Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:40 pm GMT

PDB ID	:	5MP9
EMDB ID	:	EMD-3534
Title	:	26S proteasome in presence of ATP (s1)
Authors	:	Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.; Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.
Deposited on	:	2016-12-16
Resolution	:	4.10 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:

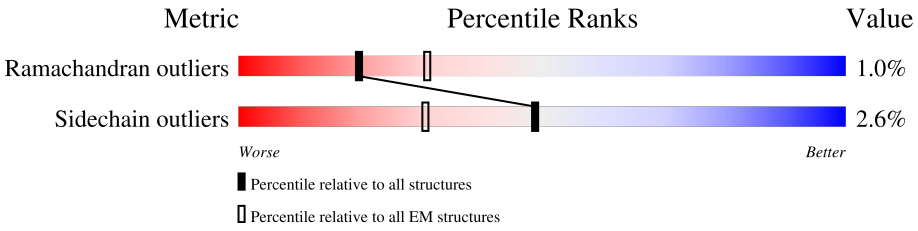
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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)
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	A	252	89% 6% ·
1	a	252	92% · ·
2	B	250	96% · ·
2	b	250	96% ·
3	C	258	90% · 5%
3	c	258	91% · 5%
4	D	254	85% 8% · 6%
4	d	254	91% · 6%
5	E	260	86% 7% · 7%

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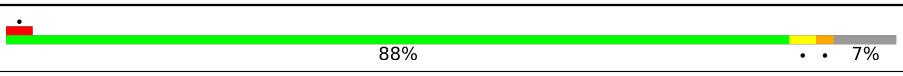
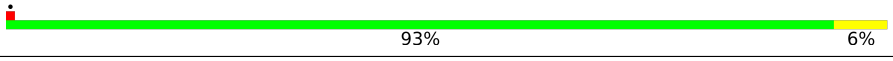
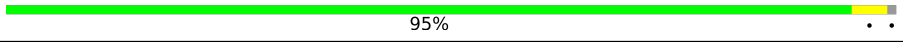
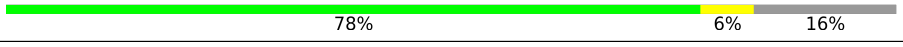
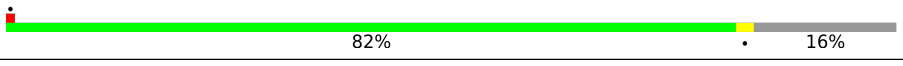
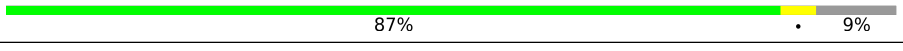
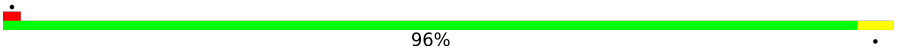
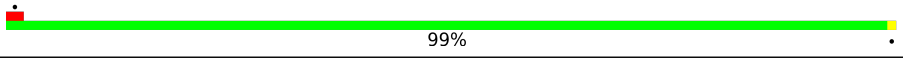
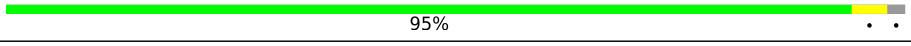
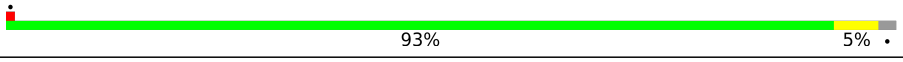
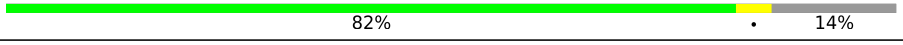
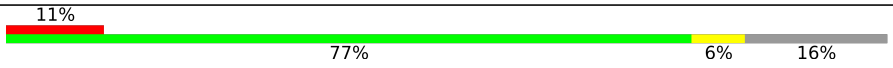
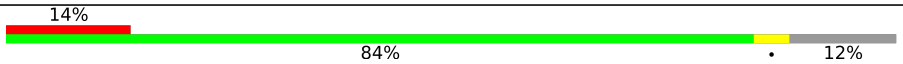
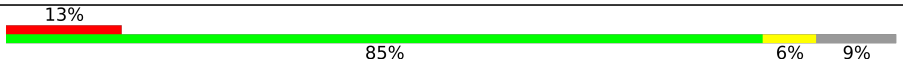
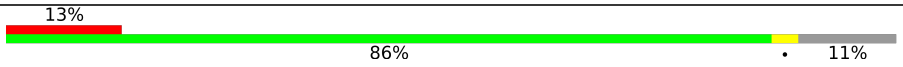
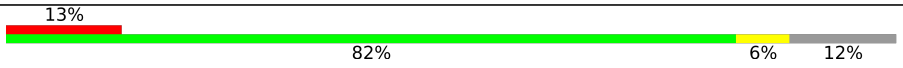
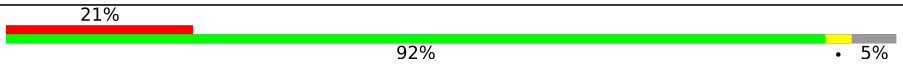
Mol	Chain	Length	Quality of chain
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	1	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	H	467	
16	I	437	
17	K	428	
18	L	437	
19	M	434	
20	J	405	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 67883 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 alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
2	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
4	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
5	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		
7	G	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	390	Total	C	N	O	S	0	0
			3053	1920	546	570	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	385	Total	C	N	O	S	0	0
			3022	1899	508	598	17		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	389	Total	C	N	O	S	0	0
			3078	1933	540	595	10		

- Molecule 18 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	388	Total	C	N	O	S	0	0
			3082	1942	548	580	12		

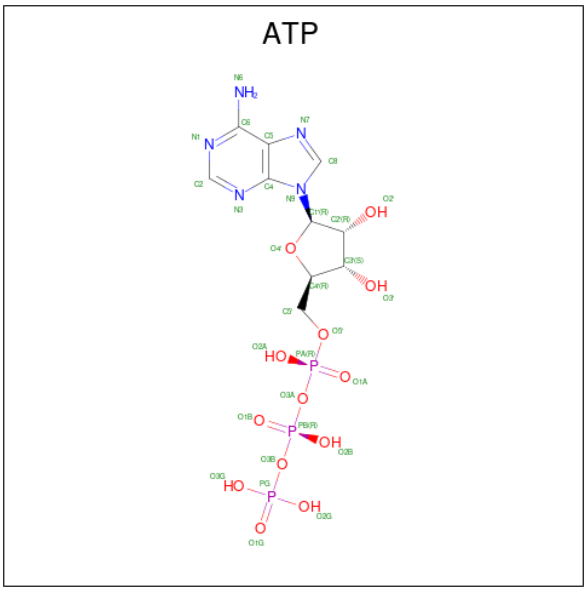
- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	381	Total	C	N	O	S	0	0
			2986	1870	524	580	12		

- Molecule 20 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	386	Total	C	N	O	S	0	0
			3033	1906	543	567	17		

- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



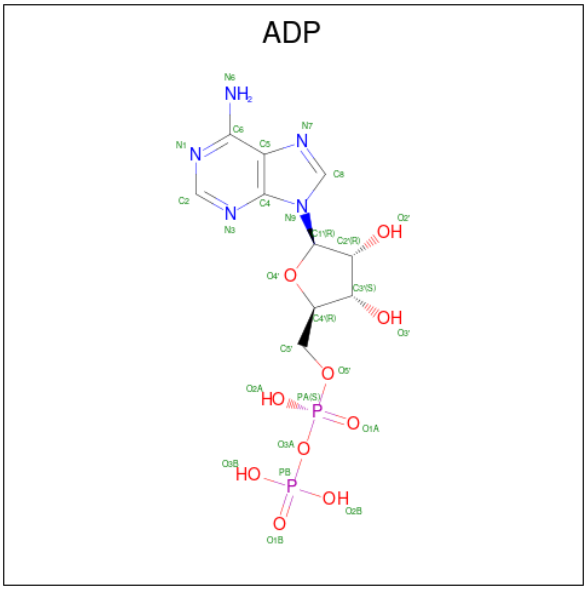
Mol	Chain	Residues	Atoms					AltConf
21	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
21	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
21	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
21	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
21	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
22	H	1	Total	Mg	0
			1	1	
22	I	1	Total	Mg	0
			1	1	
22	K	1	Total	Mg	0
			1	1	
22	L	1	Total	Mg	0
			1	1	
22	M	1	Total	Mg	0
			1	1	
22	J	1	Total	Mg	0
			1	1	

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
23	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

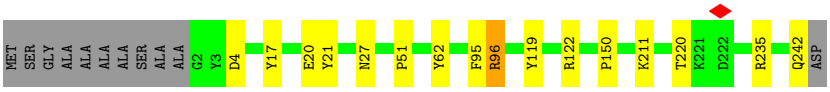
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 alpha type-1

Chain a:

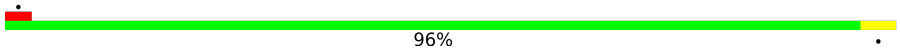
• Molecule 1: Proteasome subunit alpha type-1

Chain A:



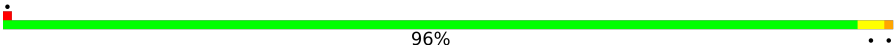
• Molecule 2: Proteasome subunit alpha type-2

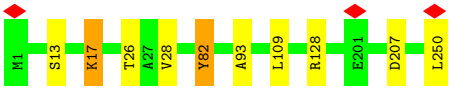
Chain b:



• Molecule 2: Proteasome subunit alpha type-2

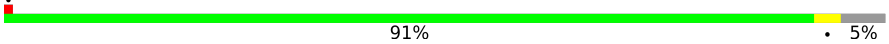
Chain B:

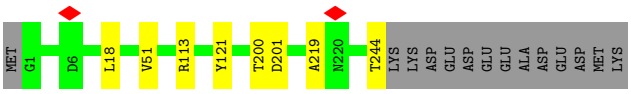




• Molecule 3: Proteasome subunit alpha type-3

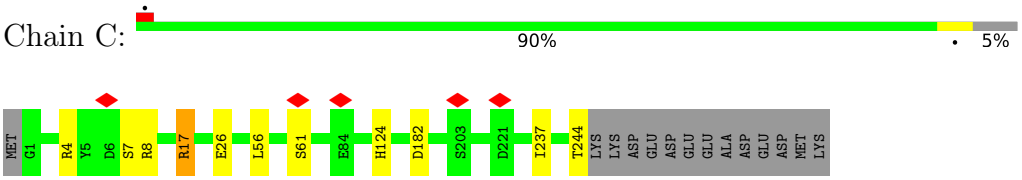
Chain c:





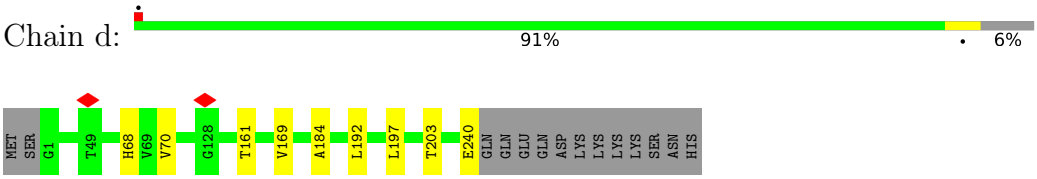
• Molecule 3: Proteasome subunit alpha type-3

Chain C:



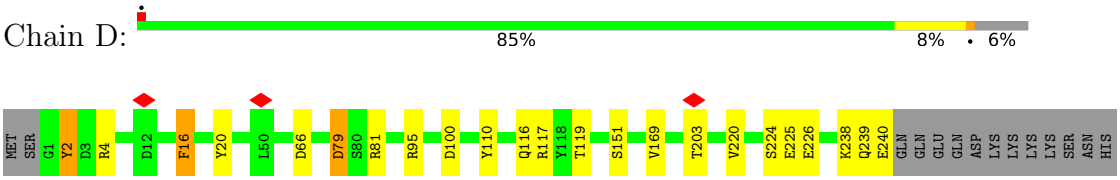
• Molecule 4: Proteasome subunit alpha type-4

Chain d:



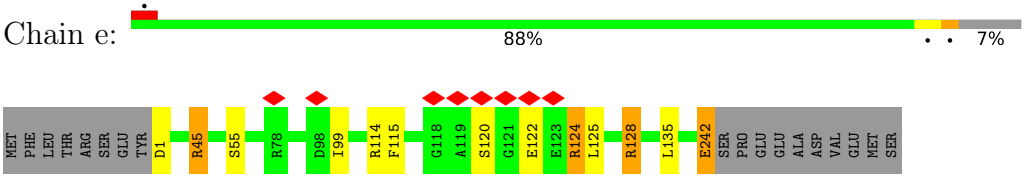
• Molecule 4: Proteasome subunit alpha type-4

Chain D:



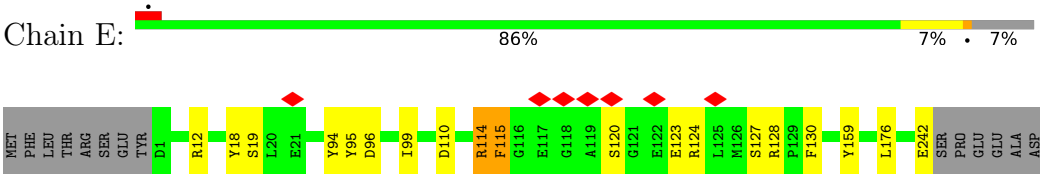
• Molecule 5: Proteasome subunit alpha type-5

Chain e:



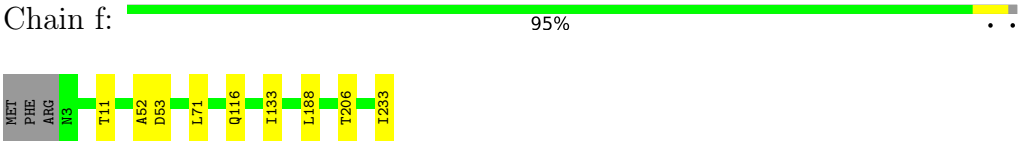
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



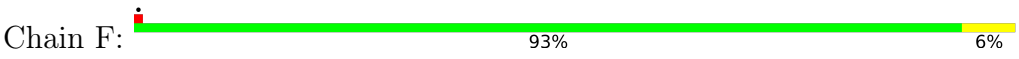
• Molecule 6: Proteasome subunit alpha type-6

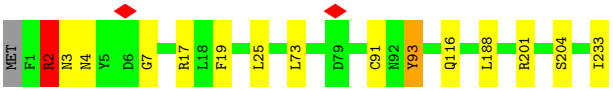
Chain f:



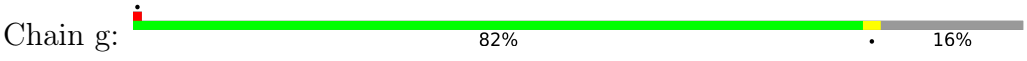
• Molecule 6: Proteasome subunit alpha type-6

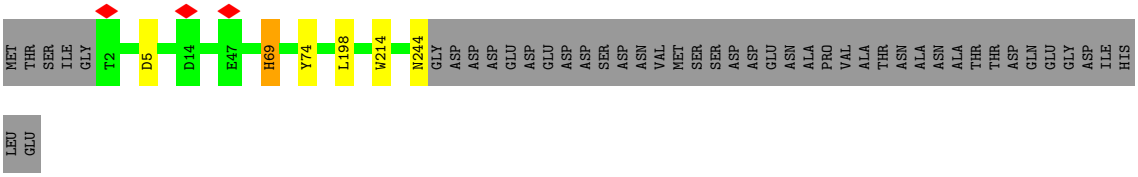
Chain F:



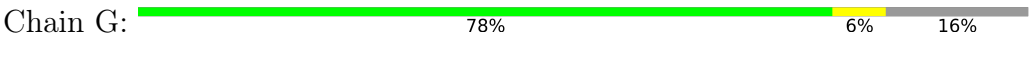


• Molecule 7: Probable proteasome subunit alpha type-7

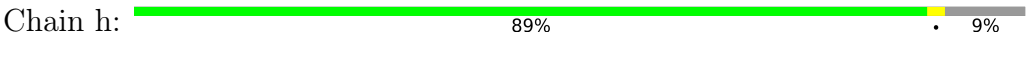




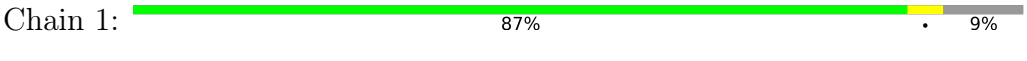
• Molecule 7: Probable proteasome subunit alpha type-7

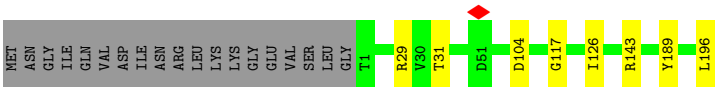


• Molecule 8: Proteasome subunit beta type-1

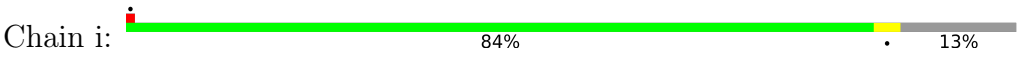


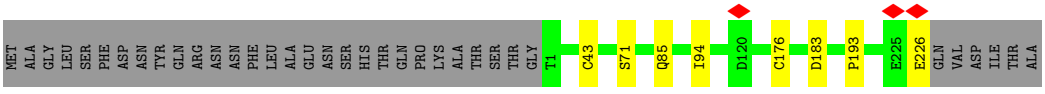
• Molecule 8: Proteasome subunit beta type-1



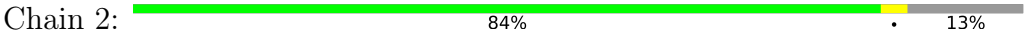


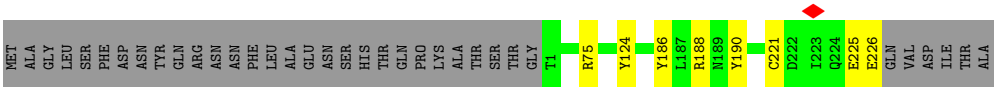
• Molecule 9: Proteasome subunit beta type-2





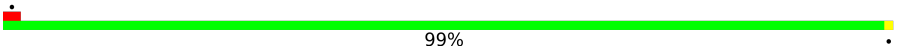
• Molecule 9: Proteasome subunit beta type-2

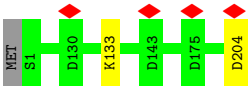




• Molecule 10: Proteasome subunit beta type-3

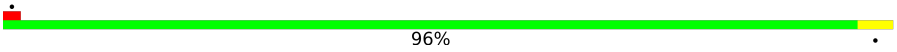
Chain j:

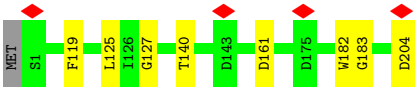




• Molecule 10: Proteasome subunit beta type-3

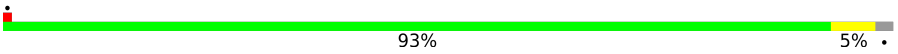
Chain 3:

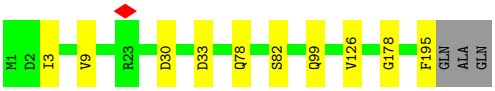




• Molecule 11: Proteasome subunit beta type-4

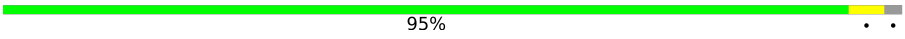
Chain k:





• Molecule 11: Proteasome subunit beta type-4

Chain 4:

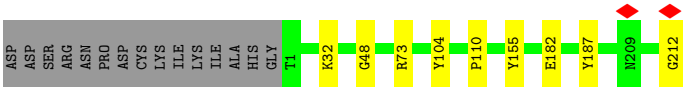


• Molecule 12: Proteasome subunit beta type-5

Chain l:

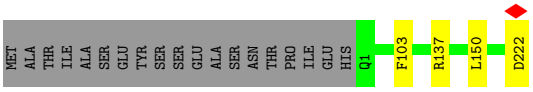
• Molecule 12: Proteasome subunit beta type-5

Chain 5:



• Molecule 13: Proteasome subunit beta type-6

Chain m:

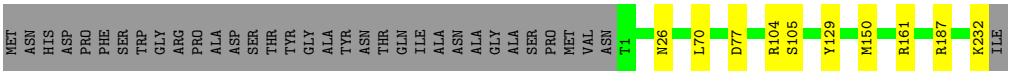


• Molecule 13: Proteasome subunit beta type-6

Chain 6:

• Molecule 14: Proteasome subunit beta type-7

Chain n:

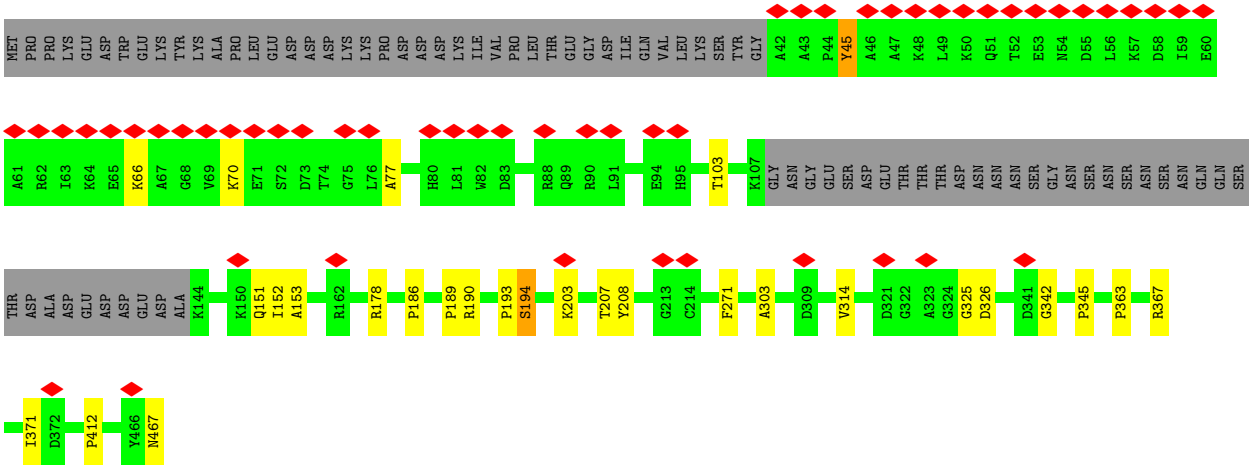


• Molecule 14: Proteasome subunit beta type-7

Chain 7:

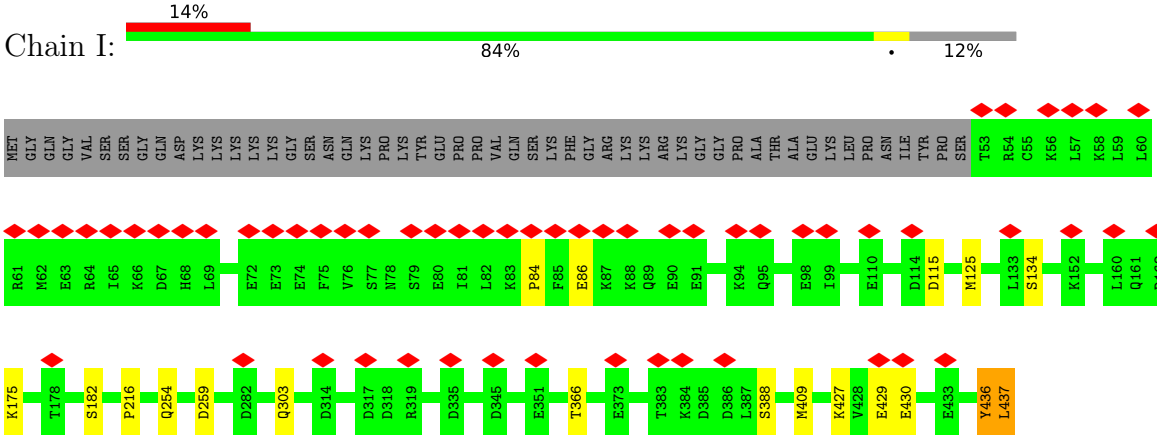
• Molecule 15: 26S protease regulatory subunit 7 homolog

Chain H:



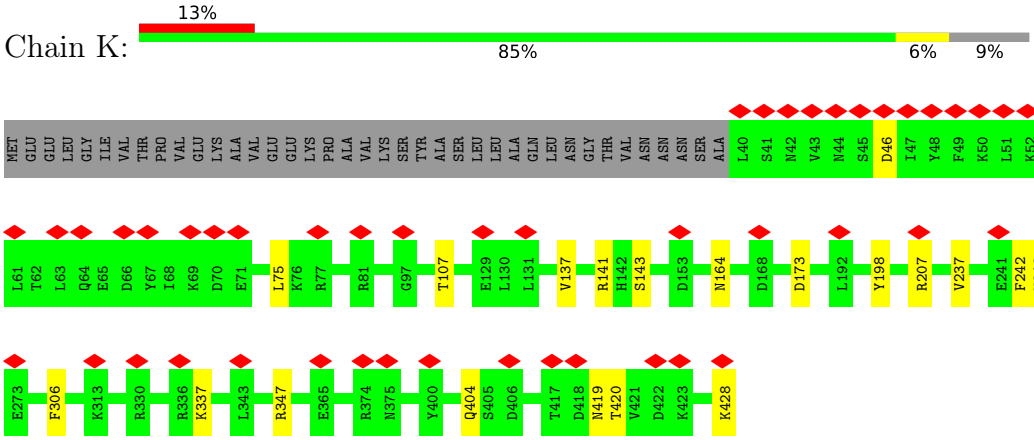
• Molecule 16: 26S protease regulatory subunit 4 homolog

Chain I:



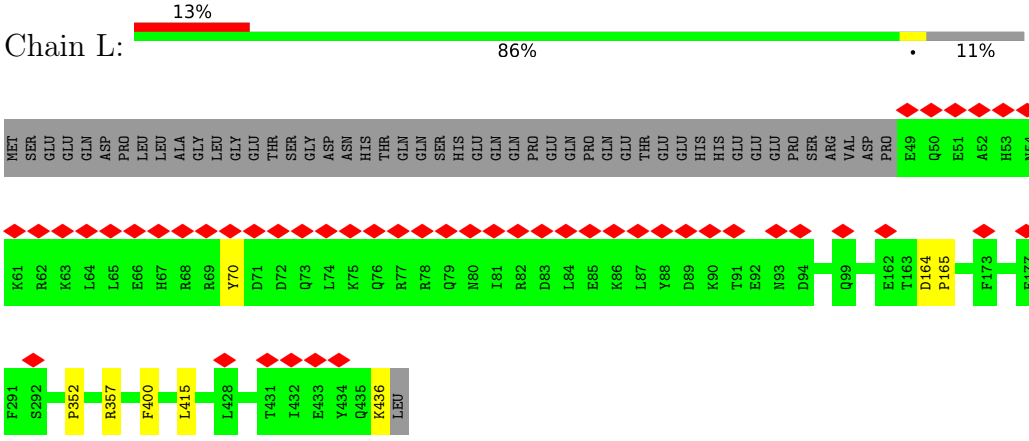
• Molecule 17: 26S protease regulatory subunit 6B homolog

Chain K:



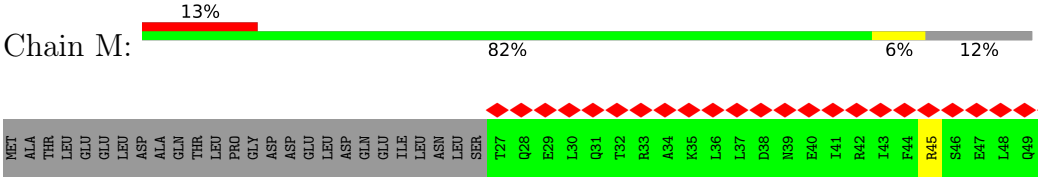
• Molecule 18: 26S protease subunit RPT4

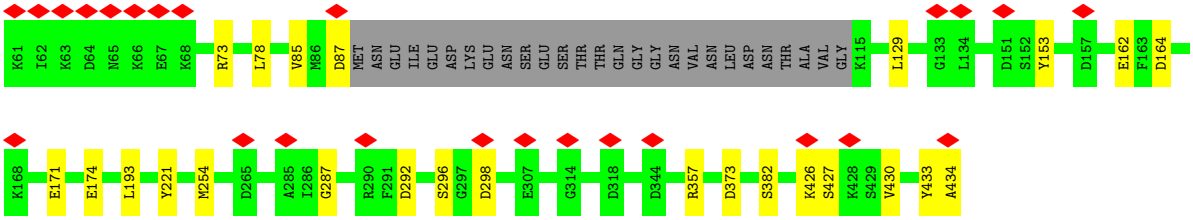
Chain L:



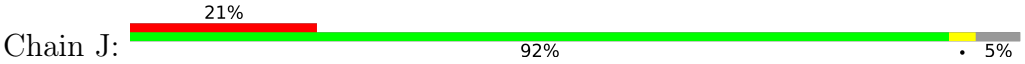
• Molecule 19: 26S protease regulatory subunit 6A

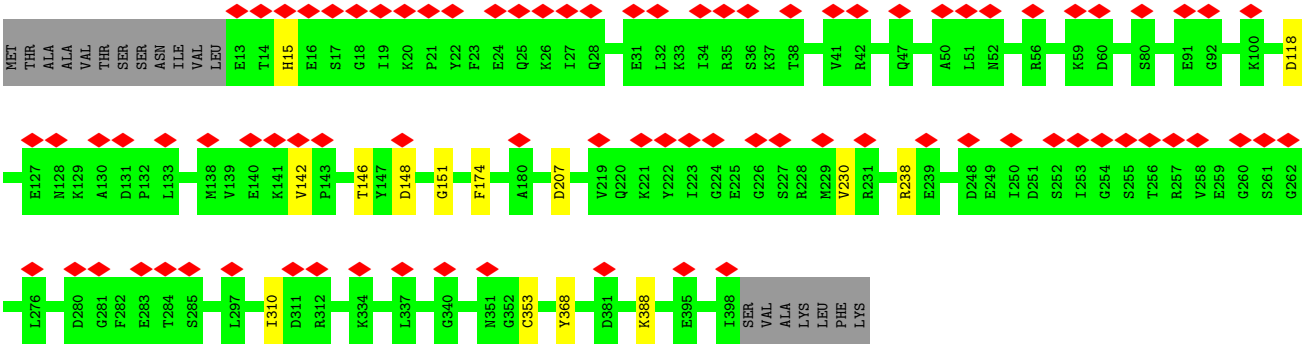
Chain M:





• Molecule 20: 26S protease regulatory subunit 8 homolog





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	286500	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.133	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.84	4/1945 (0.2%)	0.93	10/2634 (0.4%)
1	a	0.44	1/1945 (0.1%)	0.54	1/2634 (0.0%)
2	B	0.87	2/1952 (0.1%)	0.96	6/2642 (0.2%)
2	b	0.53	2/1952 (0.1%)	0.55	1/2642 (0.0%)
3	C	0.84	2/1934 (0.1%)	0.91	4/2618 (0.2%)
3	c	0.46	1/1934 (0.1%)	0.56	1/2618 (0.0%)
4	D	0.86	1/1910 (0.1%)	0.95	10/2586 (0.4%)
4	d	0.44	1/1910 (0.1%)	0.55	1/2586 (0.0%)
5	E	1.02	7/1886 (0.4%)	1.19	20/2541 (0.8%)
5	e	0.79	4/1886 (0.2%)	0.80	5/2541 (0.2%)
6	F	0.93	4/1823 (0.2%)	0.96	8/2463 (0.3%)
6	f	0.53	2/1800 (0.1%)	0.56	1/2433 (0.0%)
7	G	0.90	4/1932 (0.2%)	0.91	11/2609 (0.4%)
7	g	0.45	1/1932 (0.1%)	0.53	1/2609 (0.0%)
8	1	0.89	3/1541 (0.2%)	0.90	4/2087 (0.2%)
8	h	0.59	2/1541 (0.1%)	0.56	1/2087 (0.0%)
9	2	0.80	2/1750 (0.1%)	0.92	7/2373 (0.3%)
9	i	0.49	1/1750 (0.1%)	0.58	1/2373 (0.0%)
10	3	0.88	3/1611 (0.2%)	0.86	1/2174 (0.0%)
10	j	0.58	2/1611 (0.1%)	0.55	1/2174 (0.0%)
11	4	0.79	1/1589 (0.1%)	0.92	4/2142 (0.2%)
11	k	0.49	1/1589 (0.1%)	0.54	1/2142 (0.0%)
12	5	0.92	2/1681 (0.1%)	0.92	5/2274 (0.2%)
12	l	0.60	2/1681 (0.1%)	0.58	1/2274 (0.0%)
13	6	0.87	2/1795 (0.1%)	0.92	3/2420 (0.1%)
13	m	0.57	2/1795 (0.1%)	0.56	1/2420 (0.0%)
14	7	0.91	2/1821 (0.1%)	0.99	7/2470 (0.3%)
14	n	0.49	1/1846 (0.1%)	0.59	1/2503 (0.0%)
15	H	0.70	5/3102 (0.2%)	0.75	9/4175 (0.2%)
16	I	0.66	2/3061 (0.1%)	0.70	2/4121 (0.0%)
17	K	0.67	4/3121 (0.1%)	0.72	8/4213 (0.2%)
18	L	0.67	2/3128 (0.1%)	0.74	7/4204 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	M	0.71	3/3023 (0.1%)	0.74	7/4070 (0.2%)
20	J	0.55	0/3073	0.65	4/4129 (0.1%)
All	All	0.71	78/68850 (0.1%)	0.77	155/92981 (0.2%)

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
1	A	0	1
2	B	0	1
3	C	0	1
4	D	0	3
5	e	0	2
6	F	0	2
7	G	0	2
8	1	0	1
13	6	0	2
14	7	0	1
14	n	0	1
15	H	0	1
16	I	0	1
18	L	0	1
19	M	0	1
All	All	0	21

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	229	GLY	C-O	-14.49	1.00	1.23
12	5	212	GLY	C-O	-14.48	1.00	1.23
12	l	212	GLY	C-O	-14.48	1.00	1.23
9	2	226	GLU	C-O	-12.13	1.00	1.23
3	C	244	THR	C-O	-12.09	1.00	1.23
7	g	244	ASN	C-O	-12.09	1.00	1.23
16	I	437	LEU	C-OXT	-12.09	1.00	1.23
19	M	434	ALA	C-OXT	-12.08	1.00	1.23
11	k	195	PHE	C-O	-12.07	1.00	1.23
2	B	250	LEU	C-O	-12.07	1.00	1.23
2	b	250	LEU	C-O	-12.07	1.00	1.23
8	1	196	LEU	C-OXT	-12.07	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	244	ASN	C-O	-12.07	1.00	1.23
17	K	428	LYS	C-O	-12.07	1.00	1.23
9	i	226	GLU	C-O	-12.06	1.00	1.23
10	j	204	ASP	C-OXT	-12.06	1.00	1.23
1	a	242	GLN	C-O	-12.06	1.00	1.23
12	5	212	GLY	C-OXT	-12.06	1.00	1.23
13	6	222	ASP	C-O	-12.06	1.00	1.23
15	H	467	ASN	C-O	-12.06	1.00	1.23
3	c	244	THR	C-O	-12.05	1.00	1.23
17	K	428	LYS	C-OXT	-12.06	1.00	1.23
4	d	240	GLU	C-O	-12.05	1.00	1.23
12	l	212	GLY	C-OXT	-12.05	1.00	1.23
13	m	222	ASP	C-O	-12.05	1.00	1.23
6	F	233	ILE	C-OXT	-12.05	1.00	1.23
19	M	434	ALA	C-O	-12.05	1.00	1.23
10	3	204	ASP	C-O	-12.05	1.00	1.23
14	n	232	LYS	C-O	-12.05	1.00	1.23
11	4	195	PHE	C-O	-12.05	1.00	1.23
5	E	242	GLU	C-O	-12.05	1.00	1.23
18	L	436	LYS	C-O	-12.04	1.00	1.23
8	1	196	LEU	C-O	-12.04	1.00	1.23
13	6	222	ASP	C-OXT	-12.04	1.00	1.23
6	f	233	ILE	C-OXT	-12.04	1.00	1.23
2	b	250	LEU	C-OXT	-12.04	1.00	1.23
15	H	467	ASN	C-OXT	-12.04	1.00	1.23
8	h	196	LEU	C-OXT	-12.04	1.00	1.23
10	j	204	ASP	C-O	-12.04	1.00	1.23
13	m	222	ASP	C-OXT	-12.03	1.00	1.23
16	I	437	LEU	C-O	-12.03	1.00	1.23
8	h	196	LEU	C-O	-12.03	1.00	1.23
6	f	233	ILE	C-O	-12.02	1.00	1.23
1	A	242	GLN	C-O	-12.02	1.00	1.23
10	3	204	ASP	C-OXT	-12.02	1.00	1.23
5	e	242	GLU	C-O	-12.02	1.00	1.23
2	B	250	LEU	C-OXT	-12.00	1.00	1.23
6	F	233	ILE	C-O	-12.00	1.00	1.23
5	E	127	SER	CA-CB	8.03	1.65	1.52
5	E	124	ARG	CZ-NH1	7.50	1.42	1.33
1	A	96	ARG	NE-CZ	7.05	1.42	1.33
7	G	16	ARG	CZ-NH2	6.89	1.42	1.33
3	C	61	SER	CA-CB	6.65	1.62	1.52
15	H	178	ARG	NE-CZ	6.33	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	123	GLU	CG-CD	5.82	1.60	1.51
18	L	400	PHE	CB-CG	-5.80	1.41	1.51
9	2	75	ARG	CZ-NH2	5.64	1.40	1.33
5	e	114	ARG	CZ-NH1	5.56	1.40	1.33
1	A	20	GLU	CG-CD	5.55	1.60	1.51
15	H	45	TYR	CE2-CZ	5.49	1.45	1.38
8	1	143	ARG	CZ-NH2	5.43	1.40	1.33
4	D	4	ARG	NE-CZ	5.42	1.40	1.33
15	H	194	SER	CA-CB	5.37	1.61	1.52
17	K	141	ARG	CZ-NH1	5.31	1.40	1.33
6	F	201	ARG	CZ-NH2	5.31	1.40	1.33
7	G	28	GLU	CD-OE1	5.28	1.31	1.25
5	e	122	GLU	CG-CD	5.24	1.59	1.51
7	G	89	ARG	CD-NE	5.24	1.55	1.46
14	7	190	ARG	NE-CZ	5.13	1.39	1.33
19	M	45	ARG	CZ-NH2	5.12	1.39	1.33
5	E	19	SER	CA-CB	5.12	1.60	1.52
5	E	128	ARG	CZ-NH1	5.09	1.39	1.33
1	A	20	GLU	CD-OE2	5.06	1.31	1.25
5	E	115	PHE	CG-CD2	5.06	1.46	1.38
5	e	122	GLU	CD-OE1	5.05	1.31	1.25
10	3	119	PHE	CG-CD1	5.04	1.46	1.38
17	K	141	ARG	NE-CZ	5.03	1.39	1.33
6	F	2	ARG	CZ-NH2	5.03	1.39	1.33

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	139	TYR	CB-CG-CD2	-12.28	113.64	121.00
3	C	17	ARG	NE-CZ-NH1	-12.00	114.30	120.30
5	E	124	ARG	NE-CZ-NH2	-11.92	114.34	120.30
6	F	93	TYR	CB-CG-CD2	-11.62	114.03	121.00
2	B	82	TYR	CB-CG-CD2	-11.20	114.28	121.00
17	K	198	TYR	CB-CG-CD2	-10.62	114.63	121.00
2	B	82	TYR	CB-CG-CD1	10.53	127.32	121.00
17	K	198	TYR	CB-CG-CD1	10.37	127.22	121.00
1	A	21	TYR	CB-CG-CD1	10.35	127.21	121.00
5	E	159	TYR	CB-CG-CD2	-10.22	114.87	121.00
15	H	190	ARG	NE-CZ-NH1	9.91	125.26	120.30
12	5	187	TYR	CB-CG-CD1	9.82	126.89	121.00
1	A	21	TYR	CB-CG-CD2	-9.53	115.28	121.00
9	2	186	TYR	CB-CG-CD2	-9.23	115.46	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	115	PHE	CB-CG-CD2	9.21	127.25	120.80
5	E	110	ASP	CB-CG-OD1	9.10	126.49	118.30
20	J	238	ARG	NE-CZ-NH1	-9.09	115.76	120.30
5	E	95	TYR	CB-CG-CD1	-9.07	115.56	121.00
14	7	16	TYR	CB-CG-CD2	-9.02	115.59	121.00
11	4	139	TYR	CB-CG-CD1	8.85	126.31	121.00
4	D	4	ARG	NE-CZ-NH2	-8.82	115.89	120.30
13	6	105	TYR	CB-CG-CD1	-8.68	115.79	121.00
5	E	114	ARG	NE-CZ-NH1	8.57	124.58	120.30
4	D	2	TYR	CB-CG-CD1	-8.48	115.91	121.00
3	C	4	ARG	NE-CZ-NH1	8.37	124.48	120.30
18	L	400	PHE	CB-CG-CD1	-8.32	114.98	120.80
1	A	17	TYR	CB-CG-CD2	-8.30	116.02	121.00
19	M	45	ARG	NE-CZ-NH1	7.97	124.28	120.30
4	D	20	TYR	CB-CG-CD1	7.88	125.73	121.00
1	A	119	TYR	CB-CG-CD2	-7.86	116.28	121.00
5	e	115	PHE	CB-CG-CD2	7.72	126.20	120.80
17	K	141	ARG	NE-CZ-NH2	-7.71	116.44	120.30
18	L	194	ARG	NE-CZ-NH1	7.56	124.08	120.30
19	M	357	ARG	NE-CZ-NH2	-7.48	116.56	120.30
6	F	201	ARG	NE-CZ-NH1	7.46	124.03	120.30
6	F	201	ARG	NE-CZ-NH2	-7.46	116.57	120.30
5	E	94	TYR	CB-CG-CD1	7.40	125.44	121.00
5	E	94	TYR	CB-CG-CD2	-7.39	116.56	121.00
14	7	186	TYR	CB-CG-CD2	7.36	125.41	121.00
4	D	117	ARG	NE-CZ-NH2	-7.35	116.62	120.30
7	G	156	TYR	CB-CG-CD1	-7.34	116.60	121.00
9	2	75	ARG	NE-CZ-NH1	7.30	123.95	120.30
5	E	18	TYR	CB-CG-CD1	7.13	125.28	121.00
5	E	96	ASP	CB-CG-OD1	7.05	124.64	118.30
5	E	114	ARG	NE-CZ-NH2	-7.03	116.79	120.30
5	E	110	ASP	CB-CG-OD2	-6.98	112.02	118.30
7	G	95	PHE	CB-CG-CD1	6.94	125.66	120.80
7	G	95	PHE	CB-CG-CD2	-6.87	115.99	120.80
4	D	20	TYR	CB-CG-CD2	-6.82	116.91	121.00
14	7	143	ALA	N-CA-CB	6.80	119.62	110.10
5	E	130	PHE	CB-CG-CD1	-6.78	116.05	120.80
20	J	174	PHE	CB-CG-CD2	-6.76	116.06	120.80
7	G	89	ARG	NE-CZ-NH1	6.67	123.64	120.30
8	1	143	ARG	NE-CZ-NH1	6.62	123.61	120.30
19	M	45	ARG	NE-CZ-NH2	-6.54	117.03	120.30
14	7	181	MET	CG-SD-CE	6.51	110.62	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	128	ARG	NE-CZ-NH2	-6.51	117.04	120.30
14	7	229	GLY	CA-C-O	-6.45	109.00	120.60
12	l	212	GLY	CA-C-O	-6.45	109.00	120.60
12	5	212	GLY	CA-C-O	-6.44	109.01	120.60
7	G	89	ARG	NE-CZ-NH2	-6.39	117.10	120.30
17	K	243	VAL	CA-CB-CG2	-6.37	101.35	110.90
7	G	22	TYR	CB-CG-CD2	-6.32	117.21	121.00
12	5	187	TYR	CB-CG-CD2	-6.31	117.21	121.00
9	2	186	TYR	CB-CG-CD1	6.31	124.78	121.00
5	e	124	ARG	NE-CZ-NH2	-6.28	117.16	120.30
7	G	80	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	119	TYR	CB-CG-CD1	6.18	124.70	121.00
5	E	95	TYR	CB-CG-CD2	6.16	124.70	121.00
1	A	95	PHE	CB-CG-CD1	-5.96	116.63	120.80
15	H	271	PHE	CB-CG-CD1	5.96	124.97	120.80
20	J	368	TYR	CG-CD2-CE2	-5.90	116.58	121.30
19	M	73	ARG	NE-CZ-NH2	-5.87	117.37	120.30
7	G	11	PHE	CB-CG-CD1	-5.86	116.70	120.80
14	7	16	TYR	CG-CD1-CE1	-5.83	116.63	121.30
1	A	62	TYR	CG-CD1-CE1	-5.76	116.69	121.30
6	F	17	ARG	NE-CZ-NH1	5.76	123.18	120.30
7	G	22	TYR	CB-CG-CD1	5.73	124.44	121.00
19	M	433	TYR	CB-CG-CD1	-5.71	117.57	121.00
18	L	290	ARG	NE-CZ-NH1	5.71	123.15	120.30
11	4	23	ARG	NE-CZ-NH1	-5.70	117.45	120.30
5	e	135	LEU	CB-CG-CD2	5.69	120.68	111.00
14	7	30	TYR	CB-CG-CD2	-5.66	117.61	121.00
4	D	151	SER	N-CA-CB	5.65	118.98	110.50
13	6	16	ALA	CB-CA-C	-5.65	101.62	110.10
20	J	174	PHE	CB-CG-CD1	5.64	124.75	120.80
12	5	155	TYR	CB-CG-CD1	-5.63	117.62	121.00
5	E	12	ARG	NE-CZ-NH1	5.60	123.10	120.30
15	H	153	ALA	N-CA-CB	5.56	117.88	110.10
8	1	189	TYR	CG-CD2-CE2	-5.55	116.86	121.30
5	E	128	ARG	NE-CZ-NH1	5.55	123.07	120.30
4	D	16	PHE	CB-CG-CD2	-5.54	116.92	120.80
18	L	247	PRO	CA-N-CD	5.54	119.45	111.70
6	F	25	LEU	CB-CA-C	-5.52	99.72	110.20
2	B	93	ALA	CB-CA-C	-5.51	101.83	110.10
9	2	188	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	4	ASP	CB-CG-OD1	5.49	123.24	118.30
6	F	19	PHE	CB-CG-CD2	-5.46	116.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	93	TYR	CB-CG-CD1	5.46	124.27	121.00
9	2	124	TYR	CB-CG-CD2	-5.43	117.74	121.00
5	E	115	PHE	CB-CG-CD1	-5.39	117.02	120.80
8	1	189	TYR	CB-CG-CD1	-5.39	117.77	121.00
13	m	222	ASP	CA-C-O	-5.33	108.91	120.10
4	d	240	GLU	CA-C-O	-5.32	108.94	120.10
6	F	233	ILE	CA-C-O	-5.31	108.95	120.10
5	E	96	ASP	CB-CG-OD2	-5.30	113.53	118.30
15	H	467	ASN	CA-C-O	-5.30	108.97	120.10
1	a	242	GLN	CA-C-O	-5.29	108.98	120.10
2	b	250	LEU	CA-C-O	-5.29	108.98	120.10
8	h	196	LEU	CA-C-O	-5.29	108.98	120.10
1	A	4	ASP	CB-CG-OD2	-5.29	113.54	118.30
3	C	244	THR	CA-C-O	-5.29	108.99	120.10
11	4	195	PHE	CA-C-O	-5.29	108.99	120.10
10	j	204	ASP	CA-C-O	-5.29	108.99	120.10
5	E	242	GLU	CA-C-O	-5.29	108.99	120.10
8	1	196	LEU	CA-C-O	-5.29	109.00	120.10
2	B	250	LEU	CA-C-O	-5.29	109.00	120.10
18	L	436	LYS	CA-C-O	-5.28	109.00	120.10
1	A	242	GLN	CA-C-O	-5.28	109.01	120.10
15	H	70	LYS	N-CA-CB	5.28	120.11	110.60
5	e	242	GLU	CA-C-O	-5.28	109.01	120.10
11	k	195	PHE	CA-C-O	-5.28	109.01	120.10
19	M	221	TYR	CB-CG-CD1	-5.28	117.83	121.00
6	f	233	ILE	CA-C-O	-5.28	109.01	120.10
7	G	244	ASN	CA-C-O	-5.28	109.01	120.10
10	3	204	ASP	CA-C-O	-5.28	109.02	120.10
14	n	232	LYS	CA-C-O	-5.28	109.02	120.10
13	6	222	ASP	CA-C-O	-5.28	109.02	120.10
16	I	437	LEU	CA-C-O	-5.28	109.02	120.10
15	H	186	PRO	N-CA-CB	5.28	109.63	103.30
19	M	434	ALA	CA-C-O	-5.28	109.02	120.10
3	C	17	ARG	NH1-CZ-NH2	5.27	125.20	119.40
7	g	244	ASN	CA-C-O	-5.26	109.05	120.10
9	2	190	TYR	CB-CG-CD2	-5.26	117.84	121.00
17	K	428	LYS	CA-C-O	-5.26	109.05	120.10
3	c	244	THR	CA-C-O	-5.26	109.06	120.10
9	i	226	GLU	CA-C-O	-5.26	109.06	120.10
9	2	226	GLU	CA-C-O	-5.25	109.08	120.10
16	I	216	PRO	CA-N-CD	5.24	119.03	111.70
4	D	169	VAL	CG1-CB-CG2	-5.17	102.63	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	189	PRO	CA-N-CD	5.14	118.90	111.70
2	B	17	LYS	N-CA-CB	5.13	119.84	110.60
4	D	79	ASP	CB-CG-OD1	5.13	122.91	118.30
15	H	178	ARG	NE-CZ-NH1	-5.12	117.74	120.30
18	L	352	PRO	CA-N-CD	5.11	118.85	111.70
17	K	242	PHE	CB-CG-CD2	5.09	124.36	120.80
17	K	306	PHE	CB-CG-CD1	-5.08	117.24	120.80
15	H	345	PRO	CA-N-CD	5.07	118.80	111.70
12	5	110	PRO	CA-N-CD	5.05	118.77	111.70
5	E	159	TYR	CB-CG-CD1	5.05	124.03	121.00
2	B	28	VAL	CA-CB-CG2	-5.04	103.34	110.90
17	K	207	ARG	NE-CZ-NH1	-5.03	117.78	120.30
18	L	165	PRO	CA-N-CD	5.03	118.74	111.70
7	G	80	ASP	CB-CG-OD2	-5.02	113.78	118.30
4	D	119	THR	CA-CB-OG1	5.00	119.51	109.00

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	29	ARG	Sidechain
13	6	105	TYR	Sidechain
13	6	217	TYR	Sidechain
14	7	186	TYR	Sidechain
1	A	96	ARG	Sidechain
2	B	82	TYR	Sidechain
3	C	17	ARG	Sidechain
4	D	110	TYR	Sidechain
4	D	81	ARG	Sidechain
4	D	95	ARG	Sidechain
6	F	2	ARG	Sidechain
6	F	93	TYR	Sidechain
7	G	119	HIS	Sidechain
7	G	208	PHE	Sidechain
15	H	45	TYR	Sidechain
16	I	182	SER	Peptide
18	L	70	TYR	Sidechain
19	M	153	TYR	Sidechain
5	e	124	ARG	Sidechain
5	e	128	ARG	Sidechain
14	n	77	ASP	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/252 (95%)	228 (95%)	9 (4%)	2 (1%)	19	58
1	a	239/252 (95%)	224 (94%)	14 (6%)	1 (0%)	34	71
2	B	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	34	71
2	b	248/250 (99%)	232 (94%)	16 (6%)	0	100	100
3	C	242/258 (94%)	232 (96%)	9 (4%)	1 (0%)	34	71
3	c	242/258 (94%)	227 (94%)	13 (5%)	2 (1%)	19	58
4	D	238/254 (94%)	223 (94%)	12 (5%)	3 (1%)	12	47
4	d	238/254 (94%)	224 (94%)	12 (5%)	2 (1%)	19	58
5	E	240/260 (92%)	228 (95%)	9 (4%)	3 (1%)	12	47
5	e	240/260 (92%)	225 (94%)	12 (5%)	3 (1%)	12	47
6	F	231/234 (99%)	214 (93%)	14 (6%)	3 (1%)	12	47
6	f	229/234 (98%)	216 (94%)	11 (5%)	2 (1%)	17	54
7	G	241/288 (84%)	228 (95%)	11 (5%)	2 (1%)	19	58
7	g	241/288 (84%)	229 (95%)	11 (5%)	1 (0%)	34	71
8	1	194/215 (90%)	181 (93%)	12 (6%)	1 (0%)	29	67
8	h	194/215 (90%)	178 (92%)	15 (8%)	1 (0%)	29	67
9	2	224/261 (86%)	214 (96%)	9 (4%)	1 (0%)	34	71
9	i	224/261 (86%)	205 (92%)	17 (8%)	2 (1%)	17	54
10	3	202/205 (98%)	184 (91%)	14 (7%)	4 (2%)	7	39
10	j	202/205 (98%)	181 (90%)	21 (10%)	0	100	100
11	4	193/198 (98%)	184 (95%)	8 (4%)	1 (0%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	k	193/198 (98%)	186 (96%)	5 (3%)	2 (1%)	15 52
12	5	210/287 (73%)	195 (93%)	13 (6%)	2 (1%)	15 52
12	l	210/287 (73%)	196 (93%)	12 (6%)	2 (1%)	15 52
13	6	220/241 (91%)	207 (94%)	13 (6%)	0	100 100
13	m	220/241 (91%)	202 (92%)	18 (8%)	0	100 100
14	7	227/266 (85%)	209 (92%)	15 (7%)	3 (1%)	12 47
14	n	230/266 (86%)	211 (92%)	19 (8%)	0	100 100
15	H	386/467 (83%)	348 (90%)	26 (7%)	12 (3%)	4 31
16	I	383/437 (88%)	353 (92%)	22 (6%)	8 (2%)	7 38
17	K	387/428 (90%)	357 (92%)	24 (6%)	6 (2%)	9 43
18	L	386/437 (88%)	361 (94%)	23 (6%)	2 (0%)	29 67
19	M	377/434 (87%)	342 (91%)	26 (7%)	9 (2%)	6 35
20	J	384/405 (95%)	356 (93%)	22 (6%)	6 (2%)	9 43
All	All	8602/9546 (90%)	8015 (93%)	499 (6%)	88 (1%)	20 52

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	219	ALA
4	d	184	ALA
8	h	72	THR
4	D	203	THR
16	I	84	PRO
16	I	115	ASP
16	I	125	MET
16	I	134	SER
16	I	436	TYR
17	K	420	THR
4	d	203	THR
7	G	207	ASP
12	5	32	LYS
15	H	77	ALA
15	H	194	SER
15	H	342	GLY
16	I	86	GLU
16	I	427	LYS
17	K	143	SER

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Mol	Chain	Res	Type
18	L	357	ARG
19	M	287	GLY
19	M	296	SER
20	J	118	ASP
20	J	151	GLY
1	a	222	ASP
5	e	120	SER
7	g	69	HIS
1	A	27	ASN
2	B	17	LYS
5	E	114	ARG
7	G	59	LYS
10	3	127	GLY
14	7	86	ALA
14	7	120	GLN
15	H	412	PRO
17	K	246	TYR
17	K	419	ASN
19	M	78	LEU
19	M	164	ASP
19	M	292	ASP
20	J	353	CYS
3	c	51	VAL
5	e	45	ARG
5	e	125	LEU
6	f	52	ALA
1	A	51	PRO
4	D	100	ASP
6	F	2	ARG
6	F	7	GLY
6	F	204	SER
10	3	125	LEU
10	3	182	TRP
15	H	193	PRO
18	L	289	ARG
20	J	207	ASP
6	f	53	ASP
9	i	193	PRO
11	k	178	GLY
3	C	8	ARG
4	D	2	TYR
5	E	120	SER

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Mol	Chain	Res	Type
14	7	78	ASN
15	H	152	ILE
15	H	207	THR
15	H	371	ILE
16	I	388	SER
17	K	164	ASN
19	M	171	GLU
19	M	298	ASP
19	M	430	VAL
9	2	225	GLU
11	4	9	VAL
15	H	303	ALA
15	H	314	VAL
19	M	174	GLU
10	3	183	GLY
17	K	248	GLY
20	J	310	ILE
11	k	9	VAL
5	E	99	ILE
9	i	94	ILE
12	l	39	PRO
12	l	173	GLY
15	H	203	LYS
8	1	117	GLY
12	5	48	GLY
15	H	325	GLY
20	J	230	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	A	206/210 (98%)	201 (98%)	5 (2%)	49 69
1	a	206/210 (98%)	198 (96%)	8 (4%)	32 58
2	B	209/209 (100%)	204 (98%)	5 (2%)	49 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	209/209 (100%)	201 (96%)	8 (4%)	33	59
3	C	203/216 (94%)	197 (97%)	6 (3%)	41	64
3	c	203/216 (94%)	198 (98%)	5 (2%)	47	68
4	D	212/226 (94%)	201 (95%)	11 (5%)	23	51
4	d	212/226 (94%)	206 (97%)	6 (3%)	43	65
5	E	198/215 (92%)	196 (99%)	2 (1%)	76	85
5	e	198/215 (92%)	193 (98%)	5 (2%)	47	68
6	F	192/193 (100%)	185 (96%)	7 (4%)	35	60
6	f	190/193 (98%)	184 (97%)	6 (3%)	39	62
7	G	201/239 (84%)	196 (98%)	5 (2%)	47	68
7	g	201/239 (84%)	196 (98%)	5 (2%)	47	68
8	1	162/178 (91%)	159 (98%)	3 (2%)	57	75
8	h	162/178 (91%)	159 (98%)	3 (2%)	57	75
9	2	185/214 (86%)	184 (100%)	1 (0%)	88	93
9	i	185/214 (86%)	180 (97%)	5 (3%)	44	66
10	3	172/173 (99%)	170 (99%)	2 (1%)	71	83
10	j	172/173 (99%)	171 (99%)	1 (1%)	86	92
11	4	173/175 (99%)	170 (98%)	3 (2%)	60	78
11	k	173/175 (99%)	166 (96%)	7 (4%)	31	57
12	5	169/235 (72%)	166 (98%)	3 (2%)	59	77
12	l	169/235 (72%)	160 (95%)	9 (5%)	22	51
13	6	185/201 (92%)	180 (97%)	5 (3%)	44	66
13	m	185/201 (92%)	182 (98%)	3 (2%)	62	78
14	7	195/224 (87%)	194 (100%)	1 (0%)	88	93
14	n	198/224 (88%)	190 (96%)	8 (4%)	31	57
15	H	330/399 (83%)	323 (98%)	7 (2%)	53	72
16	I	342/385 (89%)	332 (97%)	10 (3%)	42	64
17	K	342/374 (91%)	328 (96%)	14 (4%)	30	57
18	L	332/377 (88%)	328 (99%)	4 (1%)	71	83
19	M	329/375 (88%)	319 (97%)	10 (3%)	41	64
20	J	336/352 (96%)	331 (98%)	5 (2%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7336/8078 (91%)	7148 (97%)	188 (3%)	49 67

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	5	ARG
1	a	33	SER
1	a	69	THR
1	a	117	GLN
1	a	121	GLN
1	a	122	ARG
1	a	124	TYR
1	a	200	HIS
2	b	1	MET
2	b	32	VAL
2	b	61	LEU
2	b	92	VAL
2	b	119	GLN
2	b	127	VAL
2	b	133	SER
2	b	231	LYS
3	c	18	LEU
3	c	113	ARG
3	c	121	TYR
3	c	200	THR
3	c	201	ASP
4	d	68	HIS
4	d	70	VAL
4	d	161	THR
4	d	169	VAL
4	d	192	LEU
4	d	197	LEU
5	e	1	ASP
5	e	45	ARG
5	e	55	SER
5	e	99	ILE
5	e	242	GLU
6	f	11	THR
6	f	71	LEU
6	f	116	GLN
6	f	133	ILE
6	f	188	LEU

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Mol	Chain	Res	Type
6	f	206	THR
7	g	5	ASP
7	g	69	HIS
7	g	74	TYR
7	g	198	LEU
7	g	214	TRP
8	h	30	VAL
8	h	44	CYS
8	h	62	HIS
9	i	43	CYS
9	i	71	SER
9	i	85	GLN
9	i	176	CYS
9	i	183	ASP
10	j	133	LYS
11	k	3	ILE
11	k	30	ASP
11	k	33	ASP
11	k	78	GLN
11	k	82	SER
11	k	99	GLN
11	k	126	VAL
12	l	4	LEU
12	l	25	TRP
12	l	52	CYS
12	l	69	ARG
12	l	84	SER
12	l	86	LEU
12	l	120	THR
12	l	137	TYR
12	l	187	TYR
13	m	103	PHE
13	m	137	ARG
13	m	150	LEU
14	n	26	ASN
14	n	70	LEU
14	n	104	ARG
14	n	105	SER
14	n	129	TYR
14	n	150	MET
14	n	161	ARG
14	n	187	ARG

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Mol	Chain	Res	Type
1	A	122	ARG
1	A	150	PRO
1	A	211	LYS
1	A	220	THR
1	A	235	ARG
2	B	13	SER
2	B	26	THR
2	B	109	LEU
2	B	128	ARG
2	B	207	ASP
3	C	7	SER
3	C	26	GLU
3	C	56	LEU
3	C	124	HIS
3	C	182	ASP
3	C	237	ILE
4	D	16	PHE
4	D	66	ASP
4	D	79	ASP
4	D	116	GLN
4	D	220	VAL
4	D	224	SER
4	D	225	GLU
4	D	226	GLU
4	D	238	LYS
4	D	239	GLN
4	D	240	GLU
5	E	115	PHE
5	E	176	LEU
6	F	2	ARG
6	F	3	ASN
6	F	4	ASN
6	F	73	LEU
6	F	91	CYS
6	F	116	GLN
6	F	188	LEU
7	G	5	ASP
7	G	106	PRO
7	G	161	THR
7	G	166	GLN
7	G	214	TRP
8	1	31	THR

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Mol	Chain	Res	Type
8	1	104	ASP
8	1	126	ILE
9	2	221	CYS
10	3	140	THR
10	3	161	ASP
11	4	3	ILE
11	4	126	VAL
11	4	185	ASP
12	5	73	ARG
12	5	104	TYR
12	5	182	GLU
13	6	19	ASP
13	6	34	SER
13	6	122	VAL
13	6	134	GLU
13	6	150	LEU
14	7	104	ARG
15	H	66	LYS
15	H	103	THR
15	H	151	GLN
15	H	208	TYR
15	H	326	ASP
15	H	363	PRO
15	H	367	ARG
16	I	175	LYS
16	I	254	GLN
16	I	259	ASP
16	I	303	GLN
16	I	366	THR
16	I	409	MET
16	I	429	GLU
16	I	430	GLU
16	I	436	TYR
16	I	437	LEU
17	K	46	ASP
17	K	75	LEU
17	K	107	THR
17	K	137	VAL
17	K	173	ASP
17	K	237	VAL
17	K	244	HIS
17	K	246	TYR

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Mol	Chain	Res	Type
17	K	247	LEU
17	K	264	ASN
17	K	272	ASP
17	K	337	LYS
17	K	347	ARG
17	K	404	GLN
18	L	164	ASP
18	L	183	ILE
18	L	199	LEU
18	L	415	LEU
19	M	85	VAL
19	M	87	ASP
19	M	129	LEU
19	M	162	GLU
19	M	193	LEU
19	M	254	MET
19	M	373	ASP
19	M	382	SER
19	M	426	LYS
19	M	427	SER
20	J	15	HIS
20	J	142	VAL
20	J	146	THR
20	J	148	ASP
20	J	388	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
5	e	15	GLN
5	e	91	HIS
12	l	208	ASN
14	n	194	ASN
3	C	151	ASN
4	D	229	GLN
5	E	83	HIS
6	F	147	GLN
8	1	161	GLN
9	2	200	GLN
12	5	209	ASN
16	I	376	ASN
18	L	393	ASN

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Mol	Chain	Res	Type
20	J	269	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
23	ADP	J	501	22	24,29,29	0.99	2 (8%)	29,45,45	1.28	3 (10%)
21	ATP	M	501	22	26,33,33	0.95	1 (3%)	31,52,52	1.34	5 (16%)
21	ATP	I	501	22	26,33,33	0.90	2 (7%)	31,52,52	1.33	5 (16%)
21	ATP	L	501	22	26,33,33	0.92	1 (3%)	31,52,52	1.37	4 (12%)
21	ATP	H	501	22	26,33,33	0.92	2 (7%)	31,52,52	1.46	6 (19%)
21	ATP	K	501	22	26,33,33	0.91	1 (3%)	31,52,52	1.36	5 (16%)

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
23	ADP	J	501	22	-	5/12/32/32	0/3/3/3
21	ATP	M	501	22	-	8/18/38/38	0/3/3/3
21	ATP	I	501	22	-	5/18/38/38	0/3/3/3
21	ATP	L	501	22	-	6/18/38/38	0/3/3/3
21	ATP	H	501	22	-	3/18/38/38	0/3/3/3
21	ATP	K	501	22	-	8/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	501	ADP	O4'-C1'	2.38	1.44	1.41
21	K	501	ATP	C5-C4	2.34	1.47	1.40
23	J	501	ADP	C5-C4	2.31	1.47	1.40
21	H	501	ATP	C5-C4	2.25	1.46	1.40
21	I	501	ATP	C5-C4	2.20	1.46	1.40
21	M	501	ATP	C5-C4	2.18	1.46	1.40
21	L	501	ATP	C5-C4	2.14	1.46	1.40
21	H	501	ATP	O4'-C1'	2.07	1.44	1.41
21	I	501	ATP	O4'-C1'	2.04	1.43	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	M	501	ATP	PA-O3A-PB	-3.96	119.24	132.83
21	H	501	ATP	PB-O3B-PG	-3.88	119.50	132.83
21	L	501	ATP	PA-O3A-PB	-3.82	119.72	132.83
21	K	501	ATP	N3-C2-N1	-3.59	123.06	128.68
21	L	501	ATP	N3-C2-N1	-3.51	123.20	128.68
21	I	501	ATP	N3-C2-N1	-3.36	123.43	128.68
21	H	501	ATP	N3-C2-N1	-3.32	123.48	128.68
23	J	501	ADP	N3-C2-N1	-3.25	123.60	128.68
21	M	501	ATP	C3'-C2'-C1'	2.83	105.23	100.98
21	K	501	ATP	C4-C5-N7	-2.82	106.46	109.40
21	I	501	ATP	PA-O3A-PB	-2.65	123.75	132.83
21	H	501	ATP	PA-O3A-PB	-2.60	123.92	132.83
21	I	501	ATP	PB-O3B-PG	-2.55	124.06	132.83
21	I	501	ATP	C3'-C2'-C1'	2.55	104.81	100.98
21	I	501	ATP	C4-C5-N7	-2.48	106.82	109.40
21	K	501	ATP	PB-O3B-PG	-2.40	124.58	132.83
21	L	501	ATP	PB-O3B-PG	-2.38	124.65	132.83
21	H	501	ATP	C3'-C2'-C1'	2.34	104.50	100.98
21	K	501	ATP	C3'-C2'-C1'	2.33	104.48	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	501	ATP	C4-C5-N7	-2.32	106.98	109.40
23	J	501	ADP	O3B-PB-O2B	2.24	116.20	107.64
23	J	501	ADP	C4-C5-N7	-2.19	107.11	109.40
21	M	501	ATP	C4-C5-N7	-2.19	107.12	109.40
21	M	501	ATP	N6-C6-N1	2.19	123.11	118.57
21	L	501	ATP	C4-C5-N7	-2.18	107.13	109.40
21	M	501	ATP	N3-C2-N1	-2.17	125.28	128.68
21	H	501	ATP	O3G-PG-O2G	2.05	115.48	107.64
21	K	501	ATP	C2-N1-C6	2.04	122.25	118.75

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	H	501	ATP	C5'-O5'-PA-O1A
21	I	501	ATP	C5'-O5'-PA-O2A
21	K	501	ATP	PB-O3B-PG-O2G
21	L	501	ATP	C5'-O5'-PA-O2A
21	L	501	ATP	C5'-O5'-PA-O3A
21	L	501	ATP	O4'-C4'-C5'-O5'
21	M	501	ATP	PB-O3B-PG-O2G
21	M	501	ATP	C5'-O5'-PA-O1A
23	J	501	ADP	C5'-O5'-PA-O3A
21	L	501	ATP	C3'-C4'-C5'-O5'
23	J	501	ADP	PA-O3A-PB-O1B
21	K	501	ATP	O4'-C4'-C5'-O5'
23	J	501	ADP	PB-O3A-PA-O5'
21	K	501	ATP	PB-O3B-PG-O3G
21	H	501	ATP	C5'-O5'-PA-O3A
21	I	501	ATP	C5'-O5'-PA-O3A
21	M	501	ATP	C5'-O5'-PA-O3A
21	I	501	ATP	PA-O3A-PB-O2B
21	K	501	ATP	PA-O3A-PB-O2B
21	L	501	ATP	PA-O3A-PB-O2B
21	H	501	ATP	C5'-O5'-PA-O2A
21	I	501	ATP	C5'-O5'-PA-O1A
21	M	501	ATP	C5'-O5'-PA-O2A
23	J	501	ADP	C5'-O5'-PA-O1A
21	K	501	ATP	C3'-C4'-C5'-O5'
23	J	501	ADP	C4'-C5'-O5'-PA
21	K	501	ATP	PB-O3B-PG-O1G
21	M	501	ATP	PB-O3B-PG-O1G

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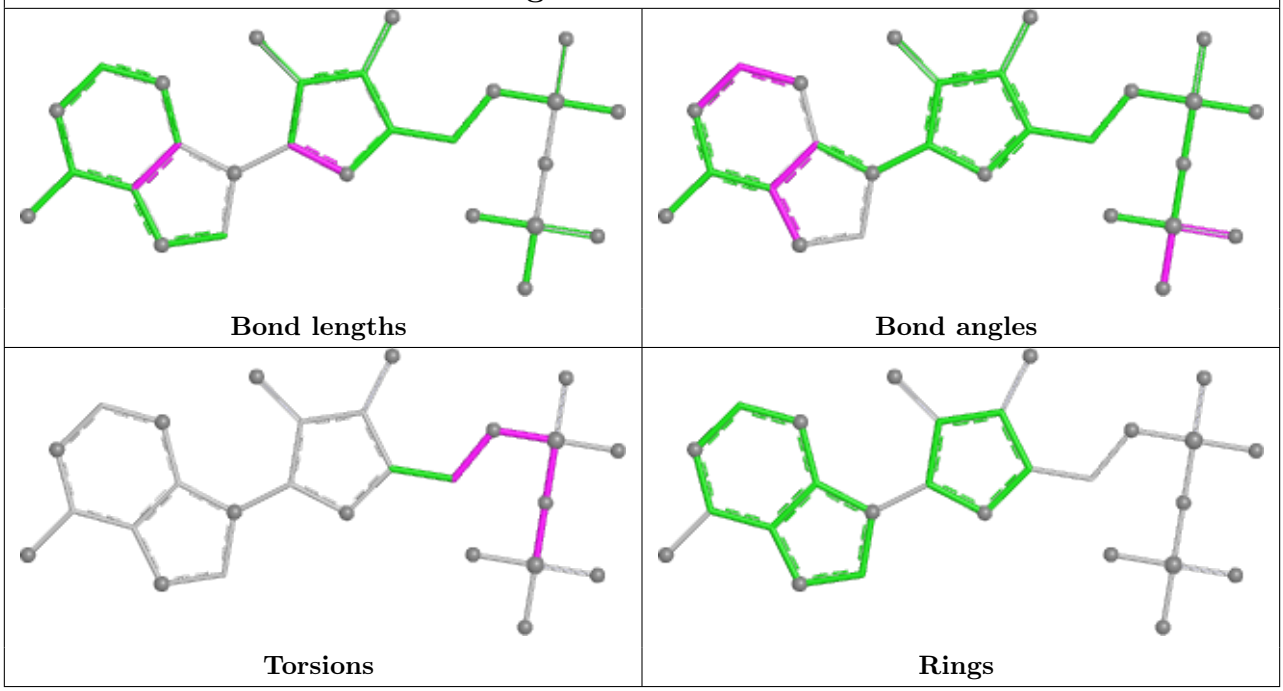
Mol	Chain	Res	Type	Atoms
21	M	501	ATP	PB-O3B-PG-O3G
21	K	501	ATP	C5'-O5'-PA-O3A
21	I	501	ATP	PA-O3A-PB-O1B
21	K	501	ATP	PA-O3A-PB-O1B
21	L	501	ATP	PA-O3A-PB-O1B
21	M	501	ATP	PA-O3A-PB-O1B
21	M	501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

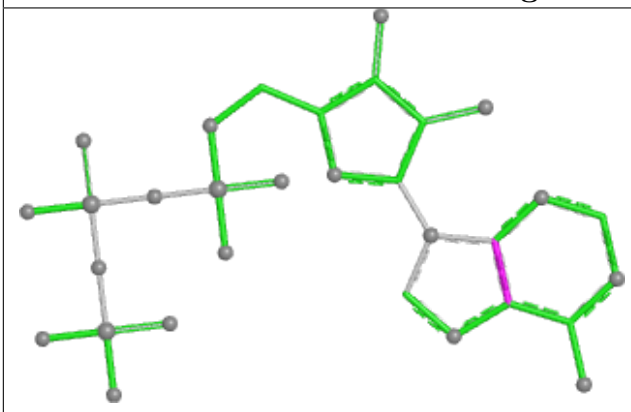
No monomer is involved in short contacts.

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.

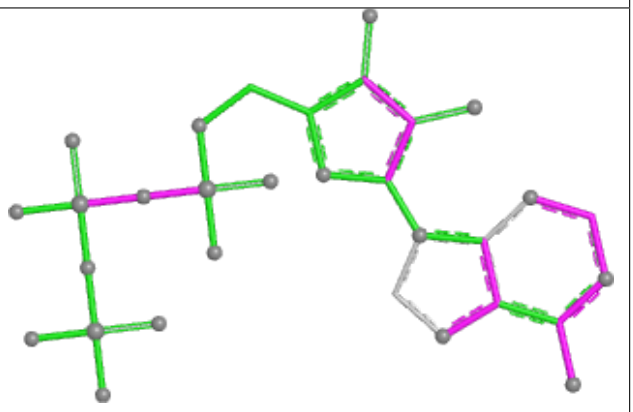
Ligand ADP J 501



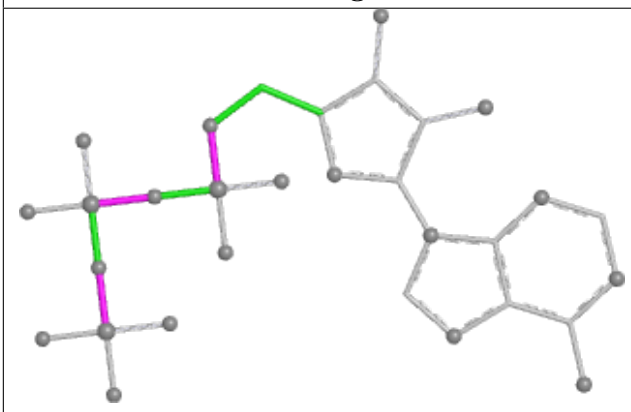
Ligand ATP M 501



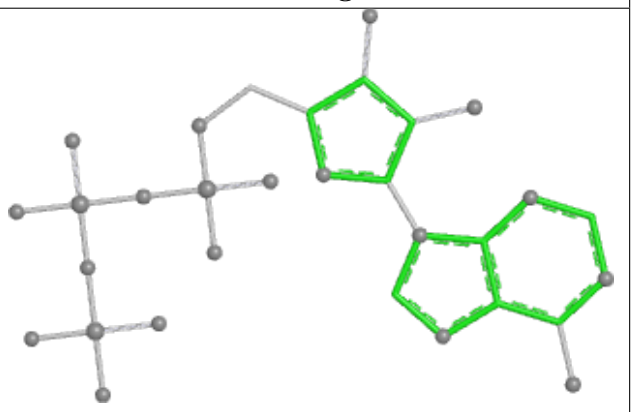
Bond lengths



Bond angles

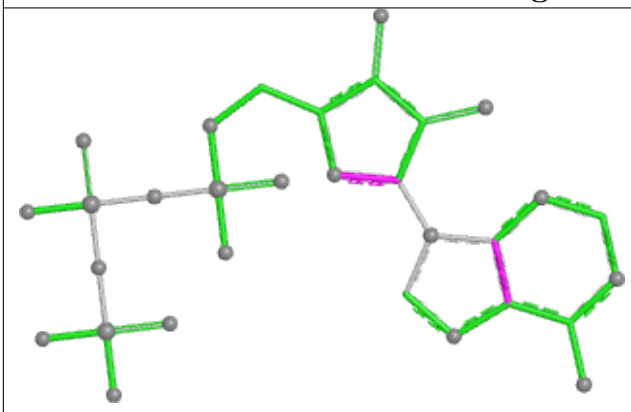


Torsions

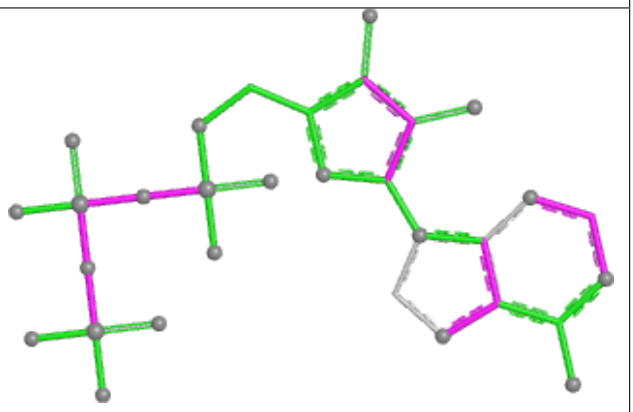


Rings

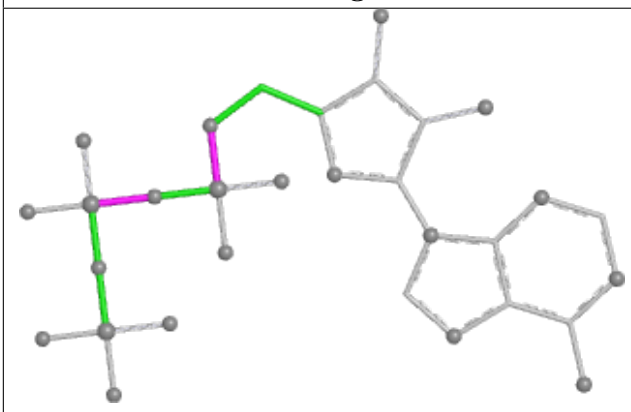
Ligand ATP I 501



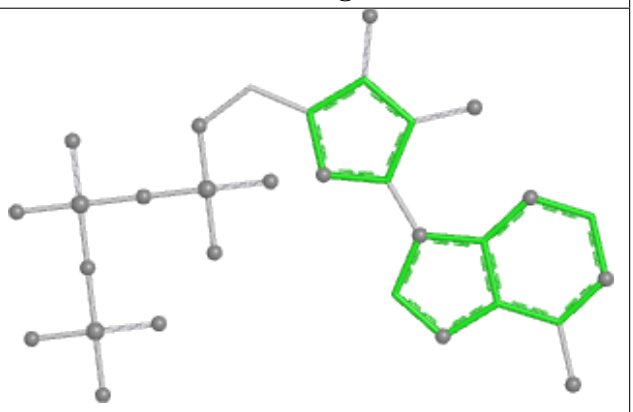
Bond lengths



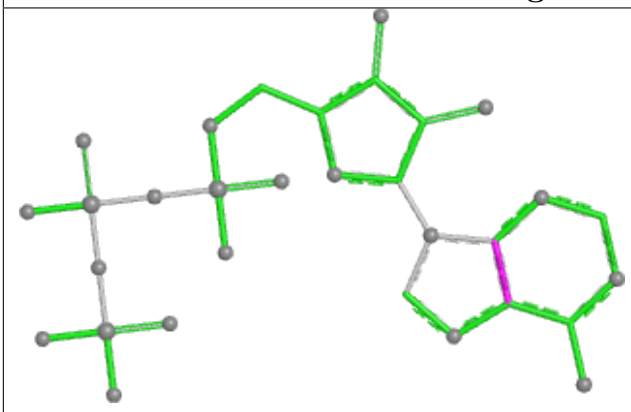
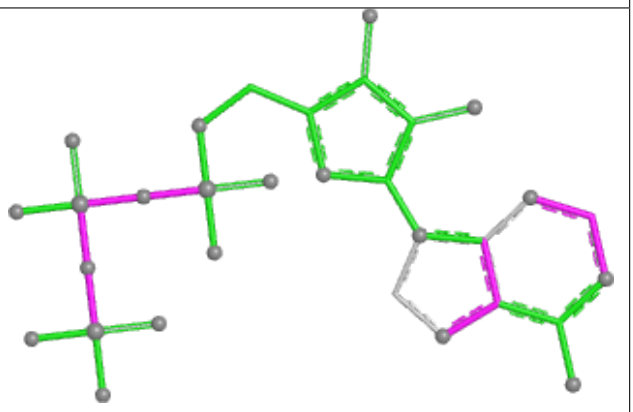
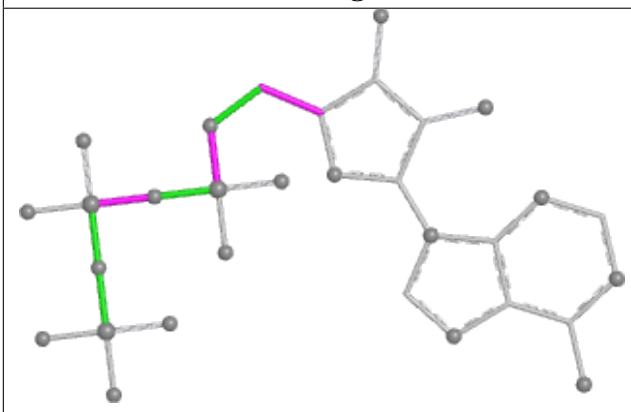
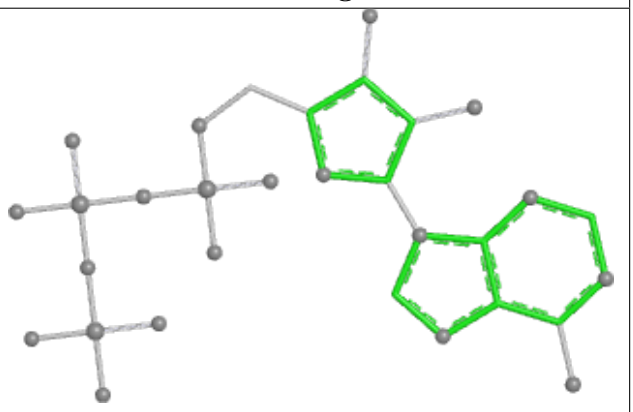
Bond angles

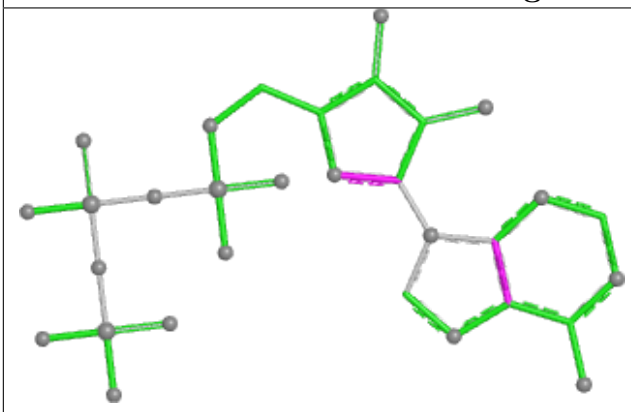
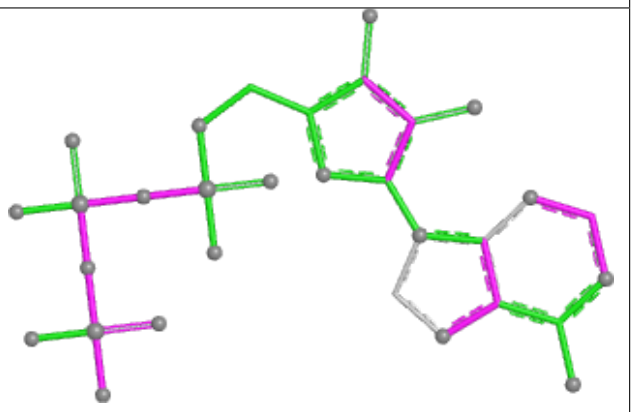
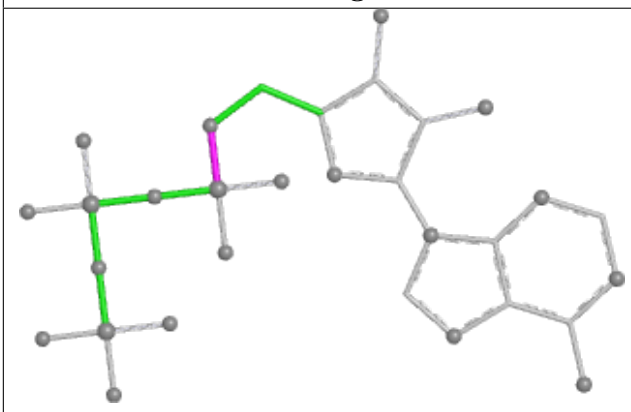
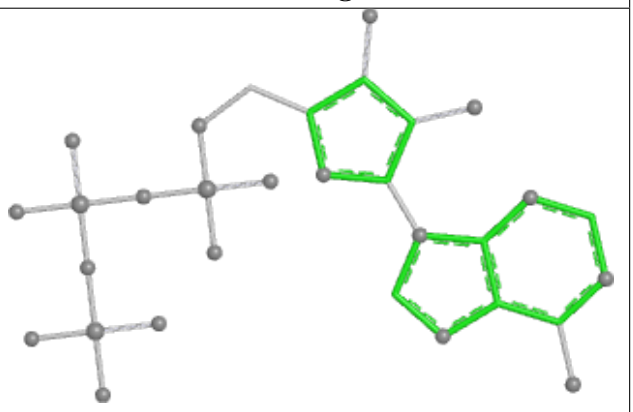


Torsions

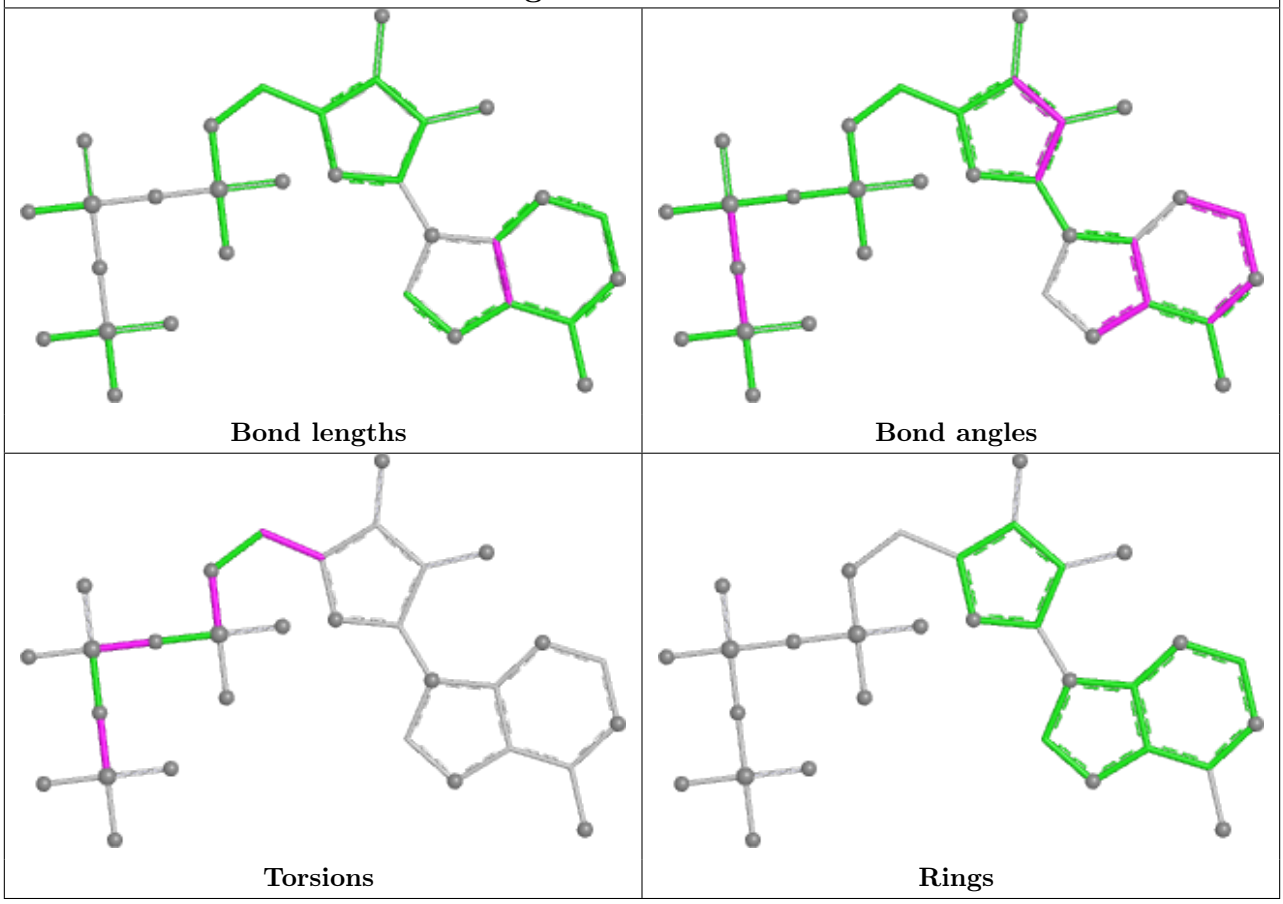


Rings

Ligand ATP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP H 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP K 501



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.

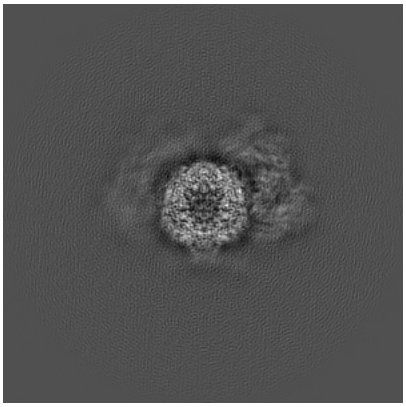
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3534. These allow visual inspection of the internal detail of the map and identification of artifacts.

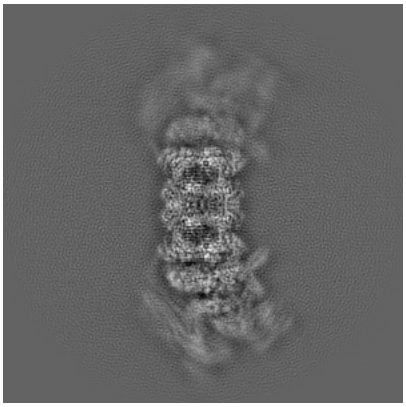
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

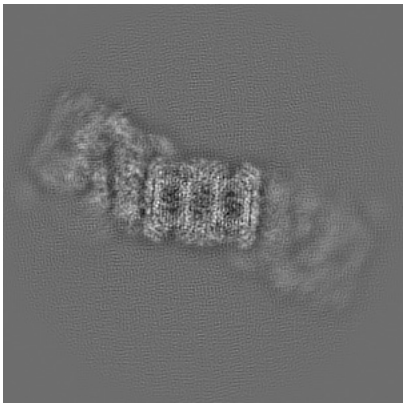
6.1.1 Primary map



X



Y

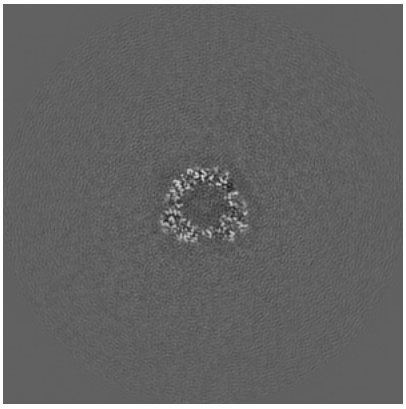


Z

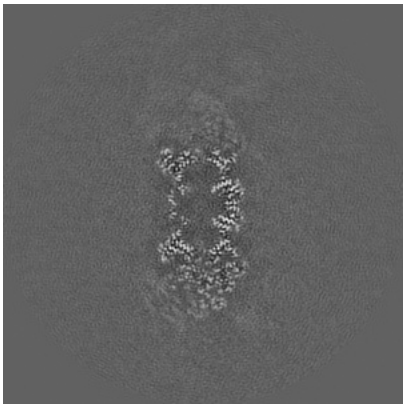
The images above show the map projected in three orthogonal directions.

6.2 Central slices

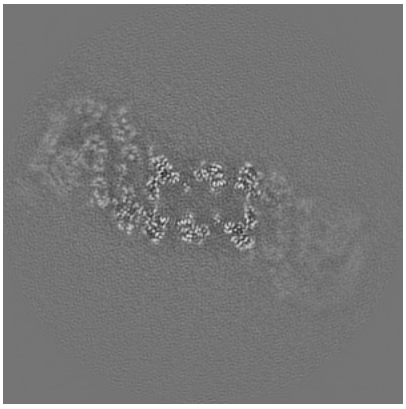
6.2.1 Primary map



X Index: 192



Y Index: 192

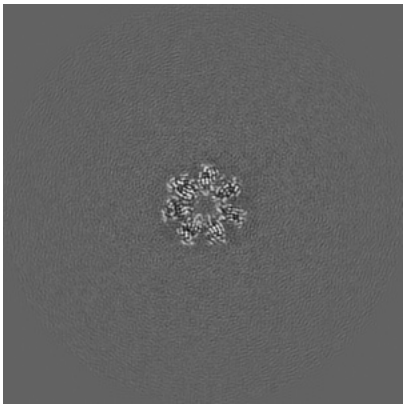


Z Index: 192

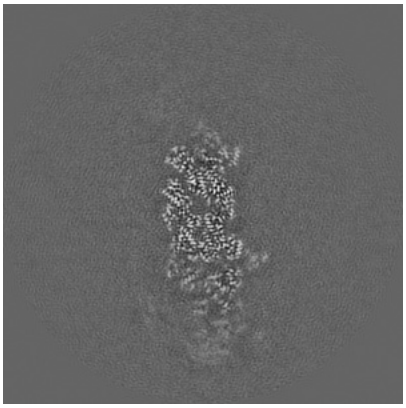
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

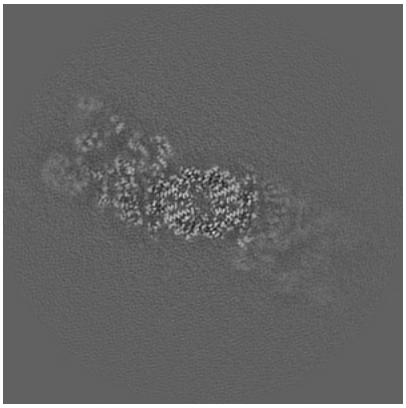
6.3.1 Primary map



X Index: 177



Y Index: 212



Z Index: 208

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

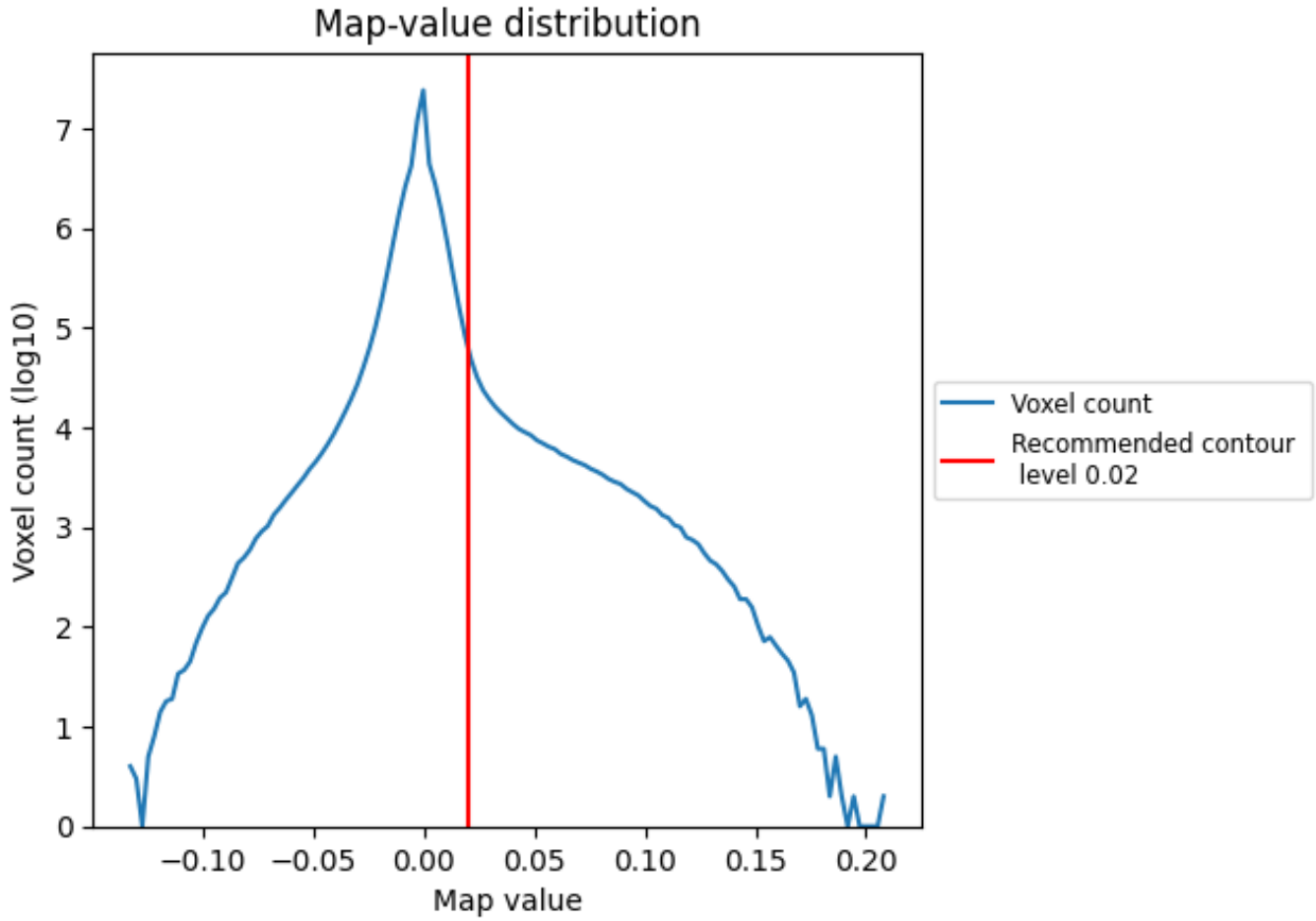
6.5 Mask visualisation (i)

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

7 Map analysis

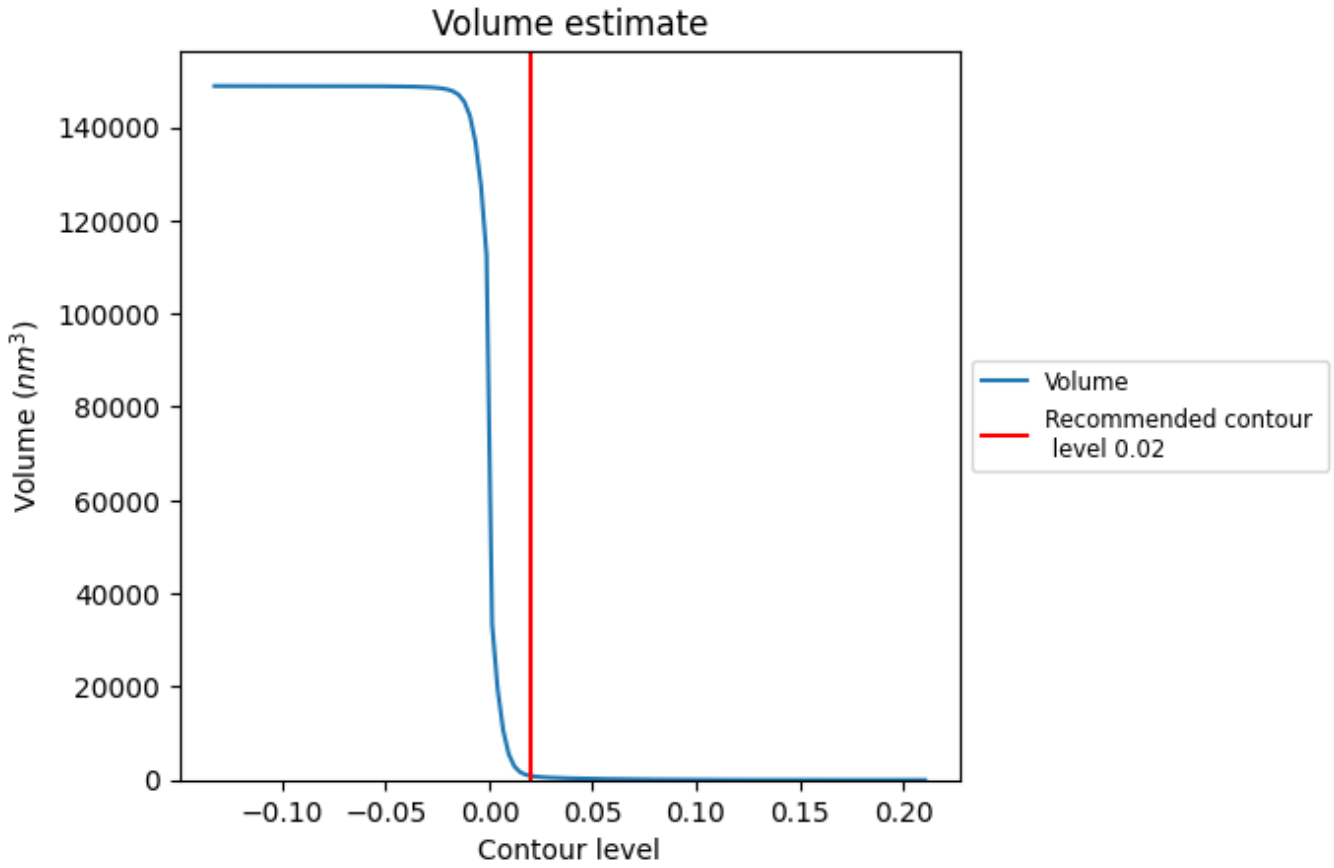
This section contains the results of statistical analysis of the map.

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.

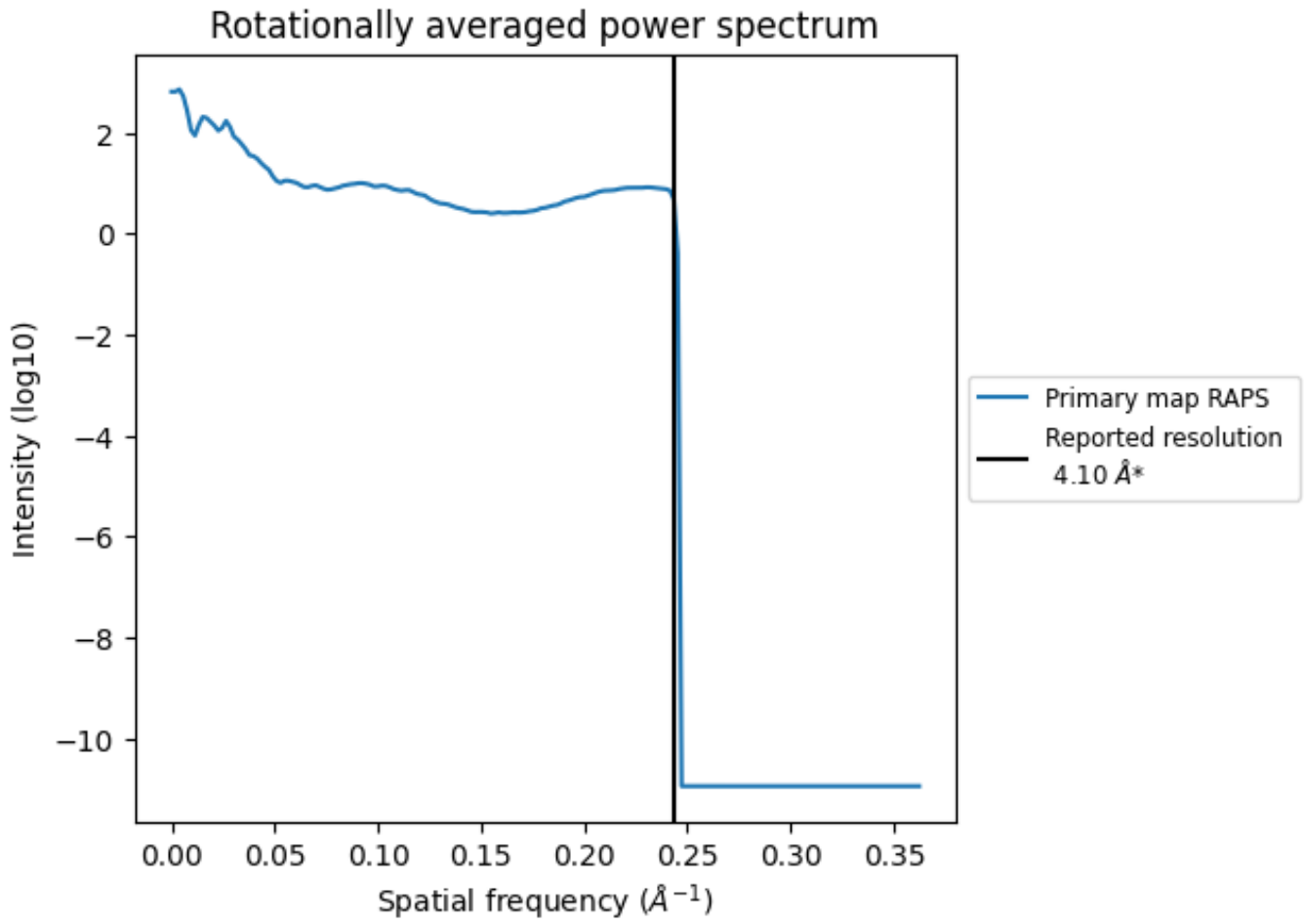
7.2 Volume estimate



The volume at the recommended contour level is 881 nm^3; this corresponds to an approximate mass of 796 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 0.244 Å^{-1}

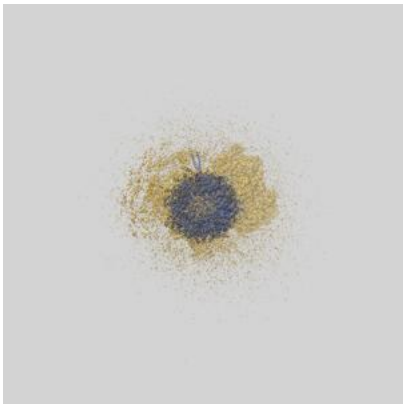
8 Fourier-Shell correlation (i)

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

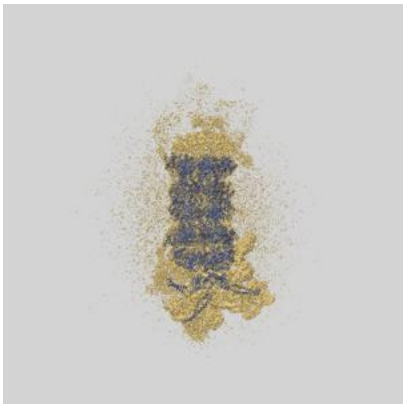
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3534 and PDB model 5MP9. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay



X

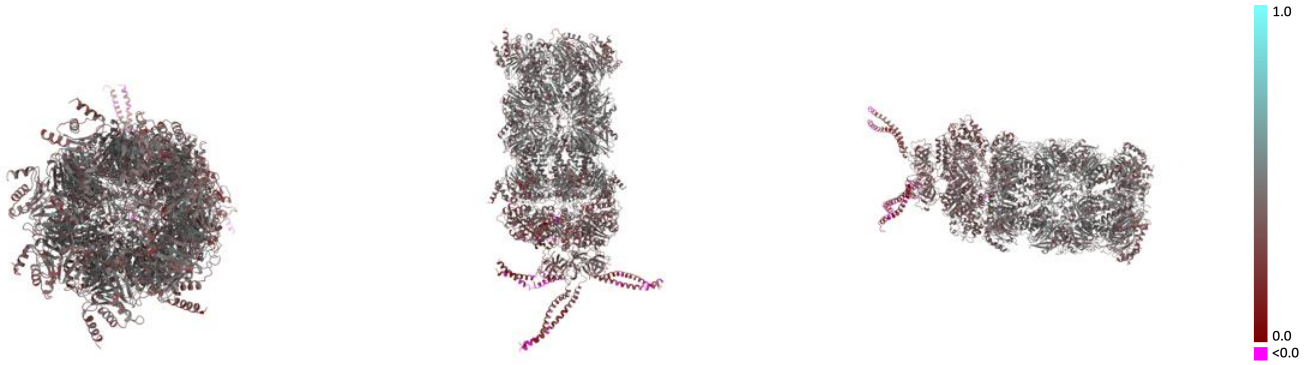


Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

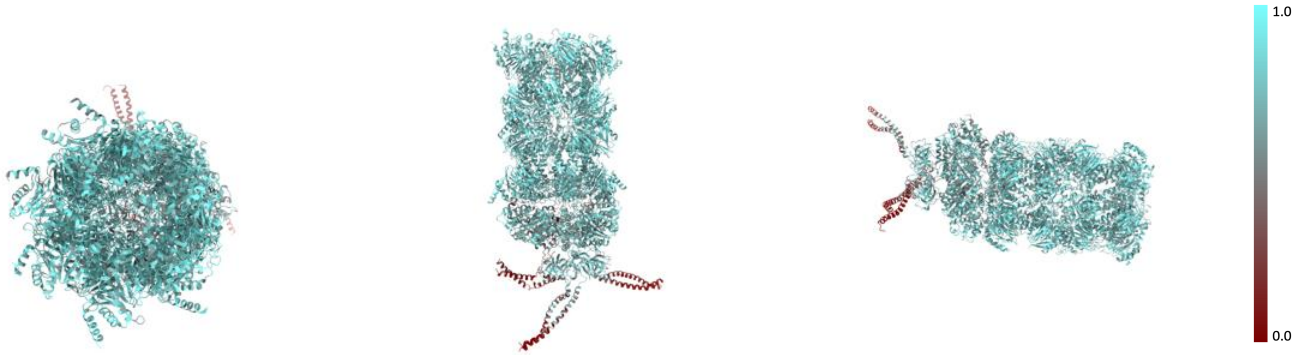
9.2 Q-score mapped to coordinate model (i)



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.

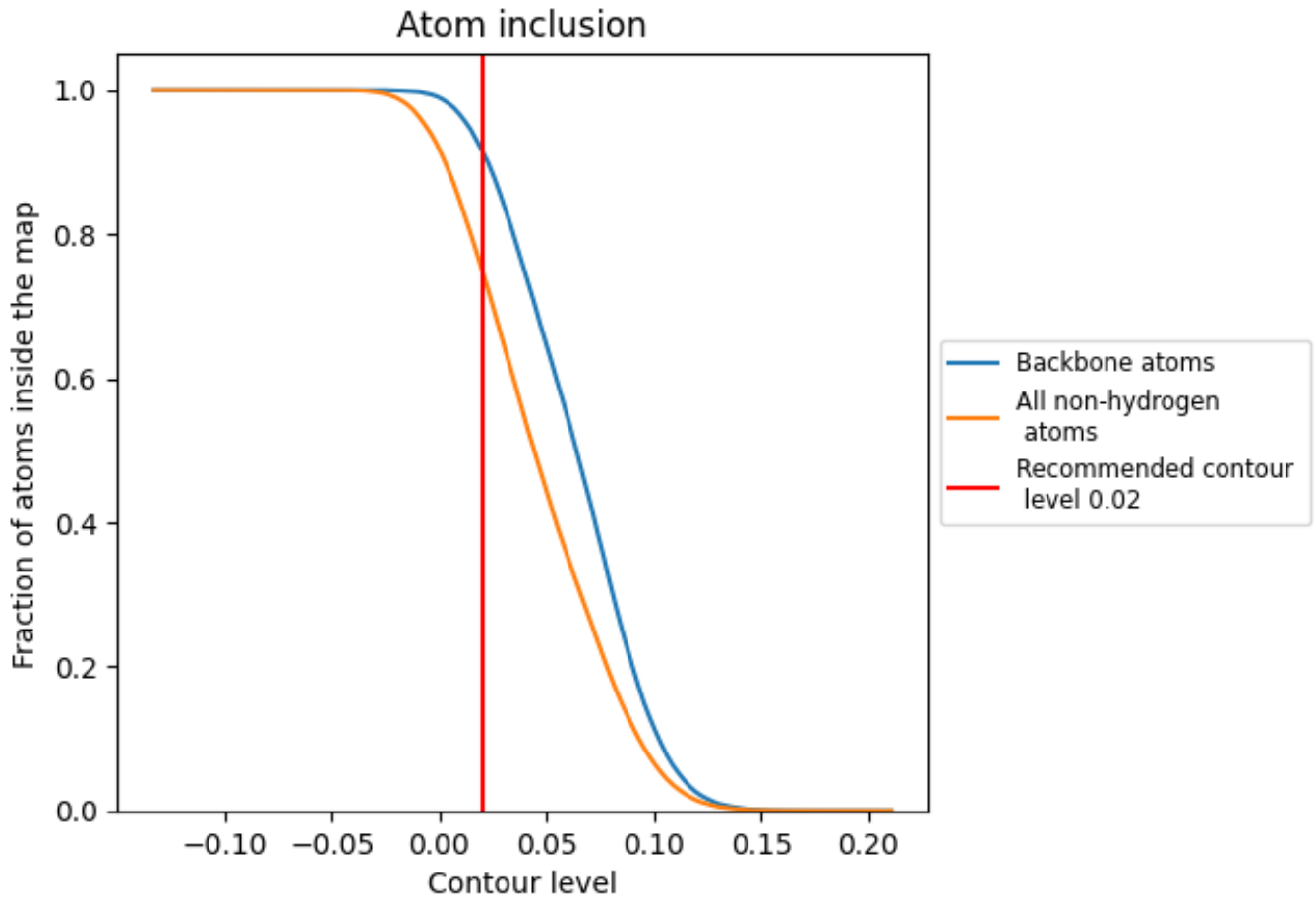
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7501	0.3940
1	0.8160	0.4380
2	0.8022	0.4330
3	0.7956	0.4410
4	0.7971	0.4300
5	0.8254	0.4320
6	0.8235	0.4400
7	0.8260	0.4380
A	0.7883	0.4190
B	0.7745	0.4130
C	0.7762	0.4060
D	0.7874	0.4100
E	0.7572	0.4040
F	0.8039	0.4290
G	0.8045	0.4240
H	0.6539	0.3470
I	0.6090	0.2990
J	0.5722	0.2810
K	0.6305	0.3180
L	0.6279	0.3290
M	0.6385	0.3460
a	0.7894	0.4070
b	0.7740	0.4040
c	0.7794	0.3940
d	0.7792	0.4080
e	0.7556	0.3920
f	0.7976	0.4080
g	0.7986	0.4090
h	0.8228	0.4400
i	0.8093	0.4360
j	0.8001	0.4370
k	0.8037	0.4340
l	0.8229	0.4360
m	0.8287	0.4380
n	0.8251	0.4370