Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 12:06 AM EST

PDB ID	:	6EF3
EMDB ID	:	EMD-9045
Title	:	Yeast 26S proteasome bound to ubiquitinated substrate (4D motor state)
Authors	:	de la Pena, A.H.; Goodall, E.A.; Gates, S.N.; Lander, G.C.; Martin, A.
Deposited on	:	2018-08-15
Resolution	:	4.17 Å(reported)
Based on initial model	:	5MPC

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:

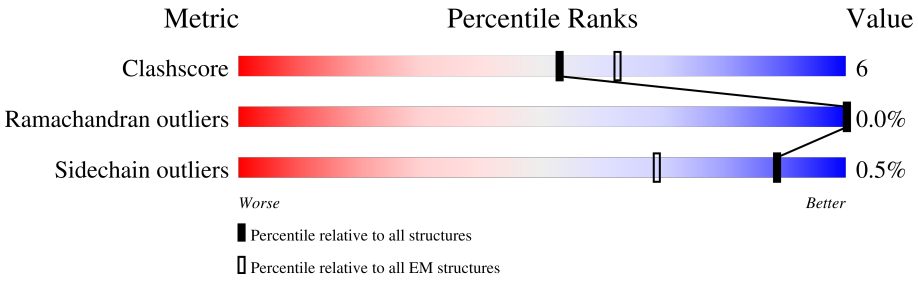
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.17 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1	215	8% 78% 13% 9%
2	2	261	7% 74% 12% 14%
3	3	205	9% 83% 16%
4	4	198	15% 83% 16%
5	5	287	9% 65% 8% 26%
6	6	241	17% 82% 9% 9%
7	7	266	6% 66% 12% 22%
8	A	252	83% 15%

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Mol	Chain	Length	Quality of chain
9	B	250	5% 81% 19%
10	C	258	7% 78% 15% 6%
11	D	254	5% 80% 15% 5%
12	E	260	83% 12%
13	F	234	87% 13%
14	G	288	77% 8% 15%
15	H	467	73% 8% 19%
16	I	437	70% 18% 12%
17	J	405	8% 80% 15% 5%
18	K	428	8% 72% 14% 14%
19	L	437	17% 71% 11% 18%
20	M	434	5% 76% 9% 15%
21	n	15	100%
22	r	306	9% 92% 8%
23	s	38	61% 100%
24	u	128	23% 59% 41%

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 44271 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 Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	196	1496	948	248	293	7	0	0

- Molecule 2 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	224	1685	1065	290	323	7	0	0

- Molecule 3 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	204	1575	1008	257	302	8	0	0

- Molecule 4 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	195	1560	992	264	298	6	0	0

- Molecule 5 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	212	1644	1045	280	312	7	0	0

- Molecule 6 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	220	1727	1101	299	323	4	0	0

- Molecule 7 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	208	Total	C	N	O	S	0	0
			1598	1011	272	309	6		

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	247	Total	C	N	O	S	0	0
			1922	1223	323	368	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1901	1211	313	374	3		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	242	Total	C	N	O	S	0	0
			1864	1183	314	364	3		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	241	Total	C	N	O	S	0	0
			1878	1175	330	369	4		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	249	Total	C	N	O	S	0	0
			1918	1201	323	387	7		

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	234	Total	C	N	O	S	0	0
			1796	1131	313	348	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	246	Total	C	N	O	S	0	0
			1903	1211	329	359	4		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	380	Total	C	N	O	S	0	0
			2889	1820	513	540	16		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	384	Total	C	N	O	S	0	0
			2871	1810	491	553	17		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	383	Total	C	N	O	S	0	0
			2918	1837	529	537	15		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	370	Total	C	N	O	S	0	0
			2761	1746	491	516	8		

- Molecule 19 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	360	Total	C	N	O	S	0	0
			2525	1603	456	457	9		

- Molecule 20 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	371	Total	C	N	O	S	0	0
			2717	1718	474	516	9		

- Molecule 21 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	n	15	Total	C	N	O	0	0
			123	82	21	20		

- Molecule 22 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	280	Total	C	N	O	S	0	0
			2088	1308	350	418	12		

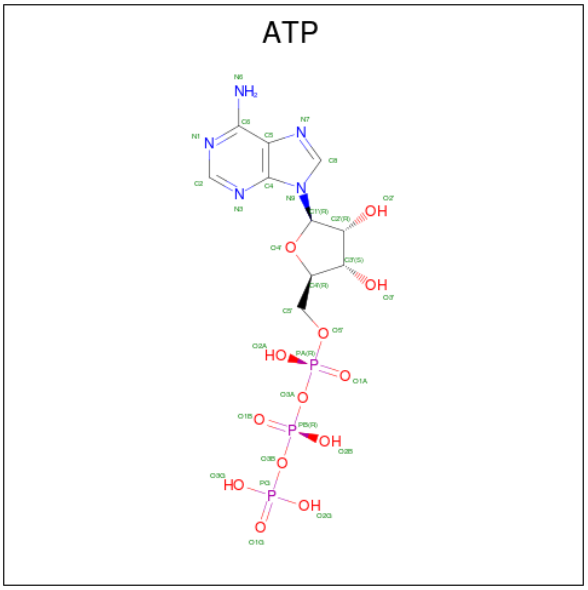
- Molecule 23 is a protein called Model substrate polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	38	Total	C	N	O	0	0
			253	155	56	42		

- Molecule 24 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	u	75	Total	C	N	O	0	0
			481	307	88	86		

- Molecule 25 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
25	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

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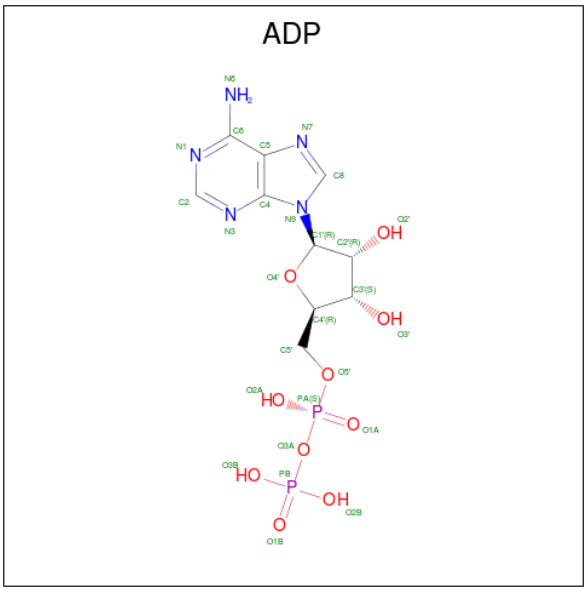
Mol	Chain	Residues	Atoms					AltConf
25	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
25	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
25	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 26 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

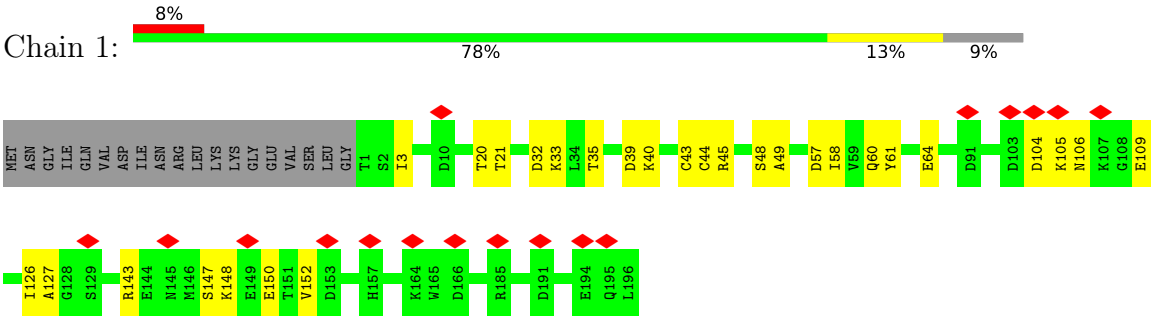


Mol	Chain	Residues	Atoms					AltConf
26	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
26	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

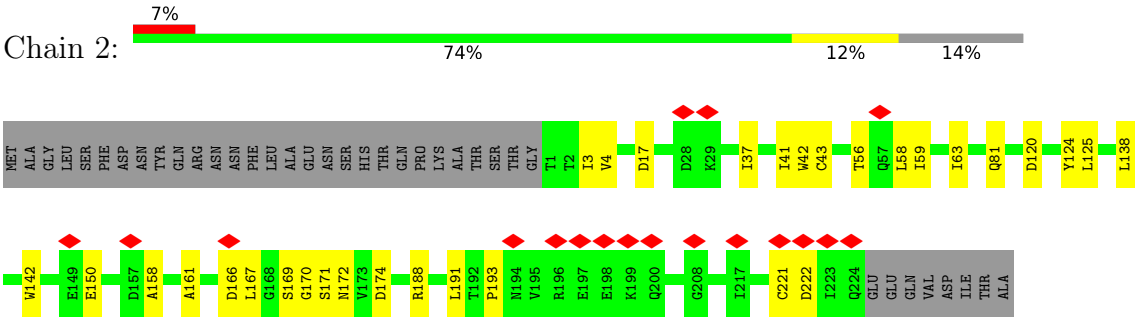
3 Residue-property plots (i)

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.

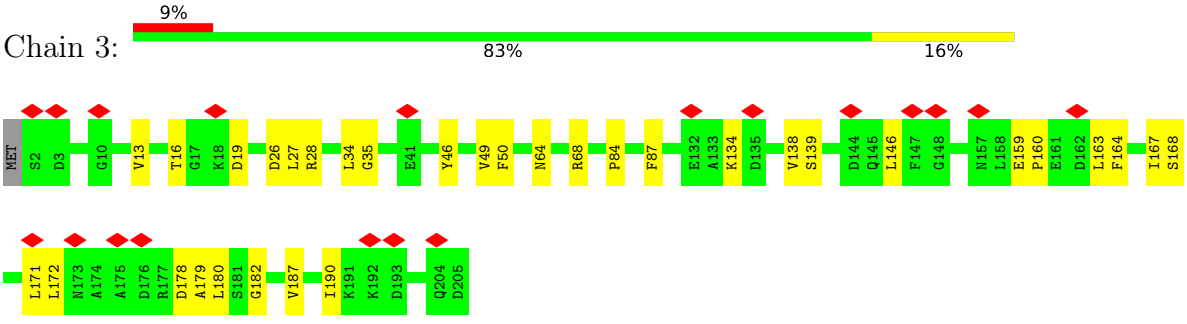
• Molecule 1: Proteasome subunit beta type-1



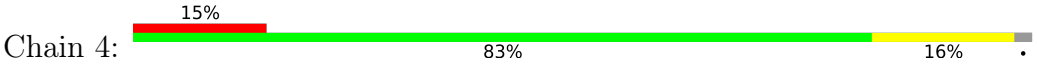
• Molecule 2: Proteasome subunit beta type-2

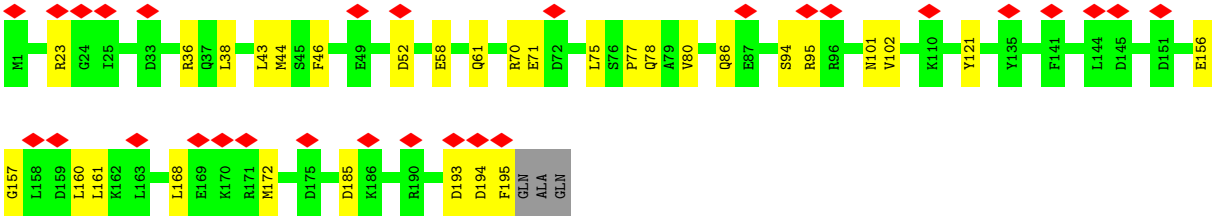


• Molecule 3: Proteasome subunit beta type-3

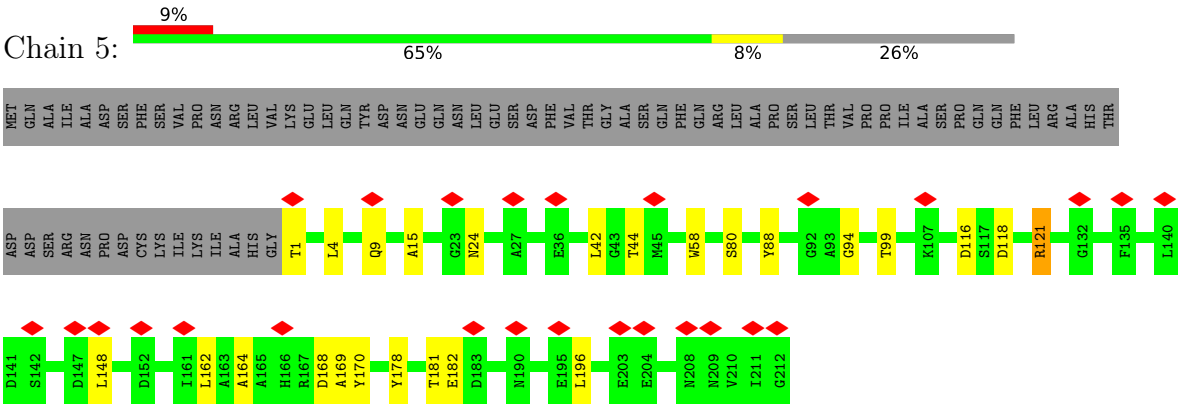


• Molecule 4: Proteasome subunit beta type-4

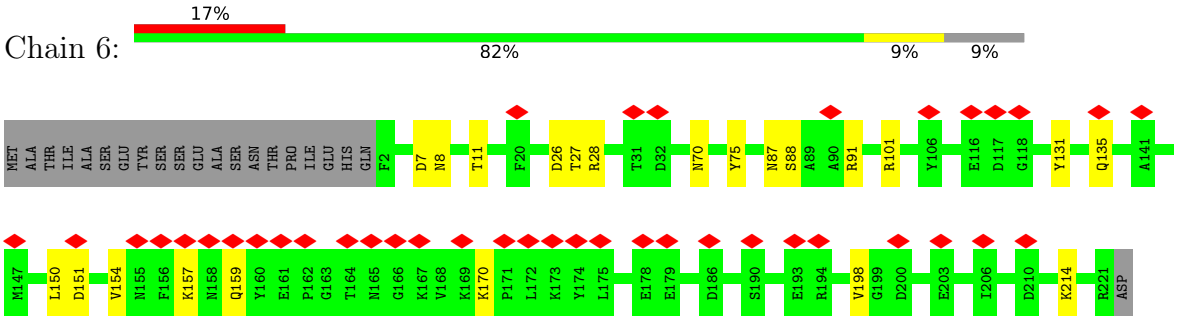




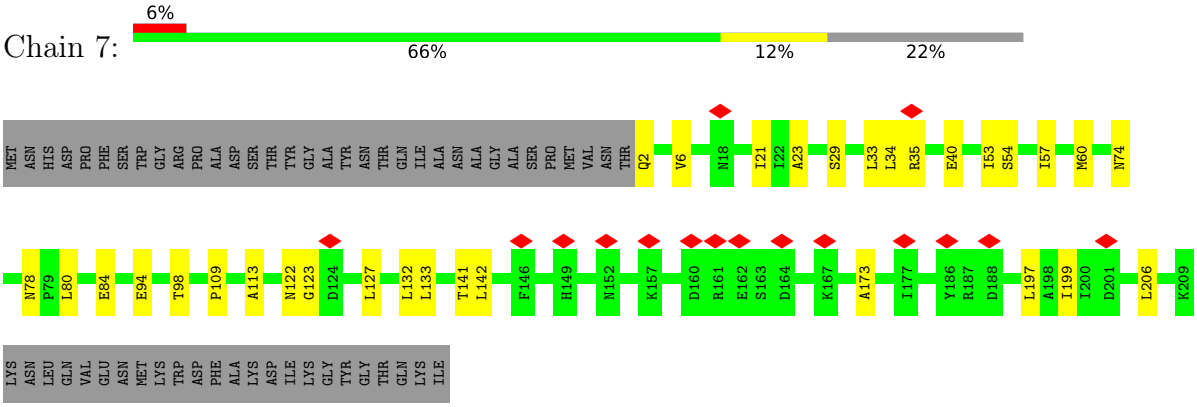
• Molecule 5: Proteasome subunit beta type-5



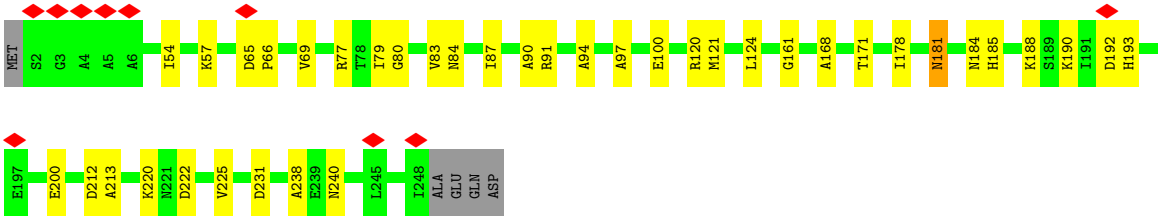
• Molecule 6: Proteasome subunit beta type-6



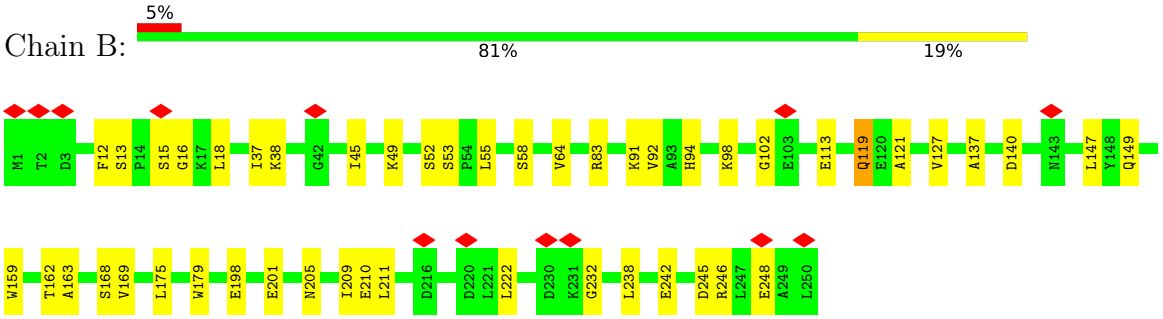
• Molecule 7: Proteasome subunit beta type-7



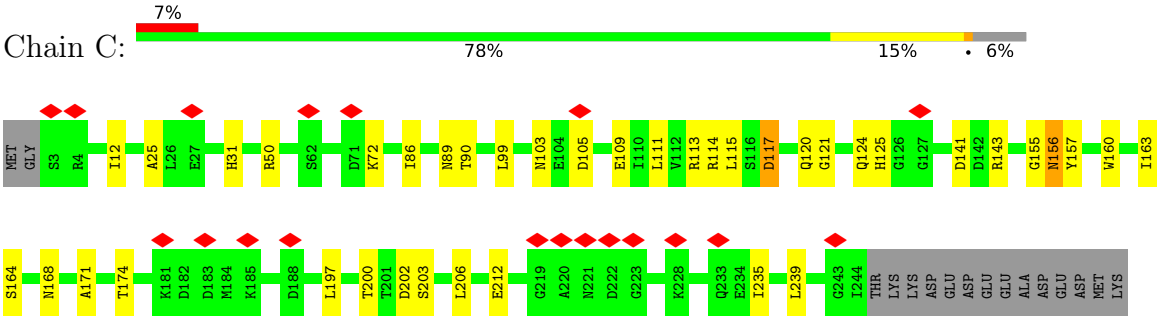
• Molecule 8: Proteasome subunit alpha type-1



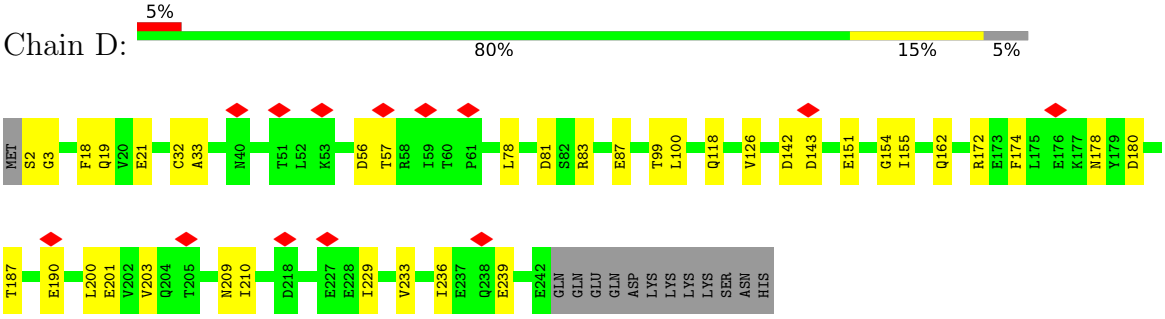
• Molecule 9: Proteasome subunit alpha type-2



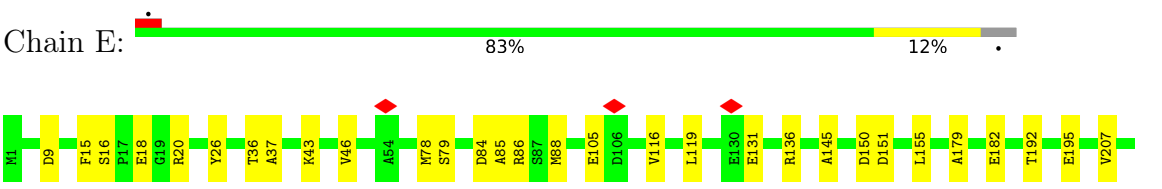
• Molecule 10: Proteasome subunit alpha type-3

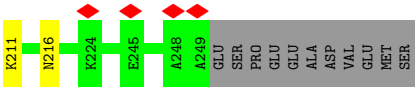


• Molecule 11: Proteasome subunit alpha type-4



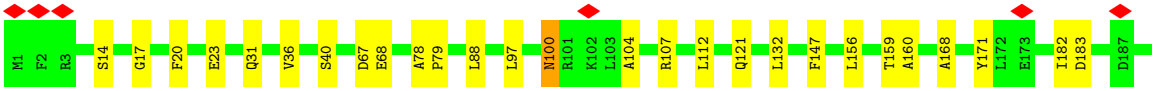
• Molecule 12: Proteasome subunit alpha type-5

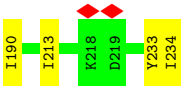




• Molecule 13: Proteasome subunit alpha type-6

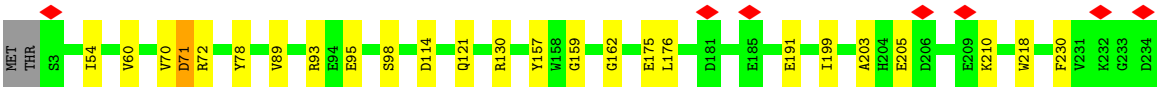
Chain F:

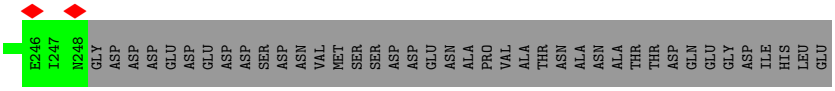




• Molecule 14: Probable proteasome subunit alpha type-7

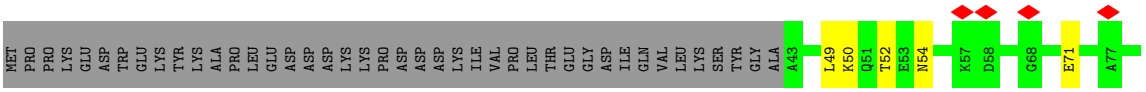
Chain G:

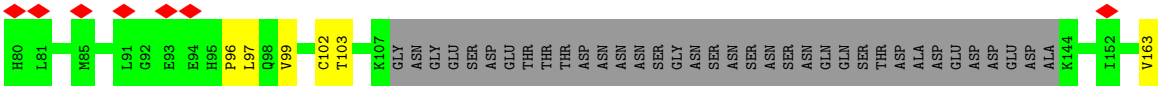


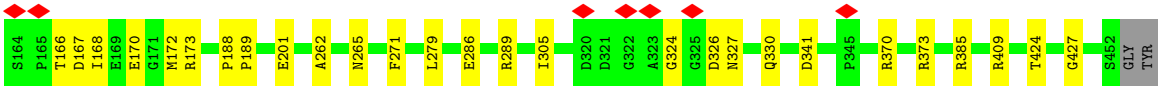


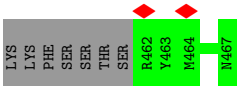
• Molecule 15: 26S proteasome regulatory subunit 7 homolog

Chain H:



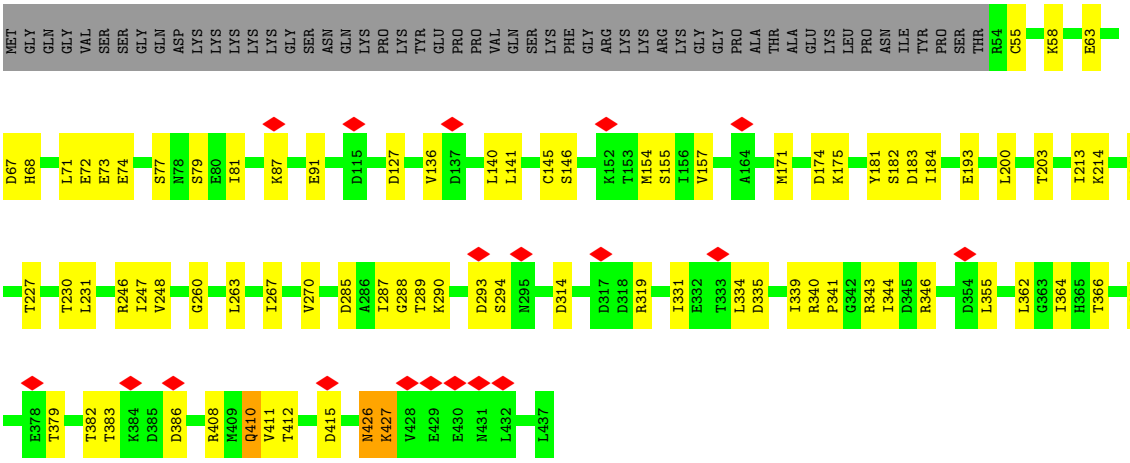






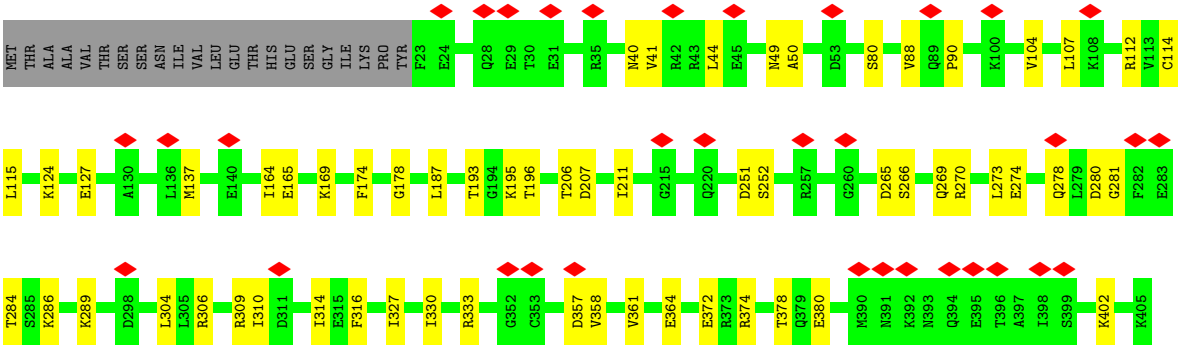
• Molecule 16: 26S proteasome regulatory subunit 4 homolog

Chain I:



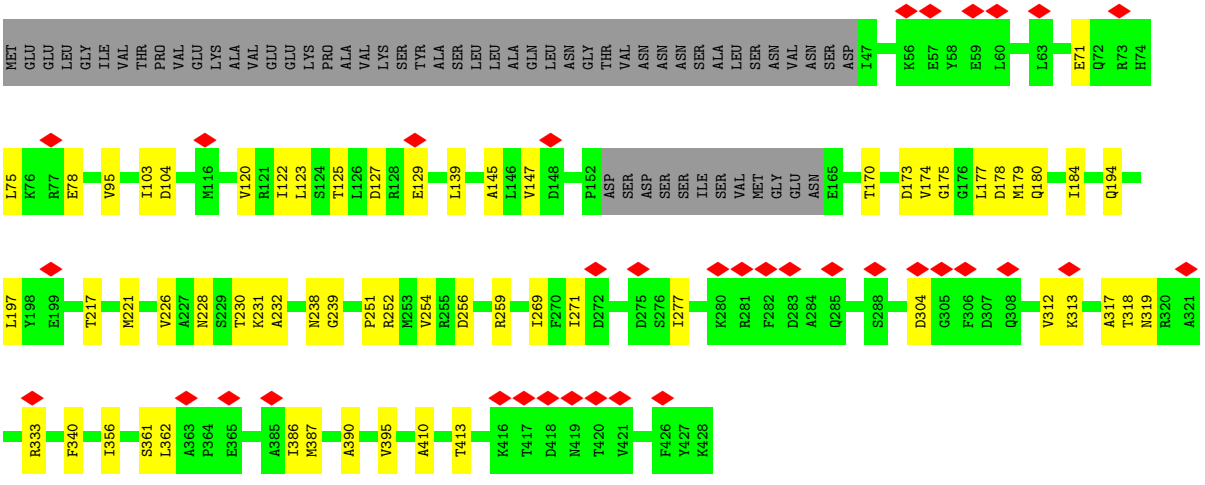
• Molecule 17: 26S proteasome regulatory subunit 8 homolog

Chain J:



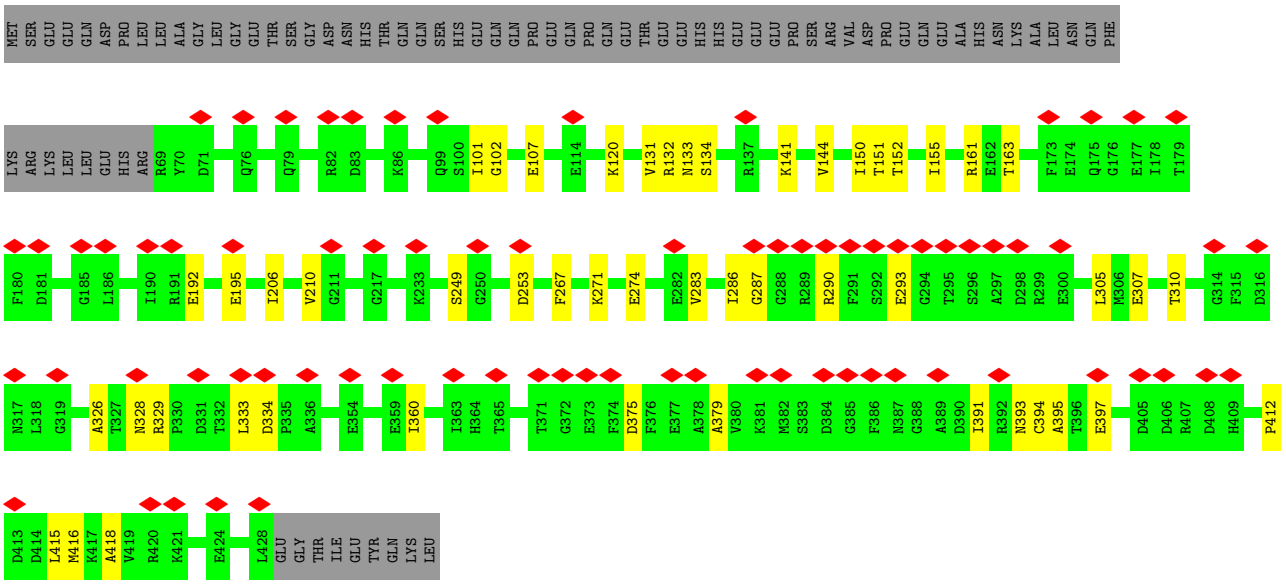
• Molecule 18: 26S proteasome regulatory subunit 6B homolog

Chain K:

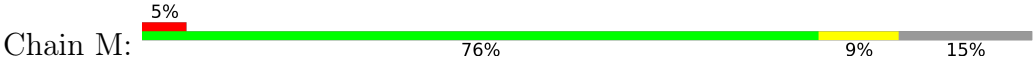


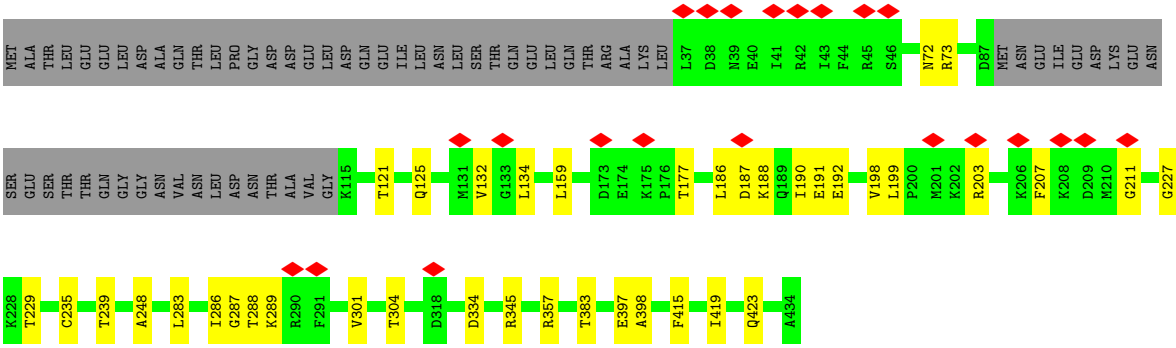
• Molecule 19: 26S proteasome subunit RPT4

Chain L:



• Molecule 20: 26S proteasome regulatory subunit 6A

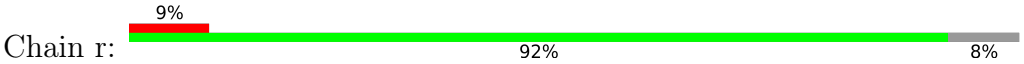


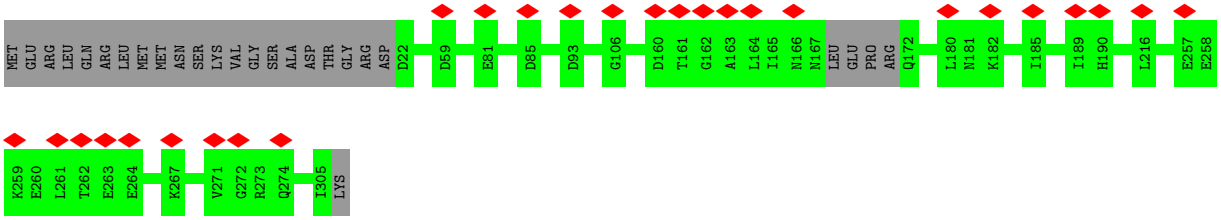


• Molecule 21: Proteasome subunit beta type-7

There are no outlier residues recorded for this chain.

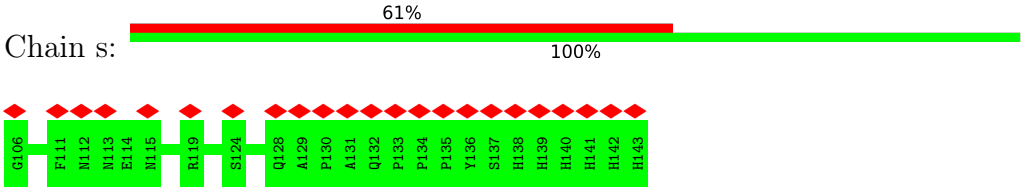
• Molecule 22: Ubiquitin carboxyl-terminal hydrolase RPN11





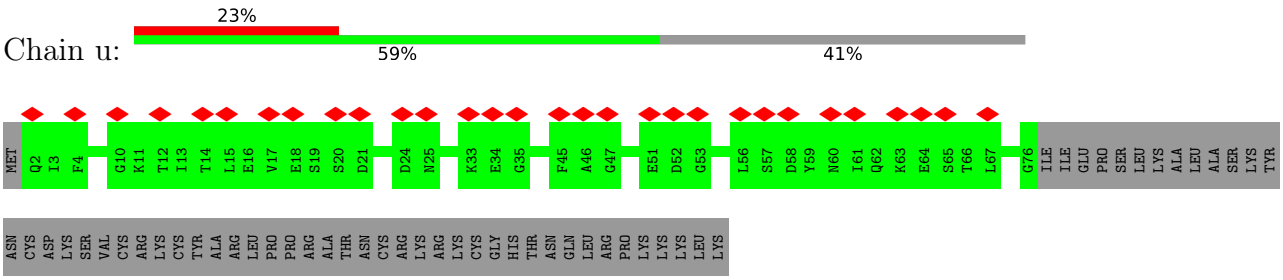
• Molecule 23: Model substrate polypeptide

Chain s:



• Molecule 24: Ubiquitin-60S ribosomal protein L40

Chain u:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48335	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed by Relion during reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	350.19998, 350.19998, 350.19998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	1	0.68	0/1525	0.64	1/2068 (0.0%)
2	2	0.63	0/1716	0.64	0/2330
3	3	0.70	0/1605	0.68	0/2167
4	4	0.63	0/1588	0.66	0/2141
5	5	0.62	1/1681 (0.1%)	0.65	0/2274
6	6	0.59	0/1765	0.61	0/2380
7	7	0.60	0/1625	0.65	0/2212
8	A	0.82	0/1960	0.68	0/2657
9	B	0.86	0/1938	0.68	0/2626
10	C	0.79	0/1894	0.70	1/2567 (0.0%)
11	D	0.83	1/1907 (0.1%)	0.71	0/2582
12	E	0.82	1/1945 (0.1%)	0.69	1/2621 (0.0%)
13	F	0.81	0/1824	0.72	0/2465
14	G	0.81	0/1943	0.68	0/2625
15	H	0.75	0/2934	0.68	1/3962 (0.0%)
16	I	0.71	0/2909	0.70	0/3936
17	J	0.67	0/2955	0.72	1/3978 (0.0%)
18	K	0.59	0/2799	0.66	0/3797
19	L	0.51	0/2561	0.64	0/3481
20	M	0.66	0/2754	0.66	0/3741
21	n	0.57	0/126	0.57	0/166
22	r	0.56	0/2119	0.62	0/2880
23	s	0.48	0/262	0.64	0/359
24	u	0.39	0/486	0.57	0/665
All	All	0.70	3/44821 (0.0%)	0.67	5/60680 (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
16	I	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	15	PHE	C-N	-5.88	1.20	1.34
5	5	58	TRP	CB-CG	-5.35	1.40	1.50
11	D	126	VAL	C-N	-5.11	1.22	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	385	ARG	NE-CZ-NH1	6.70	123.65	120.30
17	J	306	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	1	45	ARG	NE-CZ-NH1	5.48	123.04	120.30
10	C	117	ASP	CB-CG-OD1	5.41	123.17	118.30
12	E	155	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	I	410	GLN	Peptide

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	1	1496	0	1454	16	0
2	2	1685	0	1674	21	0
3	3	1575	0	1559	20	0
4	4	1560	0	1566	18	0
5	5	1644	0	1595	15	0
6	6	1727	0	1675	13	0
7	7	1598	0	1580	21	0
8	A	1922	0	1907	25	0
9	B	1901	0	1903	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	1864	0	1852	27	0
11	D	1878	0	1879	22	0
12	E	1918	0	1890	17	0
13	F	1796	0	1797	19	0
14	G	1903	0	1888	17	0
15	H	2889	0	2889	25	0
16	I	2871	0	2844	51	0
17	J	2918	0	2979	36	0
18	K	2761	0	2714	37	0
19	L	2525	0	2398	29	0
20	M	2717	0	2635	25	0
21	n	123	0	122	0	0
22	r	2088	0	1975	0	0
23	s	253	0	212	0	0
24	u	481	0	407	0	0
25	H	31	0	12	1	0
25	I	31	0	12	2	0
25	J	31	0	12	2	0
25	M	31	0	12	2	0
26	K	27	0	12	0	0
26	L	27	0	12	0	0
All	All	44271	0	43466	457	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 6.

All (457) 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)
16:I:386:ASP:O	16:I:427:LYS:NZ	2.13	0.81
2:2:37:ILE:HD11	2:2:41:ILE:HG21	1.62	0.81
3:3:46:TYR:OH	3:3:64:ASN:OD1	1.98	0.81
4:4:70:ARG:NH1	11:D:87:GLU:OE2	2.16	0.79
15:H:286:GLU:OE2	15:H:289:ARG:NH1	2.17	0.78
6:6:75:TYR:OH	12:E:105:GLU:OE2	2.05	0.74
16:I:55:CYS:SG	16:I:58:LYS:NZ	2.60	0.74
1:1:106:ASN:ND2	1:1:109:GLU:OE2	2.21	0.74
9:B:242:GLU:O	9:B:246:ARG:NH1	2.21	0.74
16:I:230:THR:OG1	25:I:501:ATP:O3G	2.05	0.74
10:C:120:GLN:NE2	10:C:124:GLN:OE1	2.22	0.73
10:C:160:TRP:CG	10:C:163:ILE:HD11	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:252:ARG:NH1	19:L:293:GLU:O	2.22	0.73
20:M:357:ARG:NH1	20:M:383:THR:OG1	2.22	0.72
3:3:68:ARG:HH12	10:C:99:LEU:HD22	1.54	0.71
14:G:114:ASP:OD1	14:G:157:TYR:OH	2.05	0.71
13:F:121:GLN:OE1	14:G:130:ARG:NH2	2.24	0.71
8:A:77:ARG:NH2	8:A:231:ASP:O	2.24	0.71
15:H:173:ARG:NH2	15:H:189:PRO:O	2.23	0.70
8:A:200:GLU:OE2	8:A:240:ASN:ND2	2.25	0.70
15:H:326:ASP:O	15:H:330:GLN:NE2	2.24	0.70
10:C:109:GLU:OE2	10:C:143:ARG:NH2	2.24	0.70
17:J:280:ASP:O	17:J:284:THR:N	2.24	0.70
12:E:18:GLU:O	13:F:31:GLN:NE2	2.27	0.68
10:C:50:ARG:NH1	10:C:212:GLU:OE1	2.28	0.66
4:4:23:ARG:NH1	5:5:118:ASP:OD2	2.27	0.66
12:E:46:VAL:HG11	12:E:145:ALA:HB1	1.78	0.66
6:6:28:ARG:NH1	6:6:198:VAL:O	2.29	0.65
8:A:188:LYS:O	8:A:190:LYS:NZ	2.22	0.65
20:M:207:PHE:O	20:M:211:GLY:N	2.28	0.65
3:3:28:ARG:NH2	3:3:34:LEU:O	2.29	0.65
16:I:408:ARG:NH2	16:I:415:ASP:OD2	2.29	0.65
5:5:4:LEU:HD21	5:5:15:ALA:HB3	1.78	0.64
7:7:2:GLN:NE2	7:7:109:PRO:O	2.31	0.64
18:K:71:GLU:O	18:K:75:LEU:N	2.31	0.64
20:M:199:LEU:O	20:M:203:ARG:N	2.30	0.63
9:B:119:GLN:NE2	10:C:86:ILE:HD11	2.14	0.63
8:A:97:ALA:HB2	8:A:121:MET:HE1	1.80	0.63
6:6:150:LEU:O	6:6:154:VAL:N	2.32	0.63
20:M:248:ALA:HB1	20:M:286:ILE:CD1	2.29	0.63
8:A:97:ALA:HB2	8:A:121:MET:CE	2.28	0.62
10:C:155:GLY:O	11:D:83:ARG:NH2	2.31	0.62
11:D:32:CYS:SG	11:D:33:ALA:N	2.70	0.62
15:H:201:GLU:N	15:H:201:GLU:OE1	2.32	0.62
16:I:340:ARG:NH1	16:I:341:PRO:O	2.32	0.62
8:A:65:ASP:N	14:G:159:GLY:O	2.33	0.62
16:I:289:THR:O	16:I:335:ASP:N	2.33	0.62
9:B:140:ASP:OD1	9:B:140:ASP:N	2.30	0.61
11:D:229:ILE:O	11:D:233:VAL:N	2.33	0.61
15:H:324:GLY:O	15:H:327:ASN:N	2.33	0.61
17:J:273:LEU:O	17:J:309:ARG:NH2	2.33	0.61
17:J:88:VAL:HG12	17:J:90:PRO:HD2	1.81	0.61
14:G:162:GLY:HA3	14:G:176:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:94:GLY:O	6:6:101:ARG:NH2	2.33	0.61
17:J:274:GLU:O	17:J:278:GLN:N	2.32	0.61
8:A:161:GLY:O	9:B:83:ARG:NH2	2.31	0.61
12:E:179:ALA:O	12:E:182:GLU:N	2.33	0.60
14:G:78:TYR:OH	14:G:89:VAL:HG13	2.02	0.60
19:L:249:SER:O	19:L:253:ASP:N	2.33	0.60
2:2:174:ASP:OD1	2:2:188:ARG:NH1	2.35	0.59
11:D:162:GLN:OE1	11:D:172:ARG:NH1	2.35	0.59
1:1:57:ASP:OD2	2:2:81:GLN:NE2	2.35	0.59
19:L:131:VAL:HG23	19:L:155:ILE:HG23	1.84	0.59
19:L:333:LEU:HD13	19:L:334:ASP:N	2.17	0.59
19:L:133:ASN:OD1	19:L:134:SER:N	2.36	0.59
1:1:143:ARG:NH2	1:1:150:GLU:OE1	2.36	0.58
8:A:83:VAL:HG11	8:A:90:ALA:HB1	1.84	0.58
12:E:131:GLU:N	12:E:131:GLU:OE1	2.36	0.58
7:7:127:LEU:HD22	7:7:142:LEU:HD13	1.85	0.58
19:L:394:CYS:SG	19:L:395:ALA:N	2.77	0.58
8:A:181:ASN:OD1	8:A:213:ALA:HB2	2.03	0.58
5:5:181:THR:OG1	5:5:182:GLU:OE1	2.22	0.58
7:7:40:GLU:N	7:7:40:GLU:OE1	2.37	0.58
19:L:107:GLU:O	19:L:120:LYS:N	2.37	0.58
6:6:91:ARG:NH2	6:6:131:TYR:OH	2.37	0.58
19:L:393:ASN:O	19:L:397:GLU:N	2.35	0.58
4:4:101:ASN:OD1	4:4:121:TYR:N	2.37	0.57
7:7:74:ASN:O	7:7:78:ASN:ND2	2.37	0.57
9:B:205:ASN:O	9:B:209:ILE:HG22	2.04	0.57
16:I:145:CYS:SG	16:I:146:SER:N	2.76	0.57
9:B:119:GLN:HE22	10:C:86:ILE:HD11	1.67	0.57
15:H:102:CYS:SG	15:H:103:THR:N	2.77	0.57
20:M:229:THR:OG1	25:M:501:ATP:O2A	2.22	0.57
10:C:89:ASN:OD1	10:C:90:THR:N	2.38	0.57
15:H:373:ARG:NH2	20:M:397:GLU:OE1	2.38	0.57
3:3:164:PHE:HE1	3:3:187:VAL:HG21	1.70	0.57
9:B:175:LEU:O	9:B:179:TRP:N	2.37	0.57
13:F:104:ALA:HB3	13:F:107:ARG:HG2	1.86	0.57
20:M:283:LEU:HD13	20:M:283:LEU:O	2.05	0.57
1:1:148:LYS:O	1:1:152:VAL:HG23	2.05	0.56
7:7:122:ASN:OD1	7:7:123:GLY:N	2.38	0.56
7:7:132:LEU:CD1	7:7:133:LEU:HD12	2.35	0.56
2:2:191:LEU:HD12	2:2:193:PRO:HD3	1.88	0.56
19:L:150:ILE:HG13	19:L:151:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:168:ALA:O	9:B:55:LEU:HD23	2.06	0.56
12:E:16:SER:OG	12:E:20:ARG:O	2.13	0.55
9:B:245:ASP:OD1	9:B:246:ARG:N	2.39	0.55
6:6:70:ASN:ND2	13:F:97:LEU:HD21	2.21	0.55
2:2:169:SER:OG	2:2:170:GLY:N	2.39	0.55
6:6:7:ASP:OD1	6:6:8:ASN:N	2.40	0.55
16:I:217:LYS:O	16:I:319:ARG:NH2	2.40	0.55
17:J:378:THR:HG23	17:J:380:GLU:H	1.70	0.55
18:K:304:ASP:OD2	18:K:333:ARG:NE	2.40	0.55
11:D:142:ASP:OD1	11:D:143:ASP:N	2.39	0.55
2:2:17:ASP:OD1	2:2:169:SER:OG	2.25	0.54
7:7:54:SER:OG	7:7:113:ALA:HB3	2.08	0.54
19:L:161:ARG:O	19:L:163:THR:HG23	2.07	0.54
2:2:150:GLU:OE1	2:2:150:GLU:N	2.40	0.54
6:6:135:GLN:N	6:6:135:GLN:OE1	2.40	0.54
12:E:84:ASP:OD1	12:E:136:ARG:NH2	2.41	0.54
12:E:150:ASP:OD1	12:E:151:ASP:N	2.40	0.54
13:F:156:LEU:HD13	13:F:159:THR:HG23	1.89	0.54
4:4:71:GLU:OE2	10:C:113:ARG:NH2	2.40	0.54
9:B:198:GLU:N	9:B:198:GLU:OE1	2.39	0.54
1:1:60:GLN:O	1:1:64:GLU:N	2.41	0.54
5:5:168:ASP:OD1	5:5:169:ALA:N	2.41	0.54
7:7:127:LEU:CD2	7:7:142:LEU:HD13	2.37	0.54
14:G:89:VAL:O	14:G:93:ARG:N	2.39	0.54
8:A:57:LYS:N	8:A:222:ASP:O	2.40	0.54
10:C:72:LYS:NZ	10:C:105:ASP:OD2	2.38	0.54
14:G:70:VAL:HG12	14:G:71:ASP:H	1.73	0.54
7:7:141:THR:C	7:7:142:LEU:HD12	2.27	0.53
9:B:49:LYS:NZ	9:B:58:SER:O	2.28	0.53
17:J:357:ASP:OD1	17:J:358:VAL:N	2.41	0.53
9:B:45:ILE:HD11	9:B:137:ALA:CB	2.38	0.53
14:G:205:GLU:N	14:G:205:GLU:OE1	2.41	0.53
10:C:168:ASN:ND2	10:C:200:THR:O	2.41	0.53
3:3:34:LEU:HD23	3:3:35:GLY:N	2.24	0.53
2:2:166:ASP:OD1	2:2:167:LEU:N	2.41	0.53
8:A:87:ILE:HD11	8:A:91:ARG:NH2	2.24	0.53
8:A:120:ARG:HH12	8:A:124:LEU:HD21	1.74	0.53
19:L:360:ILE:HG21	19:L:391:ILE:HD13	1.91	0.52
16:I:331:ILE:O	16:I:334:LEU:N	2.42	0.52
7:7:80:LEU:HD13	7:7:80:LEU:O	2.09	0.52
8:A:178:ILE:O	8:A:181:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:121:THR:HG22	20:M:125:GLN:O	2.09	0.52
1:1:35:THR:OG1	1:1:43:CYS:SG	2.42	0.52
14:G:191:GLU:N	14:G:191:GLU:OE1	2.41	0.52
20:M:198:VAL:HG23	20:M:199:LEU:HD22	1.90	0.52
3:3:168:SER:O	3:3:172:LEU:N	2.42	0.52
4:4:193:ASP:OD1	4:4:194:ASP:N	2.43	0.52
1:1:58:ILE:O	1:1:61:TYR:N	2.41	0.52
5:5:80:SER:OG	5:5:121:ARG:NH2	2.42	0.52
16:I:74:GLU:OE1	16:I:74:GLU:N	2.38	0.52
19:L:283:VAL:HG12	19:L:326:ALA:O	2.10	0.52
5:5:164:ALA:O	5:5:168:ASP:N	2.43	0.52
10:C:114:ARG:O	10:C:117:ASP:N	2.41	0.52
16:I:181:TYR:O	16:I:182:SER:OG	2.25	0.52
17:J:187:LEU:HD12	17:J:187:LEU:O	2.09	0.52
18:K:256:ASP:OD1	18:K:259:ARG:NH2	2.43	0.52
3:3:159:GLU:O	3:3:163:LEU:N	2.43	0.52
4:4:36:ARG:NE	4:4:58:GLU:OE2	2.43	0.52
6:6:151:ASP:O	6:6:157:LYS:N	2.42	0.52
12:E:85:ALA:O	12:E:88:MET:N	2.41	0.52
18:K:178:ASP:OD1	18:K:179:MET:N	2.43	0.51
16:I:339:ILE:HD12	16:I:339:ILE:O	2.10	0.51
8:A:212:ASP:OD1	8:A:213:ALA:N	2.43	0.51
12:E:116:VAL:O	12:E:119:LEU:N	2.41	0.51
2:2:124:TYR:O	2:2:125:LEU:HD22	2.10	0.51
18:K:103:ILE:HD12	18:K:104:ASP:HB2	1.91	0.51
13:F:168:ALA:O	13:F:171:TYR:N	2.44	0.51
15:H:71:GLU:N	17:J:80:SER:OG	2.44	0.51
17:J:280:ASP:OD1	17:J:281:GLY:N	2.44	0.51
9:B:168:SER:OG	9:B:169:VAL:N	2.44	0.51
12:E:207:VAL:O	15:H:409:ARG:NH2	2.40	0.51
2:2:43:CYS:SG	2:2:56:THR:HG22	2.50	0.51
10:C:12:ILE:O	11:D:19:GLN:NE2	2.36	0.51
10:C:111:LEU:O	10:C:115:LEU:N	2.38	0.50
5:5:9:GLN:NE2	5:5:148:LEU:O	2.44	0.50
19:L:267:PHE:O	19:L:271:LYS:N	2.43	0.50
17:J:251:ASP:OD1	17:J:252:SER:N	2.43	0.50
18:K:361:SER:C	18:K:362:LEU:HD12	2.31	0.50
15:H:424:THR:O	15:H:427:GLY:N	2.40	0.50
18:K:226:VAL:O	18:K:230:THR:HG22	2.12	0.50
11:D:151:GLU:OE1	11:D:155:ILE:HD11	2.10	0.50
3:3:26:ASP:OD1	3:3:27:LEU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:178:ASP:OD1	3:3:179:ALA:N	2.43	0.50
17:J:196:THR:OG1	25:J:501:ATP:O2G	2.30	0.50
14:G:70:VAL:O	14:G:72:ARG:N	2.45	0.50
18:K:386:ILE:O	18:K:390:ALA:N	2.45	0.50
5:5:4:LEU:CD2	5:5:15:ALA:HB3	2.42	0.50
19:L:101:ILE:HD12	19:L:102:GLY:O	2.11	0.50
15:H:172:MET:SD	15:H:172:MET:N	2.82	0.50
20:M:177:THR:O	20:M:177:THR:HG23	2.12	0.50
3:3:26:ASP:OD2	3:3:182:GLY:N	2.44	0.49
15:H:173:ARG:NE	15:H:188:PRO:O	2.35	0.49
1:1:20:THR:O	1:1:21:THR:OG1	2.22	0.49
11:D:78:LEU:HD11	11:D:81:ASP:OD2	2.12	0.49
5:5:1:THR:N	5:5:170:TYR:O	2.46	0.49
1:1:32:ASP:OD1	1:1:33:LYS:N	2.45	0.49
8:A:181:ASN:ND2	8:A:181:ASN:O	2.45	0.49
20:M:192:GLU:OE2	20:M:345:ARG:NH2	2.45	0.49
9:B:37:ILE:HD12	9:B:38:LYS:N	2.27	0.49
11:D:201:GLU:OE1	11:D:201:GLU:N	2.44	0.49
8:A:66:PRO:HA	8:A:69:VAL:HG12	1.95	0.49
16:I:426:ASN:ND2	16:I:426:ASN:O	2.46	0.49
4:4:43:LEU:HD22	4:4:44:MET:H	1.78	0.49
19:L:286:ILE:HD13	19:L:305:LEU:HD13	1.95	0.49
2:2:221:CYS:SG	2:2:222:ASP:N	2.82	0.49
9:B:64:VAL:HG23	9:B:210:GLU:OE2	2.12	0.49
9:B:91:LYS:O	9:B:94:HIS:N	2.46	0.49
15:H:170:GLU:N	15:H:170:GLU:OE1	2.45	0.49
16:I:285:ASP:OD2	17:J:270:ARG:NH1	2.45	0.49
17:J:372:GLU:OE1	17:J:374:ARG:NH1	2.45	0.49
18:K:78:GLU:N	18:K:78:GLU:OE1	2.46	0.48
1:1:126:ILE:O	7:7:35:ARG:NH2	2.46	0.48
16:I:355:LEU:HD23	16:I:382:THR:O	2.12	0.48
1:1:39:ASP:OD1	1:1:40:LYS:N	2.43	0.48
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.95	0.48
10:C:171:ALA:O	10:C:174:THR:N	2.47	0.48
11:D:18:PHE:O	11:D:21:GLU:N	2.46	0.48
12:E:9:ASP:OD1	12:E:26:TYR:OH	2.21	0.48
8:A:84:ASN:OD1	8:A:171:THR:HG21	2.14	0.48
16:I:246:ARG:O	16:I:247:ILE:HD13	2.12	0.48
9:B:201:GLU:N	9:B:201:GLU:OE1	2.47	0.48
17:J:187:LEU:HD13	17:J:195:LYS:HB2	1.96	0.48
5:5:116:ASP:OD1	5:5:116:ASP:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:79:SER:O	16:I:81:ILE:HD12	2.13	0.48
11:D:174:PHE:O	11:D:178:ASN:ND2	2.47	0.48
15:H:167:ASP:OD1	15:H:168:ILE:N	2.47	0.48
6:6:87:ASN:OD1	6:6:88:SER:N	2.47	0.47
10:C:156:ASN:HD22	10:C:157:TYR:N	2.11	0.47
16:I:247:ILE:HG22	16:I:248:VAL:N	2.29	0.47
14:G:218:TRP:NE1	14:G:230:PHE:O	2.44	0.47
12:E:211:LYS:O	12:E:216:ASN:ND2	2.46	0.47
13:F:14:SER:OG	13:F:17:GLY:N	2.46	0.47
16:I:73:GLU:O	16:I:77:SER:N	2.43	0.47
10:C:197:LEU:HA	10:C:200:THR:HG22	1.96	0.47
2:2:158:ALA:O	2:2:161:ALA:HB3	2.14	0.47
4:4:52:ASP:OD1	5:5:88:TYR:OH	2.25	0.47
10:C:235:ILE:O	10:C:239:LEU:N	2.48	0.47
4:4:185:ASP:OD1	4:4:185:ASP:N	2.47	0.47
13:F:67:ASP:OD1	13:F:68:GLU:N	2.45	0.47
16:I:184:ILE:HG22	25:I:501:ATP:C2	2.50	0.47
17:J:310:ILE:HD12	17:J:310:ILE:O	2.14	0.47
19:L:132:ARG:NH1	19:L:134:SER:OG	2.48	0.47
2:2:171:SER:OG	2:2:172:ASN:N	2.47	0.47
2:2:3:ILE:HD12	2:2:4:VAL:N	2.30	0.46
4:4:194:ASP:OD1	4:4:195:PHE:N	2.47	0.46
13:F:156:LEU:HA	14:G:60:VAL:HG23	1.96	0.46
16:I:71:LEU:HD12	16:I:74:GLU:OE2	2.15	0.46
20:M:248:ALA:HB1	20:M:286:ILE:HD12	1.97	0.46
10:C:202:ASP:OD1	10:C:203:SER:N	2.48	0.46
13:F:88:LEU:HD23	13:F:112:LEU:HD11	1.97	0.46
16:I:140:LEU:HD23	16:I:141:LEU:HA	1.97	0.46
16:I:314:ASP:OD1	16:I:314:ASP:N	2.48	0.46
2:2:59:ILE:O	2:2:63:ILE:HG22	2.15	0.46
8:A:184:ASN:OD1	8:A:185:HIS:N	2.48	0.46
17:J:112:ARG:NH2	17:J:127:GLU:O	2.48	0.46
18:K:230:THR:HG23	18:K:232:ALA:H	1.80	0.46
4:4:156:GLU:O	4:4:160:LEU:N	2.42	0.46
1:1:147:SER:OG	1:1:148:LYS:N	2.46	0.46
12:E:36:THR:OG1	12:E:37:ALA:N	2.49	0.46
15:H:96:PRO:C	15:H:97:LEU:HD22	2.36	0.46
3:3:68:ARG:NH1	10:C:99:LEU:HD22	2.27	0.46
4:4:157:GLY:O	4:4:161:LEU:N	2.48	0.46
18:K:184:ILE:HD13	18:K:226:VAL:HG21	1.98	0.46
20:M:73:ARG:NH2	20:M:134:LEU:HD21	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:162:LEU:HD22	5:5:196:LEU:HD12	1.97	0.45
9:B:52:SER:OG	9:B:53:SER:N	2.49	0.45
11:D:99:THR:O	11:D:100:LEU:HD22	2.16	0.45
5:5:44:THR:O	5:5:99:THR:OG1	2.15	0.45
20:M:287:GLY:O	20:M:334:ASP:N	2.44	0.45
9:B:248:GLU:OE1	9:B:248:GLU:N	2.50	0.45
15:H:279:LEU:N	15:H:279:LEU:HD12	2.32	0.45
6:6:27:THR:HG22	6:6:27:THR:O	2.16	0.45
8:A:97:ALA:O	8:A:100:GLU:N	2.44	0.45
11:D:229:ILE:HG22	11:D:233:VAL:HG23	1.98	0.45
18:K:123:LEU:HD21	18:K:147:VAL:O	2.17	0.45
8:A:54:ILE:HG13	8:A:225:VAL:HG23	1.98	0.45
10:C:160:TRP:CD1	10:C:163:ILE:HD11	2.52	0.45
9:B:13:SER:O	9:B:16:GLY:N	2.46	0.45
1:1:48:SER:OG	1:1:49:ALA:N	2.49	0.45
8:A:91:ARG:O	8:A:94:ALA:N	2.50	0.45
9:B:149:GLN:OE1	9:B:159:TRP:NE1	2.42	0.45
18:K:174:VAL:HG23	18:K:221:MET:SD	2.57	0.45
18:K:177:LEU:HD12	18:K:180:GLN:OE1	2.17	0.45
5:5:42:LEU:HD13	5:5:178:TYR:HD2	1.81	0.45
11:D:200:LEU:HA	11:D:203:VAL:HG12	1.98	0.45
16:I:373:GLU:OE2	16:I:410:GLN:NE2	2.49	0.45
1:1:3:ILE:HD11	1:1:127:ALA:HB3	1.99	0.44
9:B:12:PHE:CE1	9:B:18:LEU:HD11	2.52	0.44
18:K:356:ILE:HG21	18:K:387:MET:HG3	2.00	0.44
19:L:328:ASN:OD1	19:L:329:ARG:N	2.50	0.44
15:H:163:VAL:HG11	15:H:166:THR:OG1	2.18	0.44
16:I:260:GLY:O	16:I:263:LEU:N	2.50	0.44
3:3:179:ALA:C	3:3:180:LEU:HD12	2.38	0.44
4:4:94:SER:OG	4:4:95:ARG:N	2.48	0.44
15:H:99:VAL:HG22	16:I:127:ASP:HB2	1.99	0.44
16:I:267:ILE:HA	16:I:270:VAL:HG12	1.98	0.44
17:J:193:THR:HG21	17:J:316:PHE:HB3	1.99	0.44
17:J:327:ILE:HD12	25:J:501:ATP:N6	2.32	0.44
19:L:412:PRO:O	19:L:416:MET:N	2.44	0.44
3:3:50:PHE:CD2	3:3:190:ILE:HD11	2.53	0.44
9:B:15:SER:O	10:C:31:HIS:NE2	2.44	0.44
11:D:154:GLY:O	12:E:86:ARG:NH2	2.50	0.44
17:J:114:CYS:C	17:J:115:LEU:HD12	2.38	0.44
18:K:127:ASP:OD2	18:K:129:GLU:N	2.44	0.44
18:K:269:ILE:HD12	18:K:313:LYS:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:11:THR:N	6:6:26:ASP:OD2	2.51	0.44
10:C:121:GLY:O	10:C:125:HIS:NE2	2.51	0.44
16:I:382:THR:HG23	16:I:383:THR:N	2.33	0.44
20:M:301:VAL:O	20:M:304:THR:OG1	2.25	0.44
13:F:132:LEU:HD23	13:F:147:PHE:HB3	1.99	0.44
13:F:233:TYR:O	13:F:234:ILE:HD13	2.17	0.44
17:J:164:ILE:HD13	17:J:289:LYS:HD3	1.98	0.44
4:4:75:LEU:HD23	4:4:75:LEU:H	1.82	0.44
9:B:18:LEU:HD12	9:B:18:LEU:N	2.33	0.44
11:D:236:ILE:O	11:D:239:GLU:N	2.51	0.44
13:F:36:VAL:HG12	13:F:160:ALA:CB	2.48	0.44
16:I:81:ILE:HD12	16:I:81:ILE:N	2.32	0.44
17:J:114:CYS:SG	17:J:124:LYS:N	2.91	0.44
8:A:192:ASP:OD1	8:A:193:HIS:N	2.51	0.43
16:I:136:VAL:HG12	16:I:157:VAL:O	2.18	0.43
18:K:120:VAL:HG23	18:K:145:ALA:HA	2.00	0.43
20:M:187:ASP:OD1	20:M:188:LYS:N	2.50	0.43
17:J:137:MET:O	17:J:211:ILE:HG23	2.18	0.43
18:K:170:THR:O	18:K:173:ASP:N	2.50	0.43
9:B:45:ILE:HD11	9:B:137:ALA:HB2	2.01	0.43
12:E:79:SER:O	12:E:79:SER:OG	2.33	0.43
15:H:271:PHE:CD1	15:H:305:ILE:HD11	2.54	0.43
17:J:49:ASN:OD1	17:J:50:ALA:N	2.50	0.43
3:3:160:PRO:O	3:3:164:PHE:N	2.48	0.43
10:C:163:ILE:HG22	10:C:164:SER:N	2.33	0.43
11:D:56:ASP:OD1	11:D:57:THR:N	2.52	0.43
16:I:382:THR:HG23	16:I:383:THR:H	1.84	0.43
17:J:206:THR:OG1	17:J:207:ASP:N	2.51	0.43
18:K:123:LEU:HD23	18:K:123:LEU:H	1.81	0.43
18:K:194:GLN:HB3	18:K:197:LEU:HD23	1.99	0.43
3:3:167:ILE:O	3:3:171:LEU:N	2.49	0.43
9:B:92:VAL:HG11	9:B:113:GLU:HB3	1.99	0.43
13:F:182:ILE:HG23	13:F:182:ILE:O	2.18	0.43
14:G:199:ILE:O	14:G:203:ALA:N	2.48	0.43
16:I:193:GLU:O	16:I:346:ARG:NH1	2.51	0.43
17:J:40:ASN:O	17:J:44:LEU:N	2.52	0.43
17:J:330:ILE:O	17:J:333:ARG:NH1	2.46	0.43
4:4:38:LEU:HD23	4:4:61:GLN:CB	2.48	0.43
8:A:220:LYS:HB2	8:A:238:ALA:HB1	2.00	0.43
15:H:324:GLY:O	15:H:326:ASP:N	2.52	0.43
20:M:235:CYS:O	20:M:239:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:80:LEU:HD11	7:7:84:GLU:CG	2.48	0.43
18:K:356:ILE:HD12	18:K:356:ILE:H	1.84	0.43
19:L:333:LEU:HD13	19:L:334:ASP:H	1.81	0.43
8:A:79:ILE:HG22	8:A:80:GLY:N	2.34	0.43
9:B:162:THR:HG22	9:B:163:ALA:N	2.34	0.43
18:K:122:ILE:HD12	18:K:122:ILE:H	1.84	0.43
18:K:125:THR:O	18:K:125:THR:HG22	2.17	0.43
9:B:121:ALA:HA	9:B:127:VAL:HG11	2.01	0.43
25:H:501:ATP:O2G	16:I:343:ARG:NH2	2.48	0.43
19:L:287:GLY:O	19:L:290:ARG:N	2.52	0.43
9:B:12:PHE:HE2	10:C:25:ALA:HB2	1.84	0.42
14:G:95:GLU:O	14:G:98:SER:N	2.52	0.42
20:M:227:GLY:N	25:M:501:ATP:O1A	2.50	0.42
3:3:49:VAL:HG22	3:3:84:PRO:HG3	2.01	0.42
13:F:20:PHE:O	13:F:23:GLU:N	2.53	0.42
19:L:141:LYS:O	19:L:144:VAL:HG22	2.19	0.42
7:7:199:ILE:O	7:7:206:LEU:HD12	2.20	0.42
11:D:209:ASN:O	11:D:210:ILE:HD13	2.19	0.42
1:1:3:ILE:HD13	1:1:44:CYS:CB	2.49	0.42
11:D:180:ASP:OD1	11:D:180:ASP:N	2.52	0.42
13:F:100:ASN:O	13:F:100:ASN:ND2	2.52	0.42
16:I:184:ILE:HG21	16:I:231:LEU:HD11	2.01	0.42
18:K:410:ALA:O	18:K:413:THR:N	2.52	0.42
20:M:132:VAL:HG12	20:M:134:LEU:H	1.85	0.42
2:2:17:ASP:CG	2:2:169:SER:HG	2.22	0.42
3:3:84:PRO:O	3:3:87:PHE:N	2.53	0.42
9:B:211:LEU:HD11	9:B:238:LEU:HD12	2.00	0.42
16:I:213:ILE:HD12	16:I:214:LYS:N	2.35	0.42
18:K:312:VAL:HG12	18:K:312:VAL:O	2.19	0.42
3:3:16:THR:OG1	3:3:134:LYS:O	2.25	0.42
7:7:6:VAL:HG12	7:7:57:ILE:HD13	2.00	0.42
9:B:98:LYS:O	9:B:102:GLY:N	2.43	0.42
15:H:262:ALA:O	15:H:265:ASN:N	2.48	0.42
20:M:398:ALA:HB2	20:M:415:PHE:HA	2.01	0.42
16:I:293:ASP:OD1	16:I:294:SER:N	2.51	0.42
17:J:40:ASN:OD1	17:J:41:VAL:HG23	2.19	0.42
20:M:288:THR:OG1	20:M:289:LYS:N	2.51	0.42
2:2:120:ASP:N	2:2:120:ASP:OD1	2.51	0.42
14:G:54:ILE:HD12	14:G:210:LYS:HE3	2.02	0.42
16:I:344:ILE:HD12	16:I:344:ILE:O	2.19	0.42
18:K:251:PRO:HA	18:K:254:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:188:LYS:O	20:M:191:GLU:N	2.53	0.42
7:7:53:ILE:HG21	7:7:60:MET:CG	2.49	0.42
13:F:190:ILE:HD11	13:F:213:ILE:HD13	2.02	0.42
15:H:49:LEU:HA	15:H:52:THR:HG22	2.01	0.42
16:I:154:MET:O	16:I:155:SER:OG	2.29	0.42
18:K:174:VAL:HG22	18:K:175:GLY:N	2.34	0.42
19:L:415:LEU:HA	19:L:418:ALA:HB2	2.01	0.42
11:D:2:SER:OG	11:D:3:GLY:N	2.52	0.42
15:H:50:LYS:O	15:H:54:ASN:ND2	2.52	0.42
17:J:104:VAL:HA	17:J:107:LEU:HD13	2.02	0.42
18:K:95:VAL:HG13	18:K:139:LEU:HB2	2.02	0.42
19:L:375:ASP:O	19:L:379:ALA:N	2.52	0.42
7:7:23:ALA:HB2	7:7:197:LEU:HD12	2.01	0.41
16:I:87:LYS:O	16:I:91:GLU:N	2.46	0.41
20:M:419:ILE:HG22	20:M:423:GLN:HE22	1.85	0.41
2:2:58:LEU:HD23	2:2:59:ILE:N	2.35	0.41
17:J:174:PHE:O	17:J:178:GLY:N	2.51	0.41
18:K:177:LEU:HD11	18:K:340:PHE:HD1	1.85	0.41
1:1:104:ASP:OD1	1:1:105:LYS:N	2.53	0.41
3:3:138:VAL:O	3:3:139:SER:OG	2.29	0.41
4:4:77:PRO:O	4:4:80:VAL:N	2.54	0.41
16:I:287:ILE:HD12	16:I:288:GLY:N	2.34	0.41
4:4:46:PHE:HB3	4:4:102:VAL:HG12	2.02	0.41
6:6:159:GLN:O	6:6:170:LYS:NZ	2.51	0.41
7:7:6:VAL:HG13	7:7:29:SER:O	2.20	0.41
18:K:238:ASN:OD1	18:K:239:GLY:N	2.53	0.41
18:K:277:ILE:O	18:K:277:ILE:HD12	2.19	0.41
19:L:192:GLU:O	19:L:195:GLU:N	2.53	0.41
7:7:21:ILE:HD12	7:7:173:ALA:HB1	2.03	0.41
17:J:357:ASP:OD1	17:J:358:VAL:HG13	2.20	0.41
18:K:217:THR:O	18:K:217:THR:HG22	2.20	0.41
18:K:318:THR:OG1	18:K:319:ASN:N	2.53	0.41
19:L:271:LYS:O	19:L:274:GLU:N	2.53	0.41
3:3:13:VAL:HG12	3:3:146:LEU:HD21	2.01	0.41
7:7:33:LEU:HD23	7:7:34:LEU:N	2.36	0.41
7:7:132:LEU:HD11	7:7:133:LEU:HD12	2.01	0.41
16:I:174:ASP:OD1	16:I:175:LYS:N	2.50	0.41
16:I:411:VAL:HG12	16:I:412:THR:N	2.36	0.41
17:J:265:ASP:OD1	17:J:266:SER:N	2.54	0.41
4:4:168:LEU:O	4:4:172:MET:N	2.42	0.41
9:B:222:LEU:HD13	9:B:232:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:175:GLU:OE1	14:G:175:GLU:N	2.51	0.41
17:J:165:GLU:O	17:J:169:LYS:N	2.46	0.41
17:J:284:THR:O	17:J:286:LYS:N	2.51	0.41
17:J:361:VAL:O	17:J:364:GLU:N	2.53	0.41
16:I:68:HIS:O	16:I:72:GLU:N	2.53	0.41
16:I:227:THR:O	16:I:227:THR:HG22	2.21	0.41
18:K:395:VAL:HG23	19:L:206:ILE:HD12	2.02	0.41
19:L:206:ILE:O	19:L:210:VAL:HG12	2.20	0.41
2:2:124:TYR:C	2:2:125:LEU:HD22	2.40	0.41
15:H:341:ASP:HB3	15:H:370:ARG:HE	1.86	0.41
16:I:171:MET:SD	16:I:247:ILE:HD11	2.61	0.41
16:I:183:ASP:O	16:I:364:ILE:HD12	2.21	0.41
16:I:289:THR:HG23	16:I:290:LYS:N	2.36	0.41
18:K:271:ILE:O	18:K:317:ALA:HB3	2.21	0.41
14:G:70:VAL:HG12	14:G:71:ASP:N	2.34	0.41
2:2:41:ILE:HG22	2:2:42:TRP:N	2.36	0.40
9:B:137:ALA:HB2	9:B:147:LEU:HD12	2.02	0.40
13:F:78:ALA:HB3	13:F:79:PRO:HD3	2.03	0.40
16:I:63:GLU:O	16:I:67:ASP:N	2.54	0.40
16:I:200:LEU:O	16:I:203:THR:N	2.42	0.40
20:M:159:LEU:HD23	20:M:159:LEU:N	2.36	0.40
15:H:166:THR:OG1	15:H:167:ASP:N	2.54	0.40
19:L:151:THR:OG1	19:L:152:THR:N	2.53	0.40
2:2:138:LEU:O	2:2:142:TRP:N	2.49	0.40
7:7:94:GLU:O	7:7:98:THR:HG22	2.21	0.40
10:C:141:ASP:N	10:C:141:ASP:OD1	2.54	0.40
11:D:187:THR:HG23	11:D:190:GLU:H	1.87	0.40
12:E:192:THR:OG1	12:E:195:GLU:N	2.47	0.40
13:F:40:SER:OG	13:F:183:ASP:OD1	2.40	0.40
16:I:362:LEU:O	16:I:366:THR:OG1	2.31	0.40
16:I:379:THR:O	16:I:379:THR:HG22	2.21	0.40
17:J:314:ILE:HG21	17:J:316:PHE:CE1	2.57	0.40
17:J:273:LEU:HD11	17:J:304:LEU:HD11	2.04	0.40
19:L:307:GLU:HA	19:L:310:THR:HG22	2.03	0.40
20:M:186:LEU:O	20:M:190:ILE:HG22	2.22	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	1	194/215 (90%)	166 (86%)	28 (14%)	0	100	100
2	2	222/261 (85%)	189 (85%)	33 (15%)	0	100	100
3	3	202/205 (98%)	171 (85%)	30 (15%)	1 (0%)	29	68
4	4	193/198 (98%)	169 (88%)	24 (12%)	0	100	100
5	5	210/287 (73%)	188 (90%)	22 (10%)	0	100	100
6	6	218/241 (90%)	194 (89%)	24 (11%)	0	100	100
7	7	206/266 (77%)	183 (89%)	23 (11%)	0	100	100
8	A	245/252 (97%)	205 (84%)	40 (16%)	0	100	100
9	B	248/250 (99%)	209 (84%)	39 (16%)	0	100	100
10	C	240/258 (93%)	203 (85%)	37 (15%)	0	100	100
11	D	239/254 (94%)	206 (86%)	33 (14%)	0	100	100
12	E	247/260 (95%)	217 (88%)	30 (12%)	0	100	100
13	F	232/234 (99%)	202 (87%)	30 (13%)	0	100	100
14	G	244/288 (85%)	219 (90%)	24 (10%)	1 (0%)	34	71
15	H	374/467 (80%)	320 (86%)	54 (14%)	0	100	100
16	I	382/437 (87%)	312 (82%)	70 (18%)	0	100	100
17	J	381/405 (94%)	320 (84%)	61 (16%)	0	100	100
18	K	366/428 (86%)	307 (84%)	59 (16%)	0	100	100
19	L	358/437 (82%)	306 (86%)	52 (14%)	0	100	100
20	M	367/434 (85%)	310 (84%)	57 (16%)	0	100	100
21	n	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
22	r	276/306 (90%)	224 (81%)	52 (19%)	0	100	100
23	s	36/38 (95%)	17 (47%)	19 (53%)	0	100	100
24	u	73/128 (57%)	66 (90%)	7 (10%)	0	100	100
All	All	5766/6564 (88%)	4914 (85%)	850 (15%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	19	ASP
14	G	71	ASP

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	1	156/178 (88%)	156 (100%)	0	100	100
2	2	178/214 (83%)	178 (100%)	0	100	100
3	3	169/173 (98%)	169 (100%)	0	100	100
4	4	172/175 (98%)	170 (99%)	2 (1%)	71	83
5	5	169/235 (72%)	167 (99%)	2 (1%)	71	83
6	6	178/201 (89%)	177 (99%)	1 (1%)	86	92
7	7	172/224 (77%)	172 (100%)	0	100	100
8	A	203/210 (97%)	202 (100%)	1 (0%)	88	93
9	B	205/209 (98%)	204 (100%)	1 (0%)	88	93
10	C	193/216 (89%)	190 (98%)	3 (2%)	62	78
11	D	209/226 (92%)	208 (100%)	1 (0%)	88	93
12	E	203/215 (94%)	201 (99%)	2 (1%)	76	86
13	F	190/193 (98%)	189 (100%)	1 (0%)	88	93
14	G	201/239 (84%)	200 (100%)	1 (0%)	88	93
15	H	300/399 (75%)	300 (100%)	0	100	100
16	I	302/385 (78%)	300 (99%)	2 (1%)	84	90
17	J	306/352 (87%)	304 (99%)	2 (1%)	84	90
18	K	275/374 (74%)	273 (99%)	2 (1%)	84	90
19	L	224/377 (59%)	224 (100%)	0	100	100
20	M	269/375 (72%)	268 (100%)	1 (0%)	91	94
21	n	11/12 (92%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	r	219/268 (82%)	219 (100%)	0	100 100
23	s	20/29 (69%)	20 (100%)	0	100 100
24	u	34/116 (29%)	34 (100%)	0	100 100
All	All	4558/5595 (82%)	4536 (100%)	22 (0%)	89 93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	78	GLN
4	4	86	GLN
5	5	24	ASN
5	5	121	ARG
6	6	214	LYS
8	A	181	ASN
9	B	119	GLN
10	C	103	ASN
10	C	156	ASN
10	C	206	LEU
11	D	118	GLN
12	E	43	LYS
12	E	78	MET
13	F	100	ASN
14	G	121	GLN
16	I	426	ASN
16	I	427	LYS
17	J	269	GLN
17	J	402	LYS
18	K	228	ASN
18	K	231	LYS
20	M	72	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	41	HIS
5	5	24	ASN
7	7	112	ASN
9	B	119	GLN
10	C	103	ASN
11	D	178	ASN

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Mol	Chain	Res	Type
13	F	100	ASN
15	H	330	GLN
20	M	310	ASN
20	M	328	ASN
22	r	126	GLN
24	u	2	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	ATP	M	501	-	26,33,33	0.90	0	31,52,52	1.94	6 (19%)
25	ATP	I	501	-	26,33,33	0.88	0	31,52,52	1.83	5 (16%)
25	ATP	J	501	-	26,33,33	0.85	0	31,52,52	1.82	4 (12%)
26	ADP	K	501	-	24,29,29	0.90	0	29,45,45	1.58	5 (17%)
26	ADP	L	501	-	24,29,29	0.89	0	29,45,45	1.52	4 (13%)
25	ATP	H	501	-	26,33,33	0.92	0	31,52,52	1.93	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
25	ATP	M	501	-	-	2/18/38/38	0/3/3/3
25	ATP	I	501	-	-	3/18/38/38	0/3/3/3
25	ATP	J	501	-	-	3/18/38/38	0/3/3/3
26	ADP	K	501	-	-	0/12/32/32	0/3/3/3
26	ADP	L	501	-	-	2/12/32/32	0/3/3/3
25	ATP	H	501	-	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	M	501	ATP	PB-O3B-PG	-5.96	112.38	132.83
25	J	501	ATP	PA-O3A-PB	-5.88	112.65	132.83
25	I	501	ATP	PA-O3A-PB	-4.94	115.86	132.83
26	K	501	ADP	PA-O3A-PB	-4.84	116.22	132.83
25	H	501	ATP	PB-O3B-PG	-4.78	116.41	132.83
25	I	501	ATP	PB-O3B-PG	-4.65	116.85	132.83
25	M	501	ATP	PA-O3A-PB	-4.56	117.19	132.83
26	L	501	ADP	PA-O3A-PB	-4.56	117.19	132.83
25	J	501	ATP	PB-O3B-PG	-4.48	117.46	132.83
25	H	501	ATP	PA-O3A-PB	-4.09	118.79	132.83
25	H	501	ATP	C3'-C2'-C1'	4.00	107.00	100.98
25	H	501	ATP	N6-C6-N1	3.85	126.57	118.57
25	I	501	ATP	N3-C2-N1	-3.64	122.99	128.68
25	J	501	ATP	N3-C2-N1	-3.61	123.03	128.68
25	M	501	ATP	C3'-C2'-C1'	3.53	106.29	100.98
25	M	501	ATP	N3-C2-N1	-3.39	123.38	128.68
25	I	501	ATP	C3'-C2'-C1'	3.34	106.01	100.98
26	K	501	ADP	N3-C2-N1	-3.23	123.63	128.68
26	L	501	ADP	N3-C2-N1	-3.23	123.64	128.68
25	H	501	ATP	N3-C2-N1	-2.88	124.18	128.68
25	H	501	ATP	C5-C6-N6	-2.77	116.14	120.35
26	K	501	ADP	C3'-C2'-C1'	2.73	105.09	100.98
26	L	501	ADP	N6-C6-N1	2.61	123.99	118.57
25	J	501	ATP	C3'-C2'-C1'	2.53	104.79	100.98
26	L	501	ADP	C3'-C2'-C1'	2.50	104.73	100.98
25	I	501	ATP	C4-C5-N7	-2.33	106.97	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	M	501	ATP	N6-C6-N1	2.31	123.36	118.57
25	M	501	ATP	O3G-PG-O2G	2.27	116.31	107.64
26	K	501	ADP	N6-C6-N1	2.06	122.84	118.57
26	K	501	ADP	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	H	501	ATP	O4'-C4'-C5'-O5'
25	H	501	ATP	C3'-C4'-C5'-O5'
25	I	501	ATP	C5'-O5'-PA-O1A
25	I	501	ATP	C5'-O5'-PA-O2A
25	J	501	ATP	C5'-O5'-PA-O1A
25	J	501	ATP	C5'-O5'-PA-O2A
25	M	501	ATP	C5'-O5'-PA-O3A
26	L	501	ADP	C5'-O5'-PA-O3A
25	M	501	ATP	C5'-O5'-PA-O1A
26	L	501	ADP	C5'-O5'-PA-O1A
25	I	501	ATP	C5'-O5'-PA-O3A
25	J	501	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

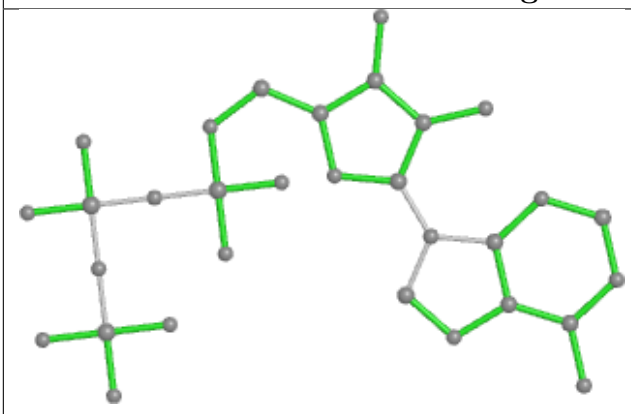
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	M	501	ATP	2	0
25	I	501	ATP	2	0
25	J	501	ATP	2	0
25	H	501	ATP	1	0

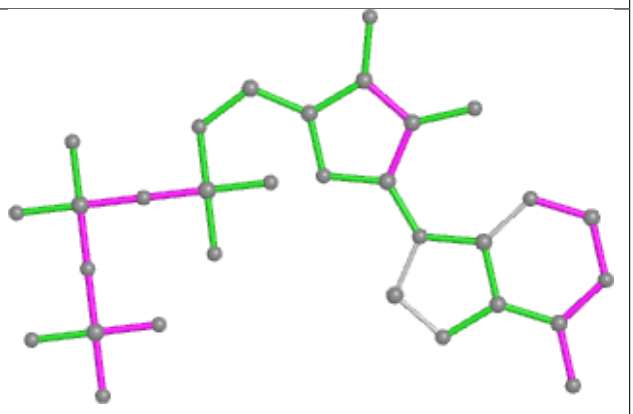
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

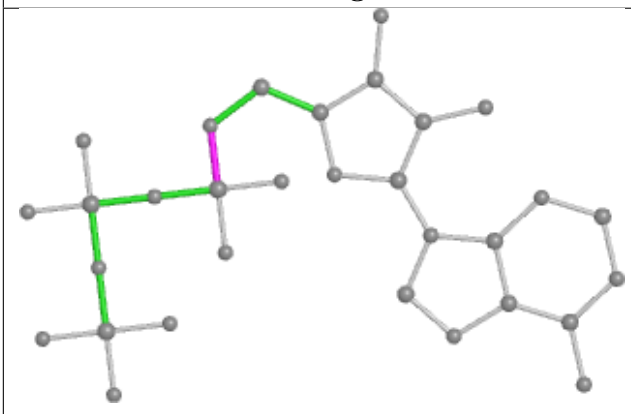
Ligand ATP M 501



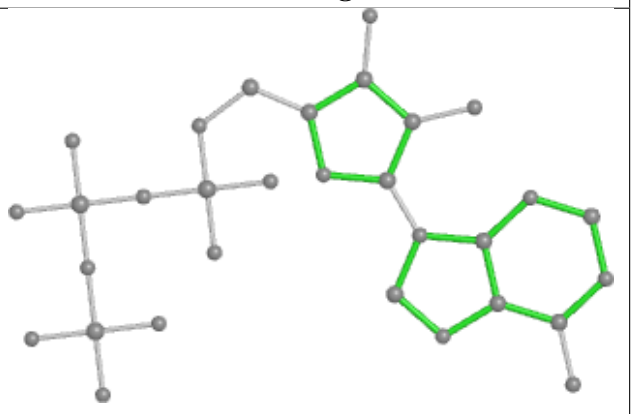
Bond lengths



Bond angles

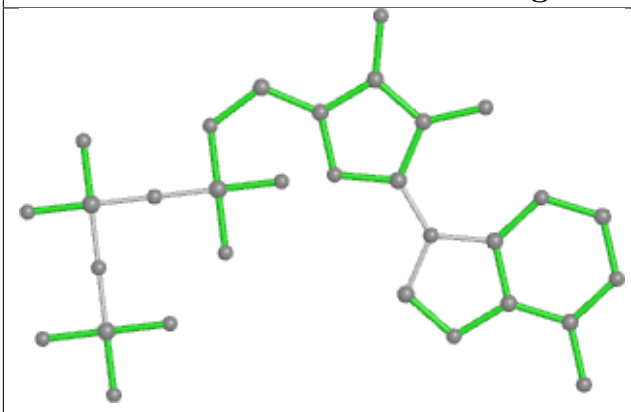


Torsions



Rings

Ligand ATP I 501



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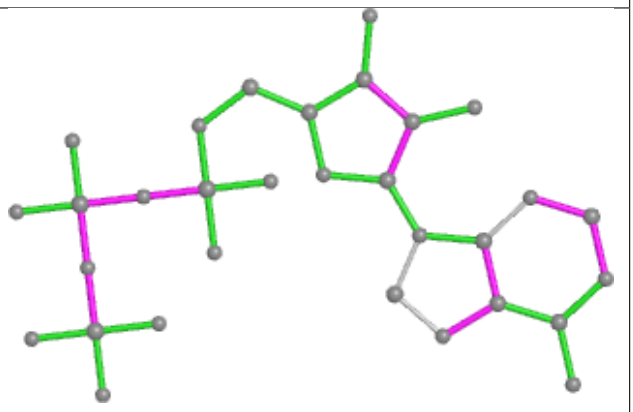

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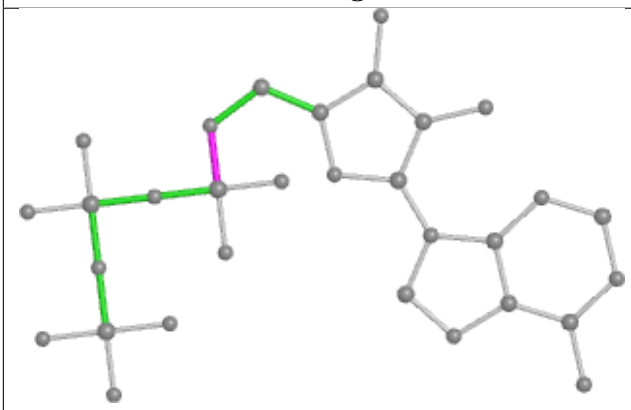

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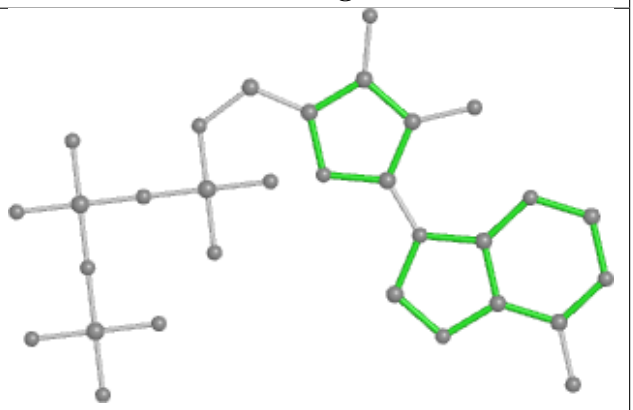
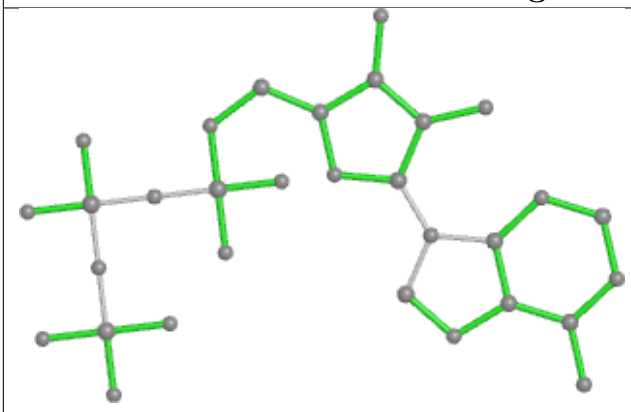
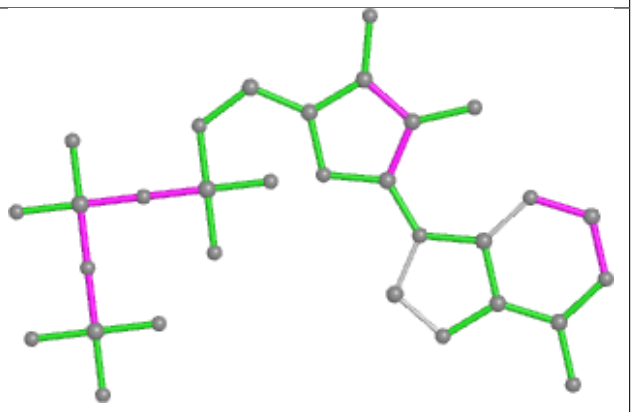


Rings

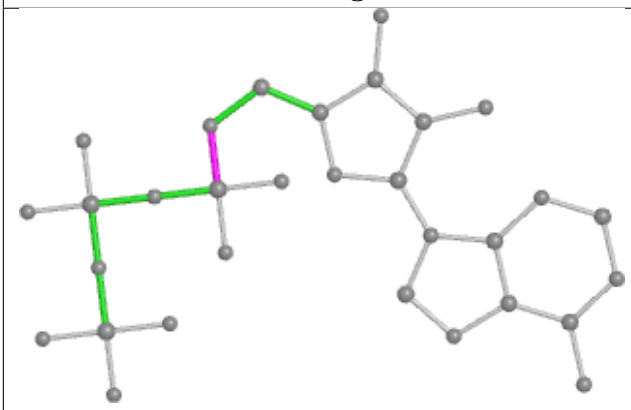
Ligand ATP J 501



Bond lengths



Bond angles



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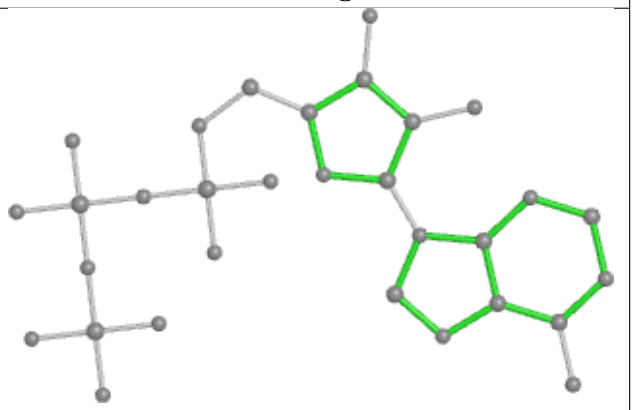
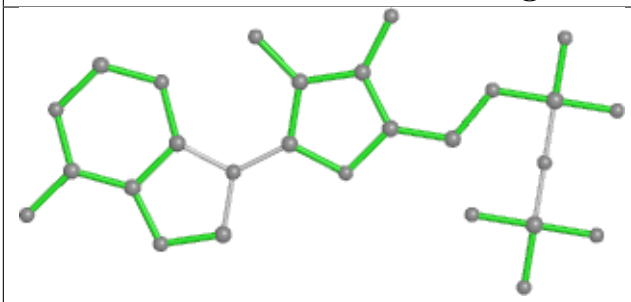
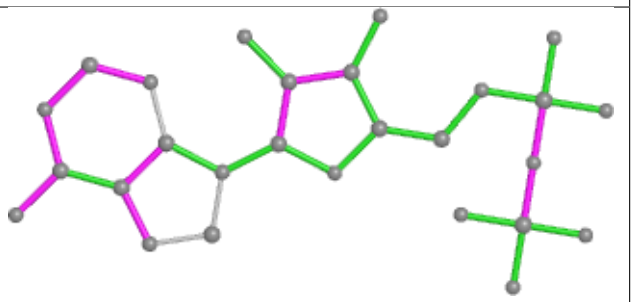


Rings

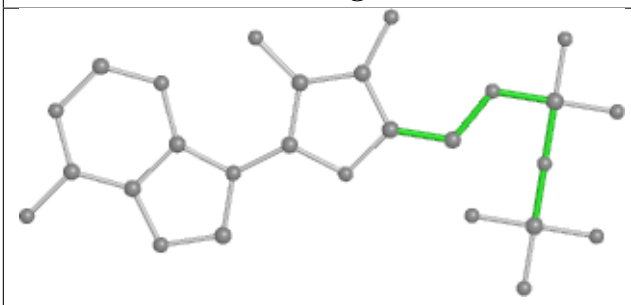
Ligand ADP K 501



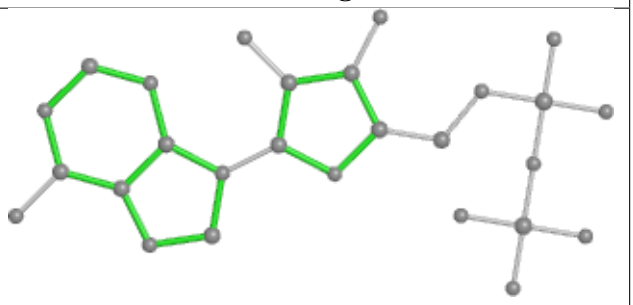
Bond lengths



Bond angles

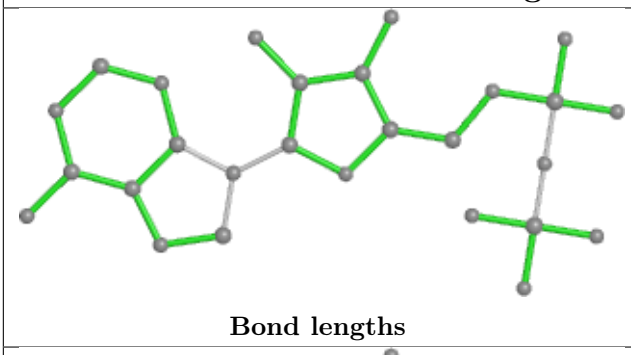


Torsions

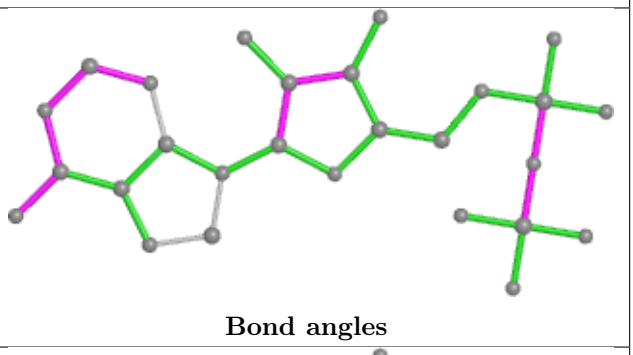


Rings

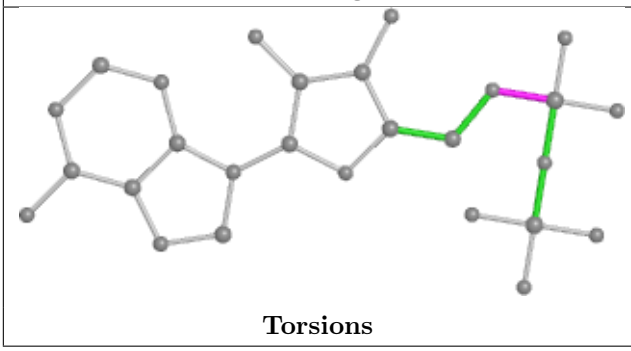
Ligand ADP L 501



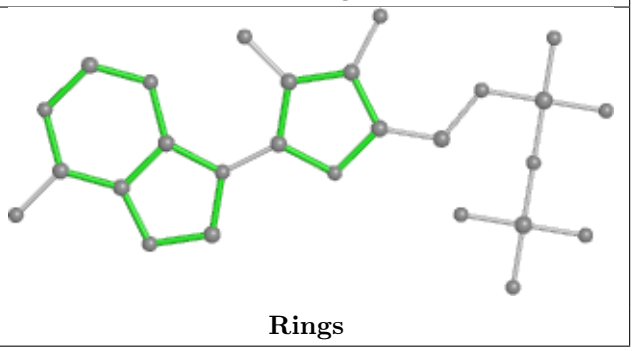
Bond lengths



Bond angles

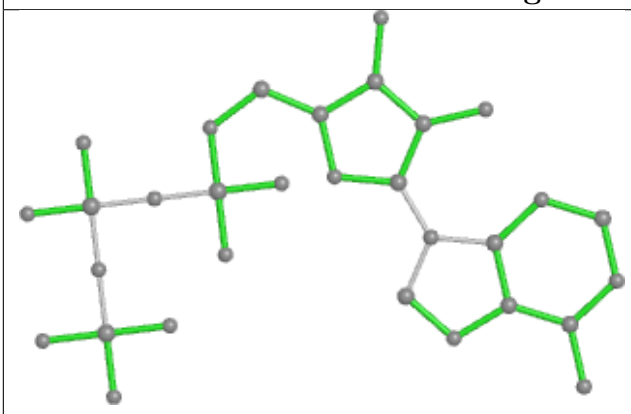


Torsions

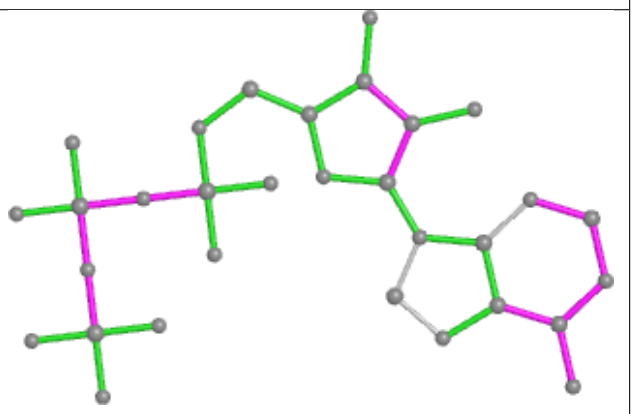


Rings

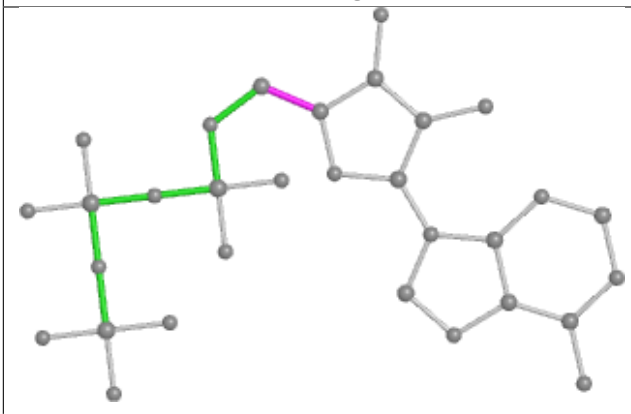
Ligand ATP H 501



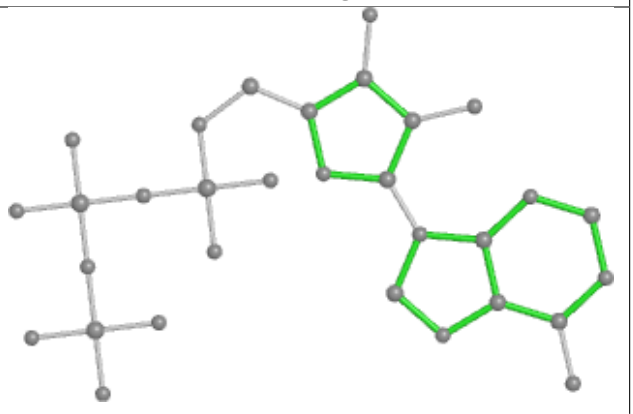
Bond lengths



Bond angles



Torsions



Rings

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.

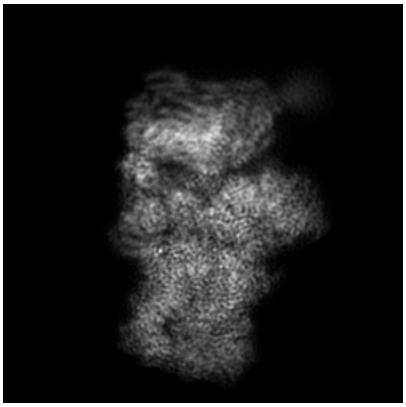
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9045. These allow visual inspection of the internal detail of the map and identification of artifacts.

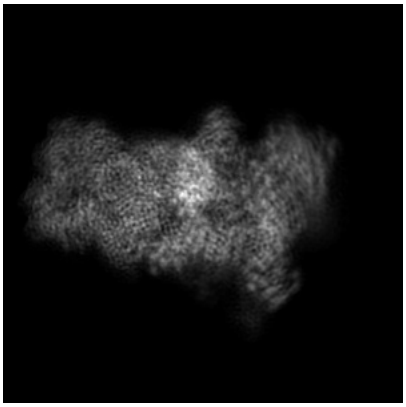
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

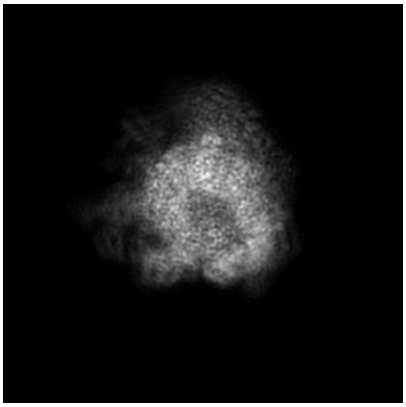
6.1.1 Primary map



X



Y



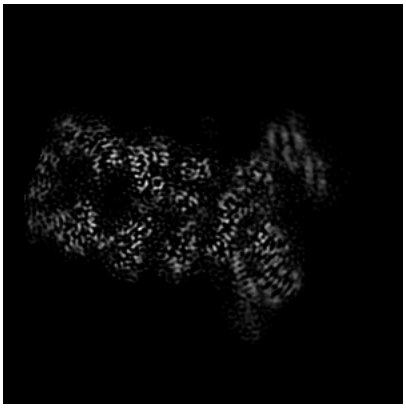
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 170



Y Index: 170

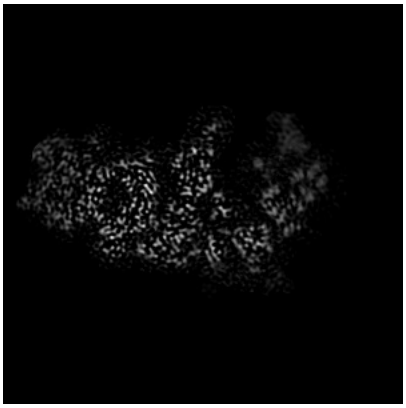
Z Index: 170

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: 175



Y Index: 189

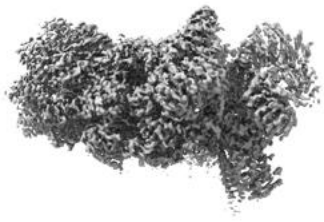
Z Index: 160

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

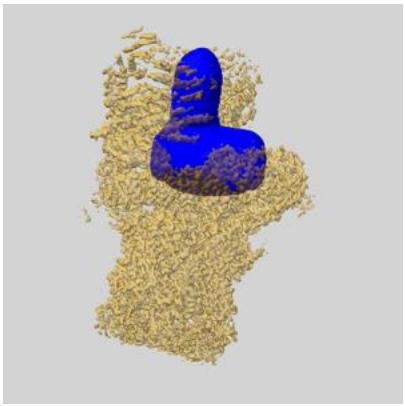
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

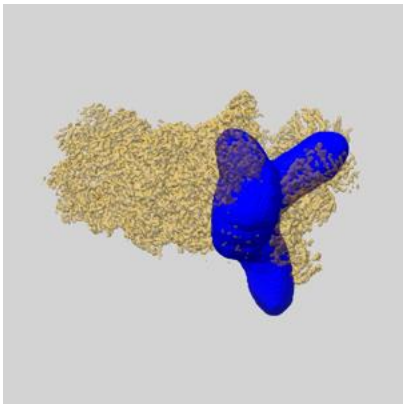
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

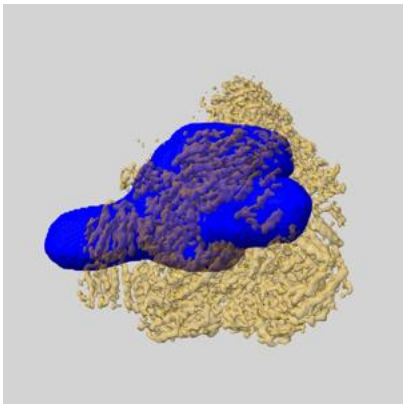
6.5.1 emd_9045_msk_3.map (i)



X

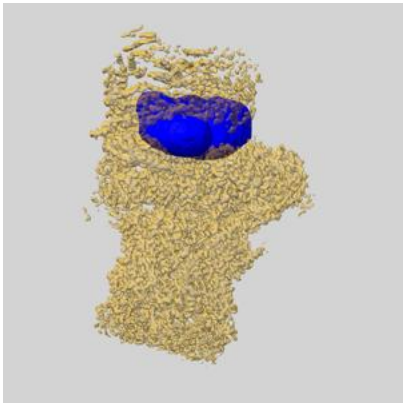


Y

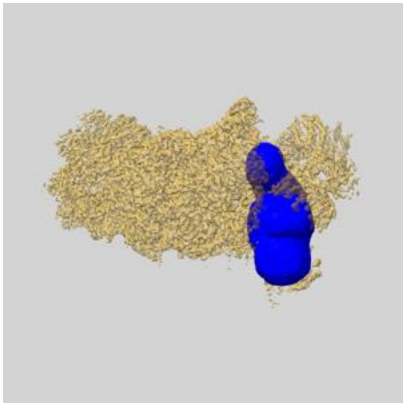


Z

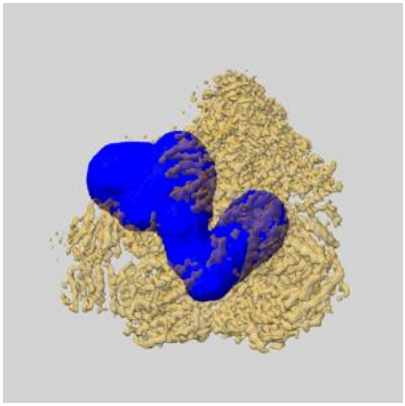
6.5.2 emd_9045_msk_2.map (i)



X

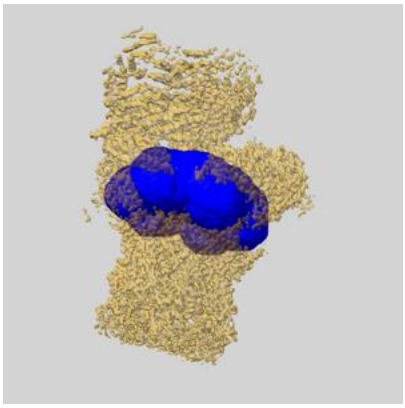


Y

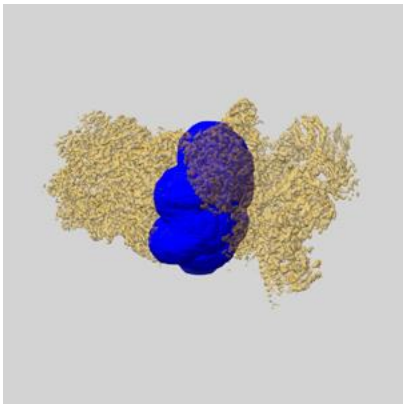


Z

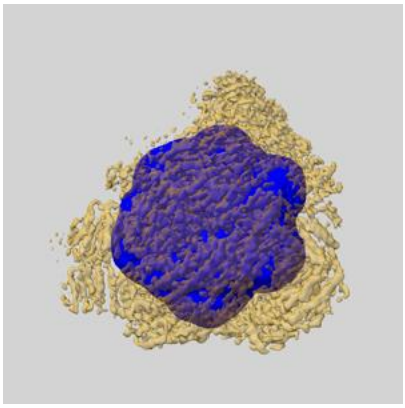
6.5.3 emd_9045_msk_6.map



X

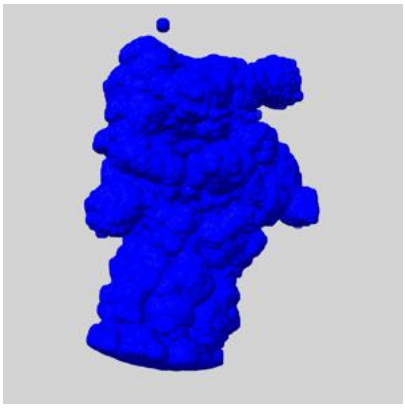


Y

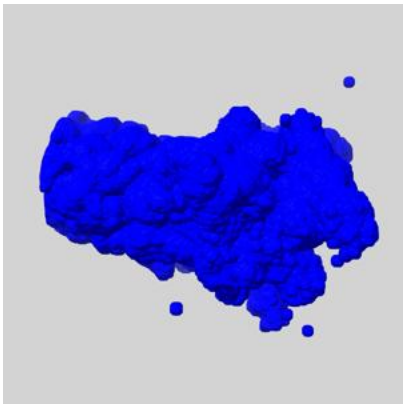


Z

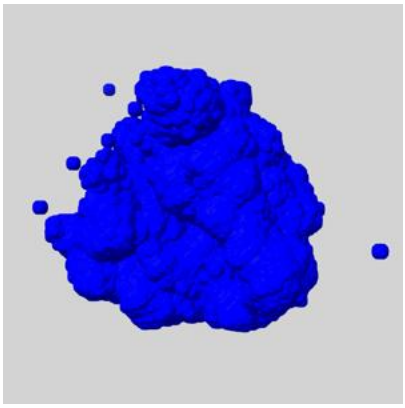
6.5.4 emd_9045_msk_1.map



X

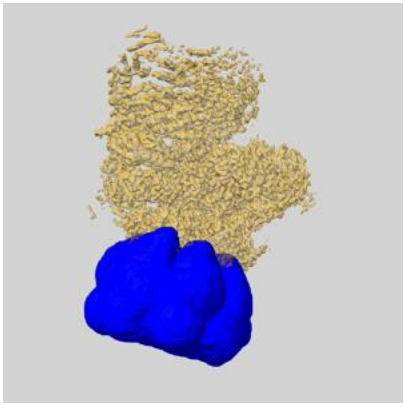


Y

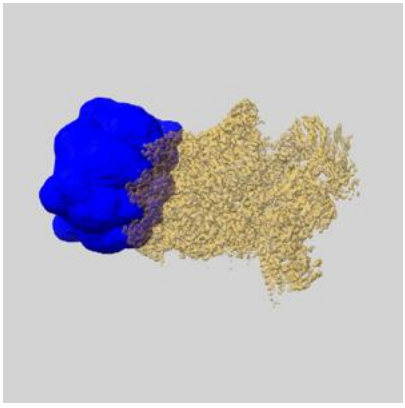


Z

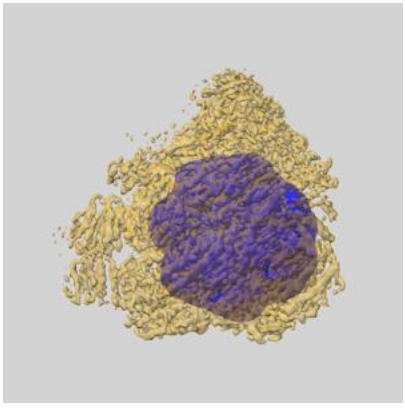
6.5.5 emd_9045_msk_5.map



X

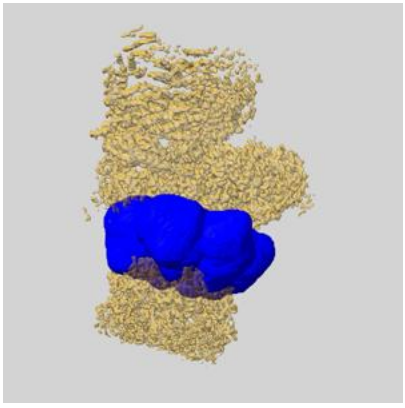


Y

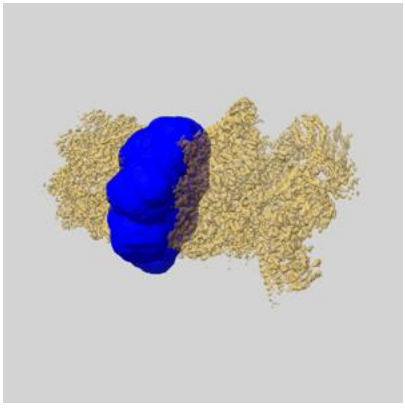


Z

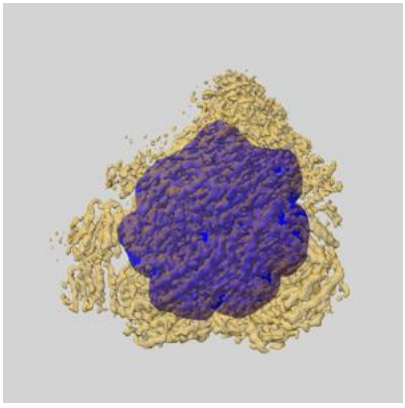
6.5.6 emd_9045_msk_4.map



X



Y

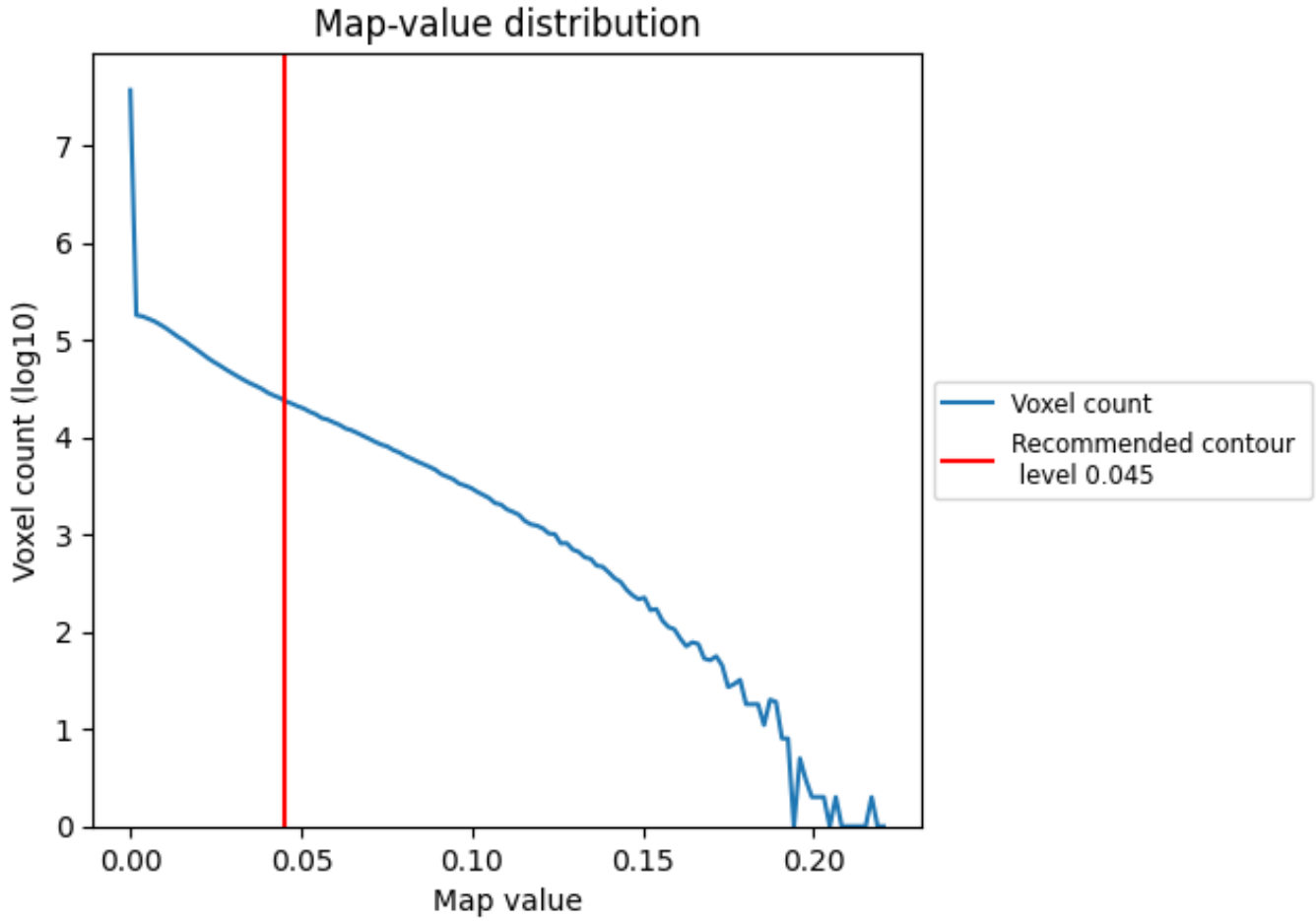


Z

7 Map analysis

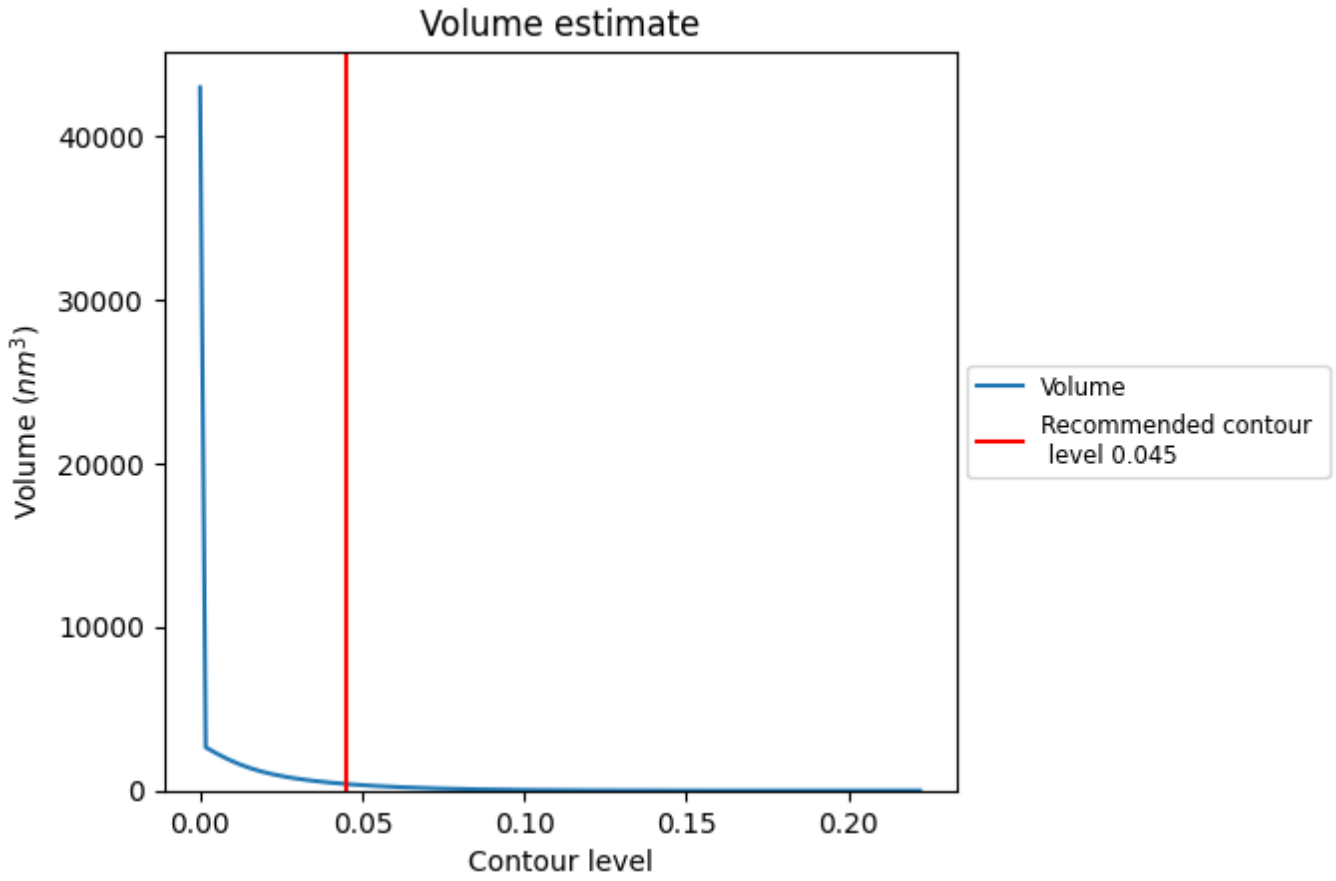
This section contains the results of statistical analysis of the map.

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.

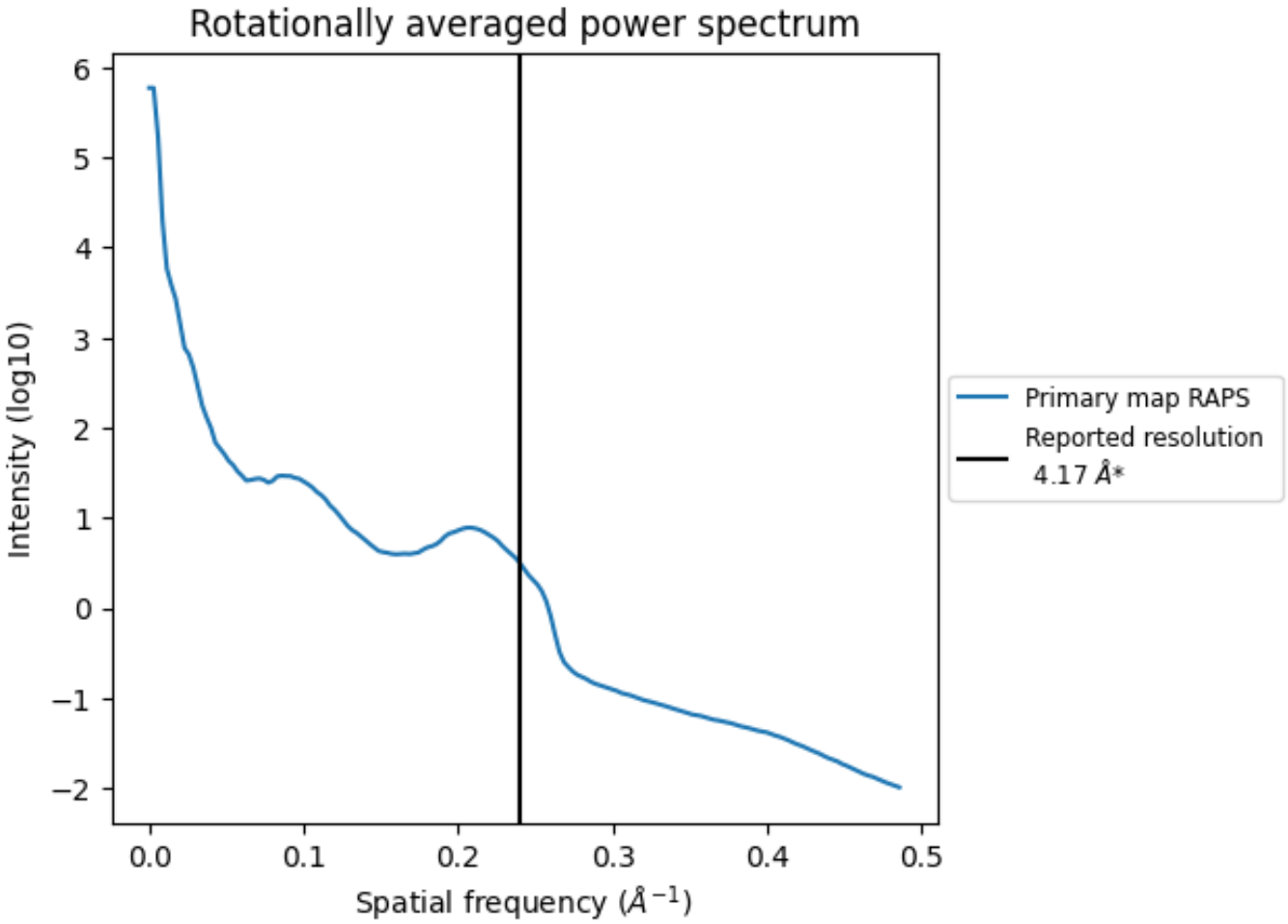
7.2 Volume estimate



The volume at the recommended contour level is 403 nm^3; this corresponds to an approximate mass of 364 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 0.240 Å^{-1}

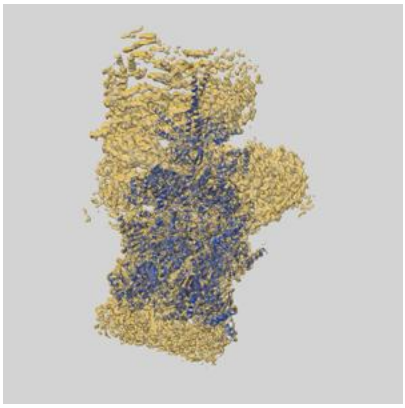
8 Fourier-Shell correlation

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

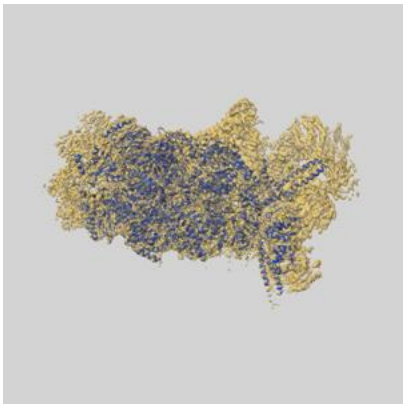
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9045 and PDB model 6EF3. Per-residue inclusion information can be found in section 3 on page 9.

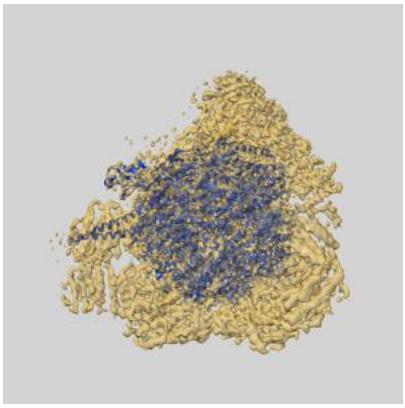
9.1 Map-model overlay



X



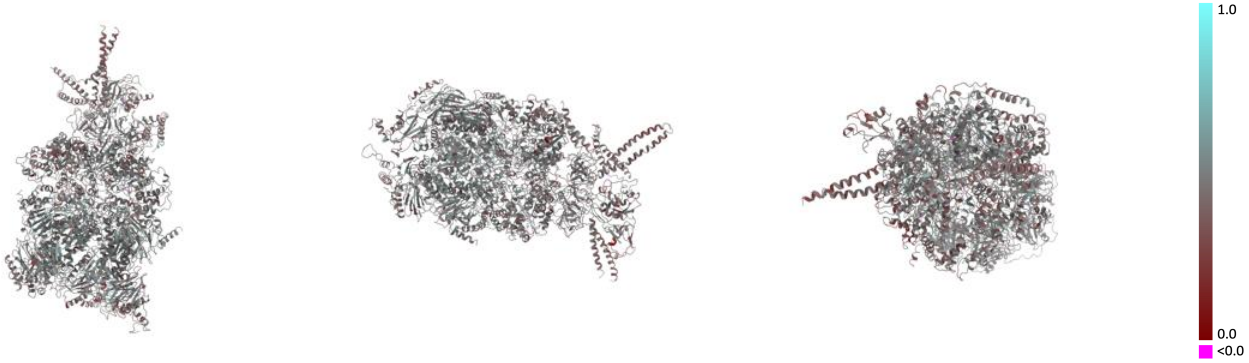
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

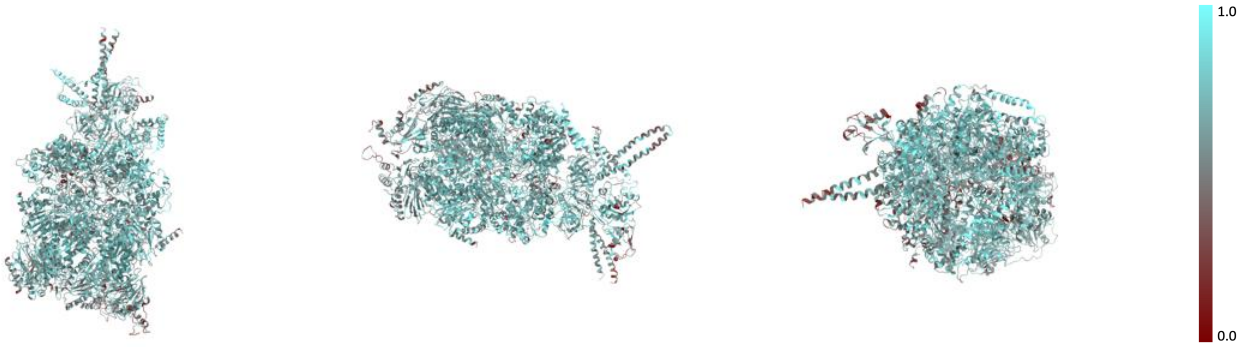
9.2 Q-score mapped to coordinate model



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.

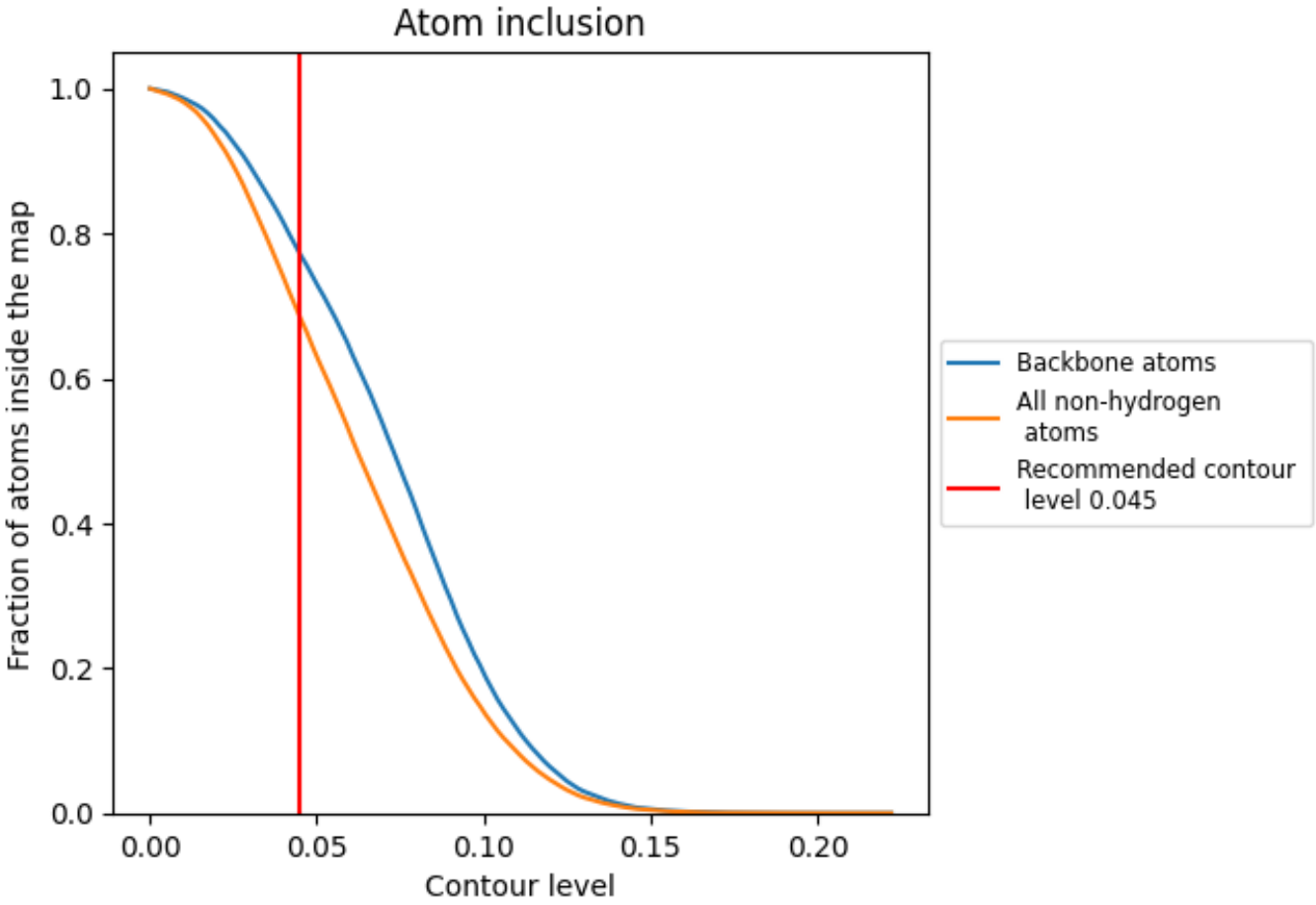
9.3 Atom inclusion mapped to coordinate model



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6838	0.4600
1	0.6751	0.4700
2	0.6538	0.4700
3	0.6542	0.4730
4	0.6189	0.4660
5	0.6203	0.4590
6	0.6099	0.4530
7	0.6447	0.4580
A	0.7211	0.4800
B	0.7301	0.4910
C	0.7244	0.4780
D	0.7113	0.4780
E	0.7266	0.4850
F	0.7489	0.4910
G	0.7259	0.4800
H	0.7221	0.4620
I	0.7336	0.4610
J	0.6900	0.4450
K	0.6756	0.4400
L	0.6067	0.4180
M	0.7036	0.4550
n	0.6446	0.4710
r	0.6820	0.4170
s	0.3586	0.3970
u	0.5272	0.4160