



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:44 PM UTC

PDB ID : 5MP9 / pdb_00005mp9
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:

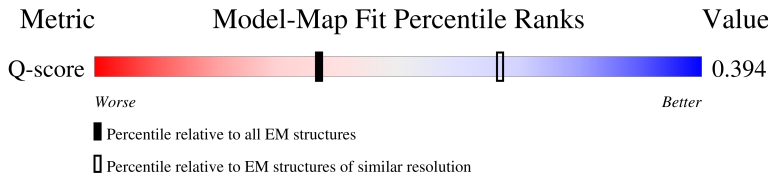
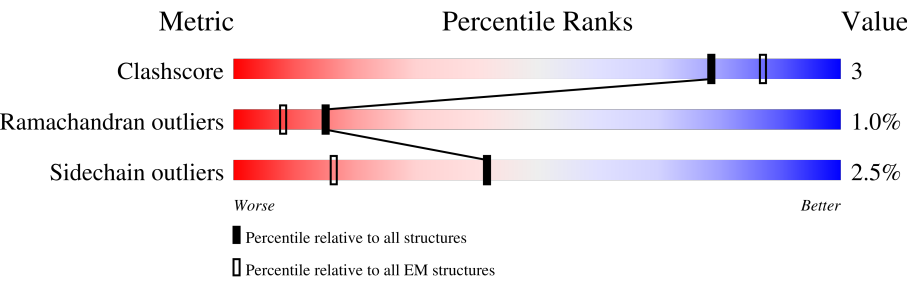
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.10 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.



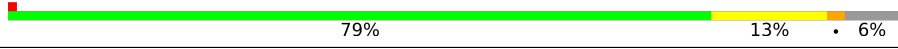
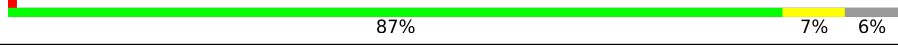
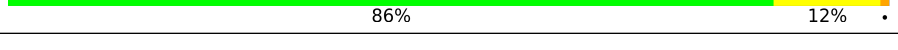
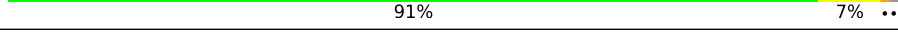
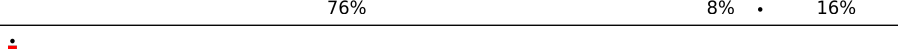
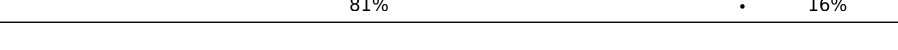
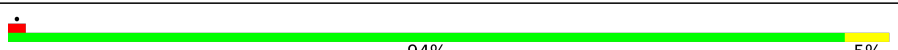
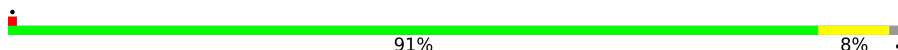
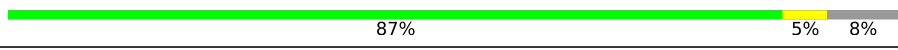
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	252	87% 7% . .
1	a	252	85% 10% . .
2	B	250	88% 12% .
2	b	250	89% 10%

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Mol	Chain	Length	Quality of chain
3	C	258	
3	c	258	
4	D	254	
4	d	254	
5	E	260	
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	l	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	

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Mol	Chain	Length	Quality of chain
16	I	437	14% 77% 10% 12%
17	K	428	13% 81% 9% 9%
18	L	437	13% 81% 7% 11%
19	M	434	13% 78% 9% 12%
20	J	405	21% 88% 7% 5%

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		

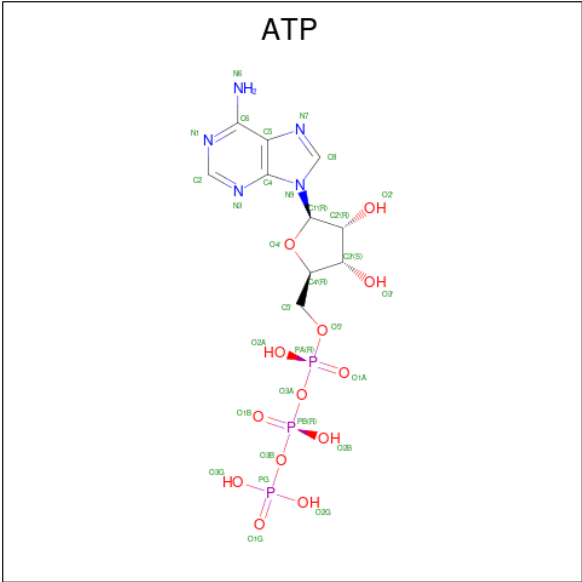
- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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 (CCD ID: 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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

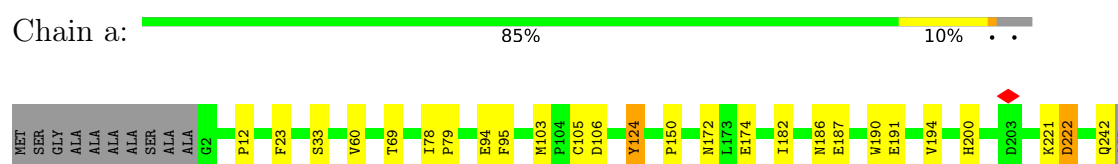


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	J	1	27	10	5	10	2	0

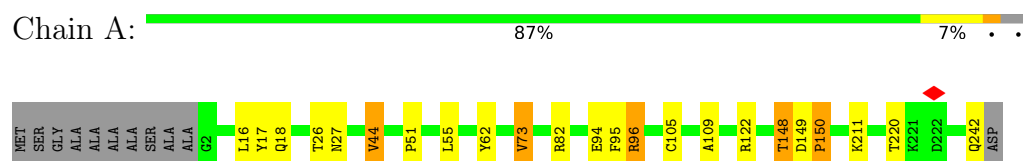
3 Residue-property plots

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.

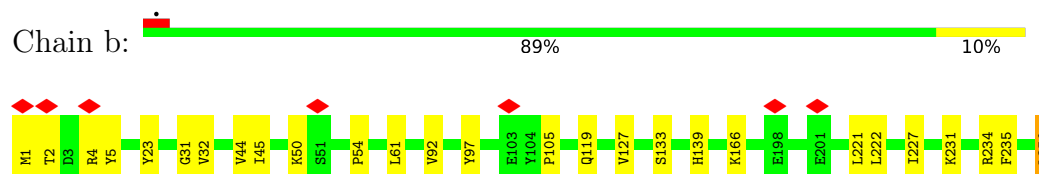
• Molecule 1: Proteasome subunit alpha type-1



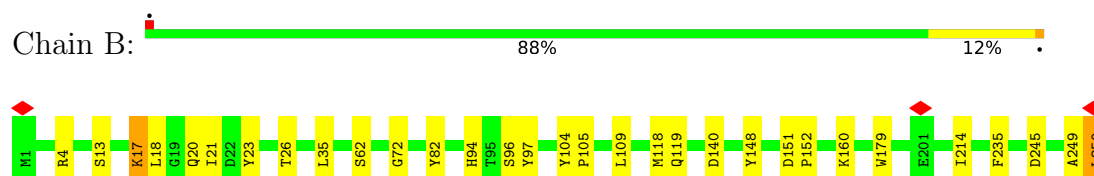
• Molecule 1: Proteasome subunit alpha type-1



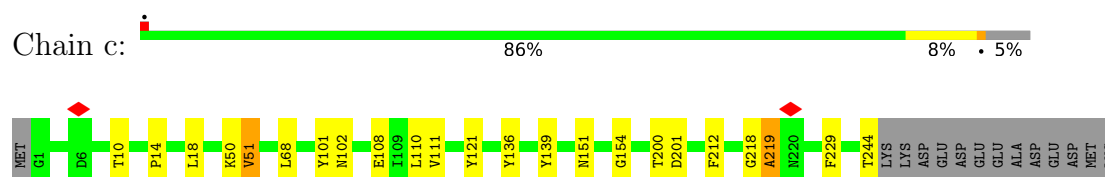
• Molecule 2: Proteasome subunit alpha type-2



• Molecule 2: Proteasome subunit alpha type-2

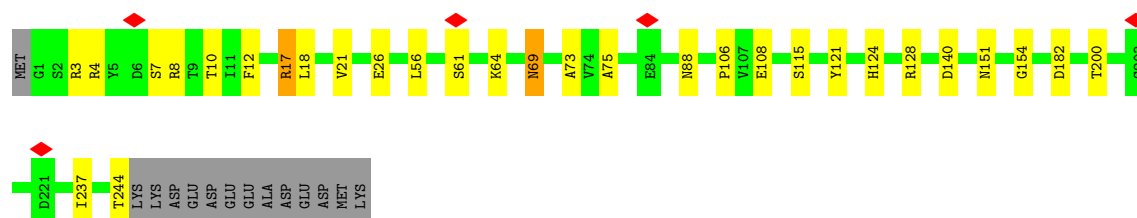


• Molecule 3: Proteasome subunit alpha type-3



- Molecule 3: Proteasome subunit alpha type-3

Chain C: 



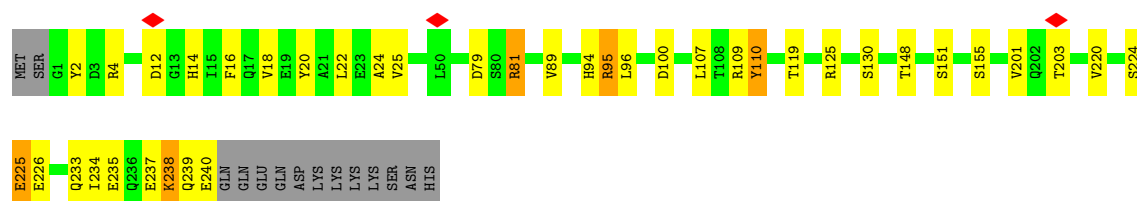
- Molecule 4: Proteasome subunit alpha type-4

Chain d: 



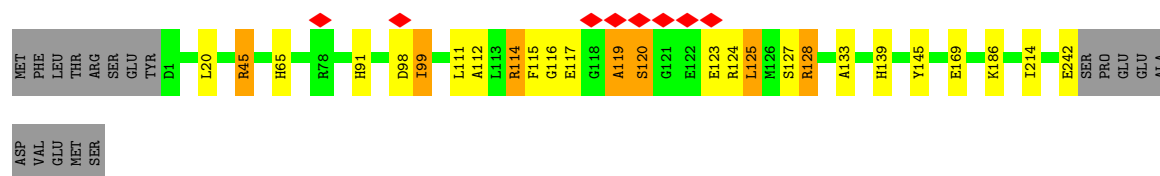
- Molecule 4: Proteasome subunit alpha type-4

Chain D: 



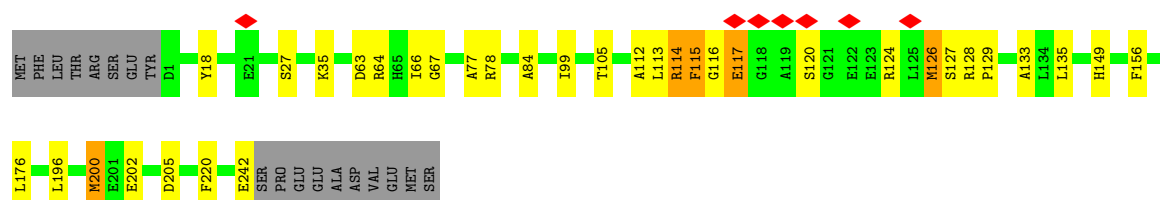
- Molecule 5: Proteasome subunit alpha type-5

Chain e: 



- Molecule 5: Proteasome subunit alpha type-5

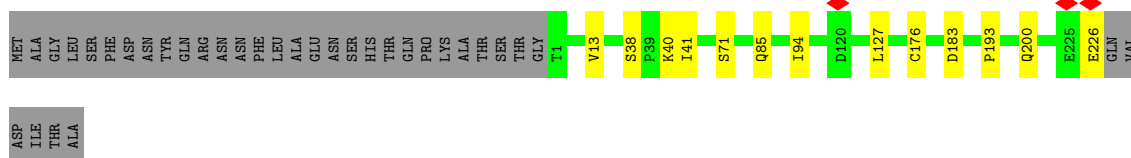
Chain E: 





• Molecule 9: Proteasome subunit beta type-2

Chain i: 82% 5% 13%



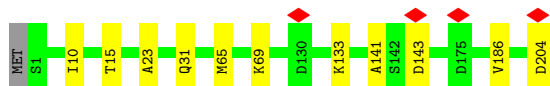
• Molecule 9: Proteasome subunit beta type-2

Chain 2: 78% 8% 13%



• Molecule 10: Proteasome subunit beta type-3

Chain j: 94% 5%



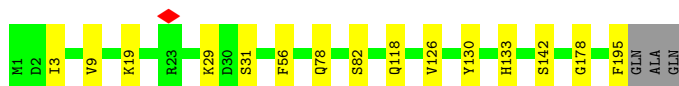
• Molecule 10: Proteasome subunit beta type-3

Chain 3: 88% 12%



• Molecule 11: Proteasome subunit beta type-4

Chain k: 91% 8%



• Molecule 11: Proteasome subunit beta type-4

Chain 4: 91% 7%



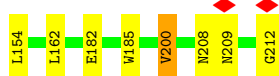
• Molecule 12: Proteasome subunit beta type-5

Chain 1: 68% 6% 26%



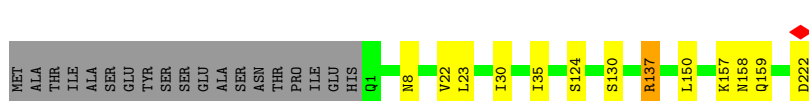
• Molecule 12: Proteasome subunit beta type-5

Chain 5: 63% 11% 26%



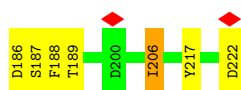
• Molecule 13: Proteasome subunit beta type-6

Chain m: 87% 5% 8%



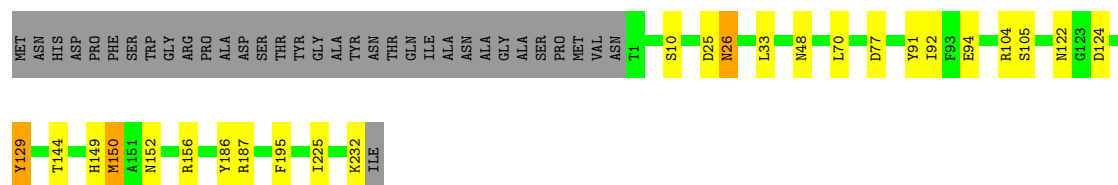
• Molecule 13: Proteasome subunit beta type-6

Chain 6: 80% 12% 8%



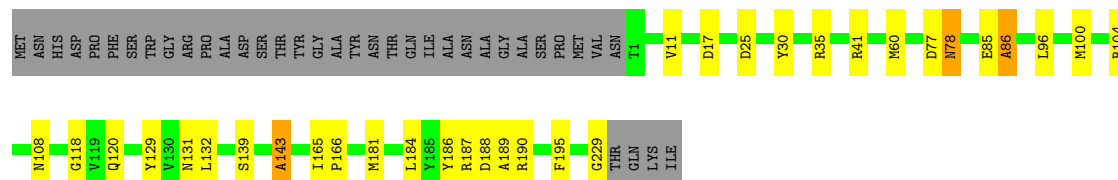
• Molecule 14: Proteasome subunit beta type-7

Chain n: 78% 8% 13%



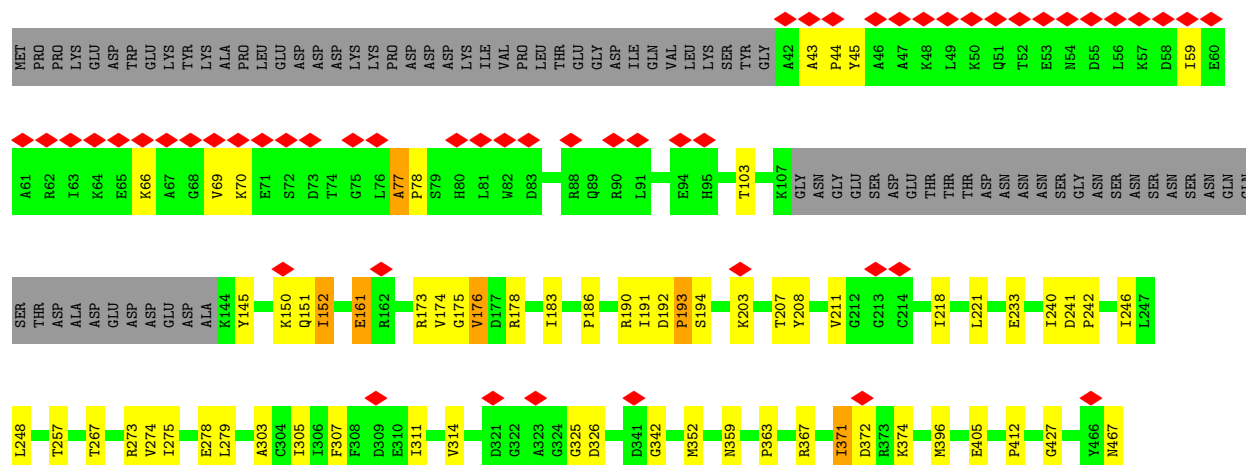
• Molecule 14: Proteasome subunit beta type-7

Chain 7: 74% 11% 14%



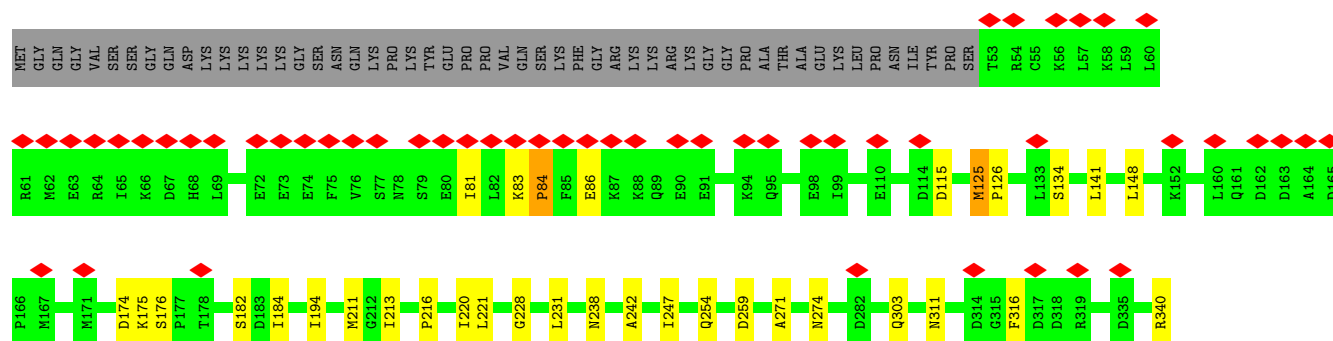
• Molecule 15: 26S protease regulatory subunit 7 homolog

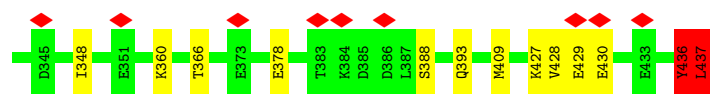
Chain H: 11% 69% 13% 16%



• Molecule 16: 26S protease regulatory subunit 4 homolog

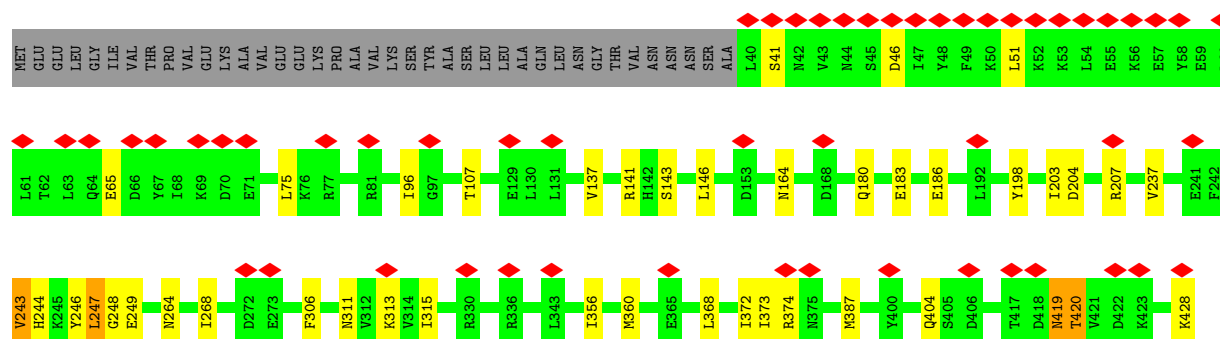
Chain I: 14% 77% 10% 12%





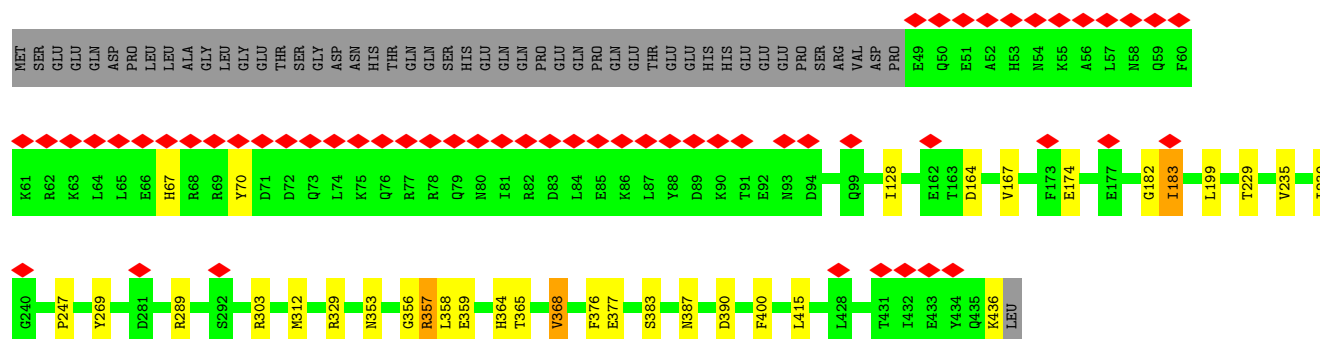
- Molecule 17: 26S protease regulatory subunit 6B homolog

Chain K: 13% 81% 9% 9%



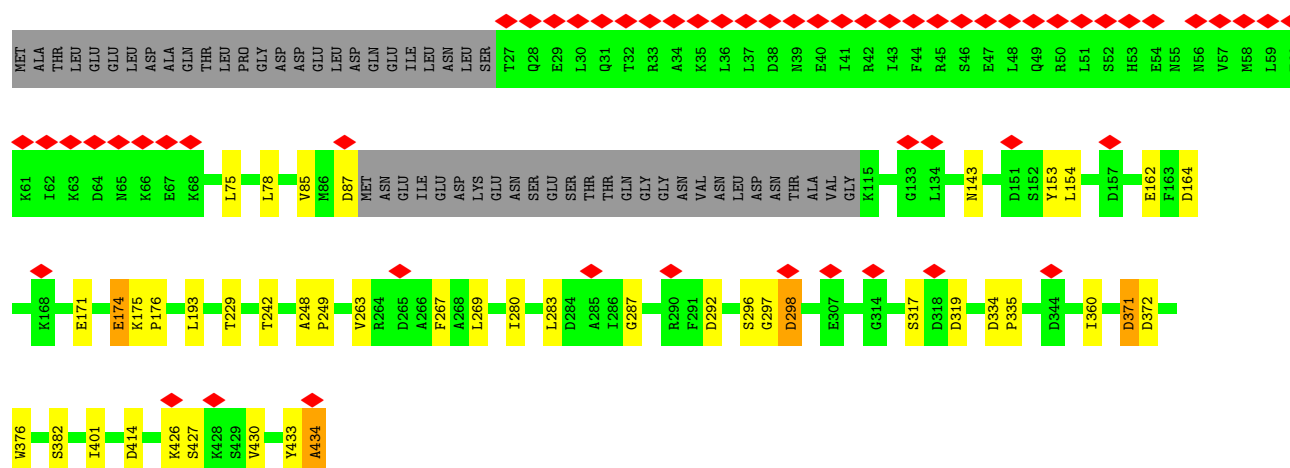
- Molecule 18: 26S protease subunit RPT4

Chain L: 13% 81% 7% 11%

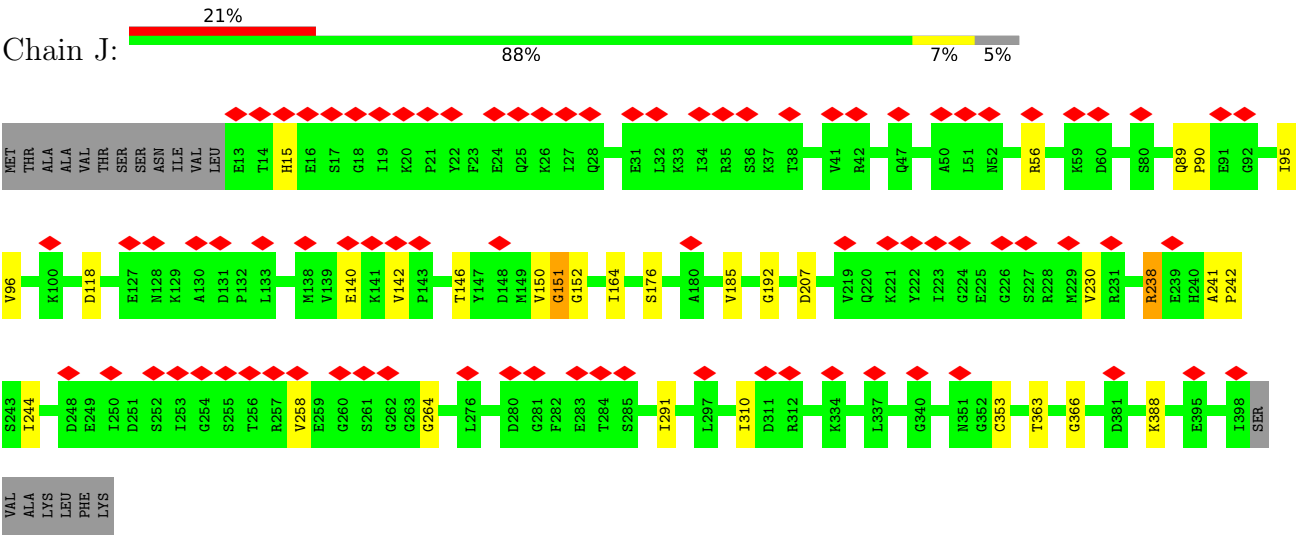


- Molecule 19: 26S protease regulatory subunit 6A

Chain M: 13% 78% 9% 12%



● Molecule 20: 26S protease regulatory subunit 8 homolog



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	14/1945 (0.7%)	1.03	9/2634 (0.3%)
1	a	0.38	1/1945 (0.1%)	0.49	1/2634 (0.0%)
2	B	1.03	7/1952 (0.4%)	1.10	16/2642 (0.6%)
2	b	0.46	2/1952 (0.1%)	0.47	0/2642
3	C	1.01	5/1934 (0.3%)	1.07	12/2618 (0.5%)
3	c	0.38	1/1934 (0.1%)	0.49	1/2618 (0.0%)
4	D	1.02	12/1910 (0.6%)	1.07	11/2586 (0.4%)
4	d	0.38	1/1910 (0.1%)	0.48	1/2586 (0.0%)
5	E	1.26	18/1886 (1.0%)	1.24	14/2541 (0.6%)
5	e	0.90	12/1886 (0.6%)	0.86	6/2541 (0.2%)
6	F	1.12	11/1823 (0.6%)	1.04	7/2463 (0.3%)
6	f	0.47	2/1800 (0.1%)	0.46	0/2433
7	G	1.03	14/1932 (0.7%)	1.00	9/2609 (0.3%)
7	g	0.37	1/1932 (0.1%)	0.46	1/2609 (0.0%)
8	1	0.99	8/1541 (0.5%)	0.97	4/2087 (0.2%)
8	h	0.51	2/1541 (0.1%)	0.48	0/2087
9	2	0.95	7/1750 (0.4%)	1.02	8/2373 (0.3%)
9	i	0.42	1/1750 (0.1%)	0.52	1/2373 (0.0%)
10	3	0.96	5/1611 (0.3%)	0.99	9/2174 (0.4%)
10	j	0.50	2/1611 (0.1%)	0.49	0/2174
11	4	0.95	5/1589 (0.3%)	0.96	3/2142 (0.1%)
11	k	0.42	1/1589 (0.1%)	0.48	1/2142 (0.0%)
12	5	1.05	9/1681 (0.5%)	0.98	5/2274 (0.2%)
12	l	0.50	2/1681 (0.1%)	0.49	0/2274
13	6	1.00	10/1795 (0.6%)	1.05	8/2420 (0.3%)
13	m	0.49	2/1795 (0.1%)	0.52	0/2420
14	7	1.03	8/1821 (0.4%)	1.03	10/2470 (0.4%)
14	n	0.42	1/1846 (0.1%)	0.56	2/2503 (0.1%)
15	H	0.75	12/3102 (0.4%)	0.84	8/4175 (0.2%)
16	I	0.69	7/3061 (0.2%)	0.71	5/4121 (0.1%)
17	K	0.71	11/3121 (0.4%)	0.69	5/4213 (0.1%)
18	L	0.69	4/3128 (0.1%)	0.77	10/4204 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	M	0.75	5/3023 (0.2%)	0.77	6/4070 (0.1%)
20	J	0.55	1/3073 (0.0%)	0.66	4/4129 (0.1%)
All	All	0.78	204/68850 (0.3%)	0.81	177/92981 (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 (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	226	GLU	C-O	-11.62	1.00	1.23
7	g	244	ASN	C-O	-11.59	1.00	1.23
3	C	244	THR	C-O	-11.59	1.00	1.23
16	I	437	LEU	C-OXT	-11.59	1.00	1.23
19	M	434	ALA	C-OXT	-11.58	1.00	1.23
11	k	195	PHE	C-O	-11.57	1.00	1.23
2	B	250	LEU	C-O	-11.57	1.00	1.23
8	1	196	LEU	C-OXT	-11.57	1.00	1.23
2	b	250	LEU	C-O	-11.56	1.00	1.23
7	G	244	ASN	C-O	-11.56	1.00	1.23
17	K	428	LYS	C-O	-11.56	1.00	1.23
9	i	226	GLU	C-O	-11.56	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	204	ASP	C-OXT	-11.56	1.00	1.23
1	a	242	GLN	C-O	-11.56	1.00	1.23
12	5	212	GLY	C-OXT	-11.56	1.00	1.23
13	6	222	ASP	C-O	-11.56	1.00	1.23
15	H	467	ASN	C-O	-11.56	1.00	1.23
17	K	428	LYS	C-OXT	-11.55	1.00	1.23
3	c	244	THR	C-O	-11.55	1.00	1.23
4	d	240	GLU	C-O	-11.55	1.00	1.23
12	l	212	GLY	C-OXT	-11.55	1.00	1.23
13	m	222	ASP	C-O	-11.55	1.00	1.23
6	F	233	ILE	C-OXT	-11.55	1.00	1.23
19	M	434	ALA	C-O	-11.55	1.00	1.23
10	3	204	ASP	C-O	-11.55	1.00	1.23
14	n	232	LYS	C-O	-11.54	1.00	1.23
5	E	242	GLU	C-O	-11.54	1.00	1.23
11	4	195	PHE	C-O	-11.54	1.00	1.23
18	L	436	LYS	C-O	-11.54	1.00	1.23
6	f	233	ILE	C-OXT	-11.54	1.00	1.23
8	1	196	LEU	C-O	-11.54	1.00	1.23
13	6	222	ASP	C-OXT	-11.54	1.00	1.23
14	7	229	GLY	C-O	-11.54	1.00	1.23
2	b	250	LEU	C-OXT	-11.54	1.00	1.23
15	H	467	ASN	C-OXT	-11.54	1.00	1.23
10	j	204	ASP	C-O	-11.53	1.00	1.23
12	5	212	GLY	C-O	-11.53	1.00	1.23
8	h	196	LEU	C-OXT	-11.53	1.00	1.23
12	l	212	GLY	C-O	-11.53	1.00	1.23
13	m	222	ASP	C-OXT	-11.53	1.00	1.23
16	I	437	LEU	C-O	-11.53	1.00	1.23
8	h	196	LEU	C-O	-11.53	1.00	1.23
6	f	233	ILE	C-O	-11.52	1.00	1.23
1	A	242	GLN	C-O	-11.52	1.00	1.23
10	3	204	ASP	C-OXT	-11.52	1.00	1.23
5	e	242	GLU	C-O	-11.52	1.00	1.23
2	B	250	LEU	C-OXT	-11.50	1.00	1.23
6	F	233	ILE	C-O	-11.50	1.00	1.23
13	6	119	LYS	C-N	9.50	1.41	1.33
15	H	176	VAL	CA-C	-8.59	1.41	1.52
1	A	96	ARG	NE-CZ	8.34	1.42	1.33
13	6	108	HIS	CA-C	-7.53	1.43	1.52
15	H	178	ARG	NE-CZ	7.48	1.41	1.33
12	5	26	VAL	CA-C	-7.33	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	135	LEU	C-N	7.30	1.40	1.33
5	e	115	PHE	CA-CB	7.25	1.63	1.53
5	E	124	ARG	CZ-NH1	7.18	1.42	1.32
10	3	188	ILE	CA-C	-7.16	1.45	1.53
17	K	368	LEU	C-N	7.15	1.43	1.34
5	E	113	LEU	CA-C	-7.03	1.44	1.52
17	K	186	GLU	CA-C	-7.00	1.43	1.52
12	5	79	ALA	CA-C	-6.95	1.43	1.52
5	e	116	GLY	N-CA	-6.84	1.38	1.45
16	I	360	LYS	C-N	6.79	1.42	1.33
14	7	108	ASN	CA-CB	6.73	1.60	1.53
1	A	16	LEU	CA-C	-6.70	1.45	1.53
6	F	21	VAL	CA-CB	-6.61	1.44	1.54
7	G	16	ARG	CZ-NH2	6.58	1.42	1.33
5	E	127	SER	CA-CB	6.53	1.65	1.53
1	A	109	ALA	N-CA	-6.53	1.38	1.46
7	G	89	ARG	CD-NE	6.50	1.55	1.46
9	2	178	MET	CA-C	-6.46	1.45	1.52
7	G	96	LYS	CA-CB	6.46	1.63	1.53
14	7	189	ALA	N-CA	-6.45	1.38	1.46
4	D	4	ARG	NE-CZ	6.41	1.40	1.33
5	E	149	HIS	CA-C	-6.35	1.45	1.52
5	E	115	PHE	CA-C	-6.34	1.44	1.52
3	C	73	ALA	CA-C	-6.28	1.45	1.52
6	F	18	LEU	CA-C	-6.27	1.44	1.52
5	E	112	ALA	CA-C	-6.26	1.44	1.52
8	1	108	GLY	CA-C	-6.23	1.45	1.52
17	K	186	GLU	C-N	6.22	1.42	1.33
17	K	141	ARG	CD-NE	6.20	1.54	1.46
1	A	95	PHE	CA-C	-6.20	1.45	1.52
1	A	17	TYR	CA-C	-6.14	1.44	1.52
7	G	22	TYR	N-CA	-6.13	1.38	1.46
7	G	82	ARG	C-N	6.13	1.42	1.33
13	6	79	HIS	C-N	6.12	1.42	1.33
15	H	175	GLY	C-N	6.11	1.42	1.33
16	I	238	ASN	N-CA	-6.09	1.38	1.46
4	D	94	HIS	ND1-CE1	6.08	1.38	1.32
5	E	116	GLY	N-CA	-6.08	1.39	1.45
5	E	112	ALA	N-CA	-6.07	1.39	1.46
14	7	190	ARG	NE-CZ	6.07	1.39	1.33
3	C	4	ARG	CD-NE	6.06	1.54	1.46
3	C	88	ASN	CA-C	-6.04	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	133	ALA	CA-C	-6.03	1.45	1.52
1	A	18	GLN	C-N	5.96	1.41	1.33
6	F	201	ARG	CA-C	-5.95	1.47	1.53
17	K	141	ARG	NE-CZ	5.95	1.39	1.33
2	B	148	TYR	CA-C	-5.94	1.45	1.52
7	G	16	ARG	CD-NE	5.92	1.54	1.46
18	L	183	ILE	CA-C	-5.91	1.46	1.52
6	F	17	ARG	NE-CZ	5.91	1.39	1.33
13	6	108	HIS	CG-ND1	5.90	1.44	1.38
12	5	26	VAL	N-CA	-5.87	1.39	1.46
5	e	128	ARG	NE-CZ	5.86	1.39	1.33
3	C	61	SER	CA-CB	5.85	1.62	1.53
1	A	148	THR	C-N	5.84	1.40	1.33
15	H	174	VAL	C-N	5.81	1.39	1.33
1	A	82	ARG	CA-C	-5.76	1.44	1.52
5	E	200	MET	C-N	5.73	1.41	1.33
12	5	140	LEU	C-N	5.72	1.41	1.34
4	D	81	ARG	NE-CZ	5.71	1.39	1.33
8	1	155	ILE	N-CA	-5.71	1.39	1.46
7	G	149	PRO	N-CA	-5.69	1.40	1.47
2	B	151	ASP	C-N	5.68	1.40	1.33
19	M	176	PRO	N-CA	-5.68	1.40	1.47
16	I	242	ALA	N-CA	-5.67	1.39	1.45
4	D	95	ARG	CD-NE	5.67	1.54	1.46
12	5	121	ARG	CA-C	5.67	1.59	1.52
4	D	20	TYR	N-CA	-5.64	1.39	1.46
5	E	124	ARG	NE-CZ	5.61	1.39	1.33
10	3	151	SER	C-N	5.60	1.41	1.33
9	2	75	ARG	NE-CZ	5.59	1.39	1.33
16	I	271	ALA	CA-C	-5.58	1.45	1.52
11	4	191	GLN	CA-C	-5.57	1.46	1.52
5	e	119	ALA	C-N	5.55	1.41	1.33
5	e	115	PHE	C-N	5.54	1.40	1.33
9	2	79	ALA	C-N	5.50	1.41	1.33
4	D	110	TYR	CA-C	-5.50	1.46	1.52
5	E	105	THR	C-N	5.48	1.41	1.33
14	7	187	ARG	NE-CZ	5.48	1.39	1.33
10	3	178	ALA	C-N	5.48	1.40	1.33
18	L	368	VAL	CA-C	-5.47	1.46	1.52
11	4	189	ILE	C-N	5.46	1.42	1.33
13	6	188	PHE	N-CA	-5.45	1.39	1.46
5	e	120	SER	N-CA	-5.45	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ARG	NE-CZ	5.45	1.39	1.33
19	M	175	LYS	C-N	5.42	1.40	1.33
4	D	201	VAL	C-N	5.41	1.40	1.33
18	L	182	GLY	C-N	5.41	1.39	1.33
9	2	151	ALA	CA-C	-5.40	1.46	1.52
8	1	178	LEU	CA-C	-5.40	1.46	1.53
7	G	82	ARG	NE-CZ	5.39	1.39	1.33
13	6	16	ALA	C-N	5.38	1.41	1.33
7	G	11	PHE	CA-CB	5.38	1.61	1.53
5	e	114	ARG	CZ-NH1	5.38	1.40	1.32
5	e	123	GLU	CA-C	-5.37	1.45	1.52
16	I	141	LEU	N-CA	5.34	1.52	1.46
14	7	184	LEU	N-CA	-5.34	1.39	1.46
9	2	75	ARG	CZ-NH2	5.33	1.40	1.33
1	A	26	THR	CA-C	5.33	1.59	1.52
5	e	123	GLU	C-N	5.32	1.41	1.33
13	6	189	THR	C-N	5.30	1.40	1.33
6	F	19	PHE	CA-CB	5.30	1.61	1.53
14	7	181	MET	CA-C	-5.30	1.45	1.52
15	H	70	LYS	C-N	5.29	1.41	1.33
13	6	106	TYR	C-N	5.28	1.40	1.33
12	5	16	VAL	CA-C	-5.26	1.46	1.52
15	H	372	ASP	N-CA	-5.26	1.40	1.46
8	1	143	ARG	NE-CZ	5.25	1.38	1.33
5	e	133	ALA	CA-C	-5.24	1.46	1.52
15	H	267	THR	N-CA	-5.23	1.40	1.46
7	G	149	PRO	C-N	5.22	1.41	1.33
4	D	22	LEU	C-N	5.22	1.41	1.34
1	A	95	PHE	N-CA	-5.21	1.40	1.46
9	2	188	ARG	NE-CZ	5.21	1.38	1.33
4	D	148	THR	CA-C	-5.20	1.46	1.52
4	D	109	ARG	CD-NE	5.19	1.53	1.46
15	H	242	PRO	CA-CB	-5.18	1.49	1.54
5	E	114	ARG	NE-CZ	5.18	1.38	1.33
4	D	94	HIS	CD2-NE2	5.17	1.43	1.37
19	M	360	ILE	CA-C	-5.17	1.46	1.52
1	A	62	TYR	CA-CB	5.16	1.61	1.53
17	K	141	ARG	CZ-NH1	5.15	1.40	1.32
2	B	62	SER	CA-C	-5.14	1.46	1.52
12	5	121	ARG	C-N	5.14	1.40	1.33
15	H	190	ARG	CA-CB	5.14	1.62	1.53
8	1	79	ALA	C-N	5.14	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	130	SER	C-N	5.13	1.40	1.33
6	F	89	GLN	C-N	5.13	1.41	1.33
8	1	143	ARG	CZ-NH2	5.13	1.40	1.33
2	B	4	ARG	C-N	5.12	1.40	1.33
7	G	106	PRO	CA-CB	5.12	1.61	1.53
15	H	242	PRO	CA-C	-5.11	1.48	1.52
6	F	169	THR	C-N	5.10	1.40	1.34
17	K	372	ILE	C-N	5.09	1.40	1.33
5	E	126	MET	CA-C	-5.08	1.46	1.52
5	E	78	ARG	NE-CZ	5.08	1.38	1.33
7	G	26	ALA	C-N	5.07	1.40	1.33
1	A	73	VAL	N-CA	-5.05	1.40	1.46
14	7	187	ARG	C-N	5.05	1.40	1.33
2	B	21	ILE	C-O	-5.05	1.17	1.24
17	K	41	SER	N-CA	-5.04	1.39	1.46
20	J	176	SER	CA-C	-5.04	1.46	1.52
5	e	125	LEU	CA-CB	5.04	1.61	1.53
6	F	77	ALA	C-N	5.03	1.39	1.33
5	E	105	THR	CA-C	-5.03	1.46	1.52
17	K	360	MET	CA-C	-5.01	1.45	1.53
11	4	139	TYR	CA-C	-5.01	1.45	1.52
6	F	201	ARG	CZ-NH2	5.00	1.40	1.33
7	G	117	GLN	CA-C	-5.00	1.45	1.52
11	4	34	LYS	C-N	5.00	1.39	1.33

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	267	PHE	CA-CB-CG	-11.17	102.63	113.80
15	H	242	PRO	N-CA-CB	10.10	108.47	103.22
15	H	241	ASP	CA-C-N	9.42	126.44	119.66
15	H	241	ASP	C-N-CA	9.42	126.44	119.66
4	D	79	ASP	CA-CB-CG	-9.17	103.43	112.60
5	E	128	ARG	N-CA-C	-9.01	100.11	108.22
3	C	200	THR	CA-C-N	8.66	131.69	120.44
3	C	200	THR	C-N-CA	8.66	131.69	120.44
3	C	151	ASN	CA-CB-CG	8.62	121.22	112.60
2	B	245	ASP	CA-CB-CG	-7.92	104.68	112.60
8	1	188	PHE	CA-CB-CG	-7.48	106.32	113.80
10	3	178	ALA	N-CA-C	7.31	119.33	111.36
13	6	188	PHE	CA-CB-CG	-7.28	106.52	113.80
2	B	151	ASP	CA-CB-CG	7.24	119.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	17	ARG	NE-CZ-NH1	-7.20	114.30	121.50
2	B	18	LEU	CA-C-N	7.12	127.88	119.98
2	B	18	LEU	C-N-CA	7.12	127.88	119.98
4	d	240	GLU	CA-C-O	-6.98	108.94	120.80
18	L	364	HIS	CA-CB-CG	-6.96	106.84	113.80
1	a	242	GLN	CA-C-O	-6.95	108.98	120.80
3	C	244	THR	CA-C-O	-6.95	108.99	120.80
11	4	195	PHE	CA-C-O	-6.95	108.99	120.80
5	E	242	GLU	CA-C-O	-6.95	108.99	120.80
18	L	436	LYS	CA-C-O	-6.94	109.00	120.80
1	A	242	GLN	CA-C-O	-6.94	109.01	120.80
5	e	242	GLU	CA-C-O	-6.93	109.01	120.80
11	k	195	PHE	CA-C-O	-6.93	109.01	120.80
7	G	244	ASN	CA-C-O	-6.93	109.01	120.80
14	n	232	LYS	CA-C-O	-6.93	109.02	120.80
7	g	244	ASN	CA-C-O	-6.91	109.05	120.80
14	n	10	SER	N-CA-C	6.91	119.22	110.24
3	c	244	THR	CA-C-O	-6.91	109.06	120.80
9	i	226	GLU	CA-C-O	-6.91	109.06	120.80
9	2	226	GLU	CA-C-O	-6.89	109.08	120.80
2	B	151	ASP	CB-CA-C	6.87	120.27	109.96
5	E	129	PRO	CA-C-O	-6.81	113.58	121.96
13	6	206	ILE	N-CA-CB	6.80	119.15	110.99
15	H	186	PRO	N-CA-CB	6.77	109.63	103.33
9	2	35	HIS	ND1-CE1-NE2	6.77	115.17	108.40
5	e	123	GLU	N-CA-C	-6.72	102.70	111.71
5	E	128	ARG	O-C-N	-6.67	115.64	121.71
4	D	119	THR	CA-CB-OG1	6.61	119.51	109.60
5	E	112	ALA	N-CA-C	6.59	118.46	111.28
6	F	39	SER	CB-CA-C	-6.58	107.59	117.07
3	C	69	ASN	CA-CB-CG	-6.51	106.09	112.60
5	e	115	PHE	CA-C-O	-6.41	113.14	120.58
10	3	143	ASP	CA-CB-CG	-6.41	106.19	112.60
18	L	182	GLY	CA-C-N	6.41	130.77	121.80
18	L	182	GLY	C-N-CA	6.41	130.77	121.80
14	7	139	SER	N-CA-C	-6.24	102.60	108.22
14	7	35	ARG	O-C-N	-6.24	115.35	122.09
16	I	194	ILE	CB-CA-C	-6.23	103.89	112.24
15	H	242	PRO	O-C-N	-6.21	118.23	121.15
10	3	152	LEU	N-CA-CB	6.18	119.77	110.19
19	M	371	ASP	CA-CB-CG	-6.15	106.45	112.60
3	C	21	VAL	CA-C-N	6.13	128.82	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	21	VAL	C-N-CA	6.13	128.82	120.54
11	4	75	LEU	N-CA-CB	6.09	118.93	109.97
9	2	205	PHE	CA-C-N	6.08	125.84	119.76
9	2	205	PHE	C-N-CA	6.08	125.84	119.76
11	4	151	ASP	CA-CB-CG	6.07	118.67	112.60
14	7	17	ASP	CA-CB-CG	6.01	118.61	112.60
7	G	79	PRO	CA-C-N	5.99	129.42	120.31
7	G	79	PRO	C-N-CA	5.99	129.42	120.31
7	G	81	GLY	N-CA-C	-5.96	105.28	112.49
7	G	119	HIS	CA-CB-CG	-5.96	107.84	113.80
4	D	12	ASP	CA-CB-CG	5.95	118.55	112.60
19	M	242	THR	N-CA-CB	5.94	118.70	109.85
14	7	108	ASN	CA-C-N	5.93	126.13	119.90
14	7	108	ASN	C-N-CA	5.93	126.13	119.90
15	H	359	ASN	CA-C-N	5.87	128.14	120.28
15	H	359	ASN	C-N-CA	5.87	128.14	120.28
16	I	174	ASP	CB-CA-C	-5.86	103.96	111.22
1	A	149	ASP	CA-C-O	-5.85	115.62	120.71
19	M	143	ASN	CA-CB-CG	-5.84	106.76	112.60
18	L	400	PHE	CA-CB-CG	-5.83	107.97	113.80
7	G	149	PRO	CA-C-N	5.81	128.54	120.29
7	G	149	PRO	C-N-CA	5.81	128.54	120.29
5	e	111	LEU	CB-CA-C	-5.76	101.22	110.79
20	J	238	ARG	NE-CZ-NH1	-5.74	115.76	121.50
10	3	35	VAL	O-C-N	5.69	127.04	121.98
12	5	117	SER	CA-C-N	5.69	128.17	120.38
12	5	117	SER	C-N-CA	5.69	128.17	120.38
8	1	186	LEU	N-CA-C	-5.68	101.12	109.81
13	6	79	HIS	CA-CB-CG	-5.67	108.13	113.80
2	B	96	SER	CA-C-O	-5.63	112.94	119.59
6	F	21	VAL	N-CA-C	-5.63	104.41	112.35
10	3	139	GLY	CA-C-N	5.63	127.76	120.44
10	3	139	GLY	C-N-CA	5.63	127.76	120.44
1	A	105	CYS	CA-C-N	5.63	128.14	120.54
1	A	105	CYS	C-N-CA	5.63	128.14	120.54
14	7	229	GLY	CA-C-O	-5.62	109.00	120.80
12	5	17	ASP	CA-CB-CG	5.62	118.22	112.60
4	D	151	SER	N-CA-CB	5.61	118.98	110.28
4	D	94	HIS	CE1-NE2-CD2	-5.61	103.39	109.00
10	3	35	VAL	CB-CA-C	-5.57	106.15	111.44
5	E	117	GLU	N-CA-C	-5.56	105.10	113.89
1	A	150	PRO	O-C-N	5.56	129.86	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	GLN	CA-C-O	-5.55	113.24	119.79
2	B	17	LYS	N-CA-CB	5.53	119.84	110.49
4	D	89	VAL	CA-C-O	-5.52	115.67	121.41
1	A	94	GLU	N-CA-C	5.48	118.77	111.75
2	B	104	TYR	CA-C-N	5.48	126.02	120.38
2	B	104	TYR	C-N-CA	5.48	126.02	120.38
9	2	150	GLU	CA-C-N	5.47	127.88	120.44
9	2	150	GLU	C-N-CA	5.47	127.88	120.44
3	C	12	PHE	CA-C-N	5.45	130.36	122.29
3	C	12	PHE	C-N-CA	5.45	130.36	122.29
14	7	188	ASP	N-CA-C	-5.44	100.84	109.59
3	C	106	PRO	N-CA-CB	5.42	108.07	103.35
12	5	200	VAL	CB-CA-C	-5.42	104.91	112.02
5	E	124	ARG	NE-CZ-NH2	-5.40	114.34	119.20
9	2	191	LEU	CB-CA-C	-5.40	101.51	110.14
6	F	209	ASN	N-CA-C	-5.38	107.08	113.97
20	J	152	GLY	CA-C-N	5.38	129.99	122.41
20	J	152	GLY	C-N-CA	5.38	129.99	122.41
5	e	127	SER	N-CA-C	-5.36	106.78	113.38
6	F	16	GLY	CA-C-O	-5.36	112.98	119.04
19	M	372	ASP	CA-CB-CG	5.36	117.96	112.60
4	D	25	VAL	CA-C-N	5.35	127.89	120.29
4	D	25	VAL	C-N-CA	5.35	127.89	120.29
2	B	105	PRO	CB-CA-C	5.33	117.43	110.92
17	K	243	VAL	CA-CB-CG2	-5.33	101.35	110.40
18	L	247	PRO	CA-N-CD	5.32	119.45	112.00
20	J	363	THR	CA-CB-OG1	5.30	117.55	109.60
18	L	376	PHE	CA-CB-CG	-5.30	108.50	113.80
2	B	96	SER	N-CA-C	-5.29	106.05	112.88
13	6	16	ALA	CB-CA-C	-5.29	101.62	110.19
5	E	77	ALA	CA-C-N	5.26	127.86	120.28
5	E	77	ALA	C-N-CA	5.26	127.86	120.28
7	G	110	ASP	CA-CB-CG	5.26	117.86	112.60
19	M	174	GLU	N-CA-CB	5.26	119.38	110.49
2	B	148	TYR	CA-CB-CG	-5.24	104.46	113.90
16	I	274	ASN	CA-CB-CG	-5.23	107.37	112.60
18	L	183	ILE	CA-C-O	-5.23	114.57	120.74
4	D	96	LEU	N-CA-CB	5.22	117.86	110.13
4	D	94	HIS	ND1-CE1-NE2	5.21	113.61	108.40
16	I	176	SER	N-CA-CB	5.21	117.55	111.09
1	A	26	THR	CA-C-N	5.21	131.49	121.54
1	A	26	THR	C-N-CA	5.21	131.49	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	119	GLN	OE1-CD-NE2	-5.21	117.39	122.60
14	7	143	ALA	N-CA-CB	5.20	119.62	111.56
5	E	18	TYR	CA-C-N	5.19	127.49	120.38
5	E	18	TYR	C-N-CA	5.19	127.49	120.38
2	B	151	ASP	CA-C-O	-5.19	115.87	121.27
10	3	187	TYR	CB-CA-C	-5.19	101.78	110.19
17	K	243	VAL	CB-CA-C	5.17	116.99	111.35
13	6	162	PRO	CA-C-N	5.17	131.03	120.80
13	6	162	PRO	C-N-CA	5.17	131.03	120.80
9	2	151	ALA	CB-CA-C	-5.16	102.75	110.90
12	5	154	LEU	O-C-N	5.16	127.38	122.07
8	1	191	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	105	CYS	CA-C-O	-5.15	115.59	121.00
6	F	25	LEU	CB-CA-C	-5.14	99.72	109.95
17	K	183	GLU	O-C-N	5.14	127.36	122.07
13	6	187	SER	N-CA-CB	5.12	117.61	109.82
10	3	105	GLY	O-C-N	-5.12	116.65	121.77
18	L	67	HIS	CE1-NE2-CD2	-5.12	103.88	109.00
18	L	174	GLU	N-CA-CB	5.12	119.14	110.49
14	7	118	GLY	O-C-N	-5.09	117.86	123.66
5	e	112	ALA	N-CA-C	5.09	121.64	110.80
2	B	94	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
17	K	183	GLU	CA-C-O	-5.09	115.48	120.82
3	C	18	LEU	CA-C-O	-5.08	115.02	120.46
17	K	198	TYR	CA-CB-CG	-5.08	104.75	113.90
4	D	18	VAL	O-C-N	-5.07	115.15	121.84
6	F	131	LEU	CA-C-O	-5.05	115.45	121.16
5	E	27	SER	CA-C-N	5.04	128.71	121.50
5	E	27	SER	C-N-CA	5.04	128.71	121.50
14	7	118	GLY	N-CA-C	5.04	118.93	110.56
6	F	11	THR	O-C-N	5.03	129.19	122.95
8	1	17	ASP	N-CA-CB	5.03	118.25	110.46
5	E	84	ALA	CA-C-O	-5.02	115.55	120.82
16	I	216	PRO	CA-N-CD	5.02	119.03	112.00
7	G	110	ASP	CA-C-O	-5.01	115.11	120.42
15	H	70	LYS	N-CA-CB	5.01	120.11	111.13
13	6	206	ILE	CA-CB-CG1	5.00	118.90	110.40

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 [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	A	1907	0	1901	1	0
1	a	1907	0	1901	17	0
2	B	1915	0	1929	11	0
2	b	1915	0	1929	25	0
3	C	1904	0	1904	12	0
3	c	1904	0	1904	12	0
4	D	1881	0	1895	8	0
4	d	1881	0	1895	6	0
5	E	1861	0	1839	11	0
5	e	1861	0	1839	19	0
6	F	1795	0	1800	11	0
6	f	1773	0	1775	5	0
7	G	1892	0	1883	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	g	1892	0	1883	3	0
8	l	1512	0	1479	9	0
8	h	1512	0	1481	7	0
9	2	1719	0	1719	37	0
9	i	1719	0	1719	5	0
10	3	1581	0	1574	10	0
10	j	1581	0	1574	6	0
11	4	1561	0	1569	4	0
11	k	1561	0	1569	7	0
12	5	1644	0	1595	15	0
12	l	1644	0	1595	5	0
13	6	1757	0	1711	11	0
13	m	1757	0	1711	9	0
14	7	1790	0	1793	15	0
14	n	1815	0	1821	45	0
15	H	3053	0	3127	31	0
16	I	3022	0	3092	36	0
17	K	3078	0	3140	16	0
18	L	3082	0	3157	20	0
19	M	2986	0	3055	18	0
20	J	3033	0	3155	13	0
21	H	31	0	12	2	0
21	I	31	0	12	7	0
21	K	31	0	12	0	0
21	L	31	0	12	2	0
21	M	31	0	12	2	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	M	1	0	0	0	0
23	J	27	0	12	1	0
All	All	67883	0	67985	383	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 3.

All (383) 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)
14:n:150:MET:SD	9:2:132:LEU:HD11	1.49	1.52
14:n:150:MET:SD	9:2:132:LEU:CD1	2.10	1.40
14:n:149:HIS:CB	9:2:132:LEU:HD23	1.69	1.23
16:I:184:ILE:HD11	16:I:231:LEU:HG	1.30	1.12
14:n:149:HIS:HB3	9:2:132:LEU:HD23	1.32	1.11
2:b:4:ARG:HH22	5:e:117:GLU:HG3	1.09	1.11
4:D:24:ALA:O	16:I:436:TYR:OH	1.70	1.08
2:b:4:ARG:HH22	5:e:117:GLU:CG	1.68	1.06
14:n:149:HIS:HB2	9:2:132:LEU:CD2	1.87	1.05
14:n:33:LEU:HD13	8:1:133:PHE:HE1	1.23	1.02
2:b:4:ARG:NH2	5:e:117:GLU:CG	2.25	0.99
2:b:4:ARG:CZ	5:e:117:GLU:OE1	2.12	0.97
14:n:149:HIS:CB	9:2:132:LEU:CD2	2.43	0.93
14:n:33:LEU:HD13	8:1:133:PHE:CE1	2.04	0.92
16:I:184:ILE:CD1	16:I:231:LEU:CD2	2.48	0.92
2:b:4:ARG:HH21	5:e:117:GLU:HB3	1.32	0.91
16:I:393:GLN:OE1	21:I:501:ATP:O2'	1.90	0.89
2:b:4:ARG:NH2	5:e:117:GLU:HB3	1.89	0.87
16:I:184:ILE:HD13	16:I:231:LEU:HD21	1.57	0.86
2:b:4:ARG:NH2	5:e:117:GLU:CB	2.38	0.85
14:n:150:MET:CG	9:2:132:LEU:HD11	2.06	0.84
2:b:4:ARG:NH2	5:e:117:GLU:HG3	1.90	0.83
16:I:184:ILE:HD13	16:I:231:LEU:CD2	2.09	0.82
18:L:377:GLU:OE1	18:L:377:GLU:N	2.14	0.80
16:I:184:ILE:HD11	16:I:231:LEU:CG	2.12	0.79
16:I:184:ILE:CD1	16:I:231:LEU:HG	2.10	0.78
19:M:371:ASP:OD1	19:M:371:ASP:C	2.29	0.75
14:n:150:MET:SD	9:2:132:LEU:HD12	2.22	0.74
2:b:250:LEU:OXT	2:b:250:LEU:HD13	1.88	0.73
15:H:246:ILE:HD11	15:H:352:MET:HE3	1.70	0.73
10:3:84:GLU:N	10:3:84:GLU:OE1	2.19	0.73
13:m:159:GLN:NE2	9:2:205:PHE:HE1	1.87	0.73
2:b:4:ARG:NH1	5:e:117:GLU:OE1	2.22	0.72
2:B:140:ASP:OD1	2:B:140:ASP:C	2.31	0.71
2:b:4:ARG:NH2	5:e:117:GLU:OE1	2.23	0.70
10:j:143:ASP:O	13:6:145:LEU:CD2	2.39	0.70
14:n:150:MET:CE	9:2:132:LEU:HD12	2.22	0.69
15:H:427:GLY:HA3	16:I:213:ILE:HD13	1.75	0.69
14:n:150:MET:CB	9:2:132:LEU:HD11	2.22	0.69
16:I:184:ILE:CD1	16:I:231:LEU:HD23	2.23	0.68
14:n:225:ILE:CG1	9:2:123:TYR:HE1	2.07	0.67
14:n:152:ASN:OD1	14:n:156:ARG:NE	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:LEU:HD12	6:F:71:LEU:C	2.20	0.66
16:I:184:ILE:CD1	16:I:231:LEU:CG	2.70	0.66
14:n:150:MET:HB2	9:2:132:LEU:HD11	1.76	0.66
14:n:149:HIS:C	9:2:132:LEU:CD2	2.69	0.66
10:3:160:GLU:OE1	10:3:160:GLU:N	2.28	0.65
16:I:378:GLU:OE1	16:I:378:GLU:N	2.30	0.65
12:5:4:LEU:C	12:5:4:LEU:HD12	2.23	0.64
6:F:233:ILE:OXT	6:F:233:ILE:HG22	1.96	0.64
13:m:35:ILE:O	14:n:156:ARG:NH2	2.32	0.63
2:b:4:ARG:NH2	5:e:117:GLU:CD	2.56	0.63
14:n:149:HIS:HB2	9:2:132:LEU:HD21	1.79	0.63
14:n:225:ILE:HG23	9:2:121:VAL:HG21	1.80	0.63
18:L:356:GLY:O	18:L:359:GLU:N	2.31	0.62
4:D:235:GLU:O	4:D:239:GLN:HB3	2.00	0.62
12:l:36:GLU:HG2	12:l:185:TRP:CZ2	2.35	0.62
14:n:150:MET:SD	9:2:132:LEU:HD13	2.32	0.61
14:n:150:MET:HE3	9:2:132:LEU:HD12	1.82	0.61
17:K:356:ILE:HG21	17:K:387:MET:HG3	1.83	0.61
20:J:140:GLU:OE1	20:J:140:GLU:HA	2.01	0.61
7:G:200:HIS:O	7:G:200:HIS:CD2	2.54	0.61
11:k:130:TYR:OH	12:5:209:ASN:ND2	2.34	0.60
12:5:38:ASN:C	12:5:38:ASN:OD1	2.41	0.60
4:D:107:LEU:O	4:D:107:LEU:HG	2.02	0.60
14:7:30:TYR:O	14:7:30:TYR:CD2	2.55	0.60
14:n:149:HIS:O	9:2:132:LEU:HG	2.01	0.60
19:M:317:SER:OG	19:M:319:ASP:OD1	2.20	0.59
2:B:97:TYR:O	2:B:97:TYR:CD2	2.56	0.59
17:K:96:ILE:HD11	18:L:128:ILE:HG13	1.84	0.59
5:E:205:ASP:OD1	5:E:205:ASP:C	2.45	0.59
2:B:35:LEU:C	2:B:35:LEU:HD12	2.28	0.59
14:n:225:ILE:HG12	9:2:123:TYR:CE1	2.37	0.59
14:7:131:ASN:OD1	14:7:131:ASN:C	2.45	0.59
16:I:247:ILE:HG23	16:I:247:ILE:O	2.02	0.59
18:L:356:GLY:O	18:L:358:LEU:N	2.35	0.59
2:B:97:TYR:CD2	2:B:97:TYR:C	2.81	0.58
15:H:371:ILE:HG22	15:H:371:ILE:O	2.02	0.58
10:3:10:ILE:HG13	10:3:10:ILE:O	2.03	0.58
16:I:148:LEU:HD22	20:J:95:ILE:HD13	1.85	0.58
5:e:91:HIS:CG	5:e:99:ILE:CG2	2.87	0.58
14:n:225:ILE:CG2	9:2:121:VAL:HG21	2.33	0.58
10:j:143:ASP:O	13:6:145:LEU:HD23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:200:HIS:O	7:G:200:HIS:CG	2.57	0.58
19:M:280:ILE:HG21	19:M:283:LEU:CD2	2.33	0.58
15:H:311:ILE:HG13	15:H:311:ILE:O	2.03	0.58
9:i:200:GLN:CG	13:6:186:ASP:OD1	2.52	0.57
6:F:233:ILE:OXT	6:F:233:ILE:CG2	2.50	0.57
15:H:240:ILE:HG23	15:H:240:ILE:O	2.05	0.57
17:K:180:GLN:N	17:K:180:GLN:OE1	2.38	0.57
5:e:99:ILE:HD13	5:e:99:ILE:H	1.70	0.56
2:B:118:MET:SD	2:B:152:PRO:HA	2.46	0.56
13:m:159:GLN:NE2	9:2:205:PHE:CE1	2.73	0.56
19:M:229:THR:OG1	21:M:501:ATP:O2A	2.24	0.56
19:M:334:ASP:HB2	19:M:335:PRO:HD2	1.88	0.56
14:n:150:MET:CE	9:2:132:LEU:CD1	2.79	0.56
12:5:104:TYR:CD1	12:5:104:TYR:C	2.82	0.56
5:e:45:ARG:HE	5:e:45:ARG:HA	1.70	0.55
16:I:436:TYR:HB3	16:I:437:LEU:HD23	1.88	0.55
14:n:225:ILE:CG1	9:2:123:TYR:CE1	2.88	0.55
3:C:3:ARG:NH2	5:E:117:GLU:OE2	2.40	0.55
1:A:44:VAL:HG21	1:A:73:VAL:HG21	1.89	0.55
16:I:184:ILE:HD12	16:I:231:LEU:HD23	1.88	0.55
14:7:132:LEU:HD23	14:7:132:LEU:H	1.72	0.55
4:D:225:GLU:OE1	4:D:225:GLU:HA	2.05	0.55
16:I:393:GLN:OE1	21:I:501:ATP:C2'	2.55	0.55
17:K:268:ILE:HG23	17:K:315:ILE:HD13	1.88	0.55
19:M:401:ILE:HG22	19:M:414:ASP:OD1	2.08	0.54
19:M:248:ALA:N	19:M:249:PRO:HD2	2.22	0.54
15:H:405:GLU:OE1	15:H:405:GLU:N	2.29	0.54
3:C:128:ARG:O	3:C:128:ARG:HG3	2.08	0.53
20:J:258:VAL:HA	20:J:264:GLY:H	1.73	0.53
15:H:173:ARG:NH1	15:H:191:ILE:HG22	2.24	0.53
18:L:235:VAL:HG22	18:L:239:ILE:HD11	1.91	0.53
20:J:244:ILE:CG2	20:J:291:ILE:HD12	2.39	0.53
21:H:501:ATP:O1G	16:I:340:ARG:NH2	2.42	0.53
5:e:65:HIS:NE2	5:e:98:ASP:HB3	2.24	0.53
14:n:186:TYR:O	8:1:29:ARG:HD3	2.09	0.53
15:H:275:ILE:HD13	16:I:311:ASN:CG	2.34	0.53
18:L:356:GLY:O	18:L:357:ARG:C	2.50	0.52
1:a:12:PRO:HA	2:b:23:TYR:CE1	2.44	0.52
9:i:200:GLN:HB2	13:6:186:ASP:OD1	2.09	0.52
19:M:280:ILE:CG2	19:M:283:LEU:HD23	2.40	0.52
1:a:60:VAL:HA	7:g:154:TRP:CZ3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:124:SER:OG	13:m:137:ARG:HD3	2.09	0.52
17:K:146:LEU:C	17:K:146:LEU:HD23	2.35	0.52
2:b:2:THR:OG1	5:e:119:ALA:HA	2.09	0.51
3:C:69:ASN:OD1	3:C:69:ASN:N	2.38	0.51
14:7:30:TYR:O	14:7:30:TYR:CG	2.63	0.51
8:h:140:LYS:HE2	8:1:161:GLN:HE21	1.75	0.51
3:C:64:LYS:O	3:C:75:ALA:HA	2.11	0.51
6:F:37:LEU:N	6:F:37:LEU:HD23	2.26	0.51
16:I:148:LEU:CD2	20:J:95:ILE:HD13	2.40	0.51
14:n:91:TYR:O	14:n:94:GLU:N	2.44	0.50
19:M:376:TRP:CD1	19:M:376:TRP:H	2.28	0.50
14:n:26:ASN:OD1	14:n:26:ASN:N	2.44	0.50
17:K:243:VAL:HG21	18:L:303:ARG:HD3	1.91	0.50
6:F:51:ASN:OD1	6:F:51:ASN:C	2.53	0.50
18:L:387:ASN:OD1	18:L:387:ASN:C	2.53	0.50
3:c:218:GLY:O	3:c:219:ALA:CB	2.59	0.50
14:n:33:LEU:CD1	8:1:133:PHE:CE1	2.89	0.50
2:b:250:LEU:OXT	2:b:250:LEU:CD1	2.59	0.50
19:M:75:LEU:HD12	19:M:75:LEU:N	2.27	0.50
9:2:14:ILE:O	9:2:14:ILE:HG23	2.11	0.50
14:n:225:ILE:HD12	8:1:30:VAL:HG11	1.94	0.50
5:E:64:ARG:O	5:E:64:ARG:HG2	2.12	0.50
15:H:257:THR:OG1	21:H:501:ATP:O2A	2.29	0.50
4:D:235:GLU:O	4:D:239:GLN:CB	2.60	0.50
10:j:31:GLN:OE1	10:j:31:GLN:HA	2.12	0.49
14:n:149:HIS:C	9:2:132:LEU:HD23	2.34	0.49
16:I:220:ILE:O	16:I:348:ILE:HG22	2.13	0.49
18:L:387:ASN:OD1	18:L:390:ASP:N	2.45	0.49
6:f:77:ALA:N	6:f:78:PRO:CD	2.76	0.49
14:n:129:TYR:C	14:n:129:TYR:CD1	2.90	0.49
1:a:221:LYS:O	1:a:222:ASP:HB2	2.11	0.49
18:L:229:THR:HG23	21:L:501:ATP:O2B	2.12	0.49
1:a:94:GLU:HA	1:a:94:GLU:OE1	2.12	0.49
13:m:124:SER:CB	13:m:137:ARG:HD3	2.43	0.49
12:5:4:LEU:HD12	12:5:4:LEU:O	2.13	0.49
19:M:229:THR:HG23	21:M:501:ATP:O2B	2.13	0.49
16:I:211:MET:HG3	16:I:213:ILE:HG23	1.95	0.49
15:H:307:PHE:C	15:H:307:PHE:CD1	2.90	0.48
18:L:167:VAL:HG12	18:L:167:VAL:O	2.12	0.48
2:b:235:PHE:CD1	2:b:235:PHE:C	2.91	0.48
13:m:8:ASN:HA	13:m:30:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:84:GLU:N	10:3:84:GLU:CD	2.70	0.48
10:3:95:TYR:O	10:3:95:TYR:CD2	2.66	0.48
2:b:97:TYR:CE2	2:b:105:PRO:HA	2.48	0.48
9:2:3:ILE:O	9:2:126:SER:HA	2.14	0.48
14:n:225:ILE:CG2	9:2:121:VAL:CG2	2.90	0.48
3:C:121:TYR:CD1	3:C:121:TYR:N	2.81	0.48
19:M:280:ILE:HG21	19:M:283:LEU:HD23	1.93	0.48
18:L:356:GLY:C	18:L:358:LEU:N	2.69	0.48
20:J:89:GLN:N	20:J:90:PRO:HD2	2.28	0.48
14:n:225:ILE:HD11	9:2:123:TYR:CD1	2.49	0.48
13:6:147:MET:HB3	13:6:148:PRO:HD3	1.95	0.48
1:a:12:PRO:HA	2:b:23:TYR:CD1	2.48	0.48
3:c:68:LEU:HD13	3:c:110:LEU:HD21	1.96	0.47
10:3:160:GLU:N	10:3:160:GLU:CD	2.72	0.47
15:H:192:ASP:N	15:H:193:PRO:CD	2.76	0.47
17:K:306:PHE:CE2	17:K:311:ASN:HB3	2.49	0.47
14:n:225:ILE:HD11	9:2:123:TYR:CE1	2.49	0.47
3:C:69:ASN:OD1	3:C:69:ASN:C	2.55	0.47
10:3:160:GLU:CD	10:3:160:GLU:H	2.20	0.47
16:I:316:PHE:CD1	16:I:316:PHE:C	2.93	0.47
2:b:4:ARG:HH21	5:e:117:GLU:CB	2.06	0.47
14:7:60:MET:SD	14:7:60:MET:C	2.97	0.47
15:H:43:ALA:N	15:H:44:PRO:CD	2.77	0.47
16:I:125:MET:HB2	16:I:126:PRO:HD3	1.95	0.47
3:c:50:LYS:O	3:c:51:VAL:HB	2.15	0.47
9:i:200:GLN:CB	13:6:186:ASP:OD1	2.62	0.47
10:j:23:ALA:HB2	10:j:186:VAL:HG13	1.97	0.47
6:F:71:LEU:HD12	6:F:71:LEU:O	2.15	0.47
8:1:193:TYR:CD1	8:1:193:TYR:C	2.93	0.47
15:H:150:LYS:C	15:H:152:ILE:H	2.23	0.47
7:G:103:ILE:HG23	7:G:103:ILE:O	2.15	0.46
10:3:95:TYR:CD2	10:3:95:TYR:C	2.93	0.46
17:K:204:ASP:OD2	17:K:207:ARG:NH1	2.46	0.46
14:7:96:LEU:O	14:7:100:MET:HG2	2.15	0.46
15:H:275:ILE:HG23	15:H:278:GLU:H	1.80	0.46
6:f:55:LEU:HD22	6:f:55:LEU:H	1.80	0.46
3:C:108:GLU:OE1	3:C:108:GLU:HA	2.14	0.46
7:G:176:VAL:HG12	7:G:176:VAL:O	2.14	0.46
14:7:25:ASP:HA	14:7:195:PHE:HA	1.98	0.46
1:a:190:TRP:O	1:a:194:VAL:HG23	2.15	0.46
19:M:334:ASP:OD1	19:M:334:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:280:ILE:CG2	19:M:283:LEU:CD2	2.93	0.46
20:J:192:GLY:N	23:J:501:ADP:O3B	2.46	0.46
20:J:244:ILE:HG21	20:J:291:ILE:HD12	1.97	0.46
15:H:374:LYS:HD2	15:H:374:LYS:N	2.31	0.46
3:c:14:PRO:HA	4:d:20:TYR:CE1	2.51	0.46
6:f:201:ARG:O	6:f:202:ASP:HB2	2.16	0.46
3:C:3:ARG:NH2	5:E:117:GLU:CD	2.74	0.46
11:4:78:GLN:CD	11:4:78:GLN:C	2.83	0.46
16:I:83:LYS:N	16:I:84:PRO:HD2	2.31	0.46
17:K:356:ILE:CG2	17:K:387:MET:HG3	2.46	0.46
14:n:122:ASN:HB2	14:n:124:ASP:OD2	2.16	0.46
16:I:393:GLN:OE1	21:I:501:ATP:C4'	2.64	0.46
16:I:393:GLN:CD	21:I:501:ATP:HO2'	2.12	0.46
12:5:55:TRP:HB2	12:5:97:MET:HE1	1.98	0.45
18:L:353:ASN:C	18:L:353:ASN:OD1	2.58	0.45
15:H:176:VAL:HG12	15:H:183:ILE:HA	1.98	0.45
3:c:10:THR:O	4:d:125:ARG:HD3	2.17	0.45
4:D:233:GLN:O	4:D:237:GLU:N	2.43	0.45
14:7:165:ILE:N	14:7:166:PRO:HD2	2.30	0.45
14:7:25:ASP:C	14:7:25:ASP:OD1	2.58	0.45
14:7:85:GLU:O	14:7:86:ALA:C	2.60	0.45
17:K:247:LEU:O	17:K:249:GLU:HG2	2.17	0.45
18:L:329:ARG:HG3	18:L:329:ARG:O	2.17	0.45
1:a:124:TYR:CD1	1:a:124:TYR:C	2.95	0.45
1:a:221:LYS:O	1:a:222:ASP:CB	2.65	0.45
11:k:29:LYS:HE2	12:l:124:GLY:HA2	1.99	0.45
4:D:234:ILE:O	4:D:238:LYS:HB3	2.15	0.45
12:5:64:ARG:O	12:5:64:ARG:HG3	2.16	0.45
1:a:78:ILE:N	1:a:79:PRO:CD	2.79	0.45
3:c:111:VAL:HG22	3:c:136:TYR:CD2	2.52	0.45
14:n:129:TYR:CE2	14:n:144:THR:HG22	2.52	0.45
8:1:14:LEU:N	8:1:14:LEU:HD12	2.32	0.45
9:2:185:GLU:HB3	9:2:187:LEU:HD21	1.98	0.45
17:K:373:ILE:HG13	17:K:374:ARG:N	2.31	0.45
14:n:149:HIS:C	9:2:132:LEU:HD21	2.40	0.45
10:3:23:ALA:HA	10:3:185:VAL:O	2.16	0.45
10:j:65:MET:HE3	10:j:69:LYS:HE2	1.98	0.45
2:B:249:ALA:C	2:B:250:LEU:O	2.56	0.45
16:I:81:ILE:HG22	16:I:84:PRO:HD2	1.99	0.45
20:J:150:VAL:O	20:J:151:GLY:C	2.59	0.45
3:c:139:TYR:CD2	3:c:139:TYR:C	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:15:ALA:HA	12:l:176:ASN:O	2.16	0.45
2:b:31:GLY:O	2:b:166:LYS:HG3	2.17	0.45
5:E:67:GLY:HA3	5:E:220:PHE:CE1	2.52	0.45
12:5:95:LEU:C	12:5:95:LEU:HD12	2.42	0.45
11:k:142:SER:HB3	12:5:135:PHE:HD2	1.82	0.44
5:E:156:PHE:O	5:E:156:PHE:CD1	2.69	0.44
8:h:59:VAL:HG22	8:h:81:VAL:HG12	1.99	0.44
16:I:393:GLN:OE1	21:I:501:ATP:H4'	2.16	0.44
12:l:41:LEU:O	12:l:42:LEU:HD23	2.16	0.44
14:n:150:MET:HB2	9:2:132:LEU:HD21	1.98	0.44
13:6:17:GLY:HA3	13:6:20:PHE:CE1	2.51	0.44
13:6:91:ARG:O	13:6:91:ARG:HG3	2.16	0.44
2:B:140:ASP:OD1	2:B:140:ASP:O	2.35	0.44
2:b:221:LEU:O	2:b:222:LEU:C	2.60	0.44
5:E:126:MET:HB2	5:E:126:MET:HE2	1.91	0.44
19:M:297:GLY:O	19:M:298:ASP:HB2	2.18	0.44
15:H:145:TYR:CD1	15:H:183:ILE:HD12	2.52	0.44
15:H:221:LEU:CD2	15:H:246:ILE:HD12	2.47	0.44
14:7:25:ASP:OD1	14:7:41:ARG:NH2	2.51	0.44
8:h:14:LEU:HD12	8:h:14:LEU:N	2.32	0.44
4:d:71:LEU:C	4:d:71:LEU:HD23	2.43	0.44
14:n:152:ASN:OD1	14:n:156:ARG:HG3	2.17	0.44
5:E:200:MET:HG2	5:E:202:GLU:H	1.83	0.44
2:B:214:ILE:O	2:B:214:ILE:HG22	2.17	0.43
3:C:10:THR:O	4:D:125:ARG:HD3	2.18	0.43
6:F:178:PHE:CD1	6:F:178:PHE:C	2.95	0.43
15:H:59:ILE:O	15:H:59:ILE:HG22	2.17	0.43
16:I:378:GLU:H	16:I:378:GLU:CD	2.21	0.43
10:3:48:VAL:HG11	10:3:86:PHE:CD2	2.54	0.43
11:4:101:ASN:HB3	11:4:133:HIS:CE1	2.54	0.43
8:h:38:HIS:CG	8:h:39:ASP:H	2.36	0.43
11:k:118:GLN:HG3	11:k:133:HIS:CE1	2.53	0.43
8:1:166:ASP:OD1	8:1:167:GLY:N	2.51	0.43
10:j:10:ILE:HG21	10:j:141:ALA:HB3	2.01	0.43
14:n:48:ASN:OD1	14:n:48:ASN:N	2.51	0.43
15:H:274:VAL:HG11	15:H:279:LEU:HD21	2.01	0.43
18:L:357:ARG:NH1	18:L:383:SER:O	2.52	0.43
8:h:71:GLY:O	8:h:72:THR:C	2.62	0.43
9:2:225:GLU:C	9:2:226:GLU:O	2.58	0.43
14:7:77:ASP:O	14:7:78:ASN:HB2	2.19	0.43
16:I:393:GLN:OE1	21:I:501:ATP:C1'	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:218:GLY:O	3:c:219:ALA:HB3	2.18	0.43
14:n:225:ILE:HG23	9:2:121:VAL:CG2	2.45	0.43
15:H:405:GLU:H	15:H:405:GLU:CD	2.18	0.43
17:K:419:ASN:O	17:K:420:THR:HB	2.19	0.43
1:a:23:PHE:CE1	1:a:150:PRO:HD2	2.54	0.43
6:f:38:ARG:HD3	6:f:39:SER:O	2.19	0.42
3:C:121:TYR:N	3:C:121:TYR:HD1	2.17	0.42
9:i:38:SER:O	9:i:40:LYS:N	2.52	0.42
3:C:140:ASP:OD1	3:C:140:ASP:C	2.62	0.42
6:F:1:PHE:CD2	6:F:1:PHE:O	2.71	0.42
9:2:113:ILE:O	9:2:113:ILE:HG23	2.18	0.42
13:m:157:LYS:O	13:m:158:ASN:HB2	2.18	0.42
19:M:248:ALA:N	19:M:249:PRO:CD	2.82	0.42
2:b:227:ILE:HG23	2:b:227:ILE:O	2.19	0.42
16:I:221:LEU:HA	16:I:348:ILE:CG2	2.49	0.42
18:L:269:TYR:CD1	18:L:269:TYR:C	2.98	0.42
15:H:248:LEU:N	15:H:248:LEU:HD12	2.34	0.42
6:F:77:ALA:N	6:F:78:PRO:HD2	2.34	0.42
15:H:405:GLU:N	15:H:405:GLU:CD	2.77	0.42
12:l:53:GLN:OE1	13:m:130:SER:HB2	2.19	0.42
14:n:25:ASP:HA	14:n:195:PHE:HA	2.00	0.42
14:7:132:LEU:HD23	14:7:132:LEU:N	2.35	0.42
15:H:192:ASP:O	15:H:193:PRO:C	2.63	0.42
4:d:107:LEU:HD13	4:d:107:LEU:O	2.20	0.42
8:h:77:THR:O	8:h:80:SER:N	2.52	0.42
9:i:200:GLN:HG2	13:6:186:ASP:OD1	2.20	0.42
11:4:52:ASP:OD1	12:5:91:LYS:NZ	2.52	0.42
15:H:161:GLU:CD	15:H:161:GLU:H	2.28	0.42
15:H:211:VAL:CG1	15:H:218:ILE:HD11	2.50	0.42
3:c:151:ASN:O	3:c:154:GLY:N	2.52	0.42
5:e:139:HIS:HB2	5:e:145:TYR:CD1	2.54	0.42
6:F:80:ALA:HB2	6:F:129:VAL:HG21	2.01	0.42
16:I:428:VAL:HG22	16:I:428:VAL:O	2.20	0.42
5:E:196:LEU:O	5:E:200:MET:HB2	2.20	0.41
9:2:104:ASP:HB2	9:2:105:PRO:HD2	2.02	0.41
16:I:228:GLY:HA2	21:I:501:ATP:O1A	2.20	0.41
3:c:101:TYR:O	3:c:102:ASN:HB2	2.20	0.41
17:K:313:LYS:O	17:K:315:ILE:HD12	2.20	0.41
2:B:23:TYR:CD1	2:B:23:TYR:N	2.84	0.41
5:E:63:ASP:C	5:E:63:ASP:OD1	2.62	0.41
12:5:162:LEU:CD2	12:5:200:VAL:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:229:THR:OG1	21:L:501:ATP:O2B	2.32	0.41
20:J:241:ALA:HA	20:J:242:PRO:C	2.44	0.41
1:a:95:PHE:CE2	1:a:103:MET:HA	2.56	0.41
7:g:72:CYS:SG	7:g:134:PHE:HB3	2.60	0.41
7:g:38:CYS:SG	7:g:43:VAL:HG23	2.60	0.41
12:5:31:VAL:O	12:5:33:LYS:N	2.53	0.41
14:7:129:TYR:CD1	14:7:129:TYR:C	2.98	0.41
3:c:212:PHE:CD2	3:c:229:PHE:CD2	3.09	0.41
11:k:56:PHE:O	11:k:56:PHE:CG	2.73	0.41
13:m:23:LEU:HD23	13:m:23:LEU:C	2.46	0.41
15:H:396:MET:HG2	16:I:213:ILE:HG22	2.03	0.41
17:K:247:LEU:C	17:K:249:GLU:H	2.28	0.41
12:5:185:TRP:CD1	12:5:185:TRP:H	2.36	0.41
12:5:208:ASN:O	12:5:209:ASN:C	2.64	0.41
19:M:433:TYR:C	19:M:434:ALA:O	2.60	0.41
20:J:95:ILE:N	20:J:95:ILE:HD12	2.36	0.41
2:b:139:HIS:CE1	2:b:234:ARG:CZ	3.04	0.41
3:c:108:GLU:OE2	3:c:108:GLU:HA	2.21	0.41
15:H:59:ILE:O	15:H:59:ILE:CG2	2.69	0.41
18:L:353:ASN:O	18:L:357:ARG:HG3	2.20	0.41
19:M:269:LEU:O	19:M:269:LEU:HG	2.20	0.41
4:d:149:GLU:HB3	4:d:150:PRO:HD2	2.03	0.41
8:h:151:THR:O	8:h:154:PHE:N	2.52	0.41
11:k:78:GLN:C	11:k:78:GLN:CD	2.89	0.41
2:B:72:GLY:HA3	2:B:235:PHE:CE2	2.56	0.41
2:B:160:LYS:HD3	2:B:179:TRP:CH2	2.56	0.41
3:C:115:SER:HB3	3:C:154:GLY:O	2.20	0.41
12:5:75:SER:HB2	12:5:78:ALA:H	1.86	0.41
15:H:305:ILE:HD12	15:H:305:ILE:N	2.35	0.41
18:L:365:THR:HA	18:L:368:VAL:HG22	2.03	0.41
1:a:95:PHE:CD2	1:a:103:MET:HA	2.56	0.41
1:a:105:CYS:O	1:a:106:ASP:C	2.64	0.41
11:4:78:GLN:C	11:4:78:GLN:OE1	2.64	0.41
14:7:11:VAL:O	14:7:143:ALA:HA	2.21	0.41
1:a:186:ASN:O	1:a:187:GLU:C	2.63	0.40
4:d:187:GLU:CD	4:d:187:GLU:H	2.29	0.40
6:f:206:THR:H	6:f:209:ASN:HB3	1.87	0.40
15:H:77:ALA:HB3	15:H:78:PRO:CD	2.51	0.40
13:6:68:PHE:O	13:6:72:VAL:HG23	2.21	0.40
15:H:273:ARG:HD2	16:I:316:PHE:CG	2.56	0.40
20:J:164:ILE:HD11	20:J:185:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:191:GLU:HA	1:a:191:GLU:OE1	2.22	0.40
5:e:114:ARG:HH11	5:e:114:ARG:HD3	1.76	0.40
11:k:19:LYS:HD3	11:k:31:SER:HA	2.03	0.40
14:n:91:TYR:O	14:n:92:ILE:C	2.64	0.40
6:F:71:LEU:HA	6:F:132:LEU:O	2.22	0.40
7:G:35:GLY:O	7:G:158:GLY:HA2	2.22	0.40
18:L:167:VAL:O	18:L:167:VAL:CG1	2.70	0.40
1:a:174:GLU:OE1	2:b:54:PRO:HG2	2.22	0.40
17:K:203:ILE:HG21	20:J:366:GLY:HA3	2.03	0.40
1:a:124:TYR:HB3	2:b:5:TYR:CD2	2.57	0.40
5:E:63:ASP:OD1	5:E:66:ILE:N	2.55	0.40
13:6:47:GLY:O	13:6:48:ASP:HB2	2.21	0.40
17:K:247:LEU:O	17:K:249:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/252 (95%)	228 (95%)	9 (4%)	2 (1%)	16	52
1	a	239/252 (95%)	224 (94%)	14 (6%)	1 (0%)	30	65
2	B	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	30	65
2	b	248/250 (99%)	232 (94%)	16 (6%)	0	100	100
3	C	242/258 (94%)	232 (96%)	9 (4%)	1 (0%)	30	65
3	c	242/258 (94%)	227 (94%)	13 (5%)	2 (1%)	16	52
4	D	238/254 (94%)	223 (94%)	12 (5%)	3 (1%)	9	41
4	d	238/254 (94%)	224 (94%)	12 (5%)	2 (1%)	16	52
5	E	240/260 (92%)	228 (95%)	9 (4%)	3 (1%)	9	41
5	e	240/260 (92%)	225 (94%)	12 (5%)	3 (1%)	9	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	231/234 (99%)	214 (93%)	14 (6%)	3 (1%)	9	41
6	f	229/234 (98%)	216 (94%)	11 (5%)	2 (1%)	14	49
7	G	241/288 (84%)	228 (95%)	11 (5%)	2 (1%)	16	52
7	g	241/288 (84%)	229 (95%)	11 (5%)	1 (0%)	30	65
8	1	194/215 (90%)	181 (93%)	12 (6%)	1 (0%)	24	61
8	h	194/215 (90%)	178 (92%)	15 (8%)	1 (0%)	24	61
9	2	224/261 (86%)	214 (96%)	9 (4%)	1 (0%)	30	65
9	i	224/261 (86%)	205 (92%)	17 (8%)	2 (1%)	14	49
10	3	202/205 (98%)	184 (91%)	14 (7%)	4 (2%)	6	33
10	j	202/205 (98%)	181 (90%)	21 (10%)	0	100	100
11	4	193/198 (98%)	184 (95%)	8 (4%)	1 (0%)	24	61
11	k	193/198 (98%)	186 (96%)	5 (3%)	2 (1%)	12	46
12	5	210/287 (73%)	195 (93%)	13 (6%)	2 (1%)	12	46
12	l	210/287 (73%)	196 (93%)	12 (6%)	2 (1%)	12	46
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%)	9	41
14	n	230/266 (86%)	211 (92%)	19 (8%)	0	100	100
15	H	386/467 (83%)	348 (90%)	26 (7%)	12 (3%)	3	25
16	I	383/437 (88%)	353 (92%)	22 (6%)	8 (2%)	5	32
17	K	387/428 (90%)	357 (92%)	24 (6%)	6 (2%)	7	37
18	L	386/437 (88%)	361 (94%)	23 (6%)	2 (0%)	24	61
19	M	377/434 (87%)	342 (91%)	26 (7%)	9 (2%)	4	30
20	J	384/405 (95%)	356 (93%)	22 (6%)	6 (2%)	7	37
All	All	8602/9546 (90%)	8015 (93%)	499 (6%)	88 (1%)	15	46

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	199 (97%)	7 (3%)	32	55
1	a	206/210 (98%)	200 (97%)	6 (3%)	37	58
2	B	209/209 (100%)	206 (99%)	3 (1%)	59	71
2	b	209/209 (100%)	198 (95%)	11 (5%)	20	44
3	C	203/216 (94%)	197 (97%)	6 (3%)	36	57
3	c	203/216 (94%)	199 (98%)	4 (2%)	48	66
4	D	212/226 (94%)	203 (96%)	9 (4%)	26	49
4	d	212/226 (94%)	204 (96%)	8 (4%)	29	51
5	E	198/215 (92%)	195 (98%)	3 (2%)	57	70
5	e	198/215 (92%)	193 (98%)	5 (2%)	42	62
6	F	192/193 (100%)	187 (97%)	5 (3%)	40	61
6	f	190/193 (98%)	181 (95%)	9 (5%)	23	47
7	G	201/239 (84%)	198 (98%)	3 (2%)	57	70
7	g	201/239 (84%)	198 (98%)	3 (2%)	57	70
8	1	162/178 (91%)	159 (98%)	3 (2%)	50	67
8	h	162/178 (91%)	160 (99%)	2 (1%)	63	73
9	2	185/214 (86%)	184 (100%)	1 (0%)	81	82
9	i	185/214 (86%)	178 (96%)	7 (4%)	29	51
10	3	172/173 (99%)	170 (99%)	2 (1%)	63	73
10	j	172/173 (99%)	170 (99%)	2 (1%)	63	73
11	4	173/175 (99%)	171 (99%)	2 (1%)	63	73
11	k	173/175 (99%)	170 (98%)	3 (2%)	53	68
12	5	169/235 (72%)	166 (98%)	3 (2%)	51	67
12	l	169/235 (72%)	162 (96%)	7 (4%)	27	50
13	6	185/201 (92%)	179 (97%)	6 (3%)	34	56
13	m	185/201 (92%)	182 (98%)	3 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	7	195/224 (87%)	194 (100%)	1 (0%)	81	82
14	n	198/224 (88%)	191 (96%)	7 (4%)	32	54
15	H	330/399 (83%)	320 (97%)	10 (3%)	36	57
16	I	342/385 (89%)	332 (97%)	10 (3%)	37	58
17	K	342/374 (91%)	331 (97%)	11 (3%)	34	56
18	L	332/377 (88%)	327 (98%)	5 (2%)	57	70
19	M	329/375 (88%)	320 (97%)	9 (3%)	39	60
20	J	336/352 (96%)	329 (98%)	7 (2%)	47	65
All	All	7336/8078 (91%)	7153 (98%)	183 (2%)	42	62

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	33	SER
1	a	69	THR
1	a	124	TYR
1	a	172	ASN
1	a	182	ILE
1	a	200	HIS
2	b	1	MET
2	b	32	VAL
2	b	44	VAL
2	b	45	ILE
2	b	50	LYS
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	121	TYR
3	c	200	THR
3	c	201	ASP
4	d	40	VAL
4	d	68	HIS
4	d	70	VAL
4	d	153	ILE
4	d	161	THR

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Mol	Chain	Res	Type
4	d	169	VAL
4	d	192	LEU
4	d	197	LEU
5	e	20	LEU
5	e	99	ILE
5	e	169	GLU
5	e	186	LYS
5	e	214	ILE
6	f	9	THR
6	f	11	THR
6	f	55	LEU
6	f	71	LEU
6	f	73	LEU
6	f	133	ILE
6	f	188	LEU
6	f	193	VAL
6	f	206	THR
7	g	5	ASP
7	g	150	SER
7	g	198	LEU
8	h	30	VAL
8	h	44	CYS
9	i	13	VAL
9	i	41	ILE
9	i	71	SER
9	i	85	GLN
9	i	127	LEU
9	i	176	CYS
9	i	183	ASP
10	j	15	THR
10	j	133	LYS
11	k	3	ILE
11	k	82	SER
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
13	m	22	VAL

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Mol	Chain	Res	Type
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	187	ARG
1	A	44	VAL
1	A	55	LEU
1	A	122	ARG
1	A	148	THR
1	A	150	PRO
1	A	211	LYS
1	A	220	THR
2	B	13	SER
2	B	26	THR
2	B	109	LEU
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	14	HIS
4	D	16	PHE
4	D	155	SER
4	D	220	VAL
4	D	224	SER
4	D	225	GLU
4	D	226	GLU
4	D	238	LYS
4	D	240	GLU
5	E	35	LYS
5	E	115	PHE
5	E	176	LEU
6	F	2	ARG
6	F	3	ASN
6	F	73	LEU
6	F	91	CYS
6	F	188	LEU

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Mol	Chain	Res	Type
7	G	5	ASP
7	G	106	PRO
7	G	161	THR
8	1	31	THR
8	1	104	ASP
8	1	126	ILE
9	2	12	VAL
10	3	140	THR
10	3	161	ASP
11	4	3	ILE
11	4	126	VAL
12	5	65	LEU
12	5	149	SER
12	5	182	GLU
13	6	19	ASP
13	6	34	SER
13	6	122	VAL
13	6	134	GLU
13	6	150	LEU
13	6	206	ILE
14	7	104	ARG
15	H	66	LYS
15	H	69	VAL
15	H	103	THR
15	H	151	GLN
15	H	161	GLU
15	H	208	TYR
15	H	233	GLU
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

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Mol	Chain	Res	Type
17	K	51	LEU
17	K	65	GLU
17	K	75	LEU
17	K	107	THR
17	K	137	VAL
17	K	237	VAL
17	K	244	HIS
17	K	247	LEU
17	K	264	ASN
17	K	404	GLN
18	L	164	ASP
18	L	183	ILE
18	L	199	LEU
18	L	312	MET
18	L	415	LEU
19	M	85	VAL
19	M	87	ASP
19	M	154	LEU
19	M	162	GLU
19	M	193	LEU
19	M	263	VAL
19	M	382	SER
19	M	426	LYS
19	M	427	SER
20	J	15	HIS
20	J	56	ARG
20	J	96	VAL
20	J	142	VAL
20	J	146	THR
20	J	238	ARG
20	J	388	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	6	HIS
1	a	75	ASN
1	a	121	GLN
1	a	172	ASN
1	a	212	ASN
1	a	242	GLN
2	b	20	GLN

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Mol	Chain	Res	Type
2	b	30	GLN
2	b	94	HIS
2	b	123	GLN
3	c	119	GLN
3	c	123	GLN
3	c	146	GLN
3	c	151	ASN
3	c	155	ASN
4	d	14	HIS
4	d	17	GLN
4	d	77	ASN
4	d	115	GLN
5	e	91	HIS
5	e	149	HIS
5	e	172	GLN
5	e	180	HIS
6	f	40	ASN
6	f	59	GLN
6	f	68	HIS
6	f	142	HIS
6	f	151	ASN
7	g	64	GLN
7	g	119	HIS
7	g	143	HIS
7	g	191	GLN
9	i	35	HIS
9	i	62	ASN
9	i	219	ASN
10	j	88	GLN
10	j	144	GLN
10	j	156	ASN
10	j	172	ASN
11	k	101	ASN
11	k	166	GLN
12	l	188	HIS
12	l	208	ASN
14	n	122	ASN
14	n	149	HIS
14	n	194	ASN
1	A	6	HIS
1	A	83	ASN
1	A	166	GLN

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Mol	Chain	Res	Type
1	A	176	HIS
1	A	242	GLN
2	B	20	GLN
2	B	149	GLN
3	C	124	HIS
3	C	146	GLN
3	C	151	ASN
3	C	226	GLN
4	D	94	HIS
4	D	115	GLN
4	D	165	ASN
4	D	202	GLN
4	D	228	ASN
4	D	229	GLN
5	E	83	HIS
5	E	139	HIS
6	F	3	ASN
6	F	118	ASN
6	F	209	ASN
7	G	17	ASN
7	G	114	GLN
7	G	191	GLN
8	1	120	HIS
8	1	161	GLN
9	2	22	GLN
9	2	172	ASN
9	2	200	GLN
10	3	63	ASN
10	3	172	ASN
11	4	61	GLN
11	4	191	GLN
12	5	29	GLN
12	5	166	HIS
12	5	209	ASN
13	6	87	ASN
13	6	155	ASN
13	6	159	GLN
13	6	195	HIS
14	7	2	GLN
14	7	74	ASN
14	7	120	GLN
14	7	122	ASN

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Mol	Chain	Res	Type
14	7	179	ASN
14	7	213	GLN
15	H	281	GLN
15	H	356	ASN
16	I	150	HIS
16	I	151	HIS
16	I	311	ASN
16	I	352	ASN
16	I	418	GLN
17	K	144	ASN
17	K	264	ASN
17	K	319	ASN
17	K	404	GLN
18	L	93	ASN
18	L	189	GLN
18	L	208	GLN
18	L	242	ASN
18	L	311	GLN
18	L	320	GLN
18	L	393	ASN
20	J	170	HIS
20	J	205	HIS
20	J	269	GLN
20	J	287	ASN
20	J	331	HIS
20	J	393	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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
21	ATP	H	501	22	32,33,33	1.37	4 (12%)	48,52,52	1.74	8 (16%)
21	ATP	K	501	22	32,33,33	1.56	8 (25%)	48,52,52	1.67	9 (18%)
23	ADP	J	501	22	28,29,29	1.47	6 (21%)	43,45,45	1.73	8 (18%)
21	ATP	L	501	22	32,33,33	1.40	7 (21%)	48,52,52	1.71	9 (18%)
21	ATP	M	501	22	32,33,33	1.56	6 (18%)	48,52,52	1.60	8 (16%)
21	ATP	I	501	22	32,33,33	1.48	8 (25%)	48,52,52	1.64	8 (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
21	ATP	H	501	22	-	4/22/38/38	0/3/3/3
21	ATP	K	501	22	-	7/22/38/38	0/3/3/3
23	ADP	J	501	22	-	5/16/32/32	0/3/3/3
21	ATP	L	501	22	-	6/22/38/38	0/3/3/3
21	ATP	M	501	22	-	8/22/38/38	0/3/3/3
21	ATP	I	501	22	-	5/22/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	501	ATP	C5-C4	4.51	1.47	1.39
23	J	501	ADP	C5-C4	4.45	1.47	1.39
21	H	501	ATP	C5-C4	4.37	1.46	1.39
21	I	501	ATP	C5-C4	4.29	1.46	1.39
21	M	501	ATP	C5-C4	4.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	501	ATP	C5-C4	4.20	1.46	1.39
21	M	501	ATP	PB-O3B	4.00	1.63	1.59
21	M	501	ATP	C5-N7	-3.24	1.33	1.39
21	K	501	ATP	PB-O3A	3.04	1.62	1.59
23	J	501	ADP	PA-O3A	3.02	1.62	1.59
21	K	501	ATP	PA-O3A	3.00	1.62	1.59
21	I	501	ATP	C5-N7	-2.72	1.34	1.39
21	M	501	ATP	C4-N9	-2.65	1.32	1.37
21	I	501	ATP	PA-O3A	2.65	1.62	1.59
21	H	501	ATP	C5-N7	-2.64	1.34	1.39
21	I	501	ATP	PB-O3B	2.64	1.62	1.59
23	J	501	ADP	C5-N7	-2.64	1.34	1.39
21	L	501	ATP	C5-N7	-2.59	1.34	1.39
21	L	501	ATP	PB-O3B	2.58	1.62	1.59
21	K	501	ATP	C5-C6	2.57	1.48	1.41
21	K	501	ATP	PB-O3B	2.56	1.62	1.59
21	K	501	ATP	C5-N7	-2.47	1.34	1.39
21	K	501	ATP	C4-N9	-2.44	1.32	1.37
21	I	501	ATP	PB-O3A	2.43	1.62	1.59
21	L	501	ATP	C5-C6	2.39	1.47	1.41
21	M	501	ATP	PB-O3A	2.37	1.62	1.59
21	H	501	ATP	C5-C6	2.36	1.47	1.41
23	J	501	ADP	C5-C6	2.32	1.47	1.41
21	I	501	ATP	C4-N9	-2.32	1.32	1.37
21	I	501	ATP	C5-C6	2.31	1.47	1.41
21	K	501	ATP	C8-N7	2.27	1.36	1.31
21	I	501	ATP	C8-N7	2.20	1.35	1.31
23	J	501	ADP	C8-N7	2.19	1.35	1.31
21	L	501	ATP	C8-N7	2.18	1.35	1.31
23	J	501	ADP	C4-N9	-2.12	1.33	1.37
21	L	501	ATP	PB-O3A	2.12	1.61	1.59
21	H	501	ATP	C8-N7	2.08	1.35	1.31
21	M	501	ATP	C8-N7	2.07	1.35	1.31
21	L	501	ATP	C4-N9	-2.06	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	H	501	ATP	C5-C4-N3	-6.05	118.39	126.72
21	L	501	ATP	C5-C4-N3	-5.86	118.64	126.72
21	M	501	ATP	C5-C4-N3	-5.80	118.74	126.72
21	I	501	ATP	C5-C4-N3	-5.39	119.30	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	501	ADP	C5-C4-N3	-5.37	119.32	126.72
21	K	501	ATP	C5-C4-N3	-5.01	119.83	126.72
21	H	501	ATP	N3-C4-N9	4.72	135.20	127.17
21	L	501	ATP	N3-C4-N9	4.64	135.05	127.17
21	M	501	ATP	N3-C4-N9	4.41	134.67	127.17
23	J	501	ADP	N3-C4-N9	4.27	134.43	127.17
21	I	501	ATP	N3-C4-N9	4.05	134.05	127.17
21	L	501	ATP	C2-N3-C4	3.90	121.35	111.83
21	H	501	ATP	C2-N3-C4	3.81	121.14	111.83
21	K	501	ATP	N3-C4-N9	3.65	133.37	127.17
21	K	501	ATP	N3-C2-N1	-3.65	123.06	128.58
21	K	501	ATP	C4-C5-N7	-3.61	106.46	110.58
21	I	501	ATP	C2-N3-C4	3.57	120.54	111.83
21	K	501	ATP	C2-N3-C4	3.56	120.52	111.83
21	L	501	ATP	N3-C2-N1	-3.56	123.20	128.58
23	J	501	ADP	C2-N3-C4	3.49	120.37	111.83
21	I	501	ATP	N3-C2-N1	-3.40	123.43	128.58
21	H	501	ATP	N3-C2-N1	-3.37	123.48	128.58
21	I	501	ATP	C4-C5-N7	-3.29	106.82	110.58
23	J	501	ADP	N3-C2-N1	-3.29	123.60	128.58
21	H	501	ATP	C4-C5-N7	-3.15	106.98	110.58
21	M	501	ATP	C2-N3-C4	3.06	119.30	111.83
23	J	501	ADP	C4-C5-N7	-3.03	107.11	110.58
21	M	501	ATP	C4-C5-N7	-3.03	107.12	110.58
21	L	501	ATP	C4-C5-N7	-3.02	107.13	110.58
21	K	501	ATP	C6-C5-N7	2.53	136.96	132.09
21	L	501	ATP	C4-N9-C8	2.47	108.34	105.74
21	K	501	ATP	C4-N9-C8	2.44	108.30	105.74
21	K	501	ATP	C5-N7-C8	2.44	107.28	103.45
21	I	501	ATP	C5-N7-C8	2.36	107.16	103.45
21	L	501	ATP	C5-N7-C8	2.36	107.16	103.45
21	H	501	ATP	C5-N7-C8	2.29	107.04	103.45
21	I	501	ATP	C4-N9-C8	2.28	108.13	105.74
23	J	501	ADP	C4-N9-C8	2.28	108.13	105.74
23	J	501	ADP	O3B-PB-O2B	2.24	116.20	107.80
21	M	501	ATP	N3-C2-N1	-2.18	125.28	128.58
21	I	501	ATP	C6-C5-N7	2.15	136.24	132.09
21	K	501	ATP	C2-N1-C6	2.14	122.25	118.73
21	H	501	ATP	C4-N9-C8	2.13	107.97	105.74
21	M	501	ATP	N6-C6-N1	2.13	123.11	118.38
21	H	501	ATP	O3G-PG-O2G	2.05	115.48	107.80
21	M	501	ATP	C5-N7-C8	2.05	106.67	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	501	ADP	C5-N7-C8	2.03	106.64	103.45
21	L	501	ATP	C6-C5-N7	2.03	136.01	132.09
21	L	501	ATP	N9-C8-N7	-2.02	111.07	113.94
21	M	501	ATP	C4-N9-C8	2.00	107.84	105.74

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	I	501	ATP	C5'-O5'-PA-O3A
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
21	M	501	ATP	C5'-O5'-PA-O3A
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	I	501	ATP	PA-O3A-PB-O2B
21	K	501	ATP	PA-O3A-PB-O2B
21	L	501	ATP	PA-O3A-PB-O2B
21	K	501	ATP	C3'-C4'-C5'-O5'
21	H	501	ATP	C5'-O5'-PA-O2A
21	H	501	ATP	C5'-O5'-PA-O3A
21	I	501	ATP	C5'-O5'-PA-O1A
21	M	501	ATP	C5'-O5'-PA-O2A
23	J	501	ADP	C5'-O5'-PA-O1A
23	J	501	ADP	C4'-C5'-O5'-PA
21	K	501	ATP	PB-O3B-PG-O1G
21	M	501	ATP	PB-O3B-PG-O1G
21	M	501	ATP	PB-O3B-PG-O3G
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

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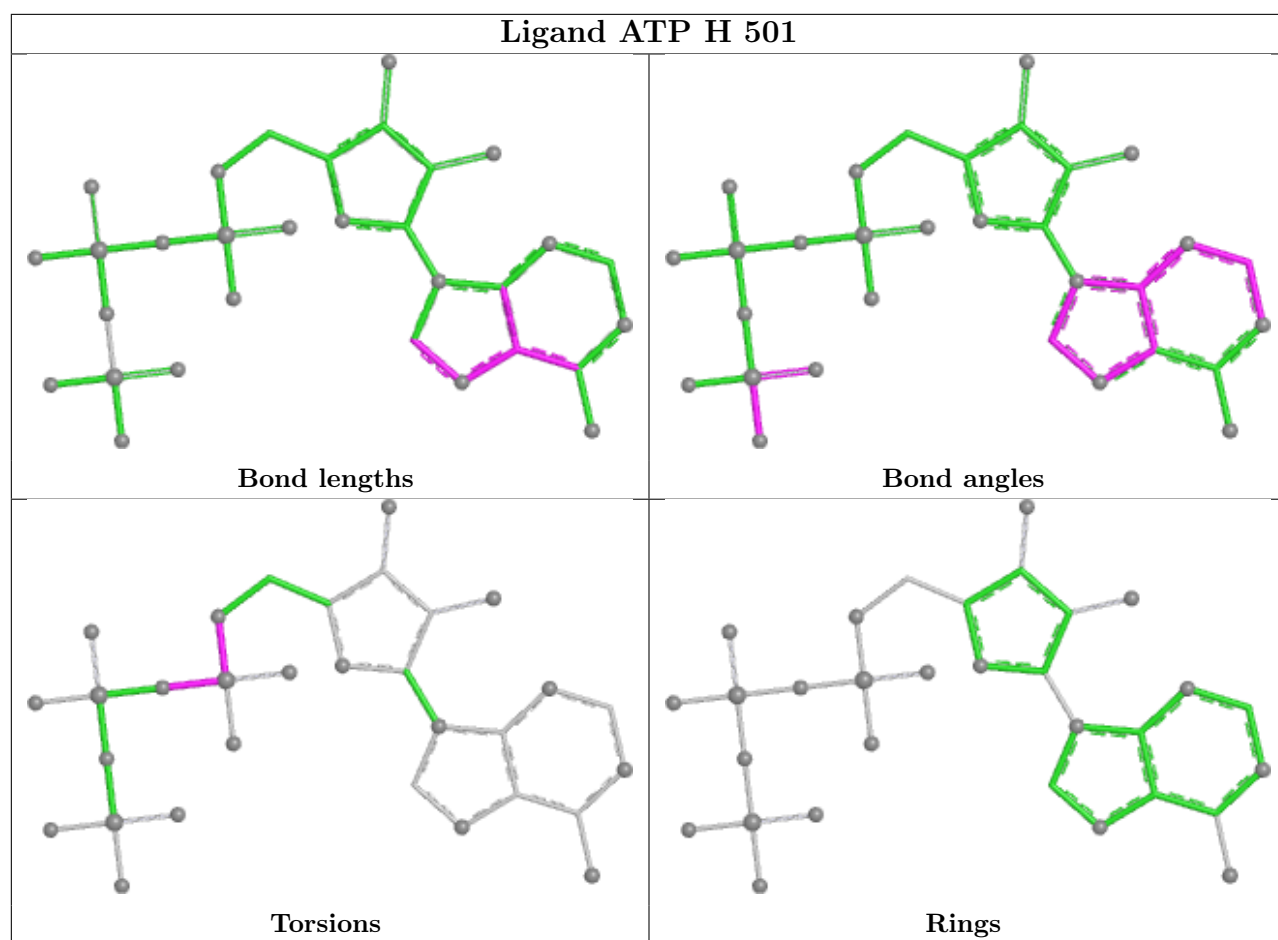
Mol	Chain	Res	Type	Atoms
21	M	501	ATP	PA-O3A-PB-O2B
21	H	501	ATP	PB-O3A-PA-O1A

There are no ring outliers.

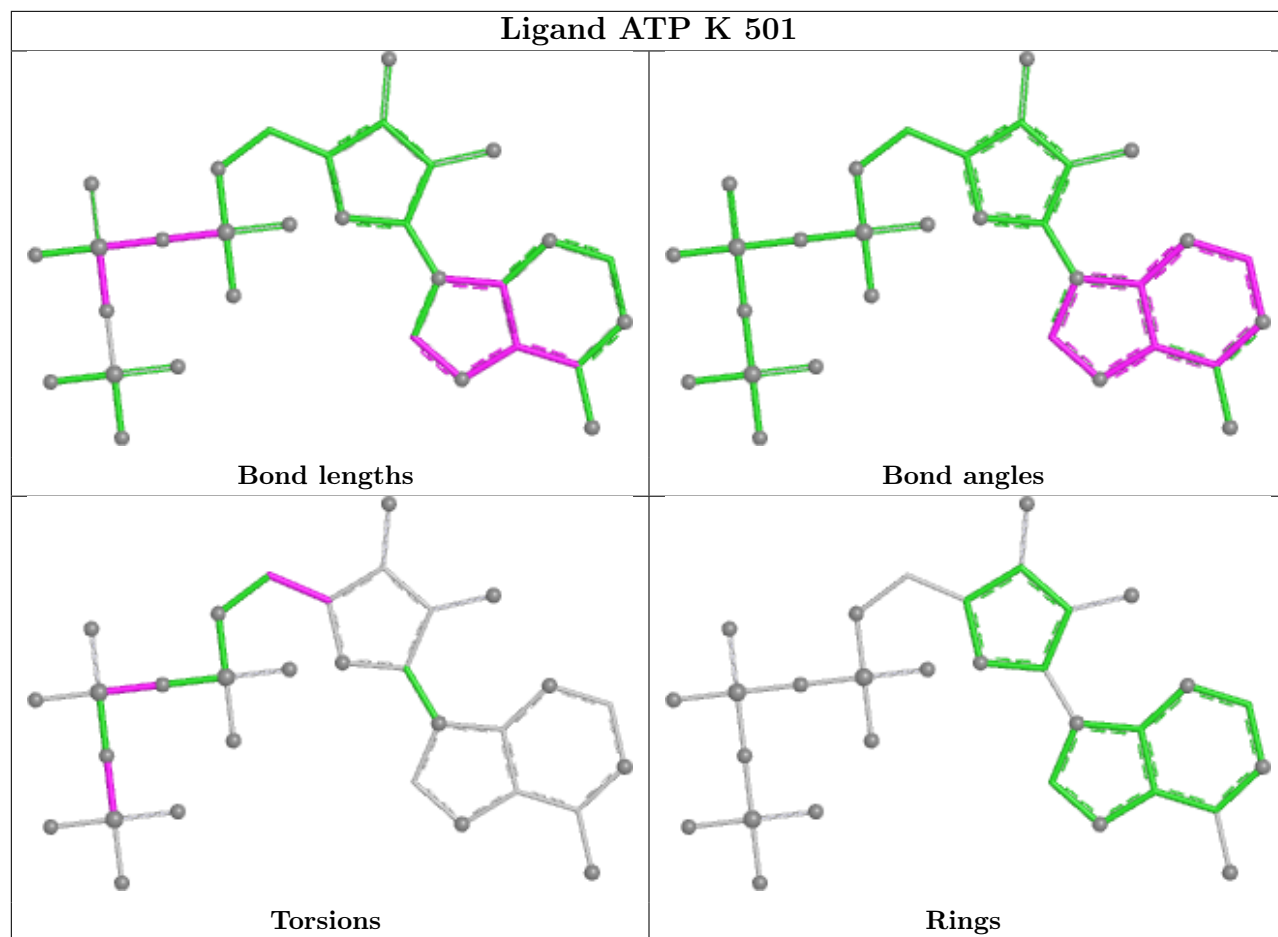
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	H	501	ATP	2	0
23	J	501	ADP	1	0
21	L	501	ATP	2	0
21	M	501	ATP	2	0
21	I	501	ATP	7	0

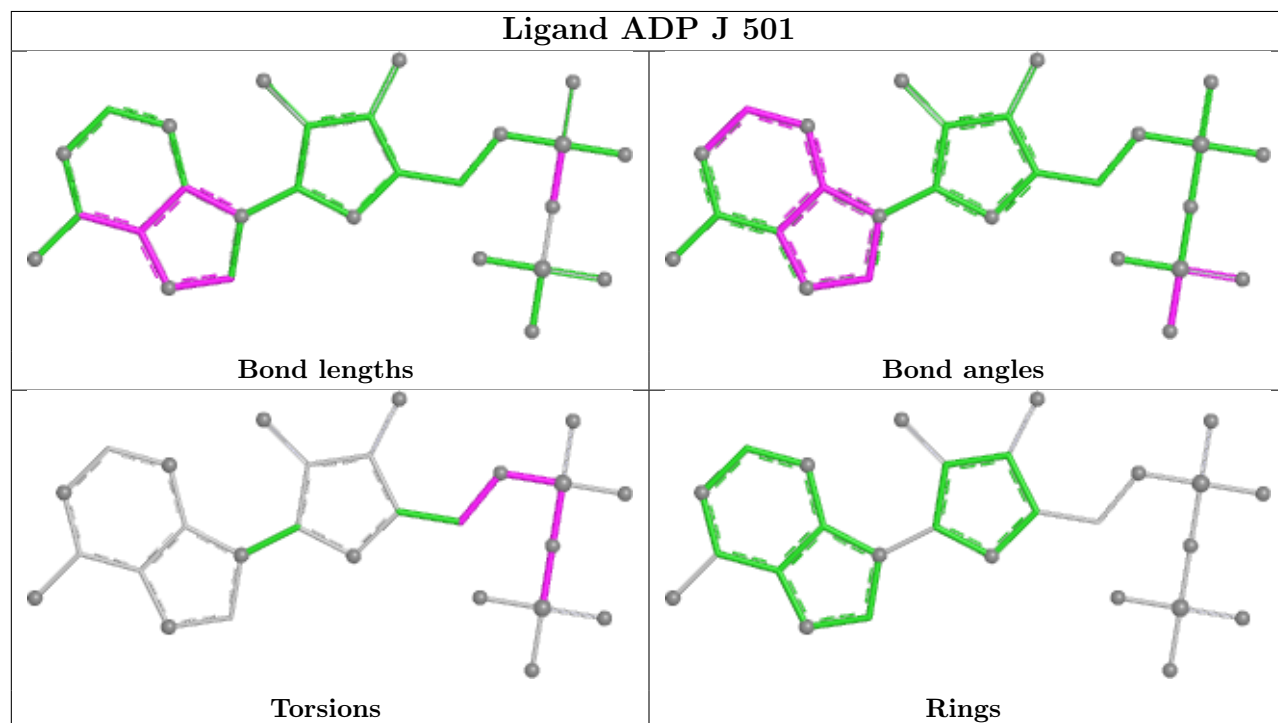
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

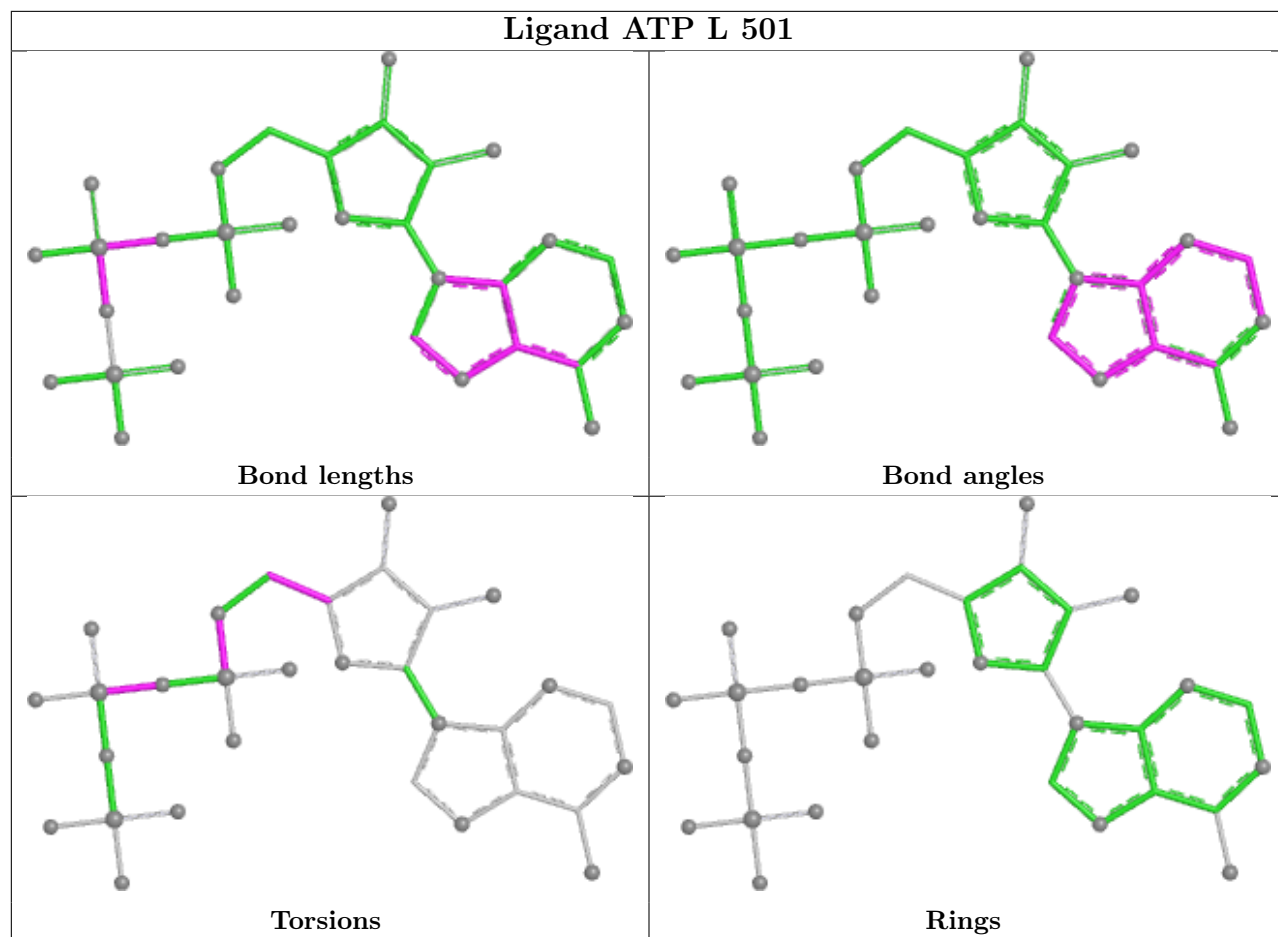


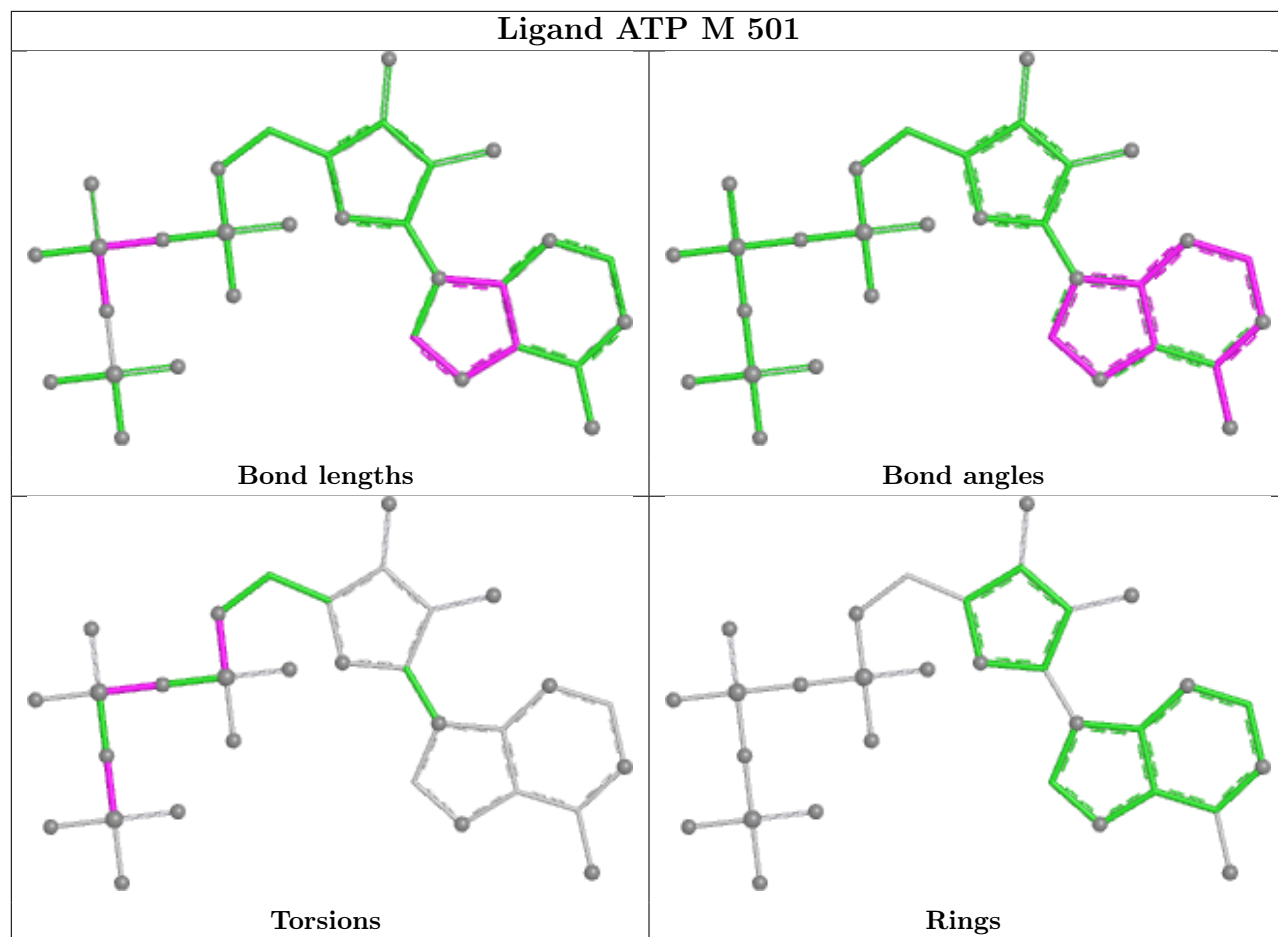
Ligand ATP K 501

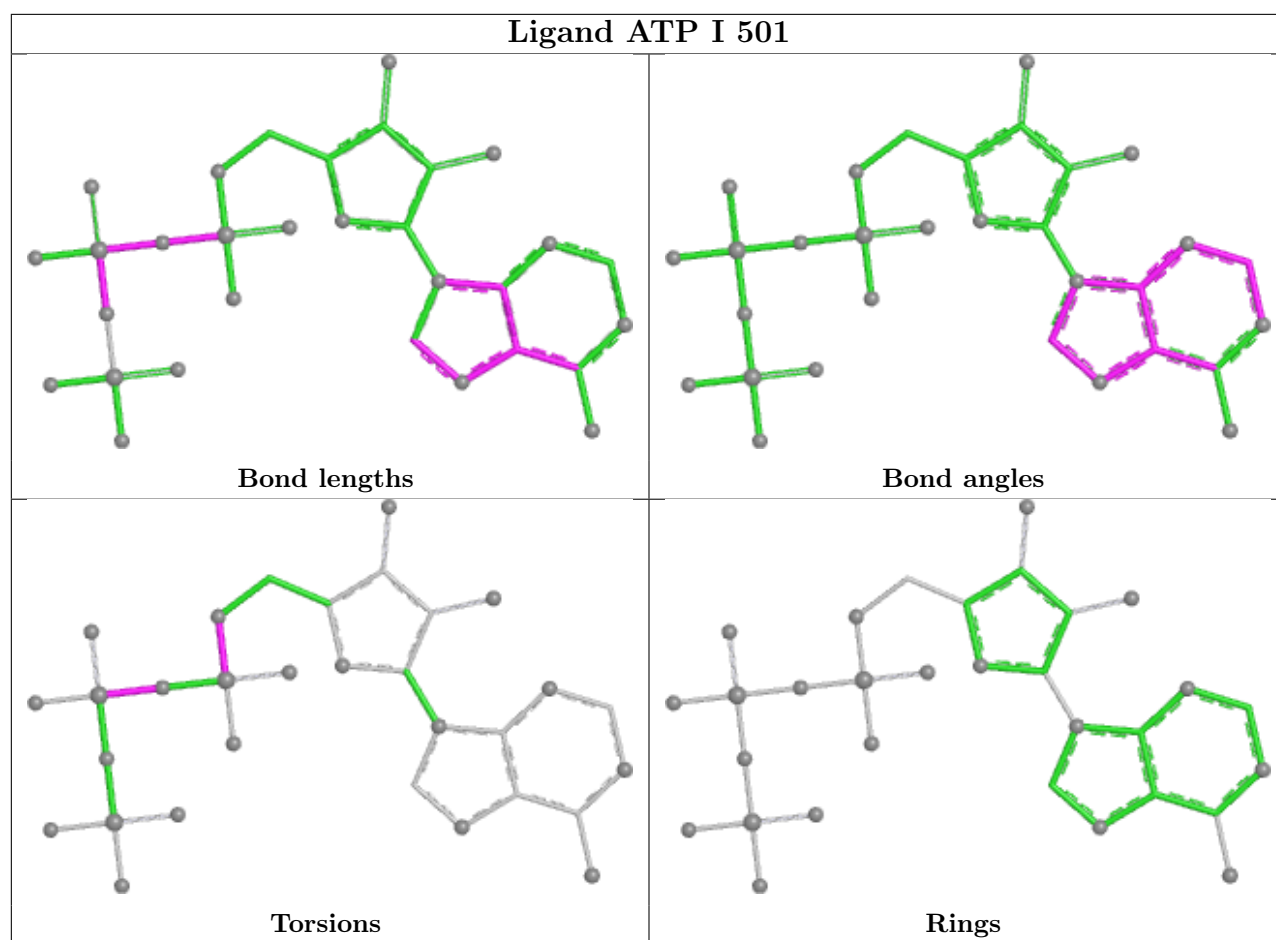


Ligand ADP J 501









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.

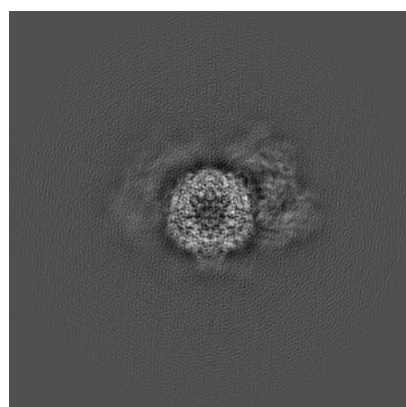
6 Map visualisation [i](#)

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.

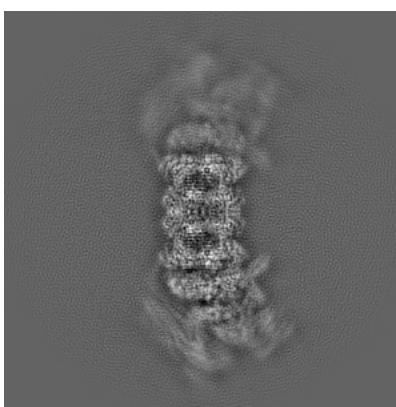
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

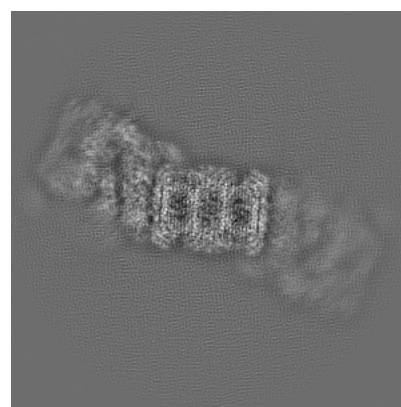
6.1.1 Primary map



X



Y

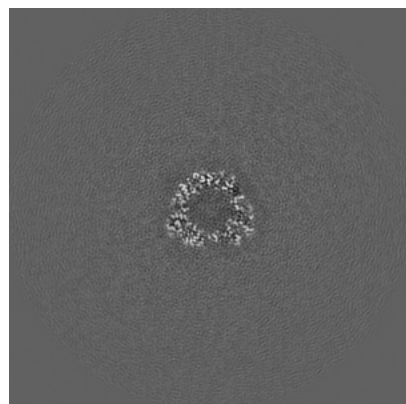


Z

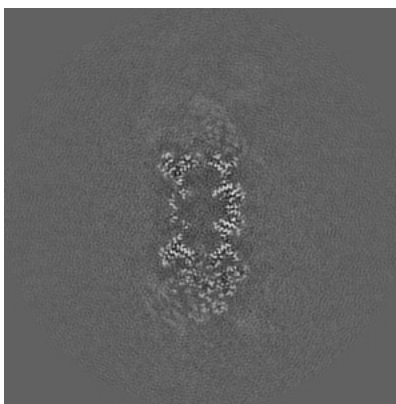
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

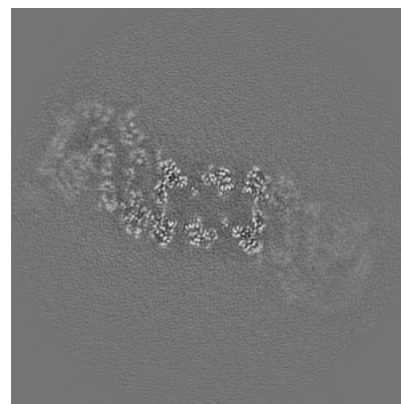
6.2.1 Primary map



X Index: 192



Y Index: 192

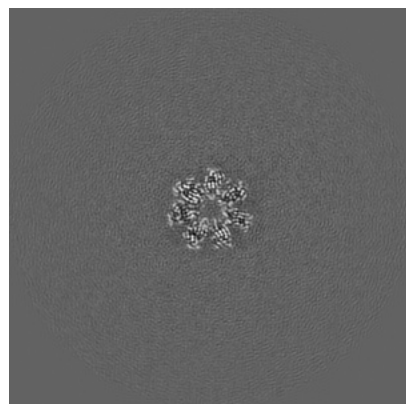


Z Index: 192

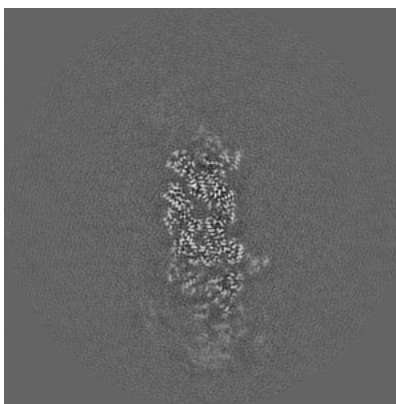
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

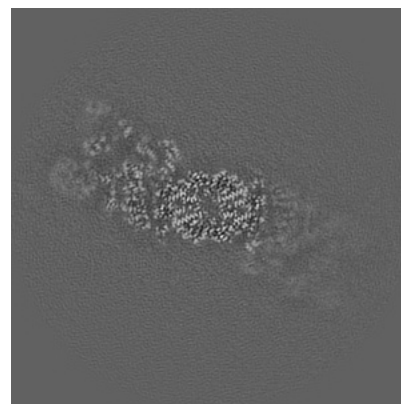
6.3.1 Primary map



X Index: 177



Y Index: 212

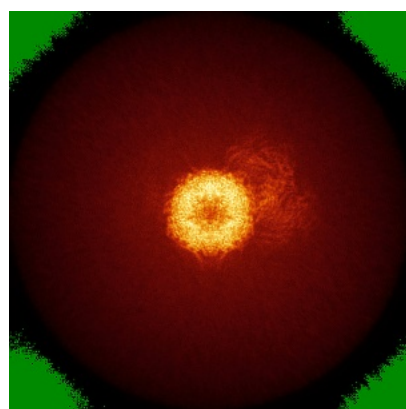


Z Index: 208

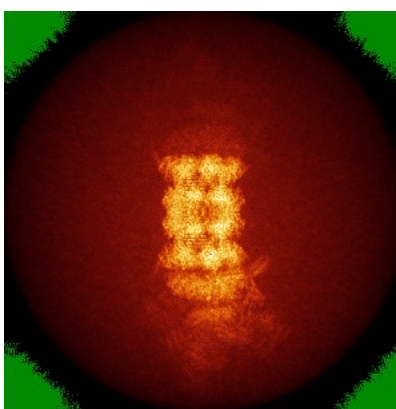
The images above show the largest variance slices of the map in three orthogonal directions.

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

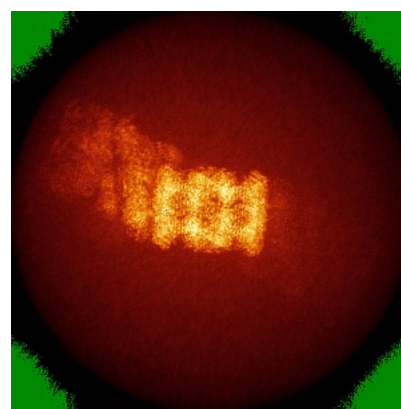
6.4.1 Primary map



X



Y

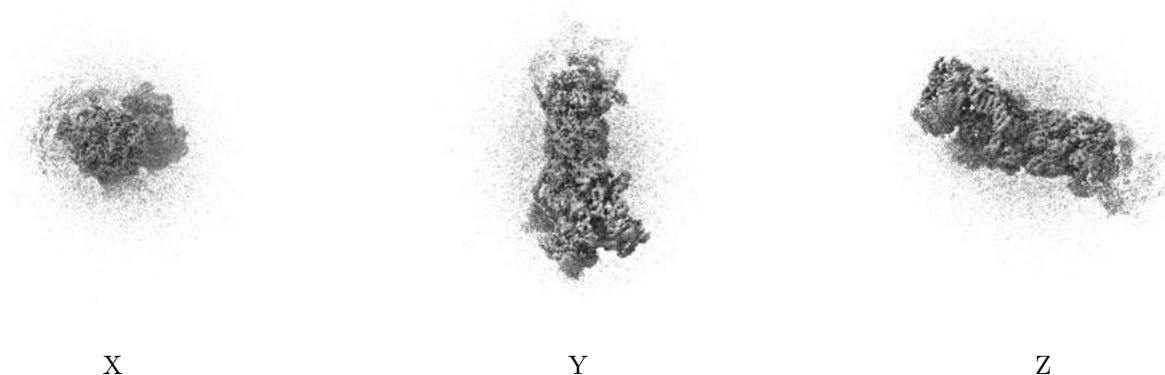


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

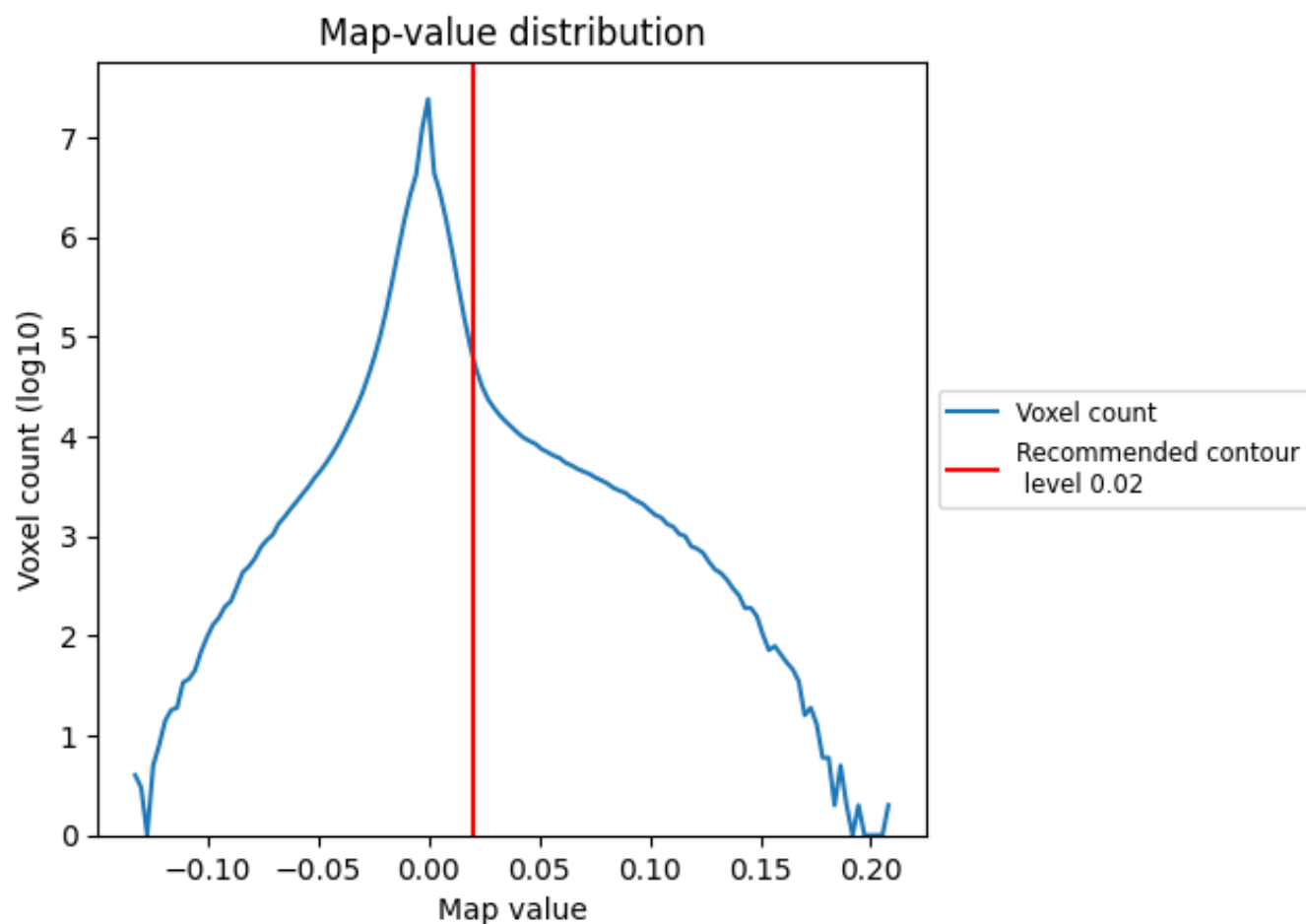
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

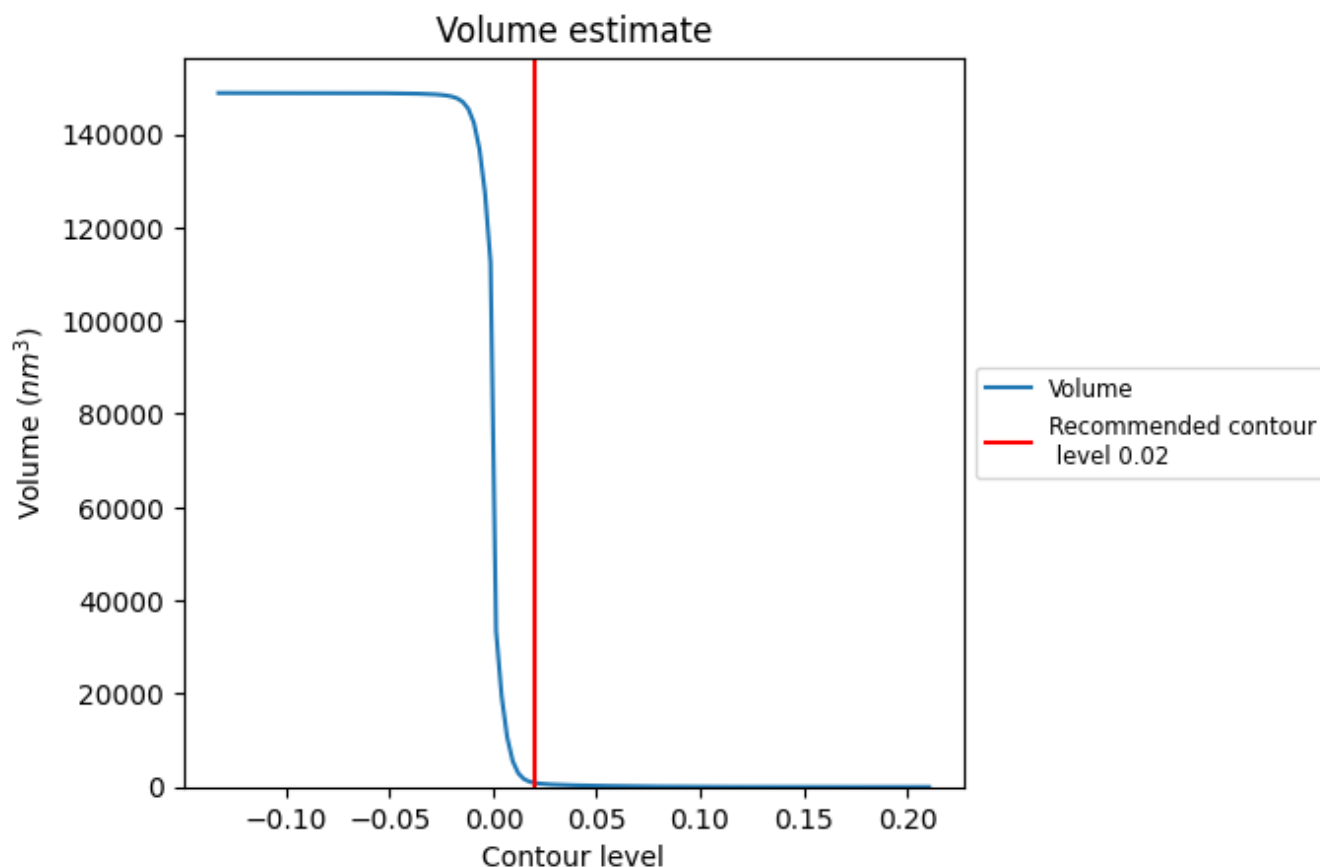
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

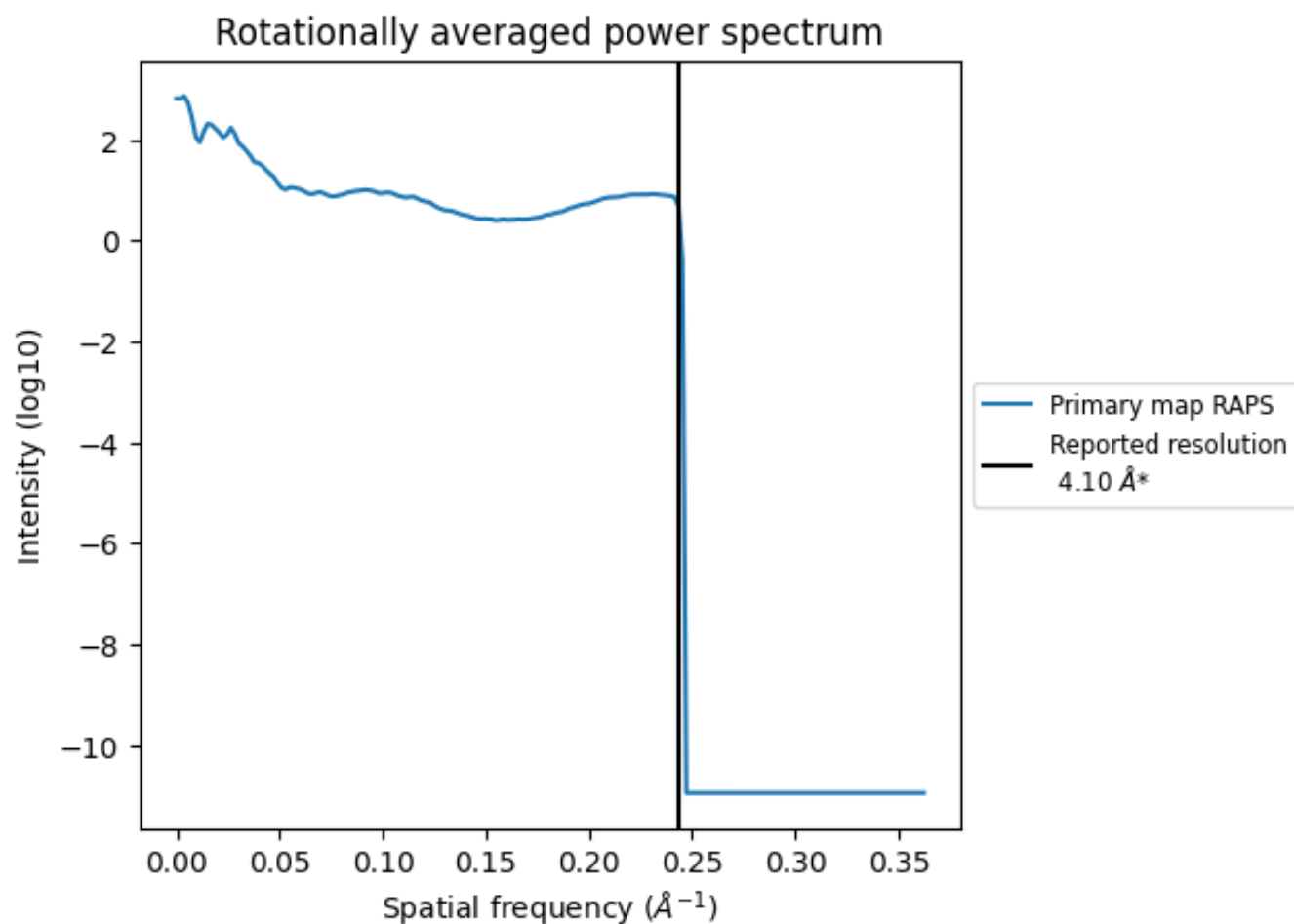
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation

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

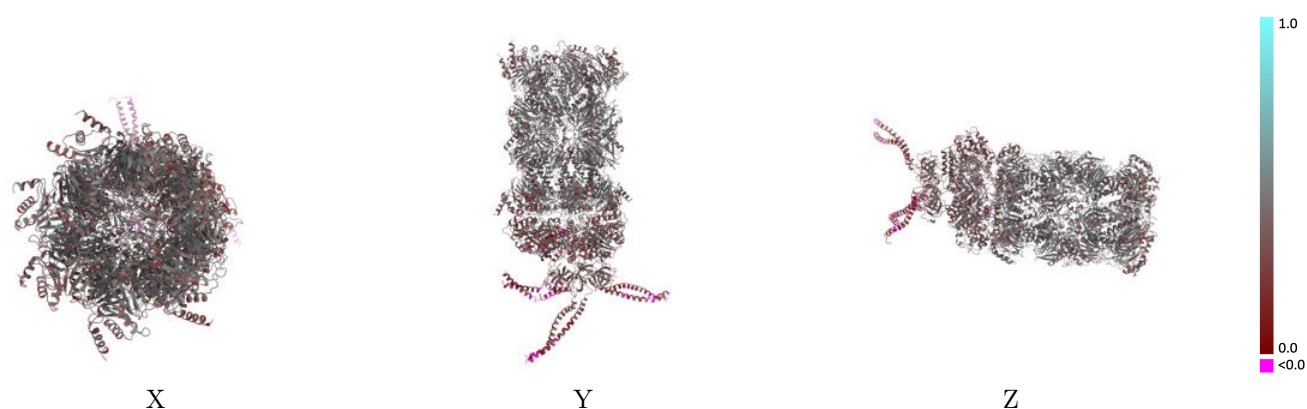
9 Map-model fit [i](#)

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 11.

9.1 Map-model overlay [i](#)

This section was not generated.

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

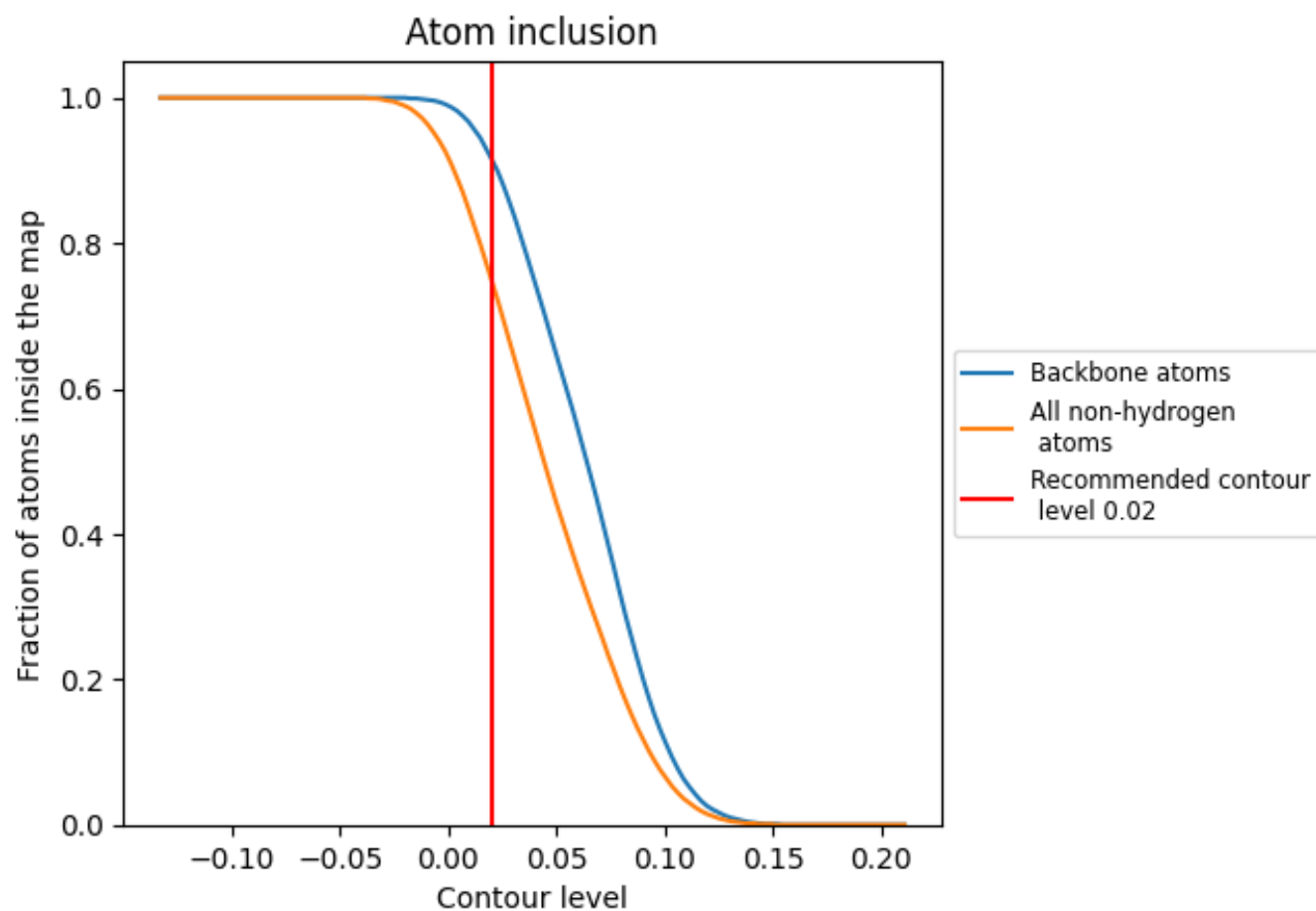


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

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	 0.7500	 0.3940
1	 0.8160	 0.4380
2	 0.8020	 0.4330
3	 0.7960	 0.4410
4	 0.7970	 0.4300
5	 0.8250	 0.4320
6	 0.8240	 0.4400
7	 0.8260	 0.4380
A	 0.7880	 0.4190
B	 0.7740	 0.4130
C	 0.7760	 0.4060
D	 0.7870	 0.4100
E	 0.7570	 0.4040
F	 0.8040	 0.4290
G	 0.8040	 0.4240
H	 0.6540	 0.3470
I	 0.6090	 0.2990
J	 0.5720	 0.2810
K	 0.6300	 0.3180
L	 0.6280	 0.3290
M	 0.6380	 0.3460
a	 0.7890	 0.4070
b	 0.7740	 0.4040
c	 0.7790	 0.3940
d	 0.7790	 0.4080
e	 0.7560	 0.3920
f	 0.7980	 0.4080
g	 0.7990	 0.4090
h	 0.8230	 0.4400
i	 0.8090	 0.4360
j	 0.8000	 0.4370
k	 0.8040	 0.4340
l	 0.8230	 0.4360
m	 0.8290	 0.4380
n	 0.8250	 0.4370

