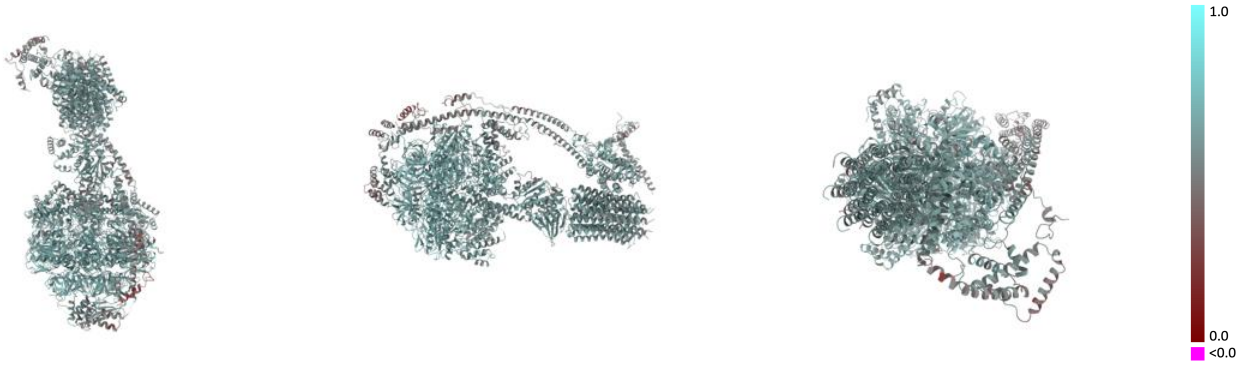
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

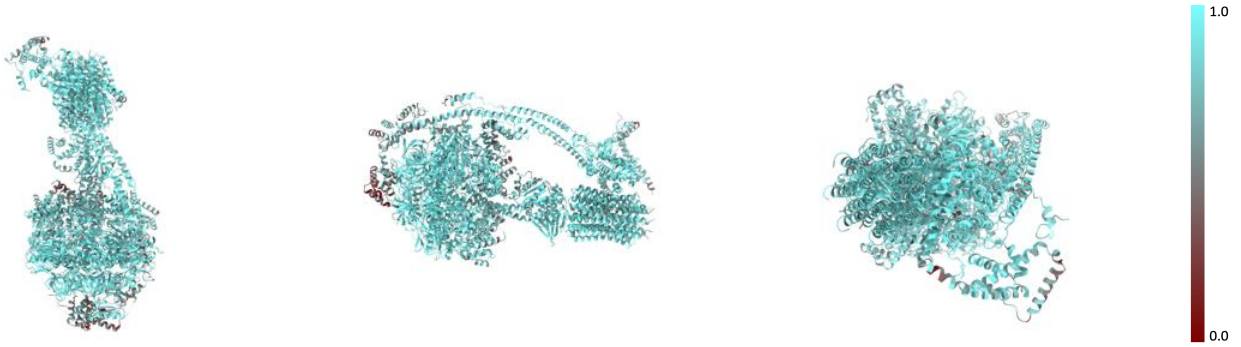
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

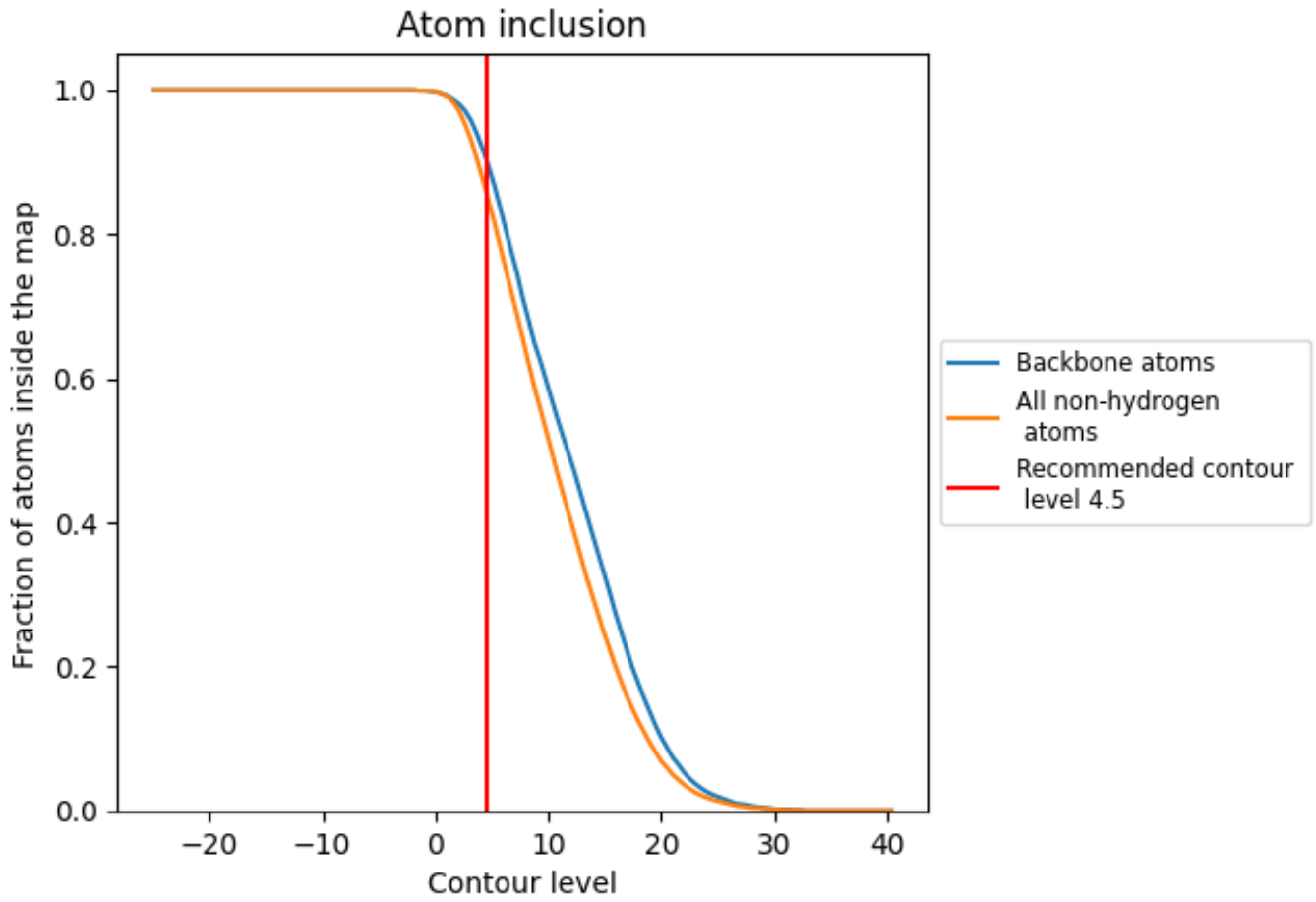
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8600	0.6010
1	0.8720	0.5900
2	0.8700	0.5840
3	0.8770	0.5940
4	0.8570	0.5810
5	0.8590	0.5800
6	0.8750	0.5830
7	0.8790	0.5840
8	0.8590	0.5720
A	0.8900	0.6350
B	0.9060	0.6320
C	0.8660	0.6170
D	0.8870	0.6330
E	0.9080	0.6370
F	0.9200	0.6430
G	0.8290	0.6020
H	0.9120	0.6010
I	0.8840	0.6040
J	0.6600	0.6030
K	0.8590	0.5360
L	0.6050	0.3970
M	0.8120	0.5140
N	0.8950	0.5920
O	0.5220	0.5170
P	0.8270	0.5590
Q	0.8610	0.5520
R	0.8660	0.5660
S	0.7160	0.4980
T	0.6840	0.4750