



Full wwPDB EM Validation Report ⓘ

Jul 8, 2026 – 07:49 PM JST

PDB ID : 9VUF / pdb_00009vuf
EMDB ID : EMD-65361
Title : Structure of human proteasome ATPase-CP intermediate assemblies with
90min rapaprotin addition
Authors : Wang, W.L.; Yin, D.Y.; Mao, Y.D.
Deposited on : 2025-07-13
Resolution : 3.10 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:

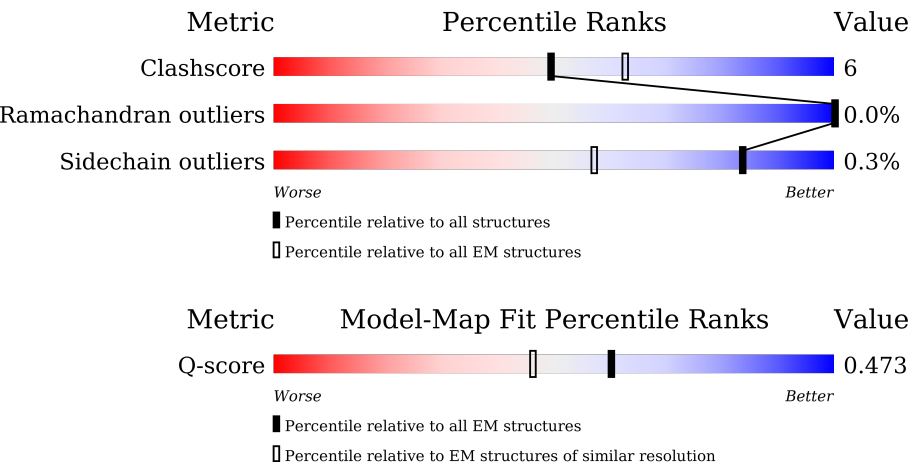
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

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 3.10 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.



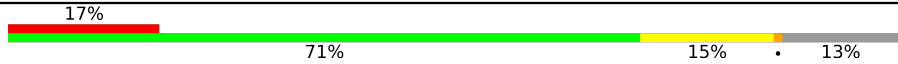
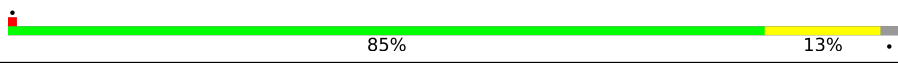
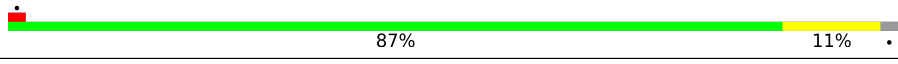
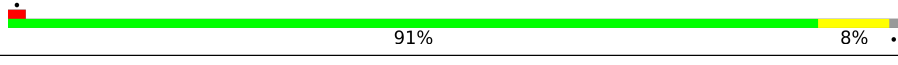
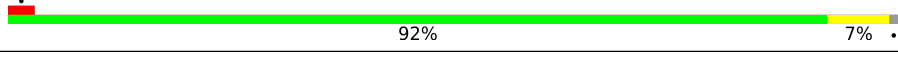
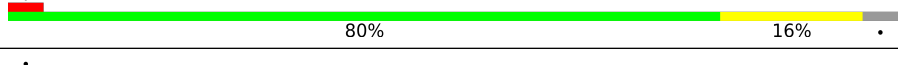
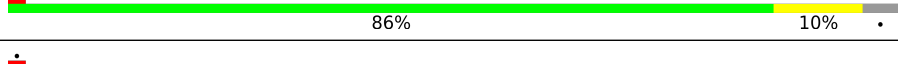
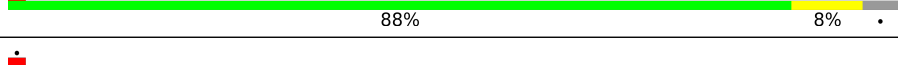
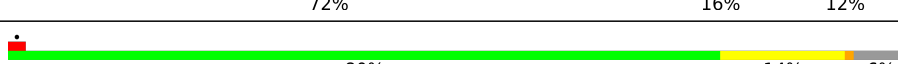
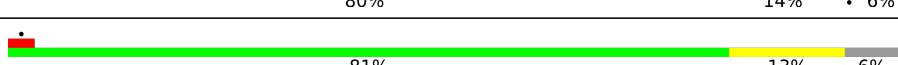
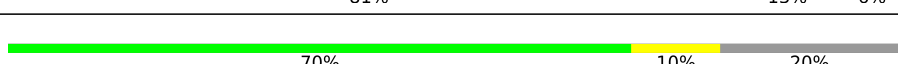
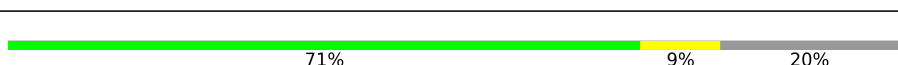
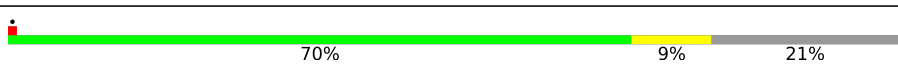
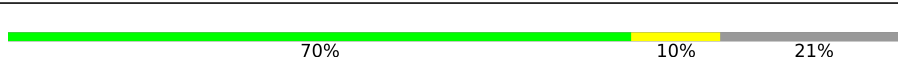
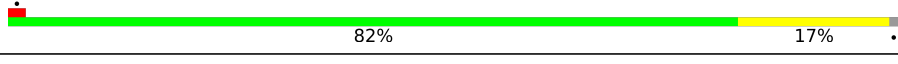
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	433	10% 71% 10% 18%
2	B	440	16% 64% 13% 23%
3	C	406	23% 62% 16% 22%
4	D	418	24% 63% 17% 19%

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Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	269	
12	l	269	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 63361 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 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	354	Total	C	N	O	S	0	0
			2776	1749	490	519	18		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	339	Total	C	N	O	S	0	0
			2638	1658	450	518	12		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	316	Total	C	N	O	S	0	0
			2464	1559	437	452	16		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	338	Total	C	N	O	S	0	0
			2666	1684	464	505	13		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	338	Total	C	N	O	S	0	0
			2664	1678	473	497	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	337	Total	C	N	O	S	0	0
			2627	1660	452	500	15		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
7	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
8	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
9	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1713	1062	311	335	5		
10	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
11	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 12 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
12	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
13	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
14	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
15	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
18	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

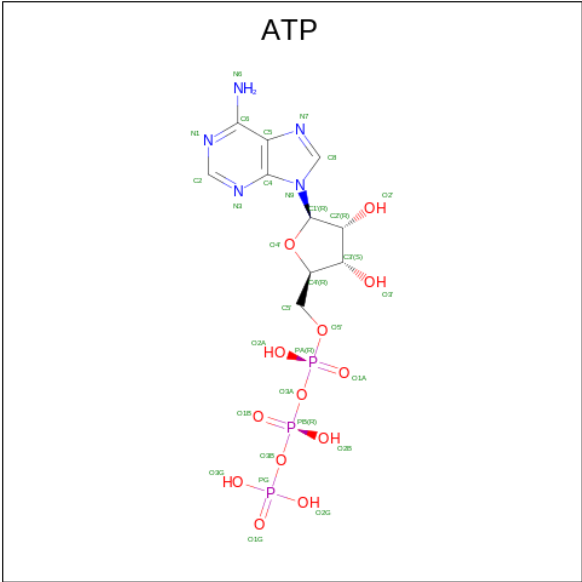
- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
19	s	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

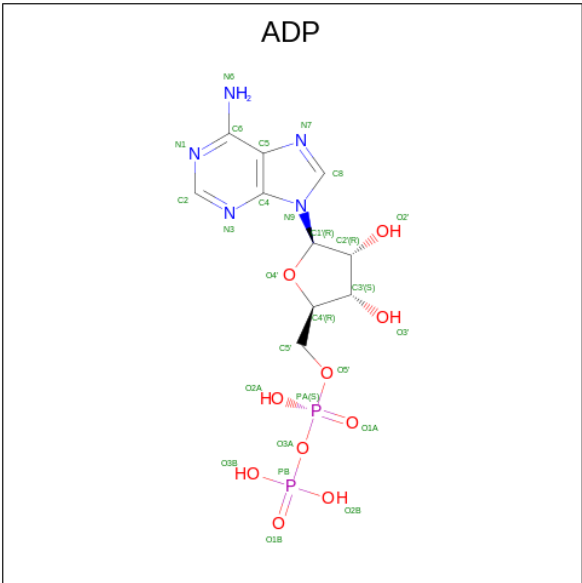
Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
20	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



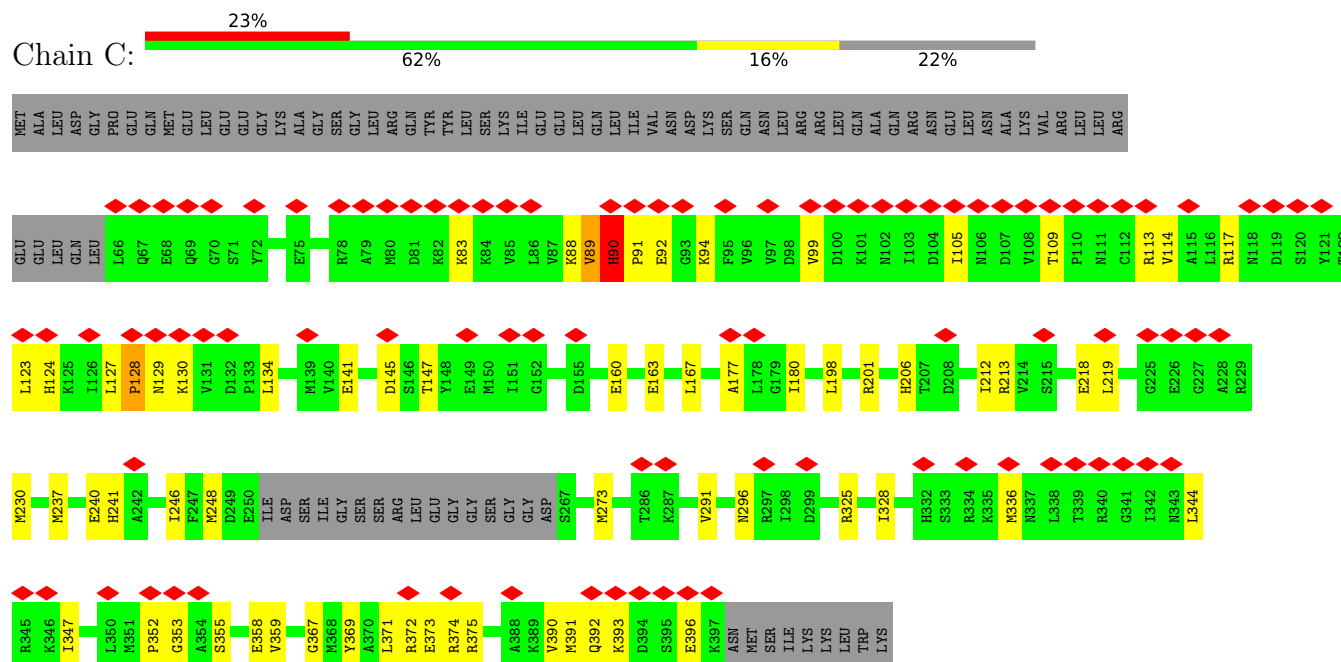
Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
21	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
21	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
21	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

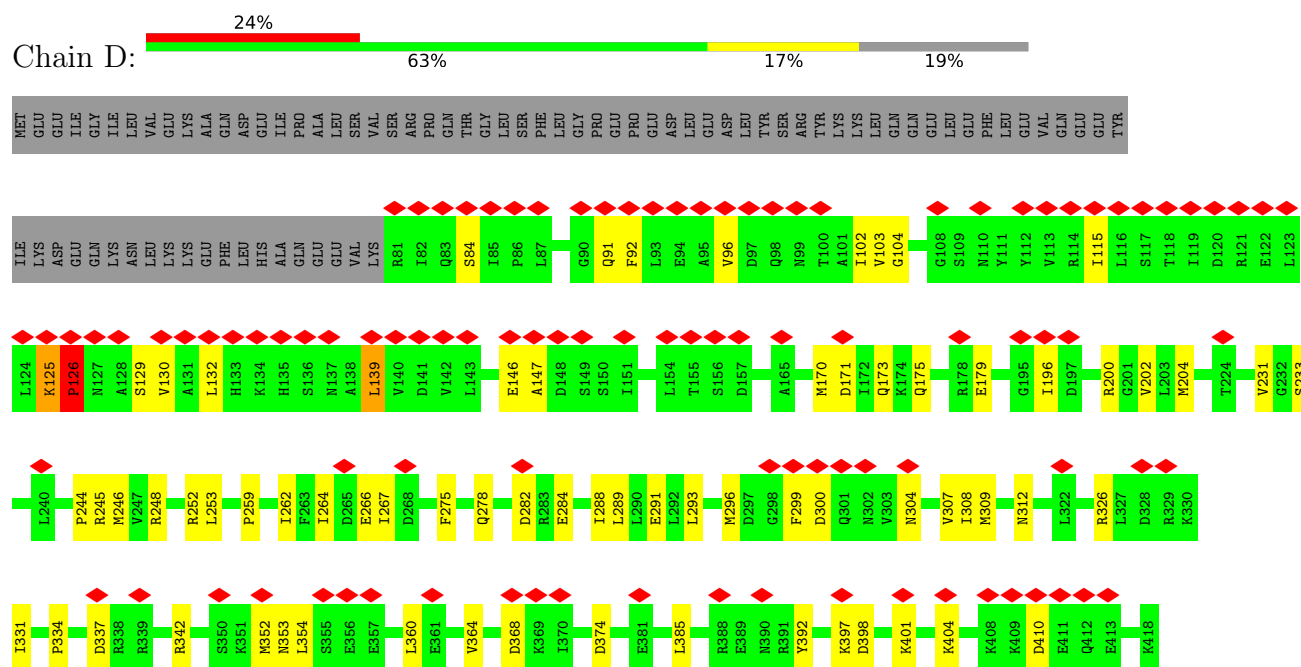


Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
22	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

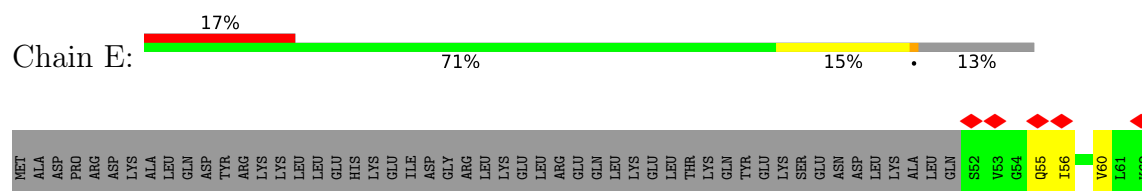
- Molecule 3: 26S proteasome regulatory subunit 8

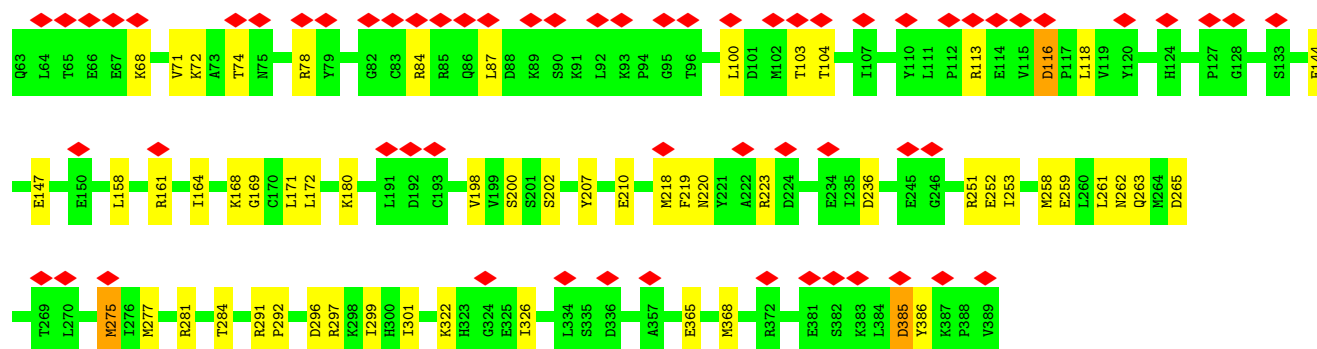


- Molecule 4: 26S proteasome regulatory subunit 6B

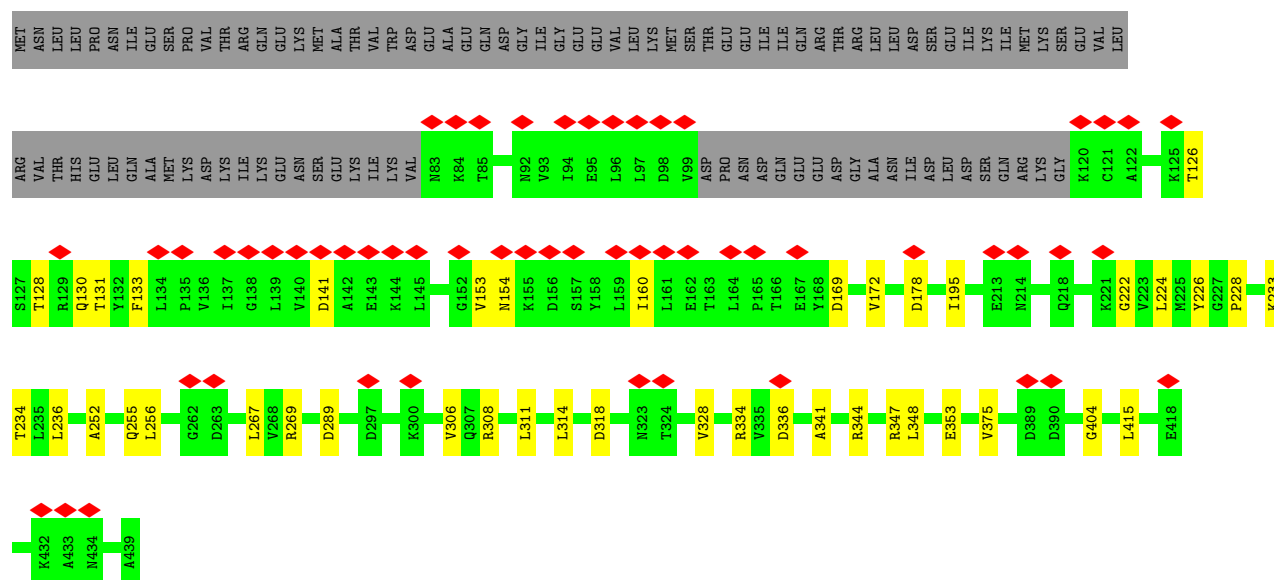


- Molecule 5: 26S proteasome regulatory subunit 10B

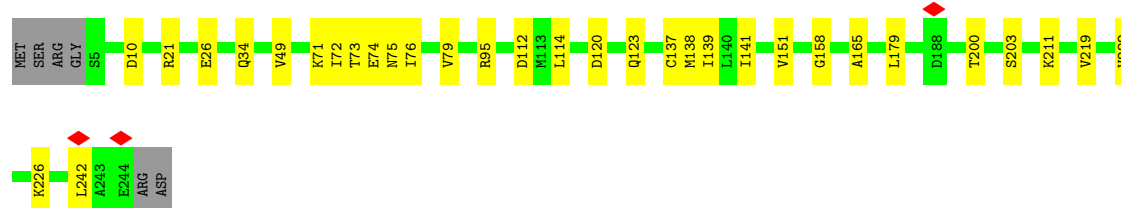
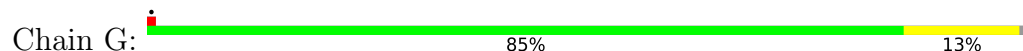




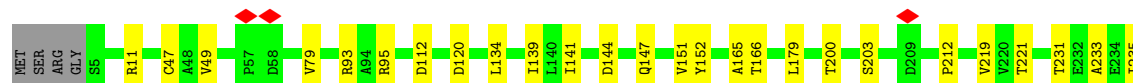
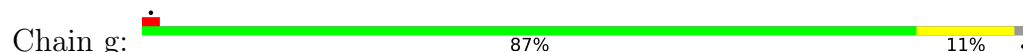
• Molecule 6: 26S proteasome regulatory subunit 6A

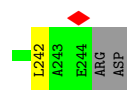


• Molecule 7: Proteasome subunit alpha type-6

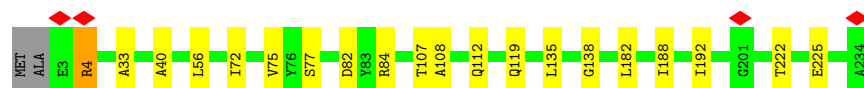
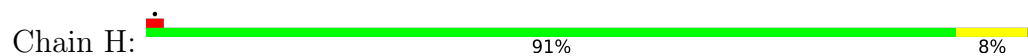


• Molecule 7: Proteasome subunit alpha type-6





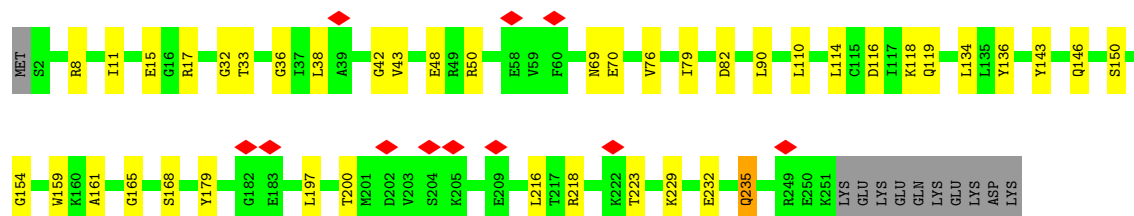
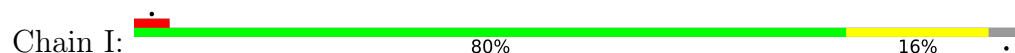
• Molecule 8: Proteasome subunit alpha type-2



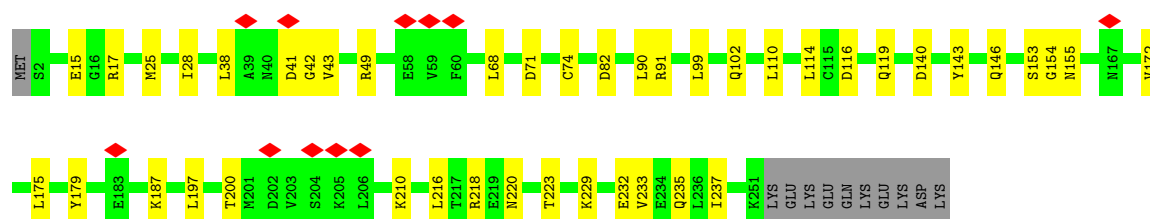
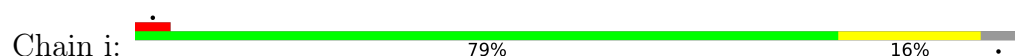
• Molecule 8: Proteasome subunit alpha type-2



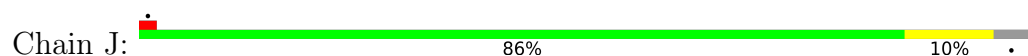
• Molecule 9: Proteasome subunit alpha type-4

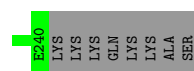


• Molecule 9: Proteasome subunit alpha type-4

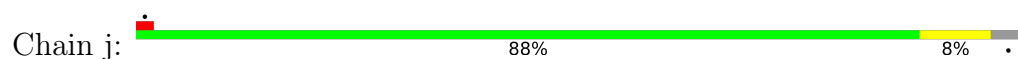


• Molecule 10: Proteasome subunit alpha type-7

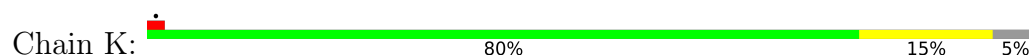




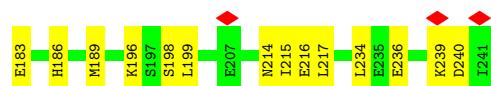
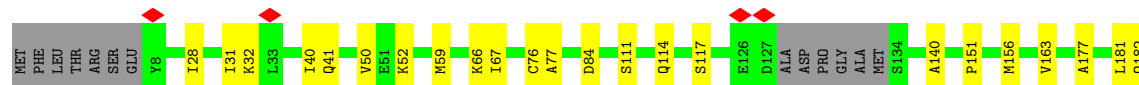
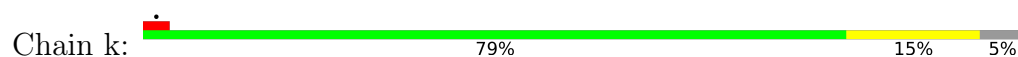
- Molecule 10: Proteasome subunit alpha type-7



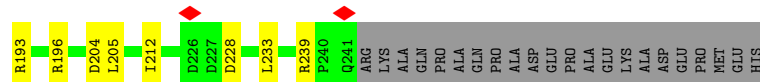
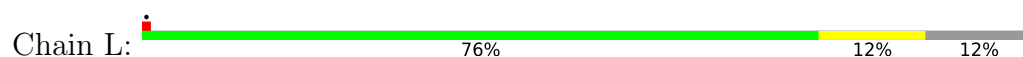
- Molecule 11: Proteasome subunit alpha type-5



- Molecule 11: Proteasome subunit alpha type-5

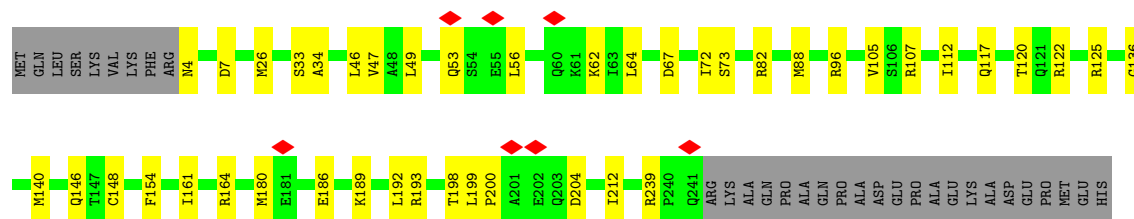


- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

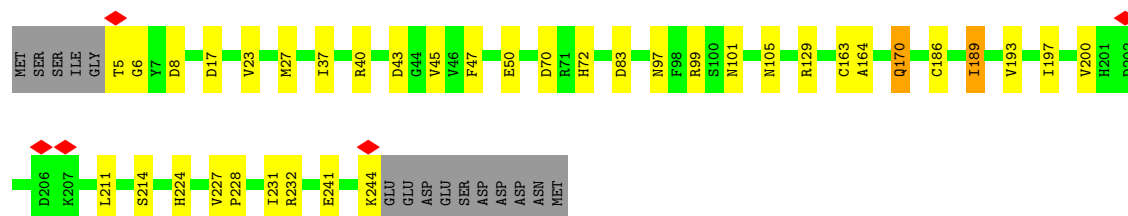
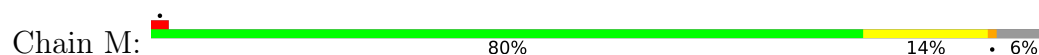


- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

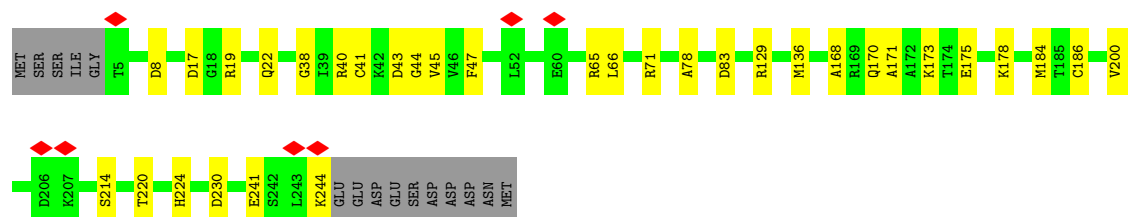
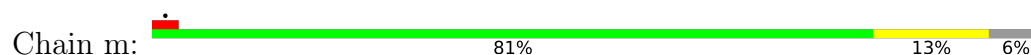




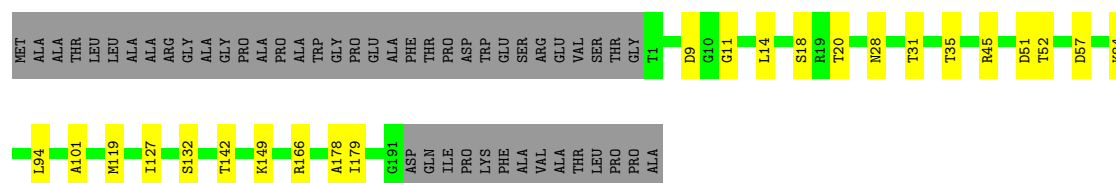
• Molecule 13: Proteasome subunit alpha type-3



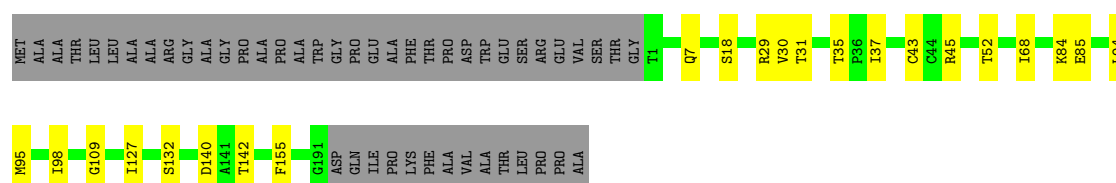
• Molecule 13: Proteasome subunit alpha type-3



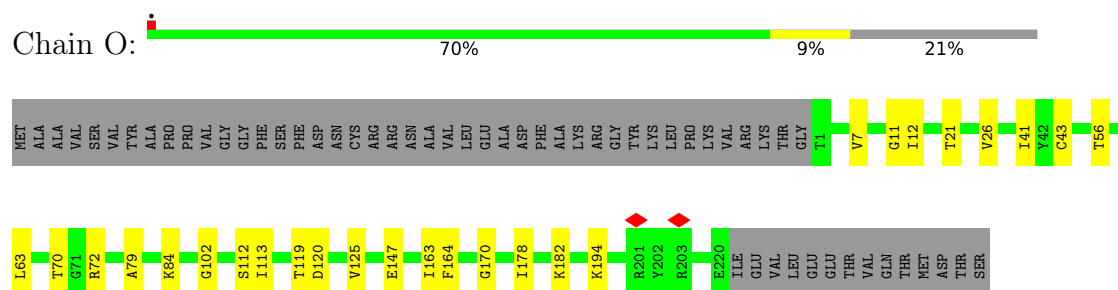
• Molecule 14: Proteasome subunit beta type-6



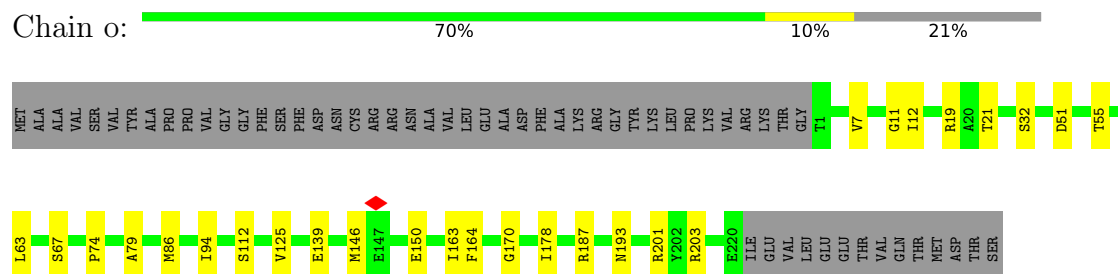
• Molecule 14: Proteasome subunit beta type-6



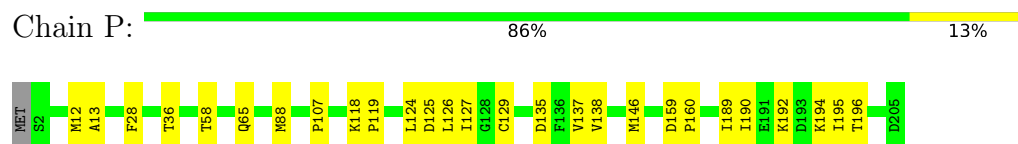
- Molecule 15: Proteasome subunit beta type-7



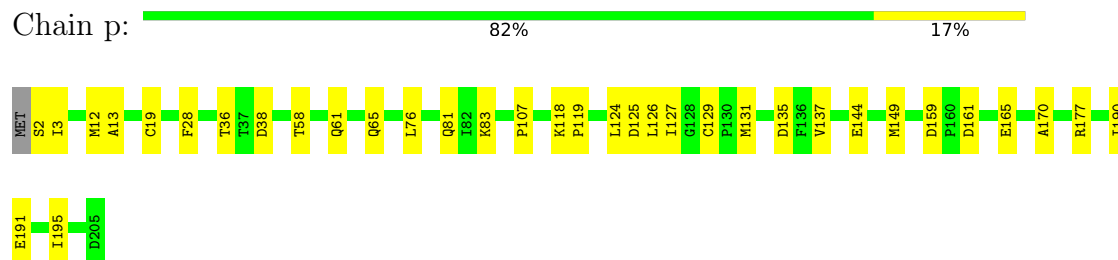
- Molecule 15: Proteasome subunit beta type-7



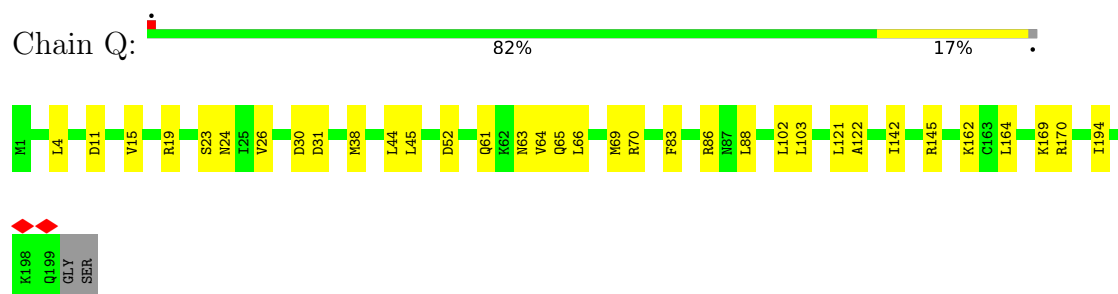
- Molecule 16: Proteasome subunit beta type-3



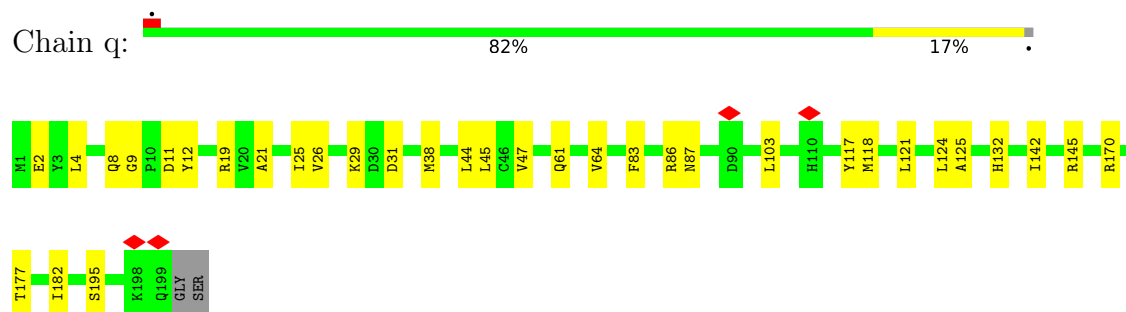
- Molecule 16: Proteasome subunit beta type-3



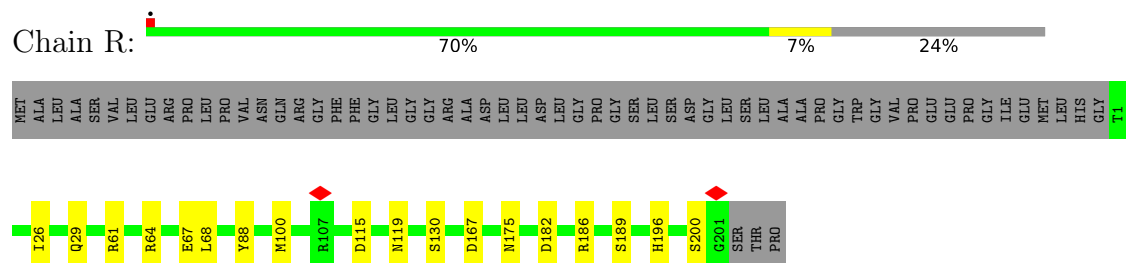
- Molecule 17: Proteasome subunit beta type-2



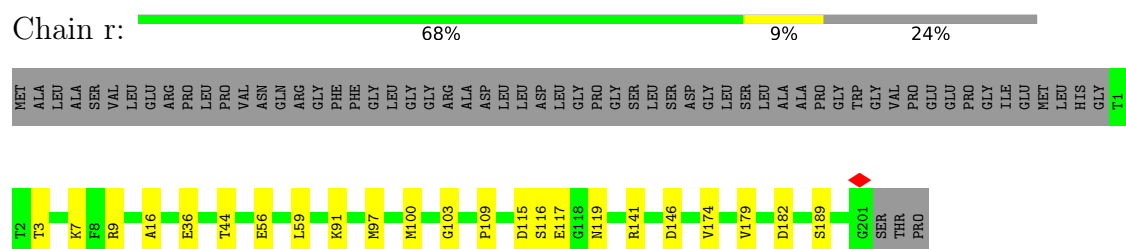
- Molecule 17: Proteasome subunit beta type-2



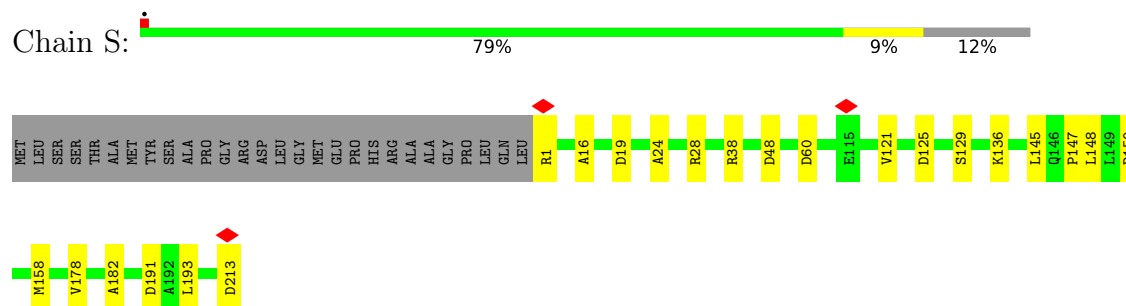
- Molecule 18: Proteasome subunit beta type-5



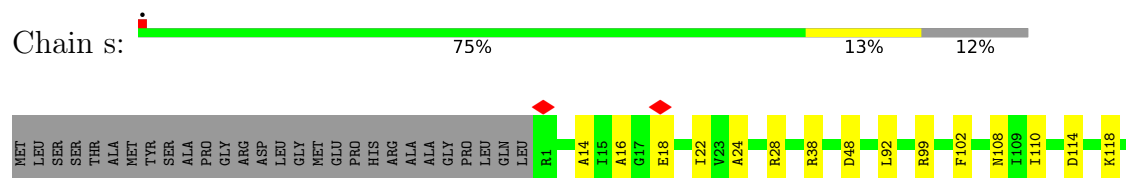
- Molecule 18: Proteasome subunit beta type-5

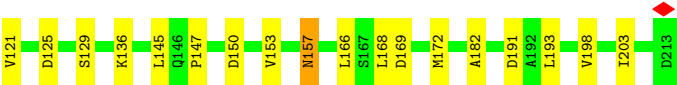


- Molecule 19: Proteasome subunit beta type-1

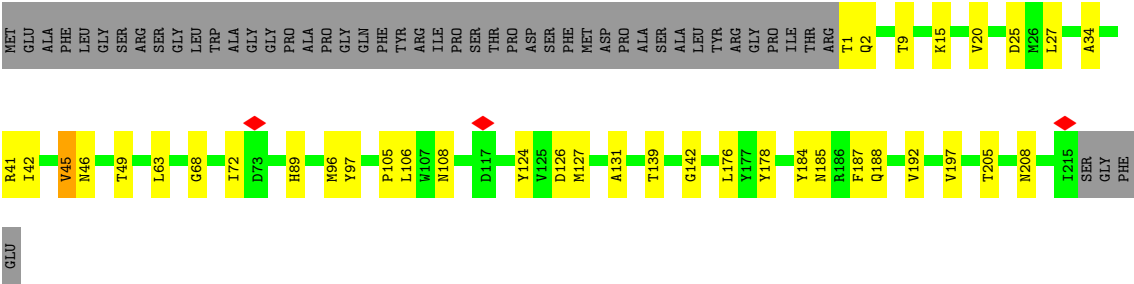


- Molecule 19: Proteasome subunit beta type-1

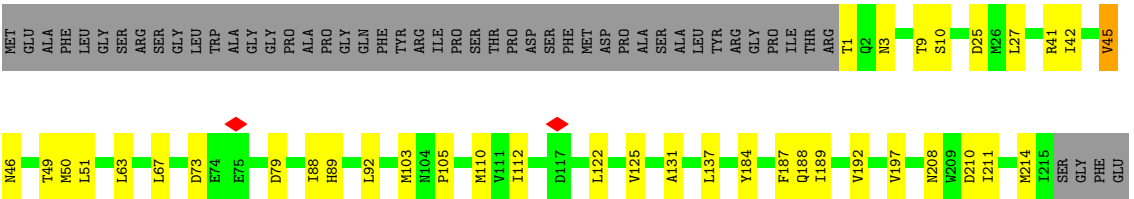




• Molecule 20: Proteasome subunit beta type-4



• Molecule 20: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	369.59998, 369.59998, 369.59998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/2823	0.55	1/3809 (0.0%)
2	B	0.19	0/2675	0.54	0/3611
3	C	0.22	0/2500	0.57	0/3366
4	D	0.22	0/2710	0.61	2/3663 (0.1%)
5	E	0.20	0/2708	0.55	0/3653
6	F	0.19	0/2665	0.50	0/3597
7	G	0.17	0/1859	0.46	0/2523
7	g	0.19	0/1859	0.51	0/2523
8	H	0.16	0/1743	0.45	0/2372
8	h	0.16	0/1743	0.47	1/2372 (0.0%)
9	I	0.17	0/1942	0.50	1/2628 (0.0%)
9	i	0.17	0/1942	0.50	0/2628
10	J	0.17	0/1737	0.48	0/2369
10	j	0.16	0/1728	0.49	0/2358
11	K	0.17	0/1747	0.49	1/2364 (0.0%)
11	k	0.18	0/1747	0.49	0/2364
12	L	0.17	0/1885	0.48	0/2552
12	l	0.18	0/1885	0.51	0/2552
13	M	0.20	0/1891	0.53	0/2552
13	m	0.17	0/1891	0.48	0/2552
14	N	0.15	0/1454	0.43	0/1967
14	n	0.19	0/1454	0.54	0/1967
15	O	0.18	0/1670	0.53	0/2265
15	o	0.16	0/1670	0.46	0/2265
16	P	0.17	0/1620	0.47	0/2184
16	p	0.18	0/1620	0.48	0/2184
17	Q	0.18	0/1603	0.50	0/2174
17	q	0.18	0/1603	0.51	0/2174
18	R	0.16	0/1579	0.46	0/2134
18	r	0.18	0/1579	0.47	0/2134
19	S	0.17	0/1671	0.44	0/2253
19	s	0.19	0/1674	0.49	0/2257

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.17	0/1700	0.46	0/2305
20	t	0.17	0/1700	0.47	0/2305
All	All	0.18	0/64277	0.50	6/86976 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	5
4	D	0	3
5	E	0	2
7	G	0	1
10	J	0	1
10	j	0	1
20	T	0	1
20	t	0	1
All	All	0	15

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	32	LYS	CB-CG-CD	5.59	124.16	111.30
1	A	400	ARG	CA-CB-CG	5.33	124.75	114.10
9	I	235	GLN	CA-CB-CG	5.20	124.49	114.10
8	h	150	ASP	CB-CA-C	5.03	116.87	109.22
4	D	126	PRO	CA-C-N	5.02	128.35	121.33
4	D	126	PRO	C-N-CA	5.02	128.35	121.33

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	127	LEU	Peptide
3	C	128	PRO	Peptide
3	C	129	ASN	Peptide
3	C	89	VAL	Peptide
3	C	90	HIS	Peptide
4	D	125	LYS	Peptide

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Mol	Chain	Res	Type	Group
4	D	126	PRO	Peptide
4	D	368	ASP	Peptide
5	E	116	ASP	Peptide
5	E	385	ASP	Peptide
7	G	222	VAL	Peptide
10	J	199	VAL	Peptide
20	T	45	VAL	Peptide
10	j	199	VAL	Peptide
20	t	45	VAL	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	2776	0	2814	33	0
2	B	2638	0	2679	42	0
3	C	2464	0	2546	39	0
4	D	2666	0	2707	50	0
5	E	2664	0	2721	42	0
6	F	2627	0	2688	30	0
7	G	1826	0	1796	21	0
7	g	1826	0	1796	18	0
8	H	1708	0	1594	14	0
8	h	1708	0	1594	9	0
9	I	1912	0	1851	29	0
9	i	1912	0	1851	28	0
10	J	1713	0	1537	21	0
10	j	1704	0	1517	12	0
11	K	1722	0	1673	25	0
11	k	1722	0	1673	22	0
12	L	1850	0	1822	22	0
12	l	1850	0	1822	28	0
13	M	1856	0	1814	23	0
13	m	1856	0	1814	21	0
14	N	1430	0	1398	14	0
14	n	1430	0	1398	14	0
15	O	1643	0	1644	18	0
15	o	1643	0	1644	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	1591	0	1609	17	0
16	p	1591	0	1609	26	0
17	Q	1570	0	1547	29	0
17	q	1570	0	1547	23	0
18	R	1548	0	1499	12	0
18	r	1548	0	1499	15	0
19	S	1641	0	1616	16	0
19	s	1644	0	1625	20	0
20	T	1667	0	1628	22	0
20	t	1667	0	1628	27	0
21	A	31	0	12	1	0
21	B	31	0	12	1	0
21	D	31	0	12	0	0
21	E	31	0	12	0	0
22	C	27	0	12	1	0
22	F	27	0	12	2	0
All	All	63361	0	62272	717	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (717) 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)
9:I:42:GLY:HA2	9:I:216:LEU:O	1.78	0.82
9:i:42:GLY:HA2	9:i:216:LEU:O	1.86	0.74
13:M:47:PHE:HB2	13:M:214:SER:HB3	1.70	0.72
11:k:236:GLU:HA	11:k:239:LYS:HE3	1.72	0.71
10:J:86:ARG:HE	10:J:114:LEU:HD11	1.58	0.68
19:s:168:LEU:HG	19:s:172:MET:HE2	1.76	0.68
10:j:86:ARG:HE	10:j:114:LEU:HD11	1.58	0.67
13:m:47:PHE:HB2	13:m:214:SER:HB3	1.77	0.66
4:D:244:PRO:HB3	4:D:291:GLU:HG3	1.77	0.66
17:Q:142:ILE:O	17:Q:145:ARG:HB3	1.95	0.66
6:F:195:ILE:HG12	6:F:236:LEU:HD21	1.78	0.66
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.61	0.65
9:I:197:LEU:HA	9:I:200:THR:HG22	1.78	0.65
15:o:55:THR:HG23	15:o:86:MET:HE1	1.78	0.65
19:S:148:LEU:HD13	19:S:178:VAL:HG23	1.78	0.64
20:t:51:LEU:HD21	20:t:110:MET:HE2	1.79	0.64
11:k:50:VAL:HG11	11:k:66:LYS:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:130:VAL:HB	4:D:139:LEU:HD13	1.80	0.64
19:S:24:ALA:HB1	19:S:193:LEU:HD11	1.79	0.63
13:M:186:CYS:HA	13:M:189:ILE:HB	1.80	0.63
12:l:120:THR:O	13:m:129:ARG:NH1	2.31	0.63
4:D:354:LEU:HD11	4:D:360:LEU:HD11	1.81	0.63
3:C:198:LEU:HD11	22:C:501:ADP:H2'	1.81	0.63
12:L:159:MET:HE3	12:L:160:SER:H	1.64	0.62
11:K:93:ARG:HH11	18:R:68:LEU:HB3	1.62	0.62
12:L:186:GLU:HA	12:L:189:LYS:HG2	1.82	0.61
17:q:117:TYR:HB3	17:q:125:ALA:HB3	1.80	0.61
10:J:88:ARG:HH11	17:Q:69:MET:HG3	1.65	0.61
4:D:204:MET:HA	4:D:331:ILE:O	2.01	0.61
17:q:142:ILE:O	17:q:145:ARG:HB3	2.00	0.61
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.64	0.61
1:A:284:ARG:O	6:F:334:ARG:NH1	2.34	0.61
5:E:169:GLY:HA3	5:E:275:MET:HB2	1.82	0.61
1:A:210:LYS:NZ	1:A:313:GLY:O	2.34	0.60
15:o:7:VAL:HG22	15:o:12:ILE:HG12	1.83	0.60
15:O:21:THR:HG22	15:O:26:VAL:HA	1.83	0.60
12:l:180:MET:SD	12:l:180:MET:N	2.72	0.60
5:E:72:LYS:HB2	5:E:78:ARG:HG2	1.81	0.60
8:H:119:GLN:NE2	9:I:82:ASP:OD1	2.34	0.60
11:k:28:ILE:O	11:k:32:LYS:NZ	2.35	0.60
19:S:1:ARG:NH1	20:T:2:GLN:OE1	2.35	0.60
7:g:165:ALA:HB1	7:g:179:LEU:HD13	1.84	0.60
18:R:64:ARG:NH1	18:R:67:GLU:OE2	2.34	0.60
19:s:92:LEU:HD21	19:s:108:ASN:HD22	1.65	0.60
4:D:84:SER:O	5:E:68:LYS:NZ	2.32	0.59
3:C:367:GLY:HA3	4:D:196:ILE:HG21	1.84	0.59
7:G:120:ASP:OD1	8:H:84:ARG:NH1	2.36	0.59
12:L:120:THR:O	13:M:129:ARG:NH1	2.35	0.59
7:g:120:ASP:OD1	8:h:84:ARG:NH1	2.35	0.59
6:F:252:ALA:HB3	6:F:255:GLN:HB2	1.83	0.59
9:I:218:ARG:NH1	9:I:223:THR:OG1	2.36	0.59
12:l:140:MET:SD	12:l:140:MET:N	2.76	0.59
11:K:20:ARG:HG2	11:K:21:LEU:H	1.68	0.59
20:T:126:ASP:OD1	20:T:127:MET:N	2.36	0.59
14:n:35:THR:OG1	14:n:45:ARG:NH1	2.36	0.59
3:C:219:LEU:HD11	4:D:289:LEU:HD23	1.85	0.58
6:F:375:VAL:HG22	6:F:415:LEU:HD12	1.84	0.58
19:S:213:ASP:OD1	15:o:193:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.35	0.58
3:C:373:GLU:HG3	3:C:375:ARG:HG3	1.84	0.58
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.37	0.58
1:A:258:ARG:HH12	6:F:255:GLN:HA	1.68	0.58
7:g:112:ASP:OD1	7:g:112:ASP:N	2.36	0.58
9:i:116:ASP:OD1	10:j:81:ARG:NH1	2.35	0.58
18:r:97:MET:HB2	18:r:116:SER:HB3	1.86	0.58
2:B:403:GLY:HA3	3:C:180:ILE:HG21	1.86	0.58
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.84	0.58
15:O:112:SER:OG	15:O:120:ASP:OD1	2.21	0.58
15:o:146:MET:HE2	15:o:150:GLU:HG3	1.86	0.58
5:E:56:ILE:HB	5:E:100:LEU:HB2	1.86	0.58
17:Q:169:LYS:HD3	17:Q:170:ARG:HG3	1.86	0.58
17:q:38:MET:HE1	17:q:44:LEU:HB2	1.86	0.58
5:E:198:VAL:HG12	5:E:200:SER:H	1.69	0.58
1:A:224:LEU:HD22	21:A:501:ATP:H2'	1.84	0.57
1:A:306:LEU:HD23	1:A:336:ARG:HB3	1.85	0.57
4:D:233:SER:OG	5:E:259:GLU:OE1	2.22	0.57
16:P:135:ASP:OD1	16:P:135:ASP:N	2.37	0.57
7:g:144:ASP:HB3	7:g:147:GLN:HB2	1.86	0.57
9:I:116:ASP:OD1	10:J:81:ARG:NH1	2.35	0.57
12:L:148:CYS:HG	12:L:150:SER:HG	1.48	0.57
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.37	0.57
13:m:175:GLU:HA	13:m:178:LYS:HZ3	1.70	0.57
14:n:7:GLN:NE2	14:n:109:GLY:O	2.38	0.57
14:n:37:ILE:HD11	14:n:43:CYS:HB3	1.87	0.57
2:B:234:LEU:HD22	21:B:501:ATP:H2'	1.86	0.57
16:P:118:LYS:HD3	16:P:119:PRO:HD2	1.86	0.57
15:o:11:GLY:HA3	15:o:178:ILE:O	2.05	0.57
7:g:49:VAL:HG22	7:g:219:VAL:HG23	1.87	0.57
9:i:68:LEU:HD11	9:i:74:CYS:HB3	1.87	0.57
19:s:92:LEU:HD13	19:s:110:ILE:HD11	1.88	0.56
9:I:154:GLY:O	10:J:81:ARG:NH2	2.37	0.56
20:T:45:VAL:HB	20:T:49:THR:HG23	1.88	0.56
7:g:231:THR:HG22	7:g:233:ALA:H	1.70	0.56
6:F:289:ASP:OD1	6:F:289:ASP:N	2.39	0.56
16:p:81:GLN:N	16:p:81:GLN:OE1	2.38	0.56
20:t:9:THR:O	20:t:41:ARG:NH2	2.39	0.56
7:G:49:VAL:HG22	7:G:219:VAL:HG23	1.87	0.56
17:Q:23:SER:OG	17:Q:24:ASN:OD1	2.22	0.56
18:R:115:ASP:HB2	18:R:119:ASN:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:154:GLY:O	10:j:81:ARG:NH2	2.38	0.56
1:A:312:ARG:HB2	1:A:315:ILE:HD12	1.86	0.56
15:O:164:PHE:O	19:s:38:ARG:NH2	2.39	0.56
12:L:7:ASP:OD1	12:L:7:ASP:N	2.40	0.55
12:l:204:ASP:OD1	12:l:204:ASP:N	2.38	0.55
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.39	0.55
11:k:41:GLN:NE2	11:k:151:PRO:O	2.39	0.55
5:E:265:ASP:OD2	5:E:291:ARG:NH2	2.39	0.55
11:K:48:LEU:HD21	11:K:77:ALA:HB2	1.87	0.55
20:t:25:ASP:OD1	20:t:41:ARG:NH1	2.39	0.55
18:R:26:ILE:HG21	18:R:29:GLN:HE21	1.72	0.55
9:i:218:ARG:NH1	9:i:223:THR:OG1	2.39	0.55
18:r:115:ASP:HB2	18:r:119:ASN:HB2	1.87	0.55
1:A:97:ARG:NH1	2:B:130:GLU:O	2.33	0.55
1:A:293:ASN:O	1:A:297:ARG:NE	2.40	0.55
18:r:3:THR:HG23	18:r:16:ALA:HB2	1.89	0.55
3:C:390:VAL:HA	3:C:393:LYS:HZ3	1.72	0.55
11:k:111:SER:HA	11:k:114:GLN:HG2	1.89	0.55
15:o:32:SER:HB2	15:o:187:ARG:HH21	1.72	0.55
16:p:135:ASP:OD1	16:p:135:ASP:N	2.35	0.55
10:J:88:ARG:NH1	17:Q:69:MET:O	2.41	0.55
20:T:9:THR:O	20:T:41:ARG:NH2	2.40	0.54
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.89	0.54
17:q:25:ILE:HG13	17:q:26:VAL:HG13	1.88	0.54
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.88	0.54
18:r:117:GLU:N	18:r:117:GLU:OE1	2.40	0.54
2:B:287:ILE:HG12	2:B:329:MET:HE3	1.88	0.54
1:A:248:LYS:NZ	4:D:278:GLN:OE1	2.40	0.54
1:A:297:ARG:HH12	6:F:306:VAL:HG21	1.72	0.54
7:G:137:CYS:SG	7:G:138:MET:N	2.80	0.54
10:J:108:THR:HG22	10:J:133:ILE:HD13	1.89	0.54
13:M:163:CYS:SG	13:M:164:ALA:N	2.81	0.54
19:s:125:ASP:OD1	19:s:129:SER:N	2.41	0.54
1:A:143:ASP:OD1	1:A:143:ASP:N	2.41	0.54
9:I:38:LEU:O	9:I:179:TYR:OH	2.26	0.54
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.41	0.54
7:g:200:THR:HG23	7:g:242:LEU:HD11	1.88	0.54
10:j:209:ALA:HB1	10:j:217:LEU:HD11	1.89	0.54
4:D:92:PHE:O	4:D:125:LYS:NZ	2.40	0.54
10:J:68:ASN:HA	10:J:211:MET:HE1	1.90	0.54
14:N:51:ASP:HB3	14:N:94:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:125:ASP:OD1	16:P:129:CYS:N	2.41	0.54
1:A:399:ALA:O	1:A:400:ARG:NH1	2.41	0.54
2:B:196:GLU:OE2	2:B:349:ARG:NH1	2.41	0.54
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.90	0.54
6:F:404:GLY:HA2	6:F:415:LEU:HD21	1.90	0.53
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.90	0.53
12:L:204:ASP:OD1	12:L:204:ASP:N	2.40	0.53
14:N:18:SER:HB2	14:N:31:THR:H	1.73	0.53
4:D:410:ASP:OD1	4:D:410:ASP:N	2.40	0.53
7:G:158:GLY:O	8:H:84:ARG:NH2	2.41	0.53
17:Q:19:ARG:HH21	17:Q:31:ASP:HB2	1.73	0.53
11:K:199:LEU:HD11	11:K:217:LEU:HD11	1.90	0.53
14:N:9:ASP:OD2	14:N:9:ASP:N	2.41	0.53
11:K:91:LYS:HG2	11:K:119:LEU:HD22	1.91	0.53
4:D:267:ILE:HD12	4:D:267:ILE:H	1.74	0.53
5:E:322:LYS:HD3	5:E:326:ILE:HG13	1.89	0.53
8:H:40:ALA:HB1	8:H:182:LEU:HB2	1.89	0.53
13:M:70:ASP:OD2	13:M:99:ARG:NH2	2.39	0.53
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.41	0.53
1:A:330:ALA:O	1:A:336:ARG:NH1	2.42	0.53
4:D:175:GLN:NE2	4:D:179:GLU:OE2	2.42	0.53
20:T:25:ASP:HA	20:T:187:PHE:HA	1.90	0.53
3:C:147:THR:OG1	3:C:206:HIS:NE2	2.41	0.53
4:D:129:SER:OG	4:D:252:ARG:NH1	2.35	0.53
9:I:90:LEU:HD13	9:I:114:LEU:HD22	1.90	0.53
12:l:105:VAL:HG21	12:l:136:GLY:HA3	1.91	0.53
13:m:168:ALA:HB1	13:m:171:ALA:HB3	1.91	0.53
2:B:133:VAL:HB	2:B:158:ALA:HA	1.91	0.53
9:I:76:VAL:HG23	9:I:134:LEU:HB3	1.90	0.53
13:M:228:PRO:HD2	13:M:231:ILE:HD12	1.90	0.53
12:L:22:ILE:HG22	12:L:26:MET:HE1	1.90	0.53
13:M:43:ASP:OD1	13:M:43:ASP:N	2.42	0.53
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.91	0.53
1:A:319:MET:HE3	1:A:337:LEU:HD11	1.91	0.52
9:I:118:LYS:NZ	9:I:150:SER:OG	2.38	0.52
16:P:12:MET:HE2	16:P:146:MET:HB3	1.89	0.52
16:P:190:ILE:HG22	16:P:195:ILE:HG13	1.91	0.52
5:E:144:GLU:O	5:E:297:ARG:NH2	2.43	0.52
17:Q:26:VAL:HG23	17:q:170:ARG:HB3	1.91	0.52
2:B:154:HIS:HD2	2:B:155:LYS:HE3	1.74	0.52
6:F:341:ALA:O	6:F:347:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:7:LYS:HE2	18:r:109:PRO:HB2	1.91	0.52
4:D:266:GLU:OE2	5:E:262:ASN:ND2	2.43	0.52
10:J:80:ALA:HA	10:J:129:ILE:HD13	1.92	0.52
14:n:84:LYS:NZ	14:n:85:GLU:OE1	2.41	0.52
20:t:45:VAL:HB	20:t:49:THR:HG23	1.92	0.52
1:A:99:THR:HG21	1:A:113:ILE:HD12	1.92	0.52
4:D:267:ILE:HD11	4:D:309:MET:HB3	1.92	0.52
5:E:252:GLU:OE1	5:E:252:GLU:N	2.39	0.52
9:i:38:LEU:O	9:i:179:TYR:OH	2.28	0.52
10:j:97:THR:OG1	10:j:98:VAL:N	2.42	0.52
16:P:159:ASP:N	16:P:159:ASP:OD1	2.43	0.52
1:A:390:THR:HA	2:B:216:ILE:HD11	1.92	0.52
11:K:50:VAL:HG11	11:K:66:LYS:HB2	1.90	0.52
20:T:192:VAL:HG12	20:T:197:VAL:HG22	1.92	0.52
17:Q:88:LEU:HB3	17:Q:122:ALA:HB2	1.91	0.52
11:k:67:ILE:HD12	11:k:216:GLU:HG3	1.92	0.52
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.44	0.51
17:Q:23:SER:OG	17:Q:24:ASN:N	2.44	0.51
1:A:213:LEU:HD22	1:A:337:LEU:HD23	1.92	0.51
5:E:220:ASN:OD1	5:E:223:ARG:NH2	2.44	0.51
4:D:353:ASN:ND2	4:D:392:TYR:O	2.44	0.51
11:K:41:GLN:NE2	11:K:151:PRO:O	2.43	0.51
5:E:368:MET:HE3	5:E:368:MET:H	1.75	0.51
5:E:385:ASP:N	5:E:385:ASP:OD2	2.42	0.51
6:F:228:PRO:O	6:F:233:LYS:NZ	2.43	0.51
15:O:11:GLY:HA3	15:O:178:ILE:O	2.10	0.51
16:P:107:PRO:HG2	16:P:124:LEU:HB2	1.92	0.51
12:l:186:GLU:HA	12:l:189:LYS:HG2	1.92	0.51
9:I:15:GLU:OE2	9:I:17:ARG:NE	2.43	0.51
11:k:182:GLN:HG2	12:l:56:LEU:HD11	1.92	0.51
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.91	0.51
2:B:104:GLY:H	2:B:154:HIS:HE1	1.59	0.51
3:C:83:LYS:HZ3	3:C:105:ILE:HB	1.76	0.51
12:L:193:ARG:HA	12:L:196:ARG:HD2	1.93	0.51
16:p:2:SER:OG	16:p:3:ILE:N	2.44	0.51
2:B:316:LEU:HD23	2:B:346:ARG:HB3	1.92	0.51
3:C:145:ASP:HA	3:C:201:ARG:HG2	1.91	0.51
4:D:401:LYS:HA	4:D:404:LYS:HE2	1.91	0.51
17:q:19:ARG:HH21	17:q:31:ASP:HB2	1.75	0.51
2:B:181:GLN:O	2:B:241:ASN:ND2	2.44	0.51
2:B:377:ASP:O	2:B:416:ASN:ND2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:392:GLN:O	3:C:396:GLU:N	2.40	0.50
9:I:69:ASN:OD1	9:I:70:GLU:N	2.40	0.50
9:I:159:TRP:HA	10:J:54:GLN:HA	1.93	0.50
19:S:60:ASP:OD1	20:T:97:TYR:OH	2.28	0.50
12:l:33:SER:O	12:l:62:LYS:NZ	2.44	0.50
20:t:25:ASP:HA	20:t:187:PHE:HA	1.93	0.50
2:B:412:MET:HE1	3:C:177:ALA:HB1	1.93	0.50
11:K:152:GLN:OE1	11:K:164:GLN:NE2	2.44	0.50
12:l:88:MET:HG2	12:l:112:ILE:HD11	1.93	0.50
13:m:65:ARG:HH21	13:m:78:ALA:HA	1.76	0.50
1:A:372:LEU:HD11	11:K:207:GLU:HA	1.93	0.50
4:D:246:MET:HE1	5:E:78:ARG:HH12	1.76	0.50
13:M:241:GLU:O	13:M:244:LYS:NZ	2.43	0.50
14:N:166:ARG:NH2	14:n:140:ASP:OD2	2.38	0.50
17:Q:44:LEU:HD11	17:Q:102:LEU:HD13	1.94	0.50
4:D:374:ASP:HB3	5:E:292:PRO:HG2	1.92	0.50
19:s:28:ARG:NH2	19:s:191:ASP:OD1	2.45	0.50
3:C:344:LEU:HA	3:C:347:ILE:HD12	1.93	0.50
11:K:111:SER:HA	11:K:114:GLN:HG2	1.94	0.50
4:D:397:LYS:NZ	4:D:398:ASP:OD1	2.44	0.50
4:D:337:ASP:OD1	4:D:337:ASP:N	2.38	0.50
12:L:117:GLN:NE2	13:M:83:ASP:OD1	2.44	0.50
12:L:140:MET:SD	12:L:140:MET:N	2.85	0.50
18:r:36:GLU:N	18:r:36:GLU:OE1	2.44	0.50
13:M:23:VAL:HG12	13:M:27:MET:HE3	1.92	0.50
20:T:68:GLY:O	20:T:72:ILE:HG13	2.12	0.50
2:B:408:ARG:NH1	3:C:163:GLU:OE2	2.45	0.49
2:B:408:ARG:NH2	3:C:160:GLU:OE2	2.44	0.49
8:h:45:VAL:HG22	8:h:212:ILE:HG22	1.94	0.49
13:m:41:CYS:N	13:m:44:GLY:O	2.42	0.49
4:D:96:VAL:HG23	4:D:102:ILE:HD11	1.94	0.49
12:l:146:GLN:HE21	12:l:154:PHE:HD2	1.58	0.49
16:p:159:ASP:OD1	16:p:159:ASP:N	2.42	0.49
2:B:108:SER:OG	2:B:153:ASN:O	2.30	0.49
6:F:336:ASP:OD1	6:F:336:ASP:N	2.40	0.49
14:n:18:SER:HB2	14:n:31:THR:H	1.78	0.49
2:B:317:ASP:HB2	2:B:346:ARG:HG2	1.93	0.49
10:J:38:ARG:NH2	10:J:182:GLU:O	2.45	0.49
11:k:76:CYS:SG	11:k:77:ALA:N	2.85	0.49
16:p:125:ASP:OD1	16:p:129:CYS:N	2.42	0.49
2:B:221:GLY:HA3	2:B:347:ILE:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:VAL:HG22	2:B:349:ARG:HB2	1.94	0.49
10:J:38:ARG:HH12	10:J:182:GLU:HA	1.78	0.49
12:L:196:ARG:O	12:L:239:ARG:NH2	2.46	0.49
20:t:1:THR:N	20:t:105:PRO:O	2.41	0.49
20:t:79:ASP:OD2	20:t:79:ASP:N	2.44	0.49
2:B:168:ASP:HB3	2:B:171:VAL:H	1.76	0.49
3:C:246:ILE:HB	3:C:291:VAL:HG12	1.95	0.49
9:i:197:LEU:HA	9:i:200:THR:HG22	1.93	0.49
16:p:118:LYS:HD3	16:p:119:PRO:HD2	1.93	0.49
7:G:21:ARG:NH2	7:G:26:GLU:OE2	2.44	0.49
17:Q:38:MET:HE1	17:Q:44:LEU:HB2	1.94	0.49
17:Q:164:LEU:HD12	17:Q:194:ILE:HD11	1.95	0.49
11:k:117:SER:HB2	12:l:82:ARG:HH12	1.78	0.49
17:q:38:MET:HB3	17:q:64:VAL:HG11	1.95	0.49
20:t:92:LEU:HG	20:t:125:VAL:HG11	1.94	0.49
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.95	0.49
4:D:91:GLN:OE1	4:D:248:ARG:NH1	2.45	0.49
4:D:173:GLN:HE22	4:D:334:PRO:HD2	1.78	0.49
8:H:75:VAL:HG12	8:H:135:LEU:HB2	1.95	0.49
9:i:90:LEU:HD12	9:i:110:LEU:HD21	1.94	0.49
13:m:40:ARG:HA	13:m:45:VAL:HA	1.94	0.49
1:A:372:LEU:HD21	11:K:207:GLU:HG3	1.94	0.49
6:F:311:LEU:HD23	6:F:314:LEU:HD12	1.95	0.48
13:M:214:SER:OG	13:M:224:HIS:NE2	2.38	0.48
5:E:158:LEU:HA	5:E:161:ARG:HG2	1.96	0.48
11:K:99:HIS:HB2	11:K:107:MET:HE2	1.95	0.48
13:M:97:ASN:O	13:M:101:ASN:HB2	2.14	0.48
5:E:116:ASP:O	5:E:118:LEU:N	2.46	0.48
12:L:105:VAL:HG21	12:L:136:GLY:HA3	1.95	0.48
18:R:182:ASP:N	18:R:182:ASP:OD1	2.43	0.48
6:F:224:LEU:HB2	6:F:348:LEU:HD23	1.95	0.48
16:P:189:ILE:HG23	16:P:196:THR:HB	1.95	0.48
16:p:107:PRO:HG2	16:p:124:LEU:HB2	1.95	0.48
16:p:83:LYS:HB3	16:p:83:LYS:HE3	1.60	0.48
16:p:190:ILE:HG22	16:p:195:ILE:HG13	1.95	0.48
19:s:18:GLU:OE1	19:s:18:GLU:N	2.40	0.48
1:A:287:ASP:OD1	1:A:287:ASP:N	2.45	0.48
5:E:202:SER:HA	6:F:269:ARG:HH22	1.78	0.48
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.96	0.48
12:l:34:ALA:HA	12:l:161:ILE:O	2.14	0.48
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:107:ARG:NH2	20:t:79:ASP:OD1	2.42	0.48
15:o:112:SER:HB3	15:o:125:VAL:HG11	1.95	0.48
2:B:265:LYS:HG2	2:B:268:ARG:HH21	1.79	0.48
12:L:50:LYS:HE2	12:L:61:LYS:HA	1.95	0.48
1:A:94:GLN:HE21	1:A:150:HIS:CE1	2.32	0.48
20:T:96:MET:HE1	20:T:106:LEU:HB2	1.96	0.48
7:g:212:PRO:HB3	7:g:235:ILE:HG22	1.96	0.48
2:B:103:ARG:HH12	2:B:151:LEU:HB3	1.78	0.48
4:D:129:SER:HG	4:D:252:ARG:HH12	1.58	0.48
10:j:80:ALA:HA	10:j:129:ILE:HD13	1.95	0.48
19:s:157:ASN:O	19:s:157:ASN:ND2	2.29	0.48
3:C:237:MET:SD	3:C:237:MET:N	2.87	0.47
3:C:352:PRO:HD2	3:C:391:MET:HE3	1.96	0.47
7:G:34:GLN:NE2	13:M:17:ASP:O	2.47	0.47
8:H:107:THR:HG21	8:H:138:GLY:HA3	1.96	0.47
9:i:15:GLU:OE2	9:i:17:ARG:NE	2.44	0.47
11:k:84:ASP:OD1	11:k:84:ASP:N	2.37	0.47
17:q:31:ASP:OD1	17:q:31:ASP:N	2.48	0.47
6:F:233:LYS:N	22:F:501:ADP:O2A	2.45	0.47
5:E:74:THR:OG1	6:F:131:THR:OG1	2.28	0.47
17:Q:38:MET:O	17:Q:65:GLN:NE2	2.48	0.47
20:T:185:ASN:OD1	20:T:205:THR:OG1	2.32	0.47
12:l:67:ASP:OD2	12:l:96:ARG:NH2	2.44	0.47
14:n:45:ARG:HD2	14:n:52:THR:HB	1.96	0.47
3:C:88:LYS:HB3	3:C:94:LYS:HG2	1.95	0.47
9:i:38:LEU:HB3	9:i:43:VAL:HG23	1.96	0.47
10:j:93:SER:HA	10:j:96:LEU:HB2	1.96	0.47
2:B:388:ASP:N	2:B:388:ASP:OD1	2.47	0.47
3:C:99:VAL:HA	3:C:123:LEU:HB2	1.96	0.47
4:D:200:ARG:HD2	4:D:299:PHE:HD2	1.79	0.47
6:F:226:TYR:CZ	6:F:353:GLU:HB2	2.50	0.47
15:O:7:VAL:HG22	15:O:12:ILE:HG12	1.96	0.47
17:Q:38:MET:HE2	17:Q:38:MET:HB2	1.75	0.47
17:Q:66:LEU:HG	17:Q:70:ARG:HD2	1.96	0.47
2:B:91:LYS:O	2:B:95:GLU:N	2.42	0.47
2:B:183:THR:OG1	2:B:184:TYR:N	2.48	0.47
11:K:38:ILE:HD12	11:K:202:LEU:HG	1.96	0.47
14:N:127:ILE:HG12	14:N:132:SER:HB2	1.96	0.47
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.95	0.47
17:Q:15:VAL:HB	17:Q:45:LEU:HD11	1.96	0.47
6:F:178:ASP:N	6:F:178:ASP:OD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:71:ASP:HB2	9:i:223:THR:HG21	1.96	0.47
1:A:278:ASP:N	1:A:278:ASP:OD1	2.46	0.47
6:F:126:THR:HG22	6:F:130:GLN:HB2	1.97	0.47
7:G:73:THR:HG23	7:G:75:ASN:H	1.80	0.47
11:K:89:ILE:HG22	11:K:93:ARG:HE	1.80	0.47
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.30	0.47
17:Q:63:ASN:HD22	17:Q:83:PHE:HZ	1.63	0.47
8:h:108:ALA:O	8:h:112:GLN:HG2	2.16	0.47
19:s:198:VAL:HG22	19:s:203:ILE:HG12	1.97	0.46
20:t:88:ILE:HG22	20:t:112:ILE:HD13	1.97	0.46
1:A:139:ARG:O	1:A:153:LEU:N	2.48	0.46
3:C:134:LEU:HD11	3:C:212:ILE:HG12	1.97	0.46
19:S:150:ASP:OD2	16:p:177:ARG:NH2	2.37	0.46
16:p:58:THR:OG1	17:q:121:LEU:O	2.25	0.46
3:C:344:LEU:HD23	3:C:347:ILE:HD12	1.97	0.46
5:E:60:VAL:HA	5:E:71:VAL:HG12	1.97	0.46
3:C:113:ARG:CZ	3:C:130:LYS:HB2	2.45	0.46
4:D:91:GLN:N	4:D:104:GLY:O	2.49	0.46
15:O:63:LEU:HD23	15:O:63:LEU:HA	1.83	0.46
19:S:147:PRO:HB2	16:p:149:MET:HE3	1.96	0.46
20:T:42:ILE:HD12	20:T:188:GLN:HG3	1.98	0.46
7:g:112:ASP:HB3	7:g:152:TYR:CZ	2.50	0.46
3:C:325:ARG:HD3	3:C:353:GLY:HA2	1.98	0.46
16:P:126:LEU:HD12	16:P:127:ILE:HG23	1.97	0.46
19:S:38:ARG:NH2	15:o:164:PHE:O	2.48	0.46
13:m:200:VAL:O	13:m:201:HIS:ND1	2.48	0.46
1:A:146:LYS:HD2	1:A:148:GLN:HG2	1.97	0.46
4:D:171:ASP:OD1	4:D:171:ASP:N	2.49	0.46
14:n:142:THR:HB	14:n:155:PHE:HE1	1.80	0.46
16:p:191:GLU:OE1	16:p:191:GLU:N	2.49	0.46
5:E:180:LYS:HG2	5:E:301:ILE:HD12	1.96	0.46
2:B:118:ASP:OD1	2:B:118:ASP:N	2.47	0.46
3:C:163:GLU:HA	3:C:167:LEU:HD13	1.97	0.46
4:D:231:VAL:HG23	5:E:262:ASN:HD22	1.80	0.46
7:G:71:LYS:O	7:G:95:ARG:NH1	2.49	0.46
14:N:35:THR:OG1	14:N:45:ARG:NH1	2.49	0.46
10:j:154:HIS:ND1	11:k:59:MET:HE1	2.30	0.46
5:E:55:GLN:N	6:F:133:PHE:O	2.48	0.46
5:E:144:GLU:OE2	5:E:297:ARG:NH1	2.49	0.46
13:M:197:ILE:HA	13:M:200:VAL:HG12	1.98	0.46
14:N:57:ASP:OD2	15:O:84:LYS:NZ	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:49:ARG:N	9:i:210:LYS:O	2.46	0.46
15:o:19:ARG:HH21	15:o:21:THR:HG21	1.80	0.46
16:p:118:LYS:HB2	16:p:118:LYS:HE2	1.69	0.46
5:E:207:TYR:HD1	5:E:210:GLU:HG3	1.80	0.46
9:I:33:THR:HB	9:I:48:GLU:HB3	1.96	0.46
17:Q:4:LEU:HD22	17:Q:45:LEU:HB3	1.97	0.46
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.97	0.46
19:s:24:ALA:HB1	19:s:193:LEU:HD11	1.98	0.46
6:F:318:ASP:OD2	6:F:344:ARG:NH2	2.44	0.45
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.98	0.45
5:E:168:LYS:N	5:E:296:ASP:OD2	2.49	0.45
11:K:37:ALA:HB2	11:K:50:VAL:HG23	1.98	0.45
19:S:48:ASP:OD1	19:S:48:ASP:N	2.48	0.45
1:A:105:ASP:OD1	1:A:105:ASP:N	2.50	0.45
5:E:103:THR:OG1	5:E:104:THR:N	2.48	0.45
6:F:318:ASP:HB3	6:F:347:ARG:HG2	1.98	0.45
13:m:71:ARG:H	13:m:71:ARG:HG3	1.59	0.45
17:q:12:TYR:HB2	17:q:182:ILE:HD11	1.99	0.45
13:m:214:SER:OG	13:m:224:HIS:NE2	2.34	0.45
17:q:2:GLU:N	17:q:2:GLU:OE2	2.49	0.45
2:B:125:THR:OG1	2:B:126:SER:N	2.49	0.45
5:E:281:ARG:HB3	5:E:386:TYR:CE2	2.51	0.45
7:G:200:THR:HG23	7:G:242:LEU:HD11	1.98	0.45
12:L:103:LEU:HD22	12:L:104:PRO:HD2	1.99	0.45
7:g:47:CYS:HB3	7:g:221:THR:HG23	1.98	0.45
17:q:177:THR:HG23	17:q:195:SER:HB3	1.98	0.45
5:E:84:ARG:HG2	5:E:87:LEU:HD23	1.98	0.45
5:E:147:GLU:HB3	5:E:297:ARG:HH22	1.81	0.45
15:O:70:THR:HB	15:O:72:ARG:HG2	1.98	0.45
10:j:137:ASP:OD2	10:j:143:ARG:NH1	2.50	0.45
13:m:241:GLU:O	13:m:244:LYS:NZ	2.41	0.45
18:r:182:ASP:OD1	18:r:182:ASP:N	2.49	0.45
2:B:117:ASP:OD1	2:B:117:ASP:N	2.50	0.45
2:B:293:LYS:HD2	2:B:293:LYS:HA	1.80	0.45
20:T:142:GLY:HA2	20:T:176:LEU:HD21	1.99	0.45
20:T:178:TYR:HH	20:T:208:ASN:H	1.62	0.45
8:h:188:ILE:O	8:h:192:ILE:HG12	2.17	0.45
11:k:117:SER:OG	11:k:156:MET:SD	2.72	0.45
5:E:219:PHE:CD1	5:E:263:GLN:HG2	2.52	0.45
14:N:119:MET:HE2	14:N:119:MET:HB3	1.86	0.45
12:l:200:PRO:O	12:l:239:ARG:NH1	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:127:ILE:HG12	14:n:132:SER:HB2	1.97	0.45
2:B:154:HIS:CD2	2:B:155:LYS:HE3	2.52	0.45
6:F:153:VAL:HG22	6:F:160:ILE:HG22	1.98	0.45
15:O:113:ILE:HG23	15:O:119:THR:HG22	1.99	0.45
7:G:72:ILE:HG21	7:G:114:LEU:HD21	1.98	0.45
9:I:136:TYR:HE2	9:I:150:SER:HB2	1.81	0.45
14:N:11:GLY:HA3	14:N:179:ILE:O	2.17	0.45
17:Q:38:MET:HG3	17:Q:61:GLN:HA	1.99	0.45
9:i:220:ASN:OD1	9:i:220:ASN:N	2.49	0.45
12:l:189:LYS:HA	12:l:192:LEU:HB2	1.98	0.45
18:r:56:GLU:HA	18:r:59:LEU:HB3	1.99	0.45
20:t:50:MET:HE2	20:t:50:MET:HB3	1.88	0.45
20:t:192:VAL:HG12	20:t:197:VAL:HG22	1.99	0.45
14:N:84:LYS:HE2	14:N:84:LYS:HB3	1.77	0.44
19:S:16:ALA:HB2	19:S:121:VAL:HG23	1.99	0.44
9:i:232:GLU:O	9:i:235:GLN:NE2	2.39	0.44
13:m:66:LEU:HD21	13:m:214:SER:HB2	1.98	0.44
16:p:126:LEU:HD12	16:p:127:ILE:HG23	1.99	0.44
3:C:336:MET:HE3	3:C:336:MET:HA	1.98	0.44
11:K:48:LEU:HD23	11:K:67:ILE:HG12	1.99	0.44
13:M:50:GLU:HB3	13:M:197:ILE:HD12	1.98	0.44
13:M:170:GLN:HE21	13:M:170:GLN:HA	1.82	0.44
15:O:147:GLU:OE2	15:O:147:GLU:N	2.47	0.44
15:o:67:SER:HB3	15:o:74:PRO:HG3	1.98	0.44
1:A:204:LEU:HD23	1:A:206:ILE:HD11	2.00	0.44
4:D:352:MET:HE1	5:E:164:ILE:HG22	1.99	0.44
12:L:84:LEU:O	12:L:88:MET:HG2	2.17	0.44
20:T:25:ASP:OD1	20:T:41:ARG:NH1	2.50	0.44
18:r:91:LYS:NZ	18:r:117:GLU:O	2.43	0.44
20:t:73:ASP:OD2	20:t:73:ASP:N	2.48	0.44
4:D:202:VAL:HG13	4:D:308:ILE:HD13	1.98	0.44
5:E:113:ARG:HH12	5:E:220:ASN:HB3	1.82	0.44
9:I:119:GLN:HG3	10:J:78:ALA:HB1	1.99	0.44
3:C:117:ARG:HH22	3:C:124:HIS:HD2	1.66	0.44
12:l:189:LYS:HG3	12:l:193:ARG:HH12	1.82	0.44
13:m:170:GLN:HA	13:m:173:LYS:HG2	1.99	0.44
4:D:282:ASP:OD2	5:E:251:ARG:NH1	2.48	0.44
11:K:146:VAL:HG11	11:K:222:PRO:HA	1.99	0.44
4:D:296:MET:HE1	4:D:326:ARG:HB3	1.98	0.44
9:i:90:LEU:HD13	9:i:114:LEU:HD22	1.99	0.44
12:l:46:LEU:HD13	12:l:73:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:20:ARG:H	11:K:20:ARG:HD2	1.82	0.44
15:O:182:LYS:HE2	15:O:182:LYS:HB3	1.86	0.44
7:g:200:THR:HA	7:g:203:SER:HB2	2.00	0.44
8:h:9:SER:OG	8:h:123:GLN:O	2.35	0.44
9:i:82:ASP:OD1	9:i:82:ASP:N	2.51	0.44
17:Q:45:LEU:HD12	17:Q:103:LEU:HD11	2.00	0.44
20:T:63:LEU:HD12	20:T:108:ASN:HD22	1.81	0.44
9:i:187:LYS:HE2	9:i:187:LYS:HB2	1.74	0.44
7:G:10:ASP:OD1	7:G:10:ASP:N	2.48	0.43
17:Q:162:LYS:O	18:r:141:ARG:NH2	2.51	0.43
20:T:46:ASN:OD1	20:T:46:ASN:N	2.51	0.43
14:n:29:ARG:NH1	15:o:139:GLU:OE2	2.50	0.43
1:A:119:ALA:HB2	6:F:128:THR:HG23	2.00	0.43
16:p:28:PHE:HD2	16:p:36:THR:HG22	1.83	0.43
4:D:259:PRO:HB3	4:D:304:ASN:HB2	2.00	0.43
6:F:222:GLY:HA2	6:F:328:VAL:O	2.19	0.43
9:I:79:ILE:HG22	9:I:82:ASP:H	1.83	0.43
10:J:81:ARG:HA	10:J:84:ILE:HD12	2.00	0.43
11:K:32:LYS:HE3	11:K:32:LYS:HA	1.99	0.43
13:M:227:VAL:HG23	13:M:232:ARG:HD2	2.00	0.43
11:k:215:ILE:HD11	11:k:234:LEU:HD21	2.00	0.43
1:A:312:ARG:HG3	1:A:315:ILE:HB	2.00	0.43
5:E:172:LEU:HD23	5:E:299:ILE:HB	1.99	0.43
15:O:112:SER:HB3	15:O:125:VAL:HG11	2.00	0.43
17:Q:38:MET:HB3	17:Q:64:VAL:HG11	2.00	0.43
1:A:271:LEU:HD12	1:A:271:LEU:HA	1.92	0.43
2:B:382:ASP:OD1	2:B:420:LYS:NZ	2.41	0.43
4:D:173:GLN:NE2	4:D:334:PRO:HD2	2.33	0.43
13:m:43:ASP:N	13:m:43:ASP:OD2	2.51	0.43
14:n:18:SER:HB2	14:n:30:VAL:HA	2.01	0.43
18:r:174:VAL:O	18:r:189:SER:HA	2.19	0.43
10:J:146:GLN:OE1	10:J:159:ASN:ND2	2.51	0.43
13:M:40:ARG:HA	13:M:45:VAL:HA	2.00	0.43
20:T:1:THR:N	20:T:105:PRO:O	2.44	0.43
8:h:161:THR:OG1	8:h:171:LYS:NZ	2.50	0.43
13:m:8:ASP:O	13:m:22:GLN:NE2	2.50	0.43
1:A:240:VAL:HG21	1:A:260:LEU:HD21	2.01	0.43
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.92	0.43
7:G:200:THR:HA	7:G:203:SER:HB2	2.01	0.43
7:g:95:ARG:NH1	14:n:68:ILE:O	2.51	0.43
7:g:165:ALA:HB3	8:h:56:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:177:ALA:O	11:k:181:LEU:HB2	2.18	0.43
12:l:164:ARG:NH1	12:l:198:THR:O	2.52	0.43
17:q:38:MET:HG3	17:q:61:GLN:HA	2.01	0.43
20:t:89:HIS:CE1	20:t:131:ALA:HB1	2.53	0.43
3:C:355:SER:OG	3:C:358:GLU:OE1	2.33	0.43
4:D:342:ARG:HB3	4:D:364:VAL:HG11	2.01	0.43
5:E:236:ASP:OD2	5:E:284:THR:OG1	2.36	0.43
12:l:26:MET:HE1	12:l:148:CYS:HB2	2.00	0.43
20:t:42:ILE:HD12	20:t:188:GLN:HG3	2.00	0.43
3:C:141:GLU:HG3	3:C:213:ARG:HD2	2.01	0.43
8:H:222:THR:OG1	8:H:225:GLU:OE1	2.35	0.43
9:I:32:GLY:H	9:I:50:ARG:HH21	1.67	0.43
19:S:145:LEU:HD21	19:S:182:ALA:HB2	2.01	0.43
11:k:196:LYS:NZ	11:k:240:ASP:OD2	2.52	0.43
12:l:198:THR:O	12:l:198:THR:OG1	2.37	0.43
17:q:11:ASP:OD1	17:q:11:ASP:N	2.52	0.43
17:q:118:MET:HE3	17:q:118:MET:HB2	1.86	0.43
20:t:208:ASN:ND2	20:t:210:ASP:OD1	2.52	0.43
2:B:124:SER:HA	2:B:130:GLU:HA	2.01	0.43
5:E:218:MET:HG3	5:E:219:PHE:HD2	1.84	0.43
6:F:169:ASP:HB2	6:F:172:VAL:HG23	2.01	0.43
13:M:8:ASP:OD1	13:M:8:ASP:N	2.52	0.43
18:R:186:ARG:HH22	18:R:189:SER:HB2	1.84	0.43
12:l:47:VAL:HG13	12:l:212:ILE:HG13	2.01	0.43
5:E:258:MET:HA	5:E:261:LEU:HB2	2.01	0.42
7:G:211:LYS:HE2	7:G:211:LYS:HB3	1.90	0.42
15:O:120:ASP:OD1	15:O:120:ASP:N	2.52	0.42
20:T:124:TYR:HE1	20:T:139:THR:HG22	1.84	0.42
7:g:11:ARG:HD3	7:g:11:ARG:HA	1.82	0.42
10:j:40:ILE:HA	10:j:211:MET:O	2.18	0.42
13:m:38:GLY:HA3	13:m:136:MET:HE1	2.01	0.42
19:s:14:ALA:HA	19:s:22:ILE:O	2.19	0.42
2:B:387:LYS:HB3	2:B:390:LEU:HD23	2.01	0.42
3:C:90:HIS:CD2	3:C:91:PRO:HD2	2.54	0.42
3:C:328:ILE:HG22	3:C:359:VAL:HG11	2.00	0.42
4:D:262:ILE:HB	4:D:307:VAL:HG22	2.01	0.42
8:H:33:ALA:O	8:H:77:SER:OG	2.34	0.42
8:H:188:ILE:O	8:H:192:ILE:HG12	2.19	0.42
15:O:163:ILE:HG12	15:O:170:GLY:HA2	2.00	0.42
16:P:13:ALA:HB3	16:P:137:VAL:HG23	2.01	0.42
9:i:99:LEU:O	9:i:102:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:153:VAL:HG13	19:s:166:LEU:HD11	2.01	0.42
4:D:115:ILE:HG22	4:D:139:LEU:HD23	2.00	0.42
4:D:264:ILE:O	4:D:309:MET:HA	2.19	0.42
5:E:365:GLU:HA	5:E:368:MET:HE1	2.00	0.42
7:g:79:VAL:HG12	7:g:139:ILE:HB	1.99	0.42
20:t:211:ILE:HA	20:t:214:MET:HE3	2.01	0.42
2:B:94:GLU:OE2	2:B:97:SER:OG	2.37	0.42
5:E:253:ILE:HG21	6:F:308:ARG:HH21	1.85	0.42
12:L:47:VAL:HG13	12:L:212:ILE:HG13	2.00	0.42
12:L:196:ARG:HE	12:L:239:ARG:HG2	1.84	0.42
11:k:40:ILE:HD12	11:k:198:SER:HB3	2.01	0.42
20:t:3:ASN:OD1	20:t:3:ASN:N	2.51	0.42
2:B:103:ARG:NH1	2:B:151:LEU:HB3	2.34	0.42
2:B:334:ILE:HD12	2:B:337:LEU:HD21	2.01	0.42
3:C:218:GLU:HB3	4:D:275:PHE:HB2	2.01	0.42
7:G:79:VAL:HG12	7:G:139:ILE:HB	2.02	0.42
16:P:58:THR:OG1	17:Q:121:LEU:O	2.23	0.42
16:P:88:MET:HE2	16:P:88:MET:HB3	1.80	0.42
11:k:163:VAL:HG11	12:l:53:GLN:HE22	1.85	0.42
16:p:12:MET:HE1	16:p:170:ALA:HB1	2.01	0.42
16:p:131:MET:HE3	16:p:131:MET:HB2	1.83	0.42
17:q:45:LEU:HB2	17:q:103:LEU:HG	2.02	0.42
19:s:48:ASP:OD1	19:s:48:ASP:N	2.48	0.42
20:t:9:THR:OG1	20:t:10:SER:N	2.50	0.42
8:H:4:ARG:HE	8:H:4:ARG:HB2	1.63	0.42
9:I:232:GLU:HA	9:I:235:GLN:HG3	2.00	0.42
11:k:52:LYS:N	11:k:214:ASN:O	2.49	0.42
18:r:100:MET:HE3	18:r:100:MET:HB2	1.90	0.42
3:C:248:MET:HE1	3:C:273:MET:HG3	2.02	0.42
9:I:8:ARG:HD3	10:J:5:ARG:HH21	1.85	0.42
9:I:36:GLY:O	9:I:161:ALA:HA	2.20	0.42
13:M:5:THR:OG1	13:M:6:GLY:N	2.51	0.42
16:p:36:THR:OG1	16:p:38:ASP:OD1	2.31	0.42
3:C:369:TYR:HD1	3:C:372:ARG:HE	1.67	0.42
11:K:236:GLU:HA	11:K:239:LYS:NZ	2.34	0.42
18:r:103:GLY:HA2	18:r:179:VAL:HG11	2.01	0.42
19:s:169:ASP:HA	19:s:172:MET:HE3	2.02	0.42
2:B:174:MET:H	2:B:174:MET:HG2	1.66	0.42
3:C:240:GLU:OE2	3:C:241:HIS:ND1	2.53	0.42
4:D:146:GLU:H	4:D:252:ARG:HH21	1.66	0.42
7:G:112:ASP:N	7:G:112:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:160:PRO:HB3	16:P:189:ILE:HD11	2.02	0.42
16:P:192:LYS:HE3	16:P:192:LYS:HB2	1.80	0.42
9:i:172:VAL:HA	9:i:175:LEU:HB2	2.01	0.42
13:m:230:ASP:OD1	13:m:230:ASP:N	2.50	0.42
16:p:61:GLN:HE22	17:q:124:LEU:HB2	1.84	0.42
18:r:9:ARG:NH2	18:r:146:ASP:OD1	2.45	0.42
19:s:147:PRO:O	19:s:150:ASP:HB2	2.20	0.42
11:K:183:GLU:HG3	11:K:184:VAL:HG13	2.00	0.42
18:R:100:MET:HB3	18:R:100:MET:HE3	1.68	0.42
20:T:27:LEU:HD11	20:T:34:ALA:HB1	2.02	0.42
11:k:186:HIS:CE1	11:k:189:MET:HG3	2.54	0.42
15:o:63:LEU:HD23	15:o:63:LEU:HA	1.85	0.42
16:p:161:ASP:O	16:p:165:GLU:HG2	2.20	0.42
17:q:21:ALA:HB3	17:q:29:LYS:HB3	2.01	0.42
4:D:284:GLU:O	4:D:288:ILE:HG12	2.20	0.41
9:I:165:GLY:N	9:I:168:SER:HB3	2.35	0.41
11:K:13:ASN:HB3	12:L:126:ARG:HB3	2.00	0.41
16:P:28:PHE:HD2	16:P:36:THR:HG22	1.85	0.41
18:R:175:ASN:OD1	18:R:175:ASN:N	2.53	0.41
7:g:93:ARG:HD2	7:g:93:ARG:HA	1.69	0.41
9:i:41:ASP:OD2	9:i:41:ASP:N	2.51	0.41
13:m:17:ASP:OD2	13:m:19:ARG:NH1	2.53	0.41
20:t:210:ASP:OD1	20:t:210:ASP:N	2.51	0.41
9:I:229:LYS:N	9:I:232:GLU:OE2	2.51	0.41
10:J:5:ARG:O	10:J:123:GLY:N	2.46	0.41
7:g:134:LEU:HD23	7:g:134:LEU:HA	1.93	0.41
12:l:4:ASN:ND2	12:l:7:ASP:OD1	2.53	0.41
12:l:49:LEU:HD21	12:l:199:LEU:HD21	2.01	0.41
17:q:4:LEU:HD21	17:q:132:HIS:HB2	2.02	0.41
20:t:103:MET:HE2	20:t:103:MET:HB2	1.91	0.41
4:D:300:ASP:OD1	4:D:300:ASP:N	2.53	0.41
11:K:91:LYS:HA	11:K:91:LYS:HD2	1.89	0.41
19:S:125:ASP:OD1	19:S:129:SER:N	2.49	0.41
20:T:89:HIS:CE1	20:T:131:ALA:HB1	2.55	0.41
14:N:149:LYS:HD2	14:N:178:ALA:HB1	2.01	0.41
18:r:44:THR:HB	18:r:100:MET:H	1.86	0.41
4:D:245:ARG:HA	4:D:248:ARG:HG2	2.02	0.41
9:I:38:LEU:HB3	9:I:43:VAL:HG23	2.02	0.41
14:N:45:ARG:HD2	14:N:52:THR:HB	2.02	0.41
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.51	0.41
4:D:115:ILE:HA	4:D:139:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:73:THR:HG22	7:G:76:ILE:HB	2.01	0.41
7:G:74:GLU:HG3	7:G:226:LYS:HD2	2.02	0.41
9:I:90:LEU:HB2	9:I:110:LEU:HD11	2.03	0.41
11:K:97:GLN:HB3	18:R:61:ARG:HG3	2.03	0.41
12:L:205:LEU:HB3	12:L:233:LEU:HD11	2.02	0.41
17:Q:30:ASP:OD1	17:Q:30:ASP:N	2.52	0.41
19:S:19:ASP:OD1	19:S:19:ASP:N	2.53	0.41
9:i:140:ASP:N	9:i:140:ASP:OD1	2.54	0.41
11:k:199:LEU:HD21	11:k:217:LEU:HD11	2.03	0.41
17:q:4:LEU:HD22	17:q:47:VAL:HG21	2.02	0.41
3:C:114:VAL:HB	3:C:123:LEU:HD21	2.02	0.41
12:L:180:MET:HE2	12:L:180:MET:H	1.86	0.41
18:R:130:SER:OG	18:R:167:ASP:OD2	2.34	0.41
9:i:91:ARG:HD3	16:p:76:LEU:HB3	2.02	0.41
19:s:114:ASP:OD1	19:s:118:LYS:N	2.42	0.41
1:A:351:ARG:NH1	1:A:378:PRO:O	2.54	0.41
4:D:147:ALA:HB3	4:D:253:LEU:HD13	2.02	0.41
4:D:385:LEU:HD21	4:D:401:LYS:HD2	2.02	0.41
6:F:234:THR:N	22:F:501:ADP:O2A	2.48	0.41
11:K:34:GLY:HA3	11:K:80:GLY:H	1.85	0.41
12:L:40:SER:HB3	12:L:187:LEU:HD22	2.03	0.41
14:N:20:THR:HB	14:N:28:ASN:HB3	2.02	0.41
10:j:67:ASP:OD1	10:j:67:ASP:N	2.54	0.41
11:k:183:GLU:H	11:k:183:GLU:HG2	1.56	0.41
15:o:201:ARG:HD2	15:o:203:ARG:H	1.86	0.41
1:A:164:MET:HB2	1:A:239:ARG:O	2.21	0.41
2:B:265:LYS:O	2:B:269:GLU:HG2	2.20	0.41
15:O:41:ILE:HG12	15:O:102:GLY:HA3	2.03	0.41
16:P:138:VAL:HB	16:P:146:MET:HE3	2.03	0.41
17:Q:88:LEU:HD23	17:Q:88:LEU:HA	1.90	0.41
9:i:229:LYS:N	9:i:232:GLU:OE2	2.53	0.41
13:m:41:CYS:HB3	13:m:186:CYS:HB3	1.70	0.41
14:n:94:LEU:C	14:n:95:MET:HE2	2.46	0.41
16:p:13:ALA:HB3	16:p:137:VAL:HG23	2.03	0.41
19:s:99:ARG:HH21	19:s:102:PHE:HD2	1.68	0.41
3:C:371:LEU:O	3:C:374:ARG:NH1	2.54	0.41
6:F:141:ASP:OD1	6:F:141:ASP:N	2.54	0.41
9:I:15:GLU:HG3	9:I:17:ARG:HG2	2.02	0.41
10:J:17:PHE:HD1	10:J:17:PHE:HA	1.79	0.41
12:L:41:LYS:HE3	12:L:41:LYS:HB2	1.78	0.41
13:M:211:LEU:HD12	13:M:211:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:136:LYS:HD2	19:S:136:LYS:HA	1.88	0.41
19:s:16:ALA:HB2	19:s:121:VAL:HG23	2.03	0.41
19:s:136:LYS:HA	19:s:136:LYS:HD2	1.93	0.41
20:t:45:VAL:HG12	20:t:46:ASN:H	1.86	0.41
2:B:205:LEU:HD23	2:B:205:LEU:HA	1.91	0.40
3:C:123:LEU:HD23	3:C:123:LEU:HA	1.92	0.40
4:D:103:VAL:HG21	4:D:132:LEU:HD21	2.02	0.40
6:F:256:LEU:HD22	6:F:267:LEU:HD23	2.02	0.40
15:O:43:CYS:SG	15:O:56:THR:OG1	2.79	0.40
15:O:163:ILE:HG23	15:O:170:GLY:HA2	2.02	0.40
17:Q:24:ASN:OD1	17:Q:24:ASN:N	2.54	0.40
20:T:15:LYS:HG2	20:T:20:VAL:HG22	2.04	0.40
8:h:222:THR:OG1	8:h:225:GLU:OE1	2.35	0.40
9:i:153:SER:OG	9:i:155:ASN:OD1	2.40	0.40
12:l:64:LEU:HD12	12:l:72:ILE:HD11	2.03	0.40
17:q:83:PHE:O	17:q:87:ASN:ND2	2.41	0.40
20:t:67:LEU:HD23	20:t:67:LEU:HA	1.95	0.40
8:H:72:ILE:HG12	8:H:107:THR:HG22	2.03	0.40
8:H:108:ALA:O	8:H:112:GLN:HG2	2.20	0.40
18:R:196:HIS:O	18:R:200:SER:HB3	2.21	0.40
19:S:28:ARG:NH2	19:S:191:ASP:OD1	2.54	0.40
14:n:52:THR:HG22	14:n:98:ILE:HD11	2.03	0.40
17:q:8:GLN:NE2	17:q:9:GLY:O	2.55	0.40
3:C:89:VAL:HB	3:C:92:GLU:HB3	2.04	0.40
14:N:14:LEU:HD11	14:N:101:ALA:HB3	2.03	0.40
12:l:122:ARG:HB2	12:l:125:ARG:HG3	2.02	0.40
13:m:184:MET:H	13:m:184:MET:HG2	1.67	0.40
15:o:51:ASP:HB3	15:o:94:ILE:HG23	2.02	0.40
2:B:332:ASN:OD1	2:B:332:ASN:N	2.54	0.40
5:E:171:LEU:HB2	5:E:277:MET:HB2	2.03	0.40
9:I:11:ILE:HG22	10:J:7:ILE:HG23	2.03	0.40
13:M:72:HIS:CE1	13:M:105:ASN:HB3	2.56	0.40
19:S:158:MET:HE3	19:S:158:MET:HB2	1.90	0.40
8:h:92:LYS:O	8:h:96:GLN:HG2	2.22	0.40
9:i:233:VAL:O	9:i:237:ILE:HG13	2.22	0.40
11:k:31:ILE:HD13	11:k:140:ALA:HB2	2.03	0.40
16:p:19:CYS:HB3	16:p:191:GLU:HB3	2.02	0.40
16:p:144:GLU:OE1	16:p:144:GLU:N	2.38	0.40
20:t:63:LEU:HD23	20:t:63:LEU:HA	1.95	0.40
2:B:254:GLU:CD	3:C:230:MET:HE1	2.47	0.40
2:B:303:ARG:H	2:B:303:ARG:HG2	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:108:THR:HG21	10:J:145:TYR:HB2	2.04	0.40
9:i:25:MET:O	9:i:28:ILE:HG22	2.22	0.40
20:t:187:PHE:HE2	20:t:189:ILE:HD11	1.87	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	352/433 (81%)	309 (88%)	43 (12%)	0	100	100
2	B	337/440 (77%)	321 (95%)	16 (5%)	0	100	100
3	C	312/406 (77%)	290 (93%)	20 (6%)	2 (1%)	21	52
4	D	336/418 (80%)	294 (88%)	41 (12%)	1 (0%)	36	67
5	E	336/389 (86%)	305 (91%)	31 (9%)	0	100	100
6	F	333/439 (76%)	304 (91%)	29 (9%)	0	100	100
7	G	238/246 (97%)	227 (95%)	11 (5%)	0	100	100
7	g	238/246 (97%)	224 (94%)	14 (6%)	0	100	100
8	H	230/234 (98%)	224 (97%)	6 (3%)	0	100	100
8	h	230/234 (98%)	222 (96%)	8 (4%)	0	100	100
9	I	248/261 (95%)	231 (93%)	17 (7%)	0	100	100
9	i	248/261 (95%)	232 (94%)	16 (6%)	0	100	100
10	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
10	j	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
11	K	224/241 (93%)	214 (96%)	10 (4%)	0	100	100
11	k	224/241 (93%)	217 (97%)	7 (3%)	0	100	100
12	L	236/269 (88%)	222 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	236/269 (88%)	221 (94%)	15 (6%)	0	100	100
13	M	238/255 (93%)	228 (96%)	10 (4%)	0	100	100
13	m	238/255 (93%)	229 (96%)	9 (4%)	0	100	100
14	N	189/239 (79%)	182 (96%)	7 (4%)	0	100	100
14	n	189/239 (79%)	180 (95%)	9 (5%)	0	100	100
15	O	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
15	o	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
16	P	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
16	p	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
17	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
17	q	197/201 (98%)	185 (94%)	12 (6%)	0	100	100
18	R	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
18	r	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
19	S	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
19	s	211/241 (88%)	207 (98%)	4 (2%)	0	100	100
20	T	213/264 (81%)	204 (96%)	9 (4%)	0	100	100
20	t	213/264 (81%)	202 (95%)	11 (5%)	0	100	100
All	All	8166/9413 (87%)	7705 (94%)	458 (6%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	90	HIS
4	D	126	PRO
3	C	128	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	301/372 (81%)	299 (99%)	2 (1%)	76	82
2	B	295/385 (77%)	294 (100%)	1 (0%)	86	87
3	C	270/352 (77%)	268 (99%)	2 (1%)	76	82
4	D	292/366 (80%)	289 (99%)	3 (1%)	68	79
5	E	294/341 (86%)	293 (100%)	1 (0%)	86	87
6	F	285/379 (75%)	284 (100%)	1 (0%)	84	86
7	G	193/210 (92%)	193 (100%)	0	100	100
7	g	193/210 (92%)	192 (100%)	1 (0%)	81	85
8	H	164/191 (86%)	163 (99%)	1 (1%)	78	83
8	h	164/191 (86%)	164 (100%)	0	100	100
9	I	193/221 (87%)	193 (100%)	0	100	100
9	i	193/221 (87%)	193 (100%)	0	100	100
10	J	154/211 (73%)	154 (100%)	0	100	100
10	j	152/211 (72%)	151 (99%)	1 (1%)	76	82
11	K	186/203 (92%)	186 (100%)	0	100	100
11	k	186/203 (92%)	186 (100%)	0	100	100
12	L	198/230 (86%)	196 (99%)	2 (1%)	68	79
12	l	198/230 (86%)	198 (100%)	0	100	100
13	M	192/212 (91%)	190 (99%)	2 (1%)	68	79
13	m	192/212 (91%)	191 (100%)	1 (0%)	81	85
14	N	148/181 (82%)	147 (99%)	1 (1%)	76	82
14	n	148/181 (82%)	148 (100%)	0	100	100
15	O	177/228 (78%)	176 (99%)	1 (1%)	78	83
15	o	177/228 (78%)	177 (100%)	0	100	100
16	P	173/174 (99%)	172 (99%)	1 (1%)	78	83
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	164/171 (96%)	164 (100%)	0	100	100
17	q	164/171 (96%)	164 (100%)	0	100	100
18	R	153/202 (76%)	153 (100%)	0	100	100
18	r	153/202 (76%)	153 (100%)	0	100	100
19	S	174/199 (87%)	174 (100%)	0	100	100
19	s	175/199 (88%)	174 (99%)	1 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	175/215 (81%)	175 (100%)	0	100	100
20	t	175/215 (81%)	175 (100%)	0	100	100
All	All	6624/7891 (84%)	6602 (100%)	22 (0%)	84	87

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

Mol	Chain	Res	Type
1	A	143	ASP
1	A	403	ILE
2	B	125	THR
3	C	109	THR
3	C	296	ASN
4	D	139	LEU
4	D	170	MET
4	D	312	ASN
5	E	275	MET
6	F	154	ASN
8	H	4	ARG
12	L	126	ARG
12	L	228	ASP
13	M	170	GLN
13	M	189	ILE
14	N	142	THR
15	O	194	LYS
16	P	194	LYS
7	g	166	THR
10	j	85	ASN
13	m	220	THR
19	s	157	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	117	GLN
1	A	296	GLN
1	A	379	ASN
2	B	131	HIS
2	B	154	HIS
2	B	368	HIS

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Mol	Chain	Res	Type
3	C	124	HIS
3	C	171	HIS
3	C	392	GLN
4	D	187	HIS
4	D	304	ASN
4	D	353	ASN
4	D	414	HIS
5	E	129	ASN
5	E	190	GLN
5	E	262	ASN
5	E	316	HIS
6	F	321	GLN
6	F	417	HIS
7	G	12	HIS
8	H	95	GLN
8	H	214	ASN
9	I	40	ASN
9	I	95	GLN
9	I	109	GLN
9	I	166	ASN
9	I	167	ASN
10	J	120	GLN
10	J	122	ASN
10	J	175	ASN
11	K	41	GLN
11	K	98	ASN
11	K	152	GLN
11	K	164	GLN
11	K	214	ASN
13	M	170	GLN
14	N	110	GLN
14	N	158	ASN
15	O	80	ASN
15	O	116	HIS
15	O	165	ASN
15	O	193	ASN
17	Q	27	GLN
17	Q	63	ASN
17	Q	65	GLN
17	Q	71	ASN
17	Q	168	GLN
17	Q	174	ASN

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Mol	Chain	Res	Type
18	R	70	ASN
19	S	131	GLN
19	S	160	ASN
7	g	92	GLN
7	g	150	GLN
7	g	224	ASN
8	h	63	HIS
9	i	40	ASN
9	i	146	GLN
9	i	167	ASN
10	j	116	GLN
11	k	41	GLN
11	k	97	GLN
11	k	155	HIS
11	k	178	GLN
12	l	4	ASN
12	l	146	GLN
12	l	166	GLN
12	l	185	ASN
13	m	97	ASN
15	o	35	HIS
15	o	165	ASN
16	p	93	ASN
17	q	193	ASN
18	r	70	ASN
19	s	108	ASN
19	s	163	HIS

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

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	ATP	B	501	-	29,33,33	0.27	0	44,52,52	0.44	1 (2%)
21	ATP	A	501	-	29,33,33	0.29	0	44,52,52	0.46	1 (2%)
21	ATP	D	501	-	29,33,33	0.29	0	44,52,52	0.52	1 (2%)
22	ADP	F	501	-	27,29,29	1.35	4 (14%)	42,45,45	1.95	10 (23%)
21	ATP	E	401	-	29,33,33	0.27	0	44,52,52	0.46	1 (2%)
22	ADP	C	501	-	27,29,29	1.36	4 (14%)	42,45,45	2.00	9 (21%)

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	B	501	-	-	4/22/38/38	0/3/3/3
21	ATP	A	501	-	-	7/22/38/38	0/3/3/3
21	ATP	D	501	-	-	9/22/38/38	0/3/3/3
22	ADP	F	501	-	-	7/16/32/32	0/3/3/3
21	ATP	E	401	-	-	7/22/38/38	0/3/3/3
22	ADP	C	501	-	-	7/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	ADP	C5-C4	4.60	1.47	1.39
22	F	501	ADP	C5-C4	4.49	1.47	1.39
22	C	501	ADP	C5-C6	2.68	1.48	1.41
22	F	501	ADP	C5-C6	2.62	1.48	1.41
22	F	501	ADP	C8-N7	2.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	ADP	C8-N7	2.31	1.36	1.31
22	C	501	ADP	C5-N7	-2.26	1.34	1.39
22	F	501	ADP	C5-N7	-2.20	1.34	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	501	ADP	C5-C4-N3	-6.61	118.12	126.75
22	F	501	ADP	C5-C4-N3	-6.14	118.74	126.75
22	C	501	ADP	N3-C4-N9	5.20	135.66	127.08
22	F	501	ADP	N3-C4-N9	4.74	134.90	127.08
22	C	501	ADP	C2-N3-C4	3.98	121.14	111.75
22	F	501	ADP	PA-O3A-PB	-3.93	119.34	132.83
22	F	501	ADP	C2-N3-C4	3.77	120.66	111.75
22	C	501	ADP	PA-O3A-PB	-3.23	121.75	132.83
22	C	501	ADP	C4-C5-N7	-3.21	106.71	110.62
22	F	501	ADP	C4-C5-N7	-3.20	106.72	110.62
22	C	501	ADP	N3-C2-N1	-3.07	123.80	128.60
22	F	501	ADP	N3-C2-N1	-3.00	123.91	128.60
22	C	501	ADP	C5-N7-C8	2.74	107.41	103.51
22	F	501	ADP	C5-N7-C8	2.60	107.20	103.51
22	C	501	ADP	C3'-C2'-C1'	2.59	106.35	101.43
22	F	501	ADP	C4-N9-C8	2.40	108.33	105.73
22	F	501	ADP	C3'-C2'-C1'	2.29	105.79	101.43
22	C	501	ADP	C4-N9-C8	2.28	108.19	105.73
22	F	501	ADP	C6-C5-N7	2.11	135.95	132.02
21	A	501	ATP	PB-O3B-PG	2.05	139.85	132.83
21	B	501	ATP	PB-O3B-PG	2.03	139.78	132.83
21	D	501	ATP	PB-O3B-PG	2.02	139.76	132.83
21	E	401	ATP	PB-O3B-PG	2.02	139.74	132.83

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	501	ATP	C5'-O5'-PA-O1A
21	A	501	ATP	C3'-C4'-C5'-O5'
21	B	501	ATP	PB-O3B-PG-O3G
21	B	501	ATP	C5'-O5'-PA-O1A
21	B	501	ATP	C5'-O5'-PA-O2A
21	D	501	ATP	C5'-O5'-PA-O3A
21	E	401	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
22	C	501	ADP	C5'-O5'-PA-O1A
22	C	501	ADP	C3'-C4'-C5'-O5'
22	F	501	ADP	C5'-O5'-PA-O1A
22	F	501	ADP	C5'-O5'-PA-O3A
22	F	501	ADP	O4'-C4'-C5'-O5'
22	F	501	ADP	C3'-C4'-C5'-O5'
21	D	501	ATP	O4'-C4'-C5'-O5'
22	C	501	ADP	O4'-C4'-C5'-O5'
21	D	501	ATP	O4'-C1'-N9-C4
21	A	501	ATP	O4'-C4'-C5'-O5'
21	E	401	ATP	O4'-C4'-C5'-O5'
21	E	401	ATP	C3'-C4'-C5'-O5'
21	D	501	ATP	O4'-C1'-N9-C8
21	D	501	ATP	C3'-C4'-C5'-O5'
22	F	501	ADP	C2'-C1'-N9-C8
21	A	501	ATP	C5'-O5'-PA-O3A
22	C	501	ADP	C5'-O5'-PA-O3A
22	C	501	ADP	PB-O3A-PA-O1A
21	A	501	ATP	C5'-O5'-PA-O2A
21	D	501	ATP	C5'-O5'-PA-O1A
21	D	501	ATP	C5'-O5'-PA-O2A
21	E	401	ATP	C5'-O5'-PA-O2A
22	C	501	ADP	C5'-O5'-PA-O2A
21	A	501	ATP	PG-O3B-PB-O2B
22	F	501	ADP	C2'-C1'-N9-C4
21	E	401	ATP	PA-O3A-PB-O1B
22	F	501	ADP	O4'-C1'-N9-C8
21	A	501	ATP	PB-O3B-PG-O2G
21	B	501	ATP	C5'-O5'-PA-O3A
21	E	401	ATP	C5'-O5'-PA-O3A
21	D	501	ATP	PA-O3A-PB-O1B
21	E	401	ATP	PA-O3A-PB-O2B
22	C	501	ADP	PB-O3A-PA-O2A
21	D	501	ATP	C2'-C1'-N9-C8

There are no ring outliers.

4 monomers are involved in 5 short contacts:

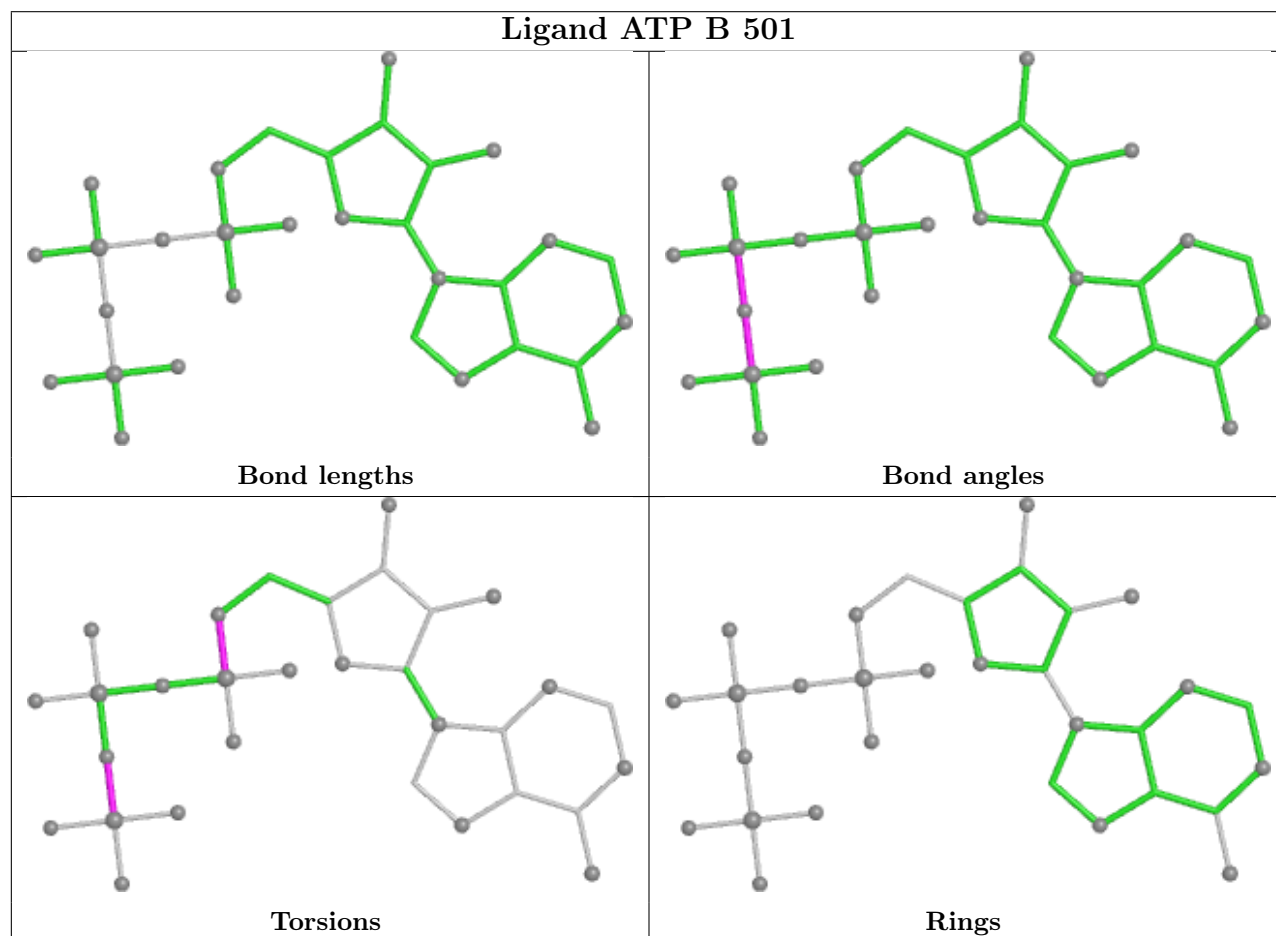
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	501	ATP	1	0
21	A	501	ATP	1	0
22	F	501	ADP	2	0

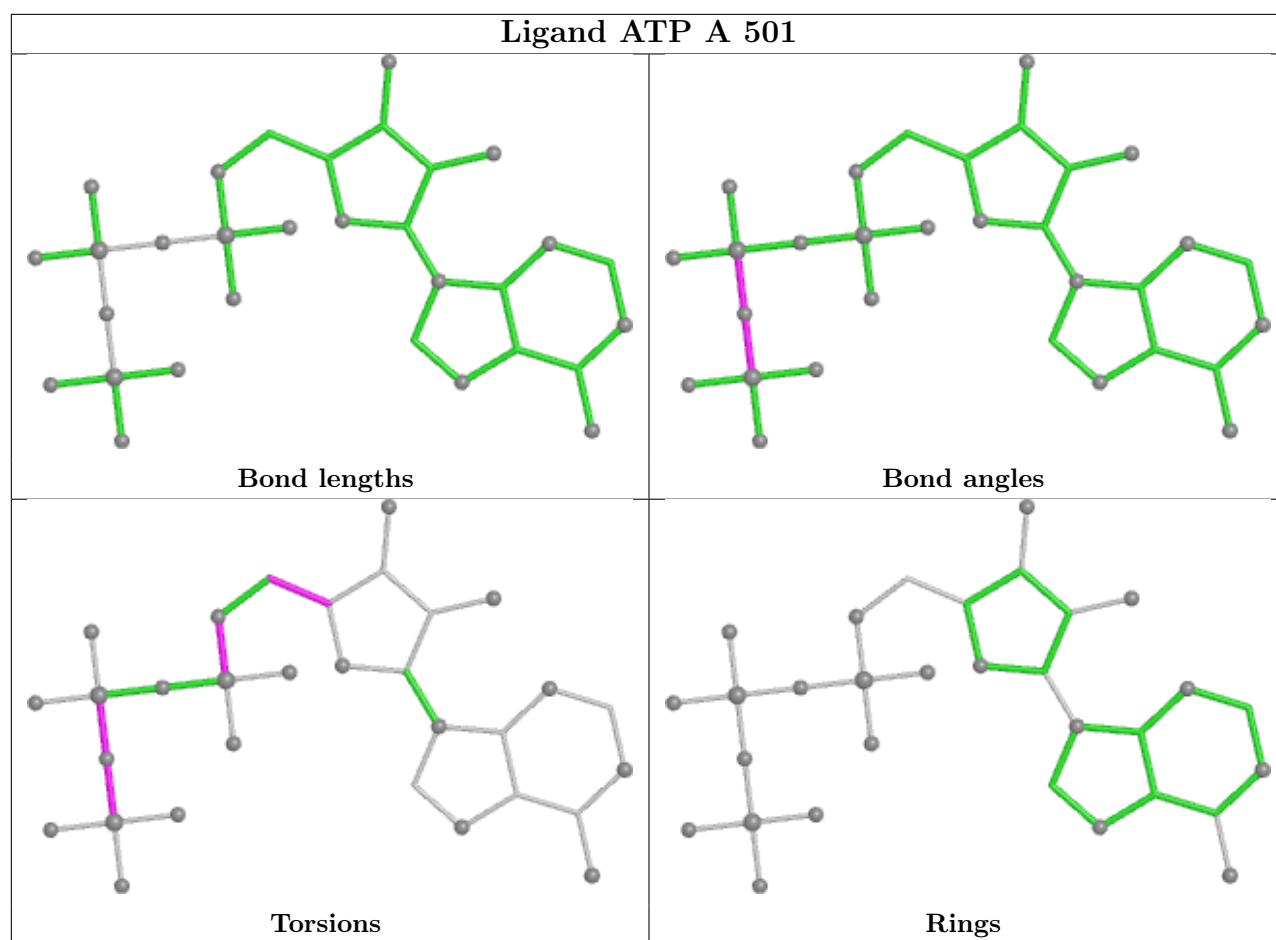
Continued on next page...

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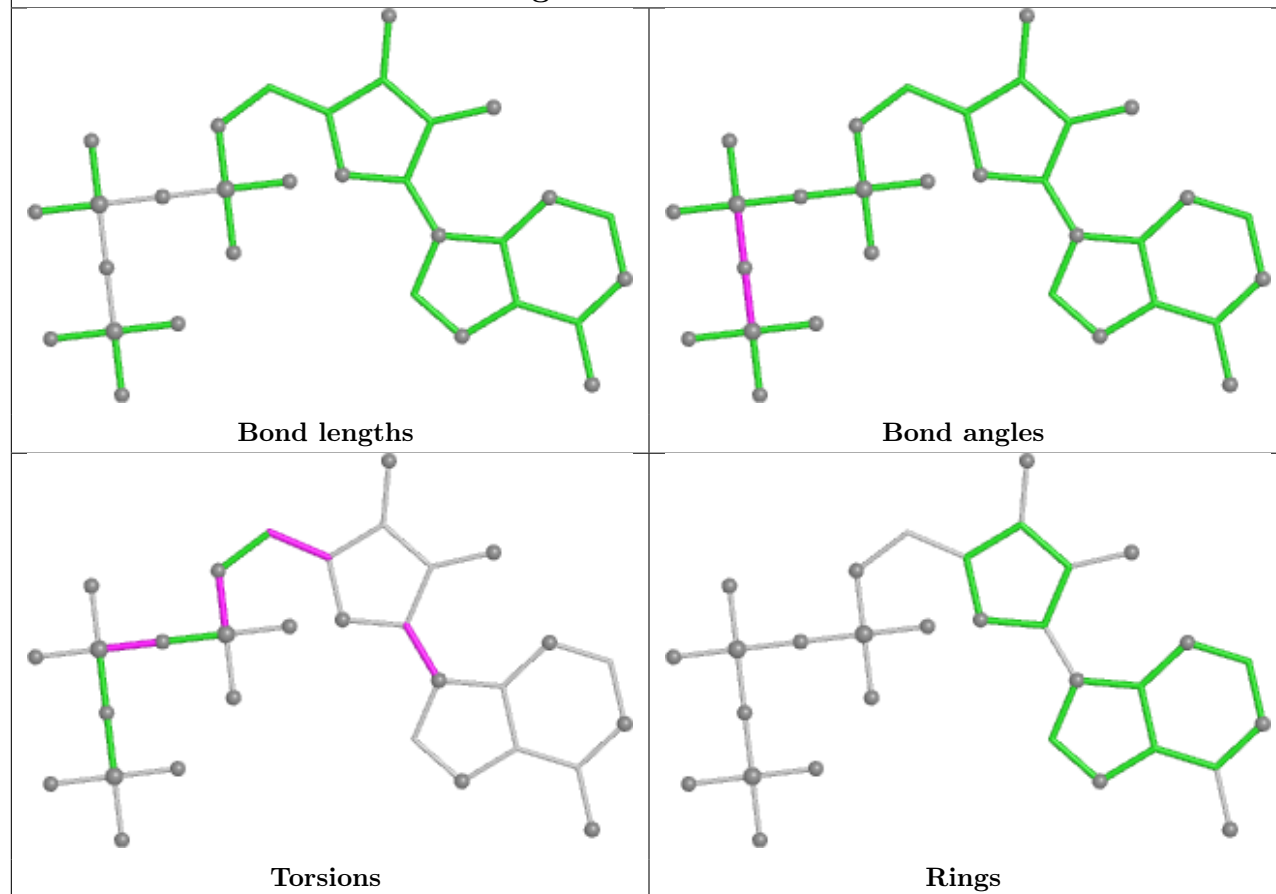
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	501	ADP	1	0

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

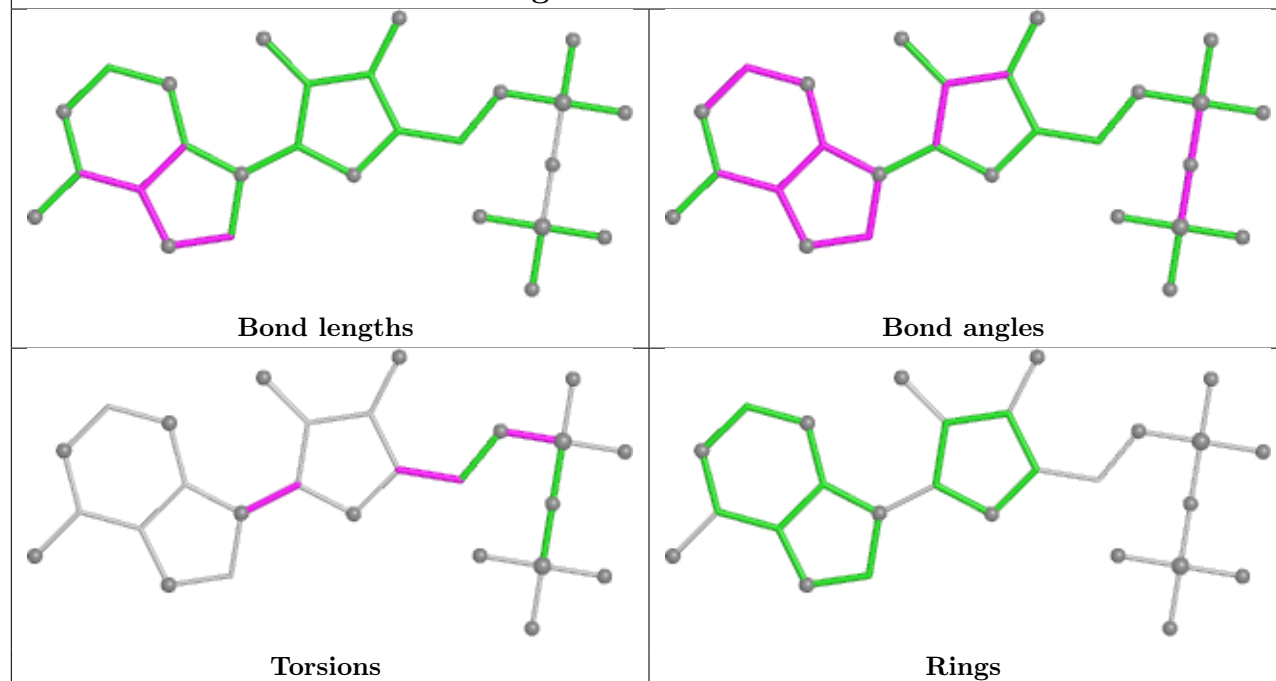




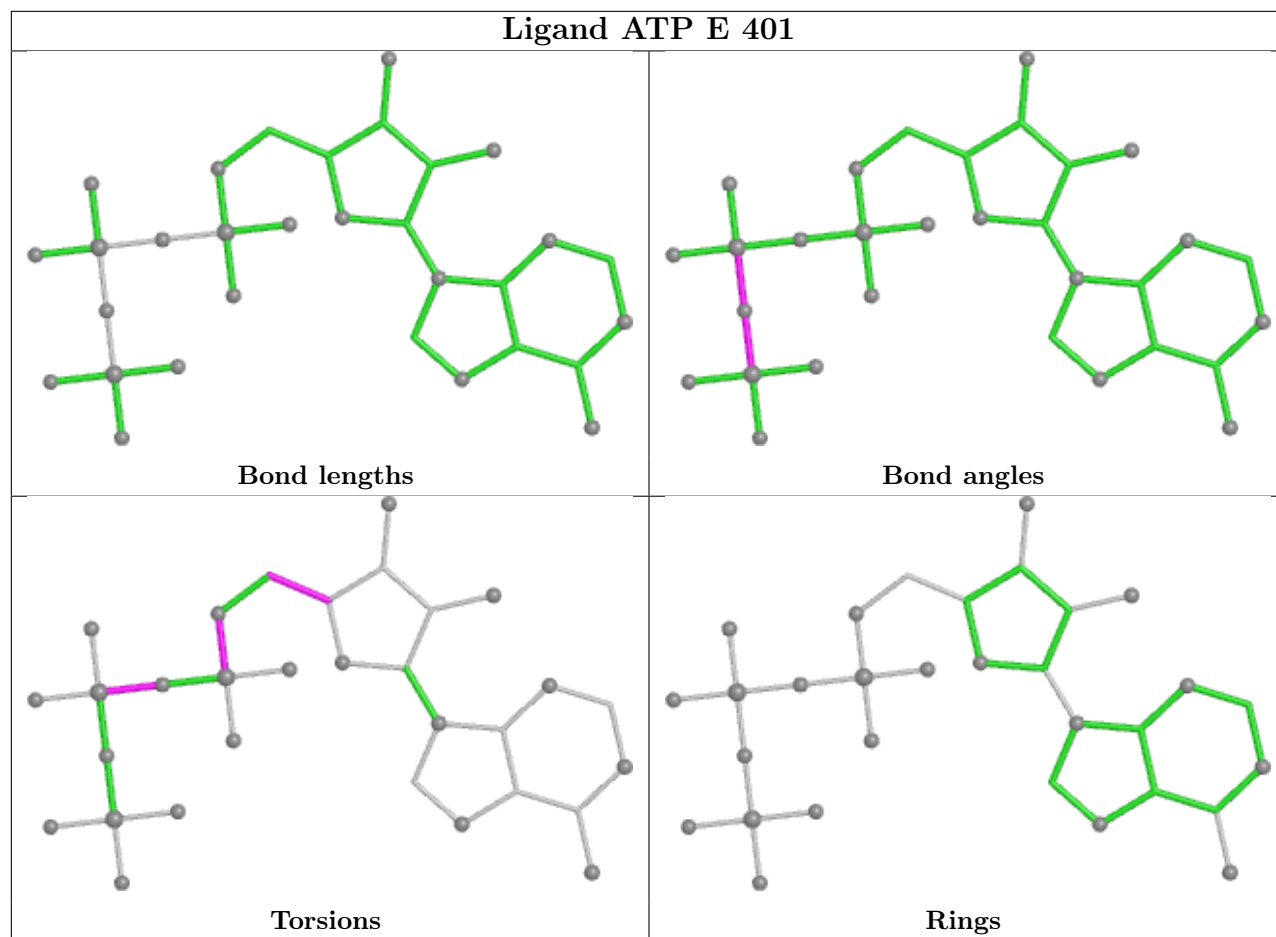
Ligand ATP D 501



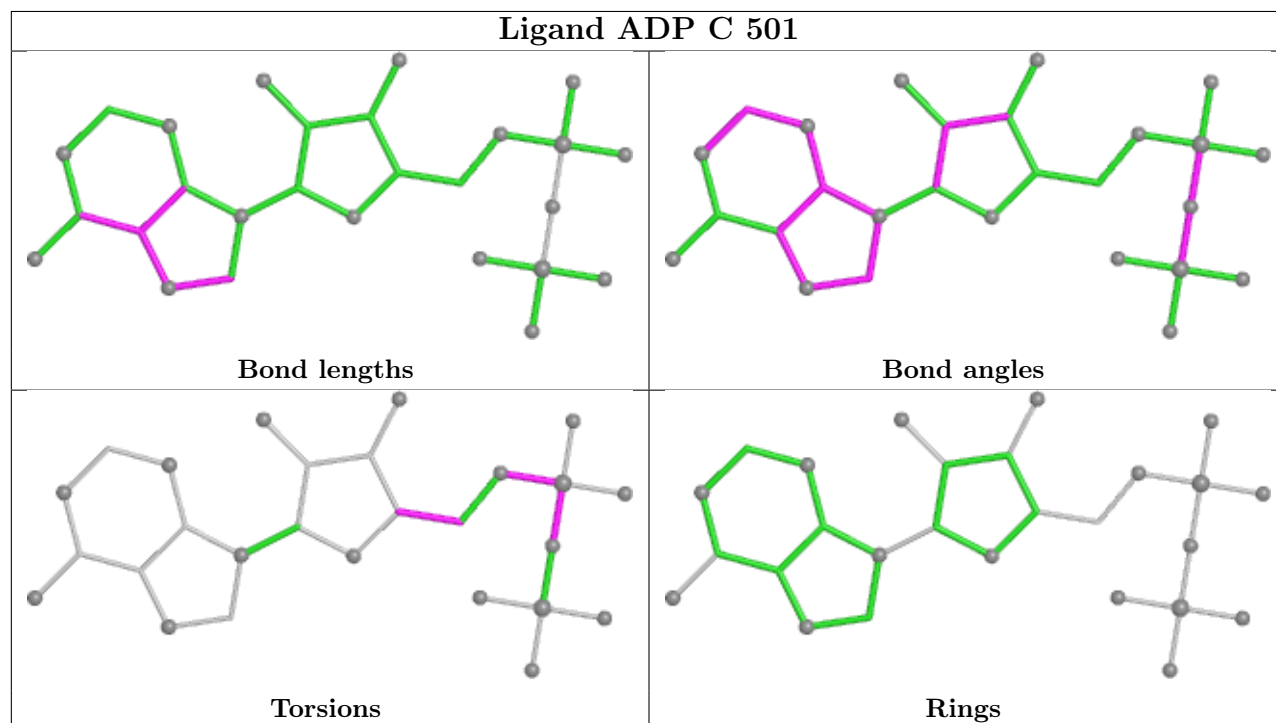
Ligand ADP F 501



Ligand ATP E 401



Ligand ADP C 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

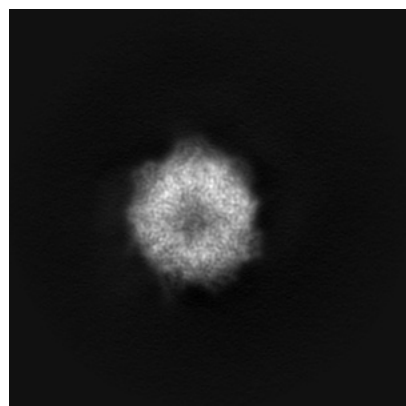
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65361. These allow visual inspection of the internal detail of the map and identification of artifacts.

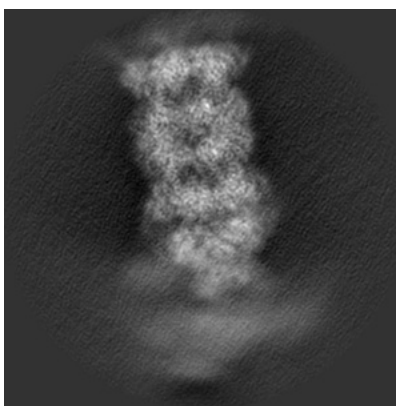
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

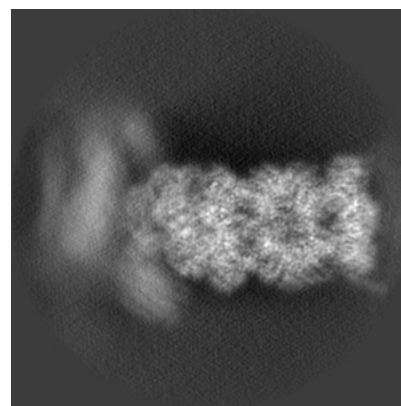
6.1.1 Primary map



X

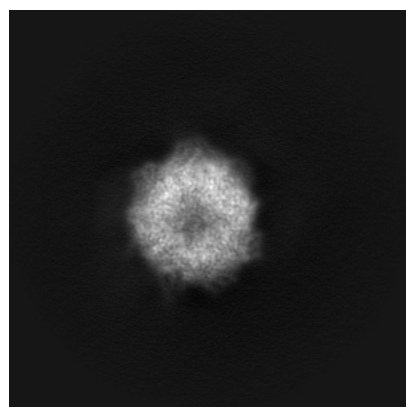


Y

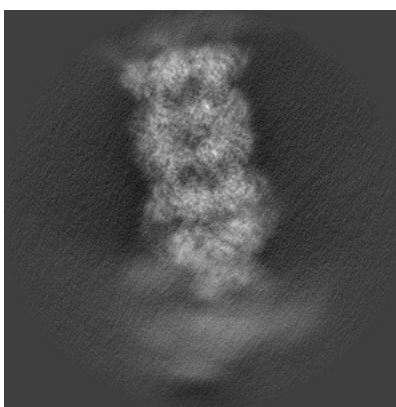


Z

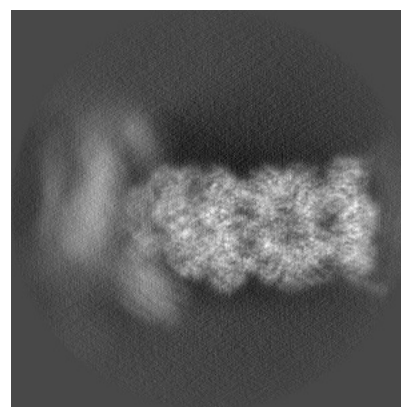
6.1.2 Raw map



X



Y

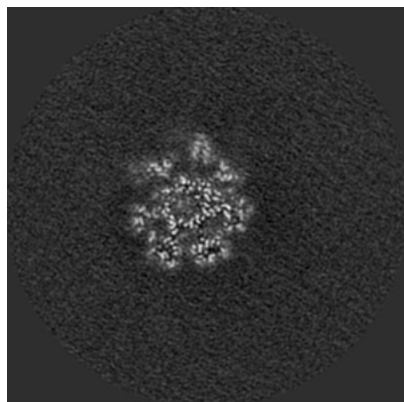


Z

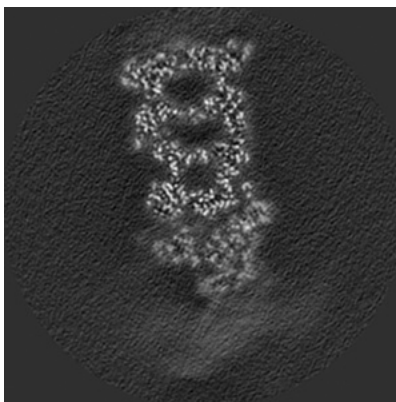
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

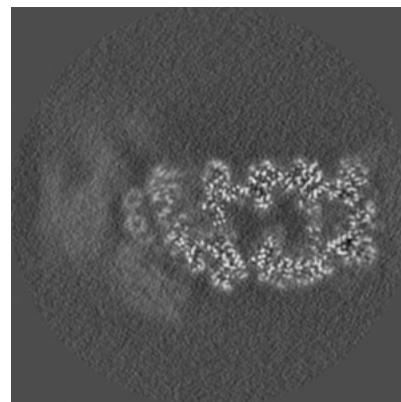
6.2.1 Primary map



X Index: 220

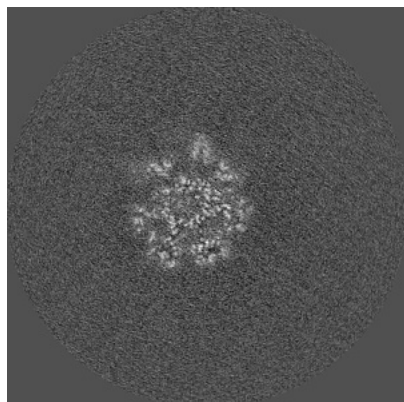


Y Index: 220

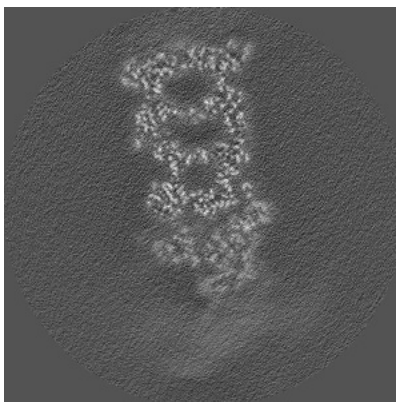


Z Index: 220

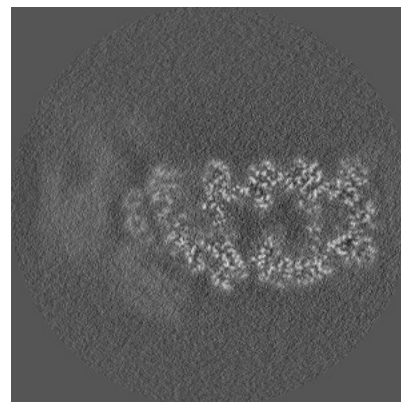
6.2.2 Raw map



X Index: 220



Y Index: 220

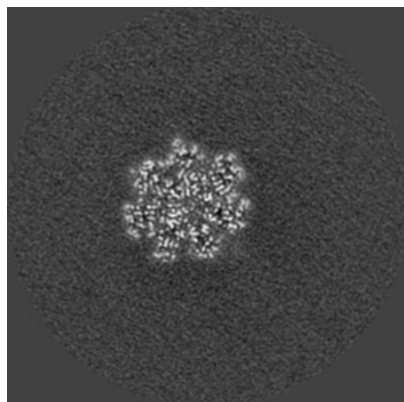


Z Index: 220

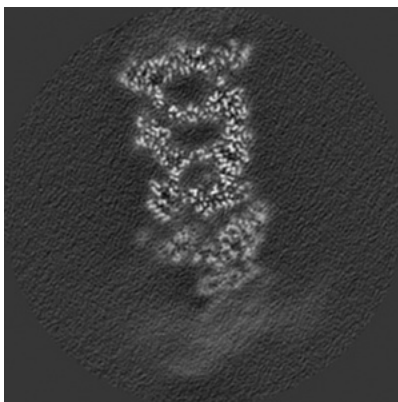
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

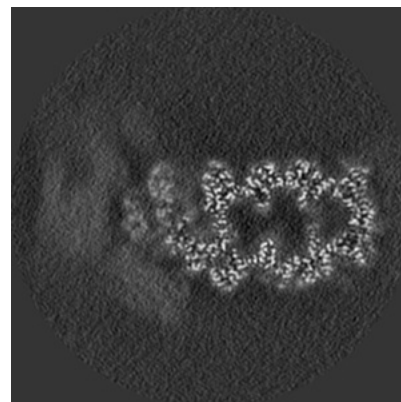
6.3.1 Primary map



X Index: 236

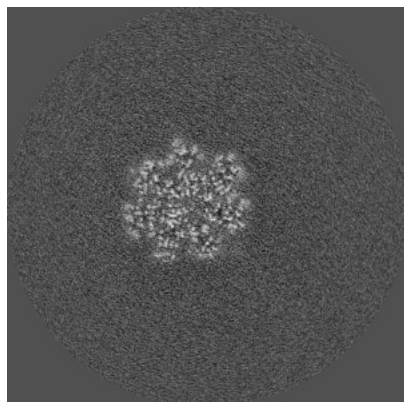


Y Index: 223

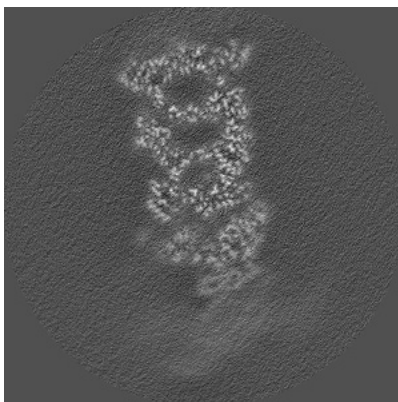


Z Index: 217

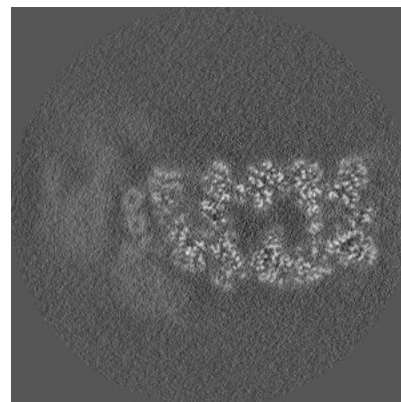
6.3.2 Raw map



X Index: 236



Y Index: 223

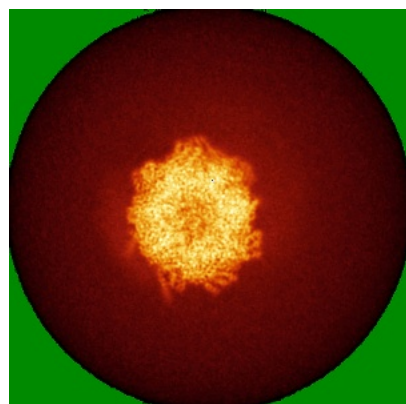


Z Index: 222

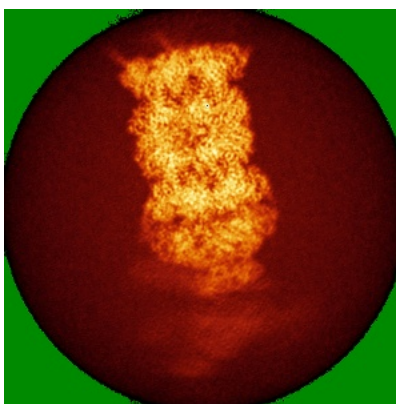
The images above show the largest variance slices of the map in three orthogonal directions.

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

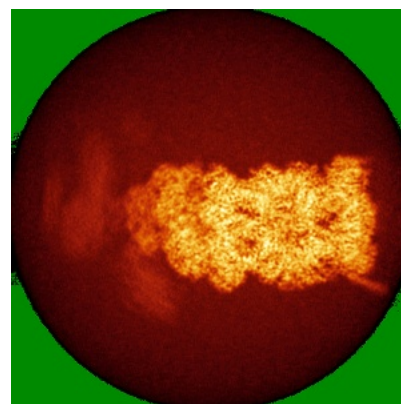
6.4.1 Primary map



X

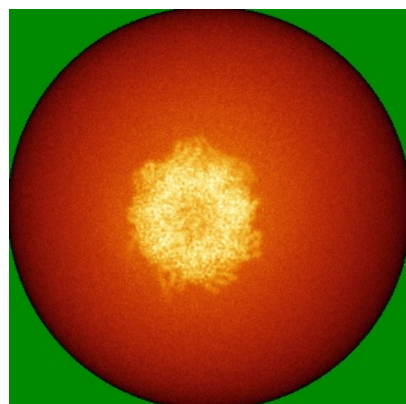


Y

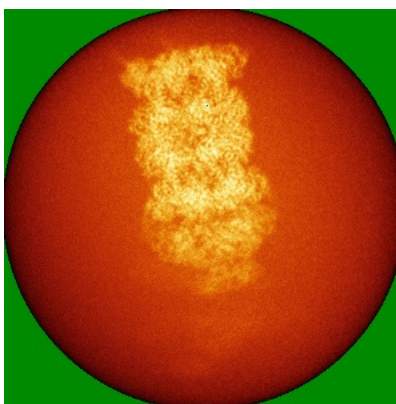


Z

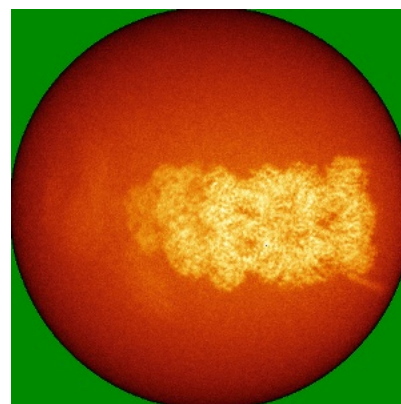
6.4.2 Raw map



X



Y

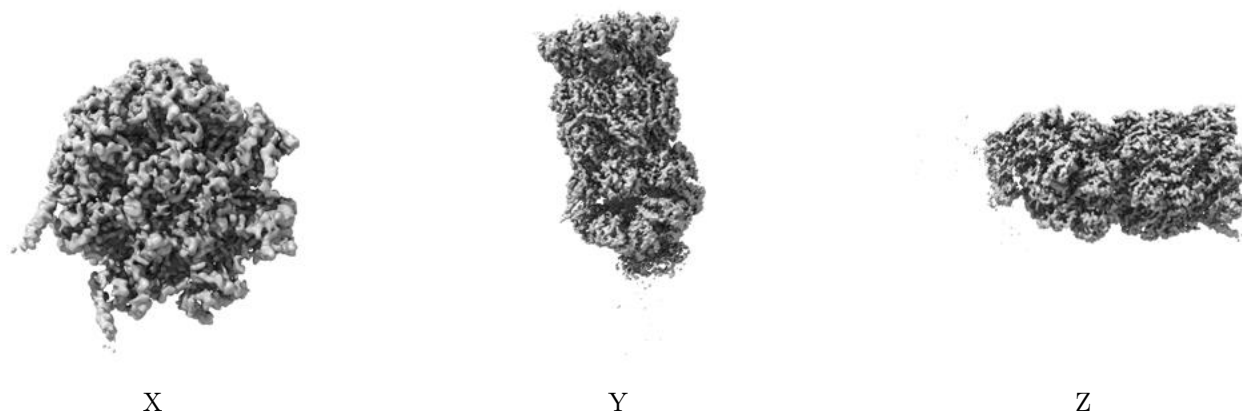


Z

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.

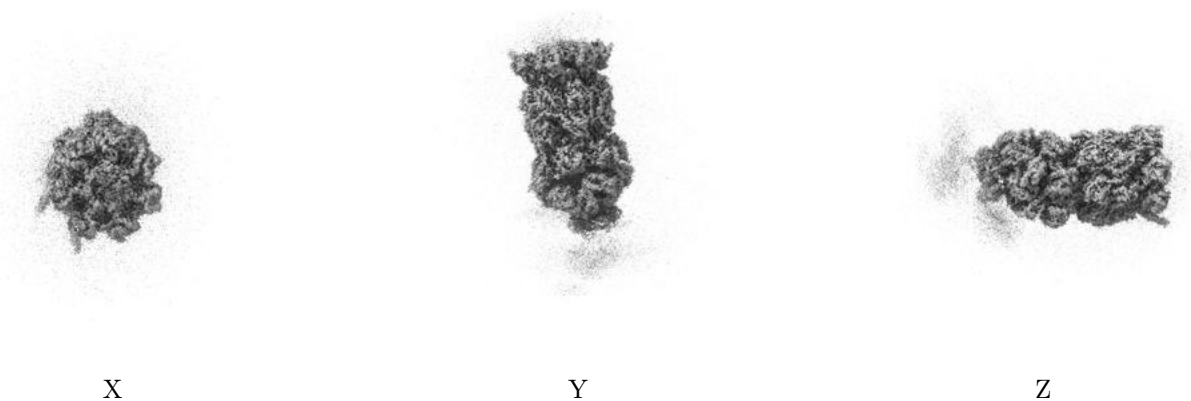
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

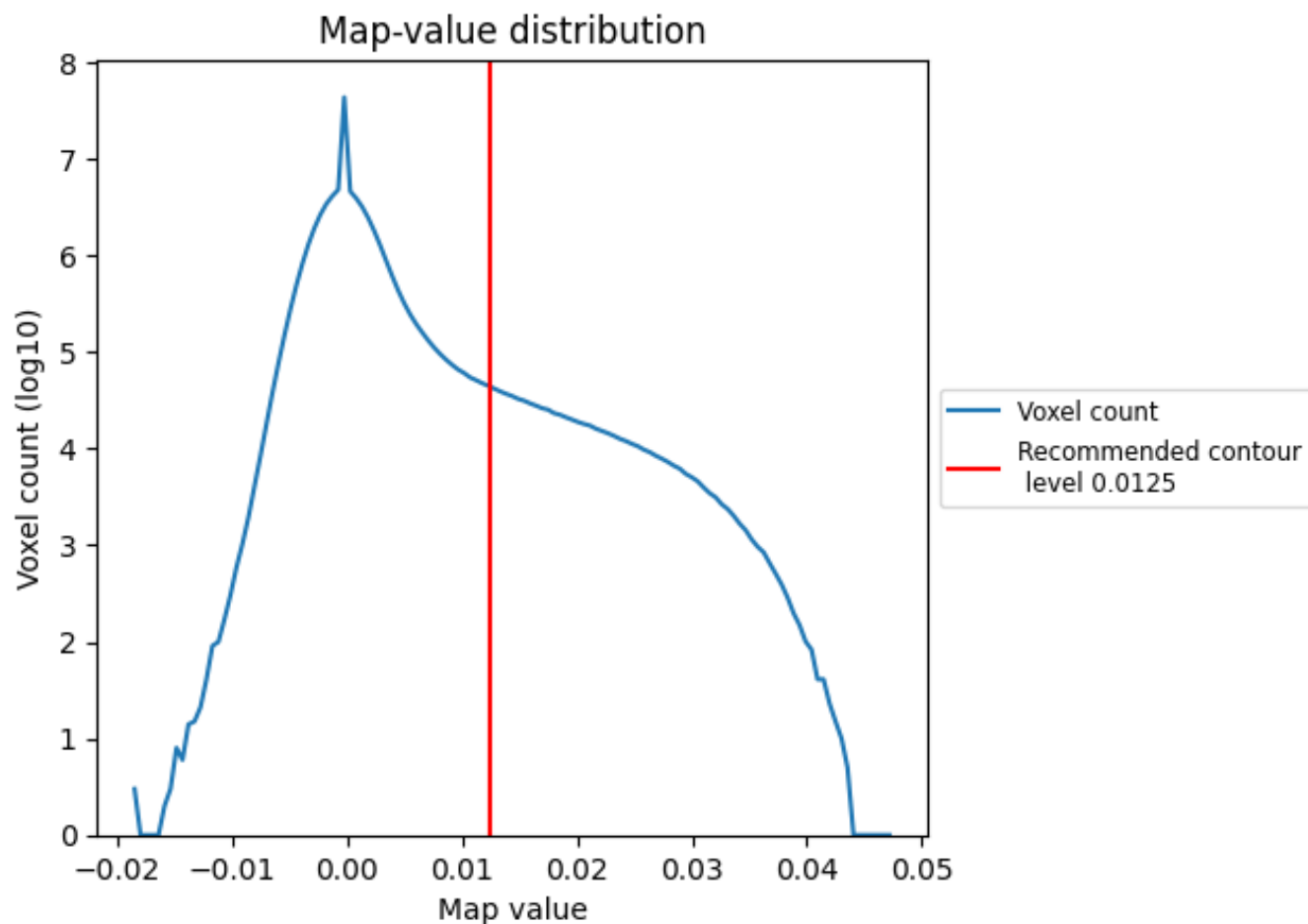
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

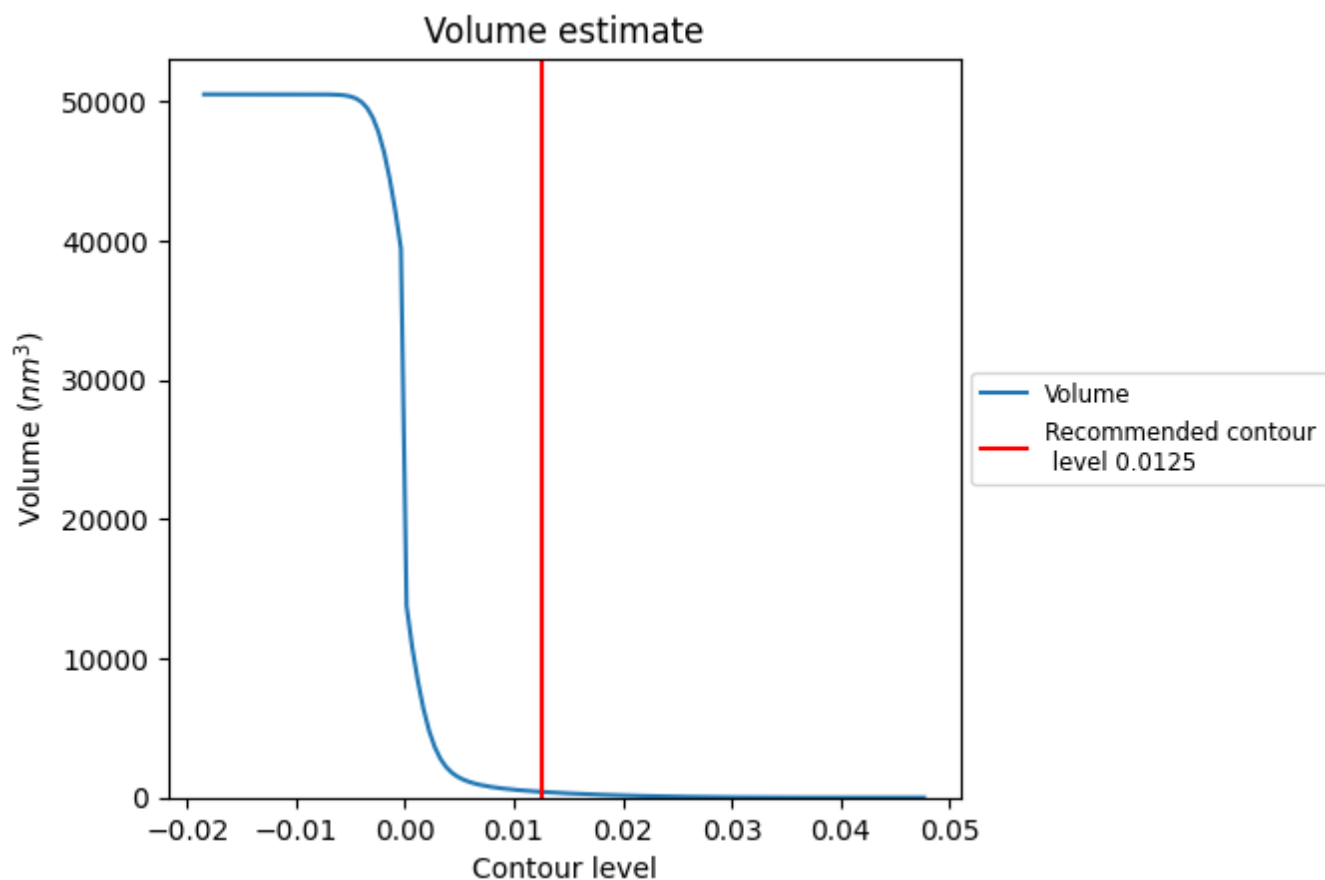
This section contains the results of statistical analysis of the map.

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.

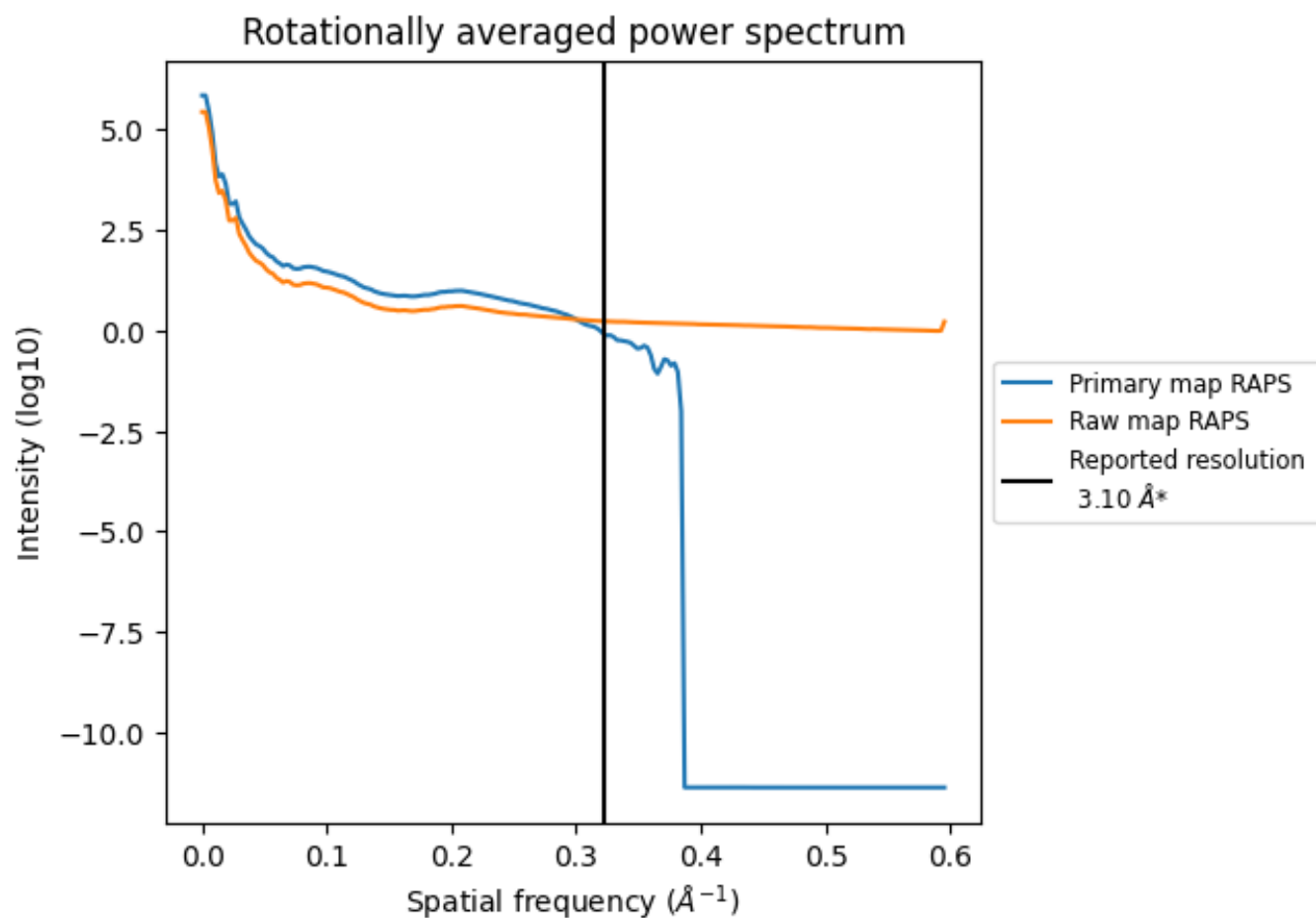
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm³; this corresponds to an approximate mass of 373 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 ⓘ

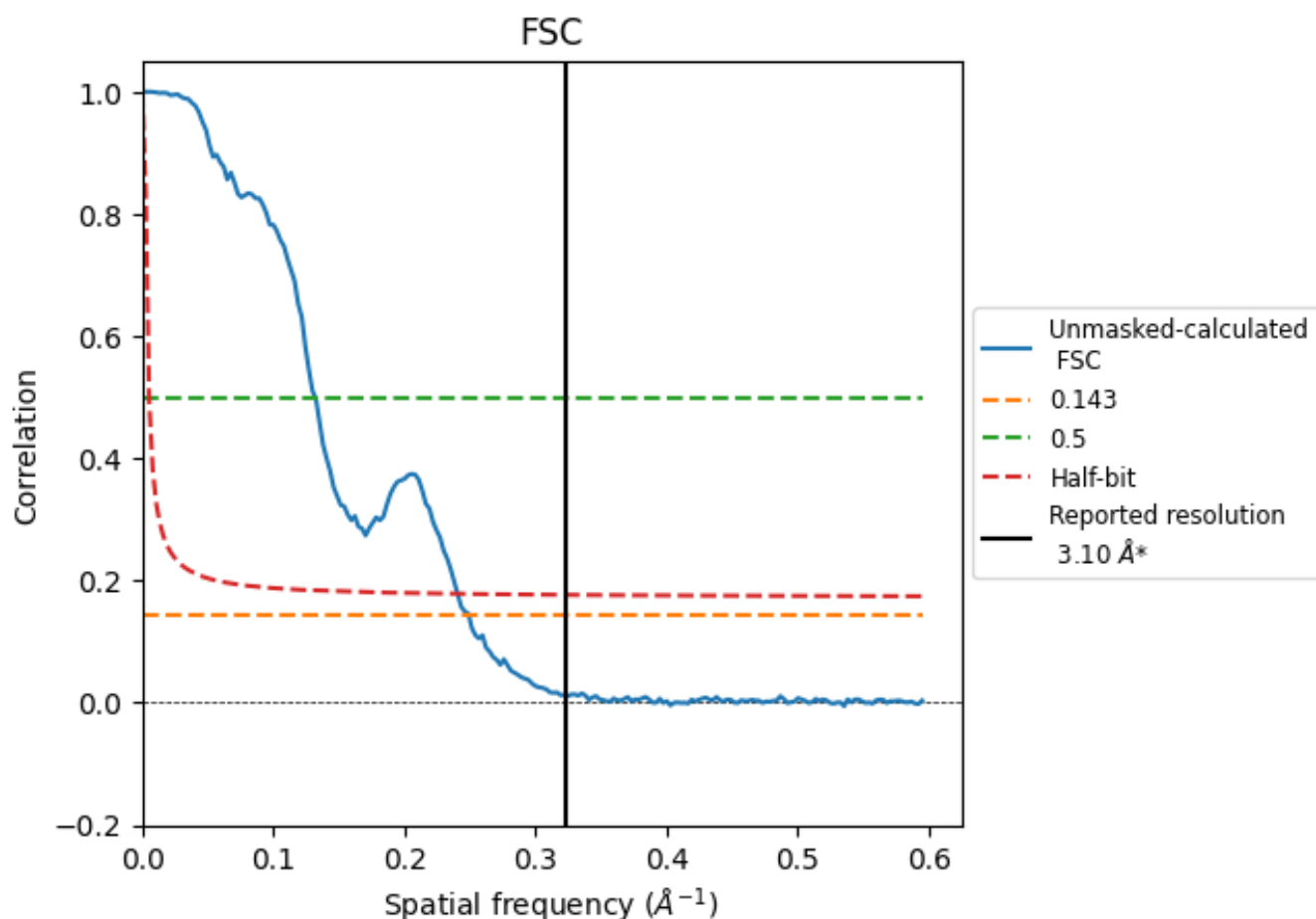


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

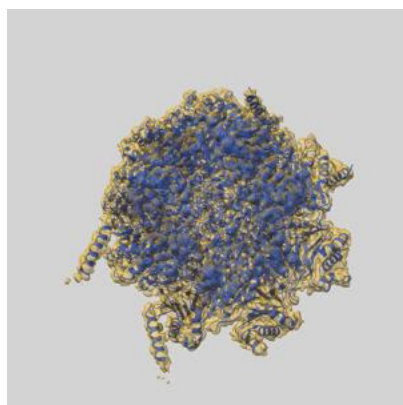
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.58	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.1 by more than 10 %

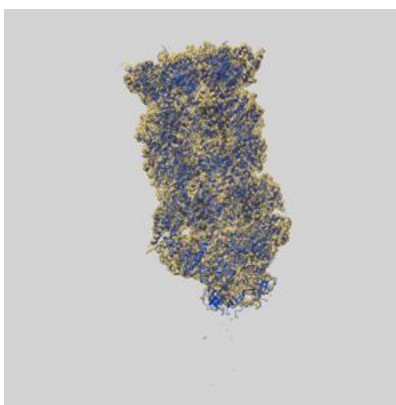
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65361 and PDB model 9VUF. Per-residue inclusion information can be found in section 3 on page 11.

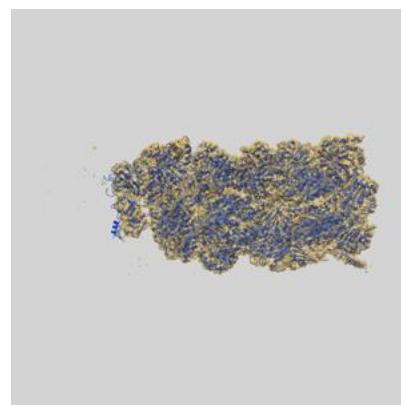
9.1 Map-model overlay [i](#)



X



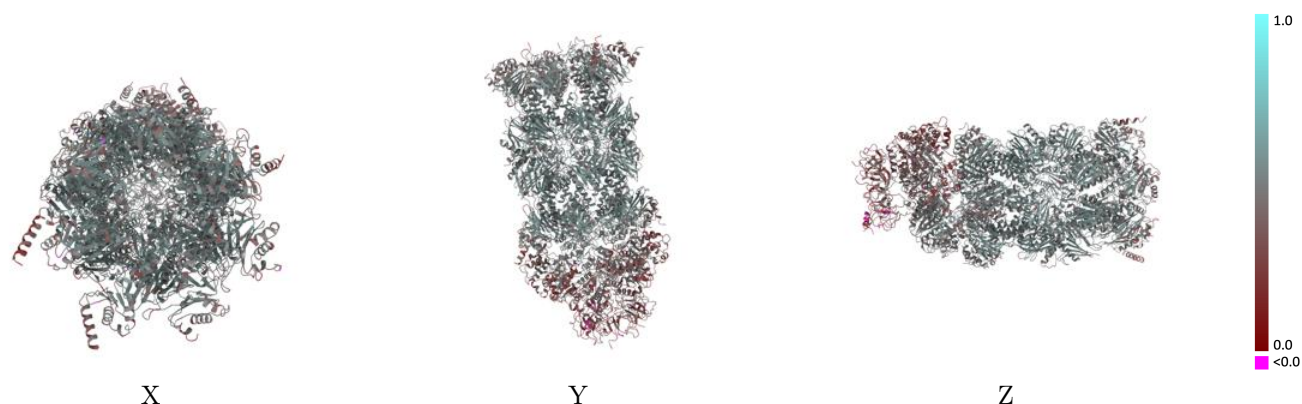
Y



Z

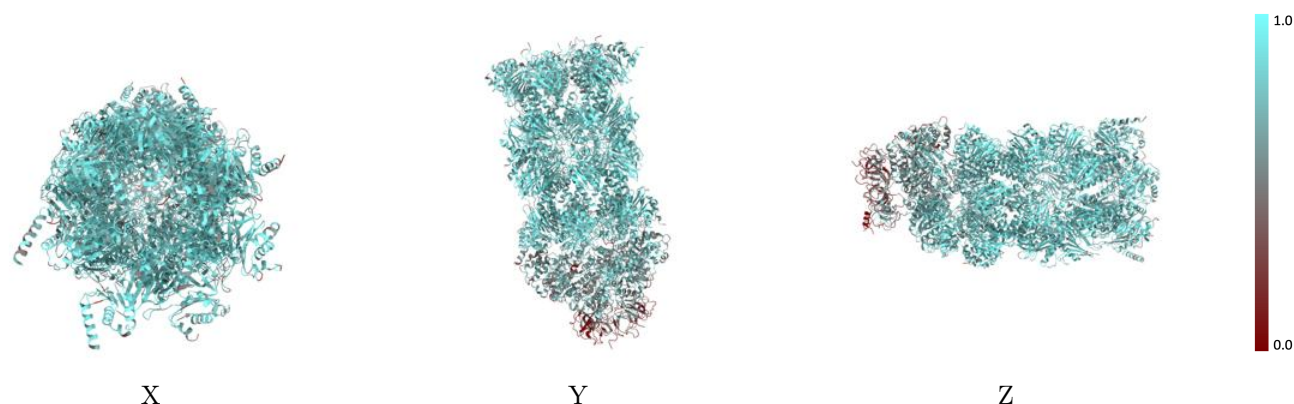
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



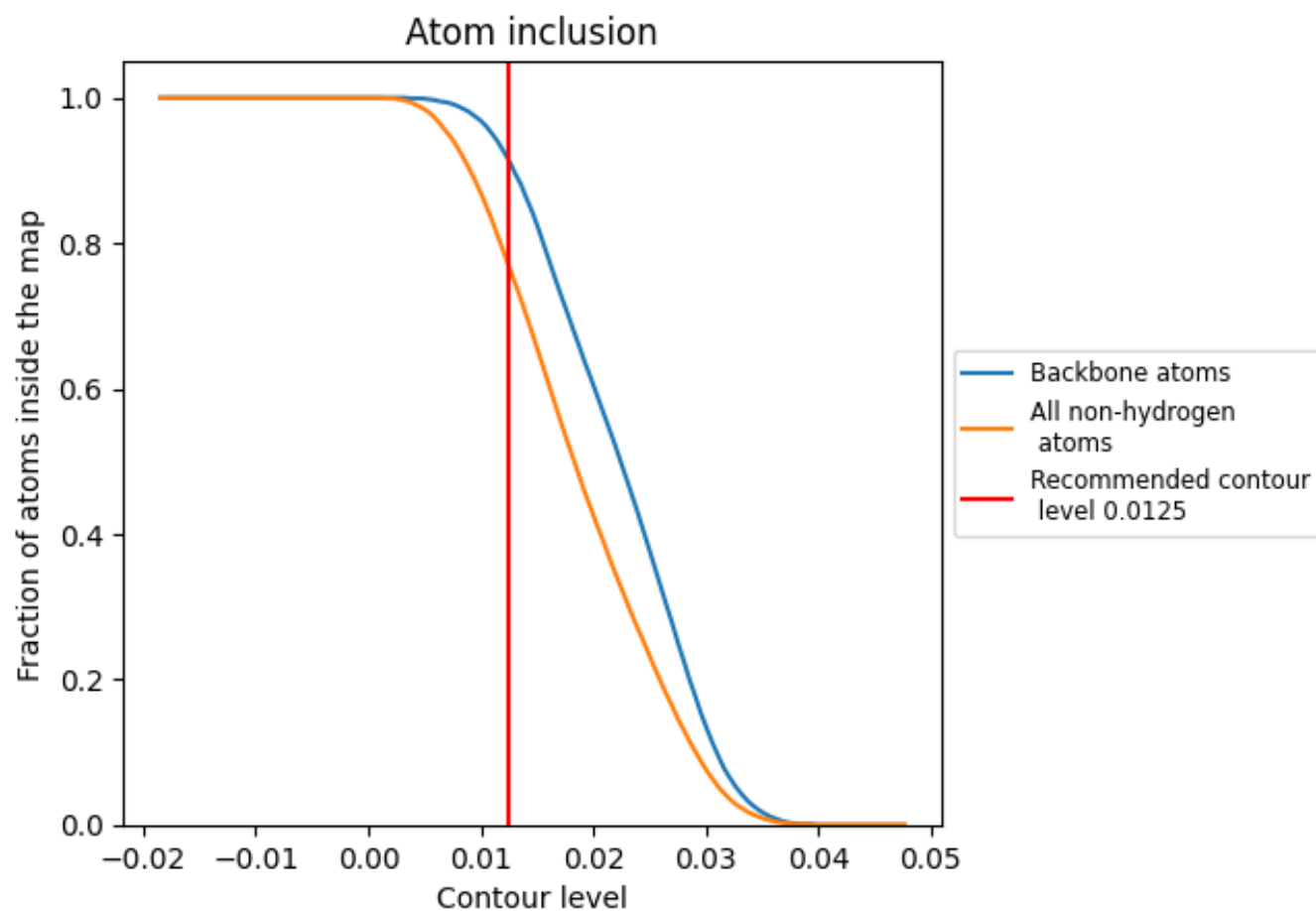
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 77% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.4730
A	 0.6750	 0.4370
B	 0.5820	 0.3780
C	 0.5160	 0.3440
D	 0.5300	 0.3290
E	 0.5840	 0.3400
F	 0.6470	 0.4120
G	 0.8350	 0.5110
H	 0.8630	 0.5290
I	 0.8010	 0.4880
J	 0.8340	 0.5050
K	 0.8000	 0.5130
L	 0.8430	 0.5090
M	 0.8200	 0.4900
N	 0.8750	 0.5360
O	 0.8550	 0.5260
P	 0.8620	 0.5370
Q	 0.8530	 0.5290
R	 0.8660	 0.5360
S	 0.8510	 0.5150
T	 0.8630	 0.5280
g	 0.7880	 0.4760
h	 0.7930	 0.4830
i	 0.7610	 0.4590
j	 0.8000	 0.4680
k	 0.7700	 0.4700
l	 0.7950	 0.4750
m	 0.7850	 0.4700
n	 0.8600	 0.5280
o	 0.8480	 0.5230
p	 0.8430	 0.5290
q	 0.8420	 0.5180
r	 0.8740	 0.5290
s	 0.8480	 0.5220
t	 0.8650	 0.5300

