



## Full wwPDB EM Validation Report ⓘ

Jun 9, 2026 – 08:52 PM JST

PDB ID : 9VUG / pdb\_00009vug  
EMDB ID : EMD-65362  
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 : 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](mailto: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>.

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

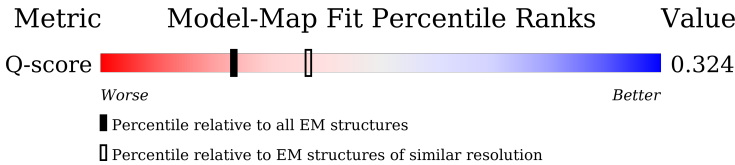
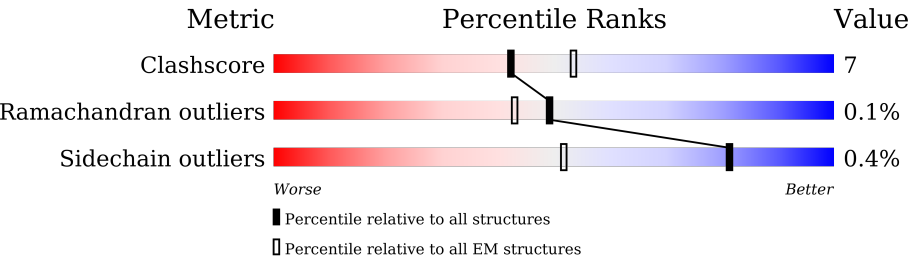
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 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  $\geq 3$ , 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	
2	B	440	
3	C	406	
4	D	418	







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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	
21	f	908	

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 68847 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	380	Total	C	N	O	S	0	0
			2893	1817	515	543	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	370	Total	C	N	O	S	0	0
			2806	1763	478	553	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	319	Total	C	N	O	S	0	0
			2486	1572	441	456	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	333	Total	C	N	O	S	0	0
			2625	1658	455	499	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	336	Total	C	N	O	S	0	0
			2651	1670	471	494	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
			2628	1660	452	501	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	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	230	Total	C	N	O	S	0	0
			1688	1070	284	329	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	248	Total	C	N	O	S	0	0
			1895	1195	324	368	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
			1704	1056	308	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
			1729	1086	284	349	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
			1585	1010	262	294	19		
16	p	204	Total	C	N	O	S	0	0
			1585	1010	262	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
			1641	1036	282	313	10		

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

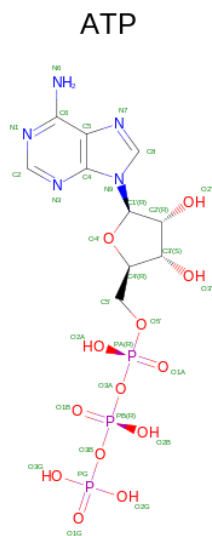
Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
20	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	f	689	Total	C	N	O	S	0	0
			5319	3343	904	1037	35		

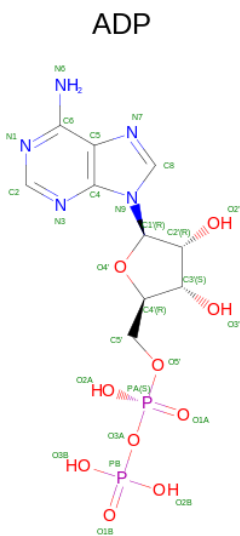
- Molecule 22 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





Id	Chain	Residues	Atoms					AltConf
22	A	1	Total 31	C 10	N 5	O 13	P 3	0
22	C	1	Total 31	C 10	N 5	O 13	P 3	0
22	D	1	Total 31	C 10	N 5	O 13	P 3	0
22	F	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).

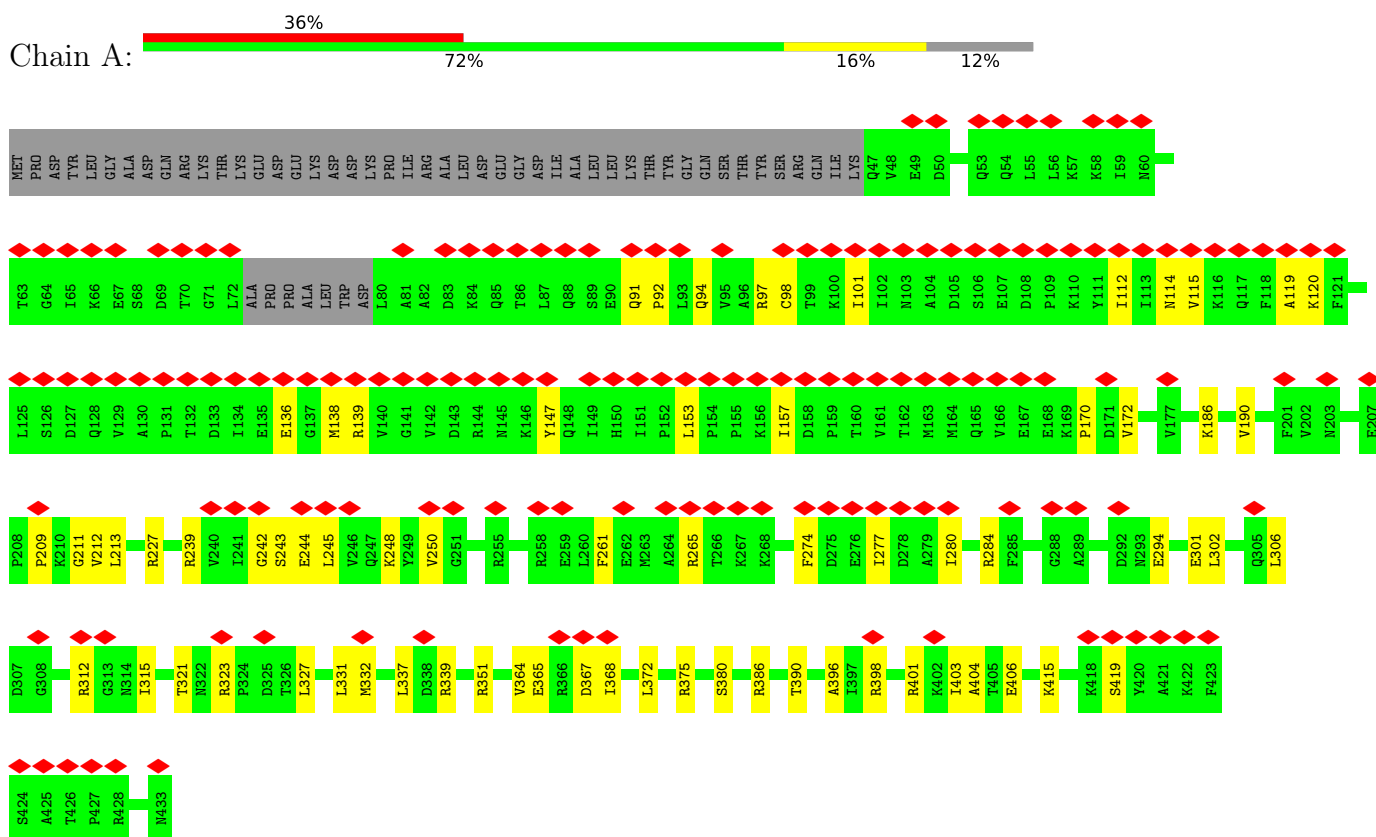


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	D	1	27	10	5	10	2	0

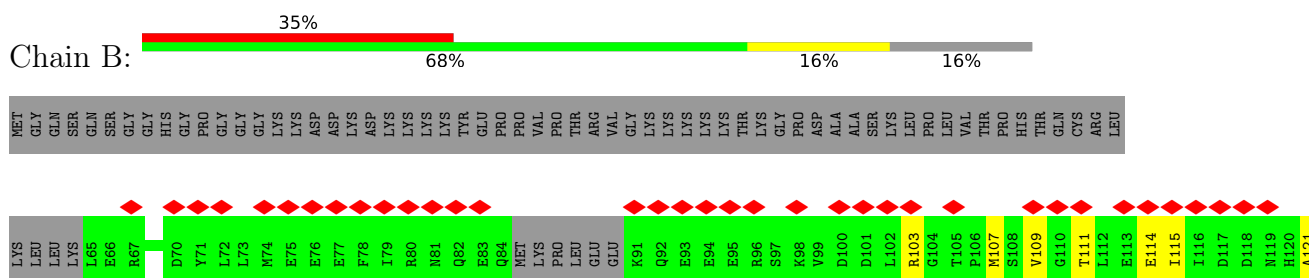
### 3 Residue-property plots

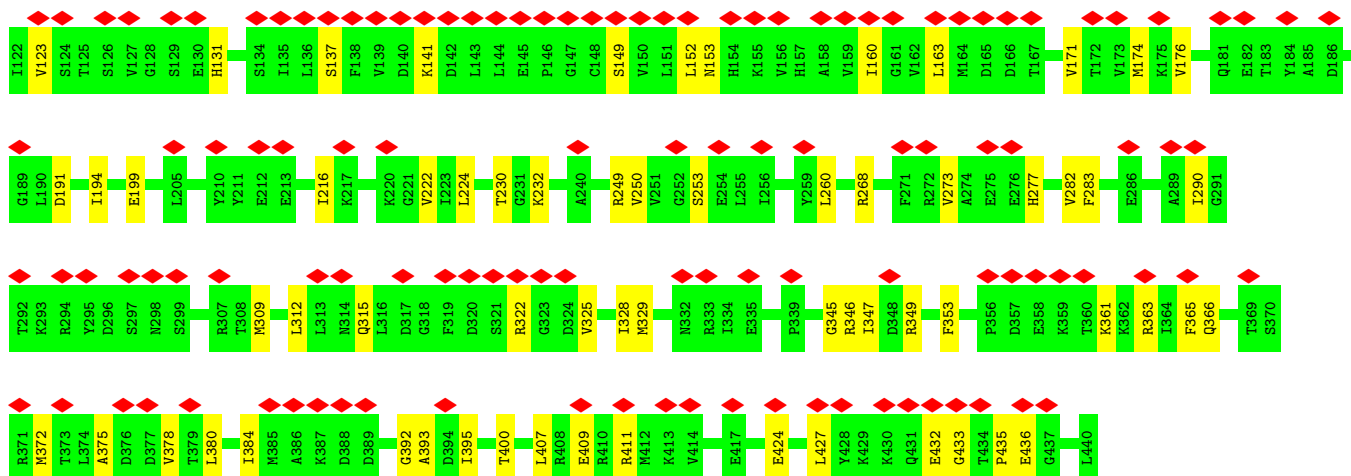
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S proteasome regulatory subunit 7

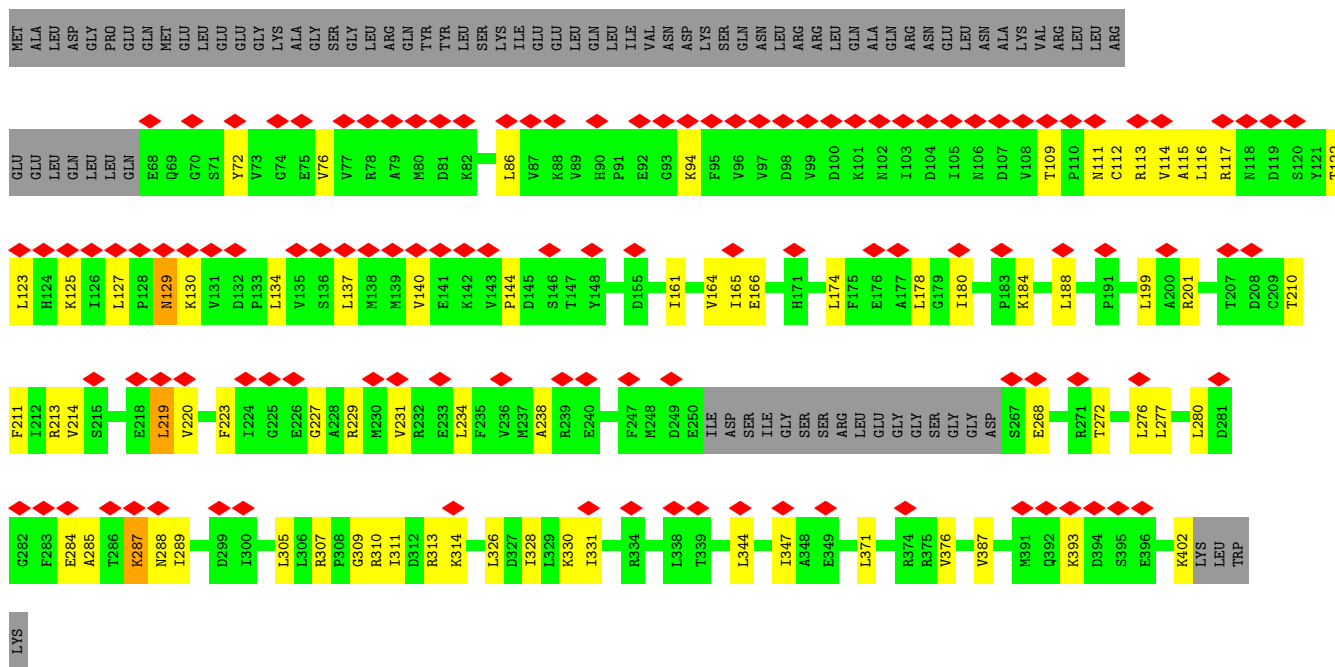


#### • Molecule 2: 26S proteasome regulatory subunit 4

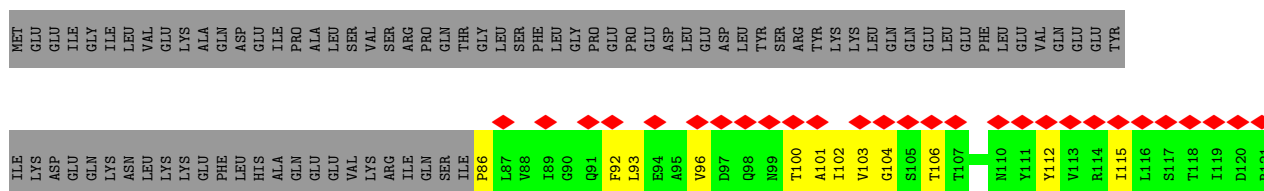


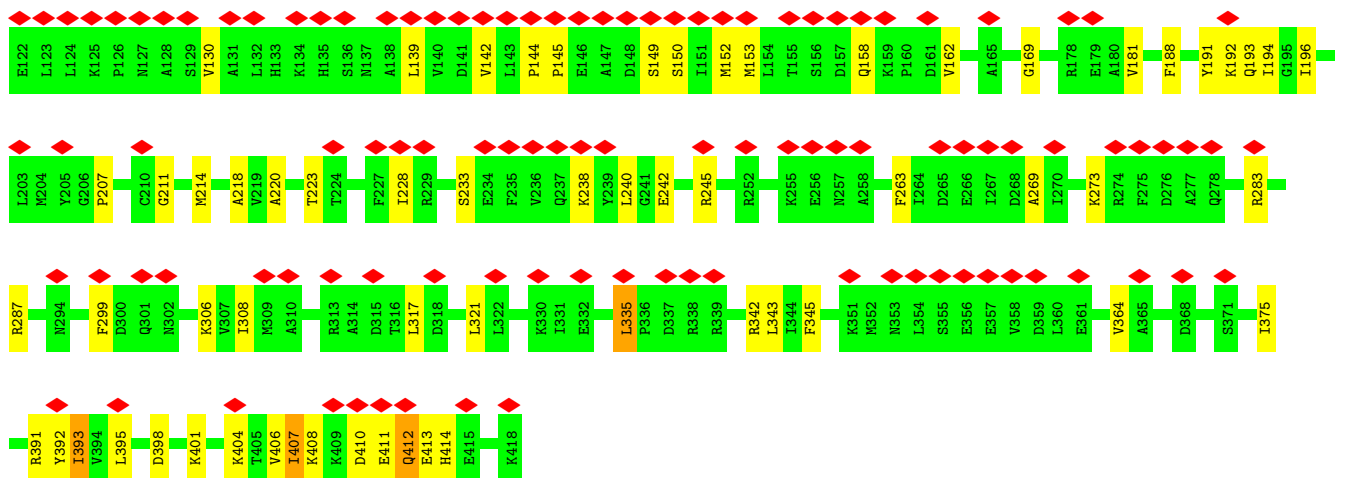


• Molecule 3: 26S proteasome regulatory subunit 8

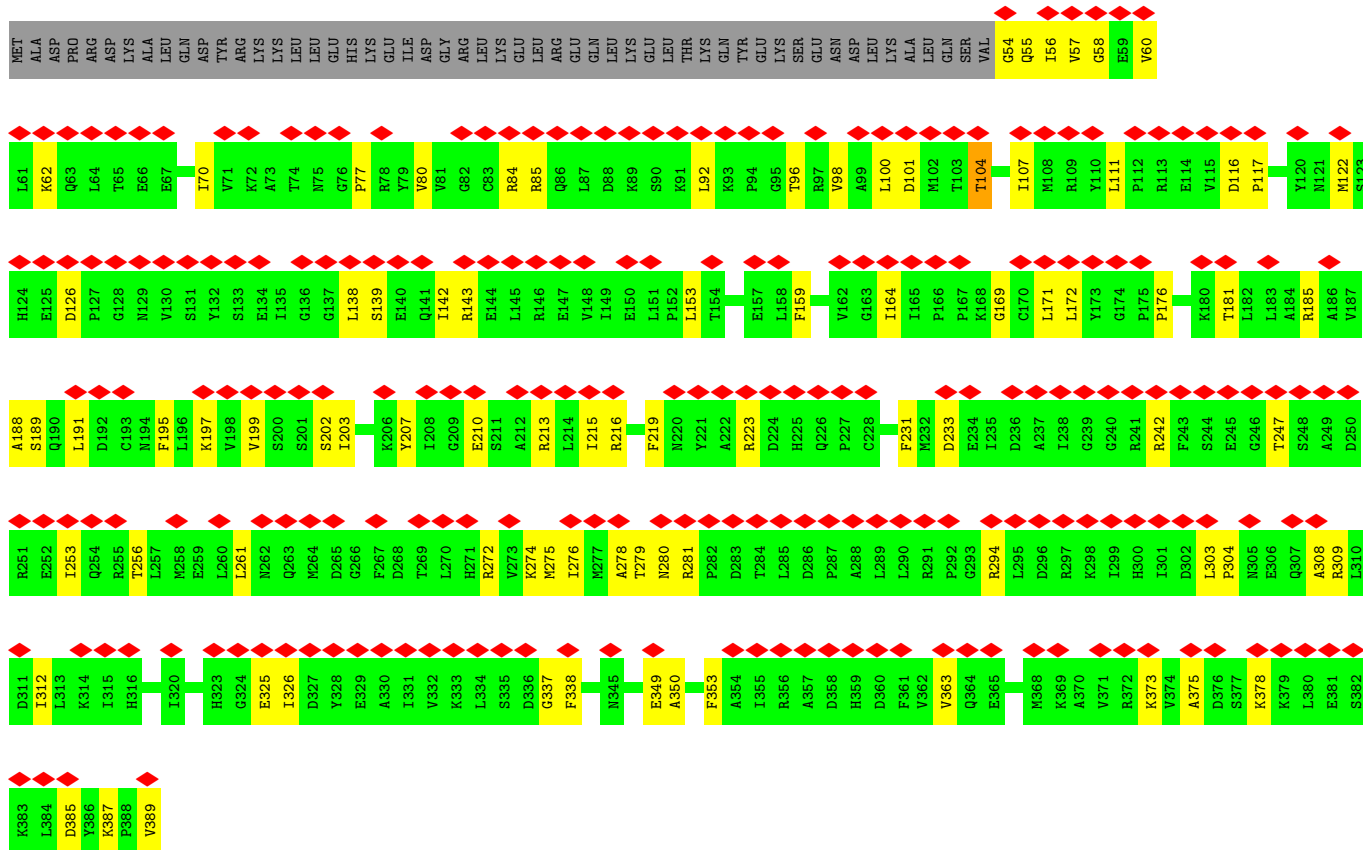


• Molecule 4: 26S proteasome regulatory subunit 6B

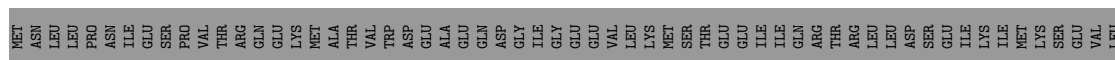


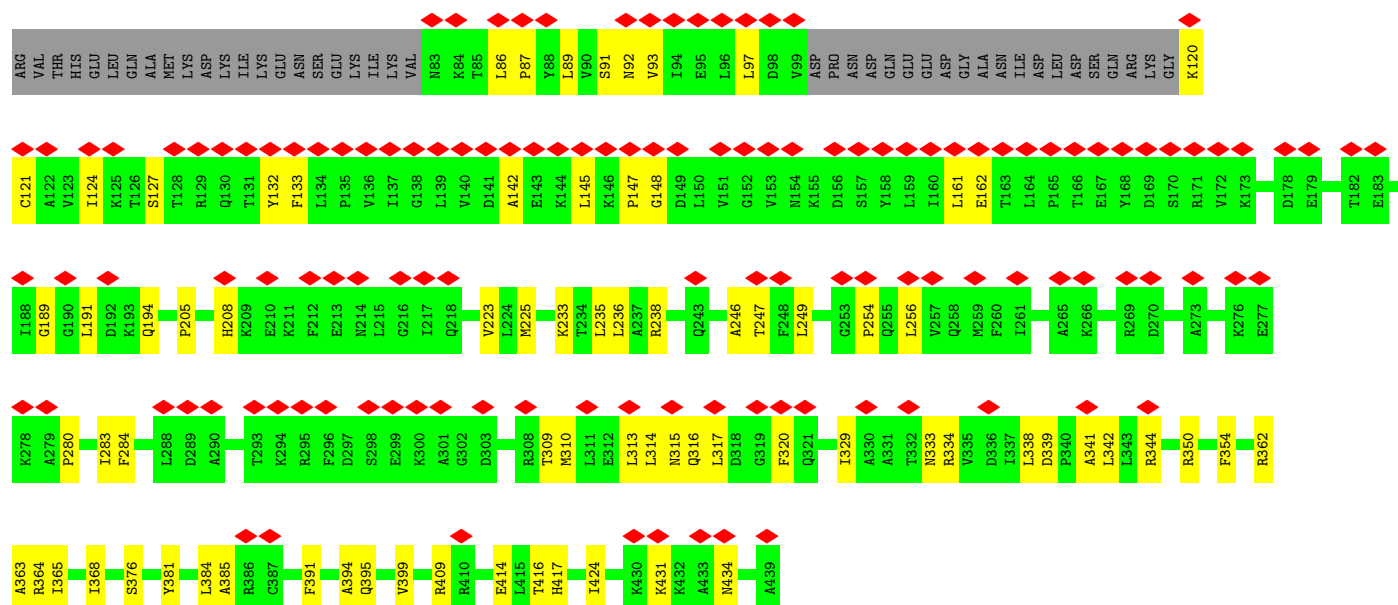


• Molecule 5: 26S proteasome regulatory subunit 10B

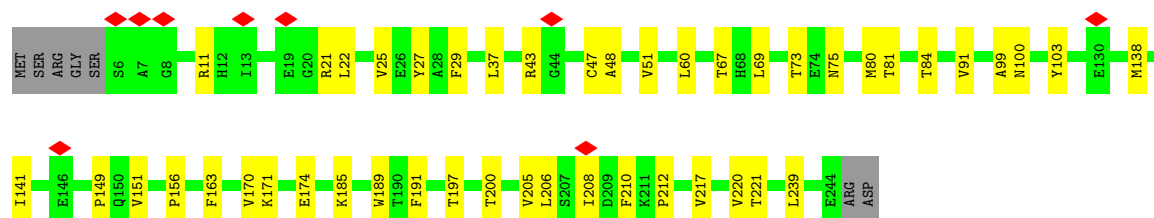
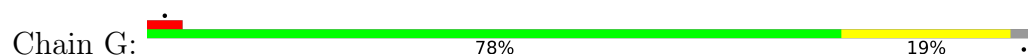


• Molecule 6: 26S proteasome regulatory subunit 6A

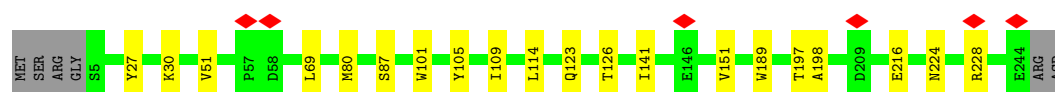
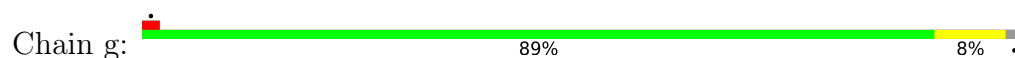




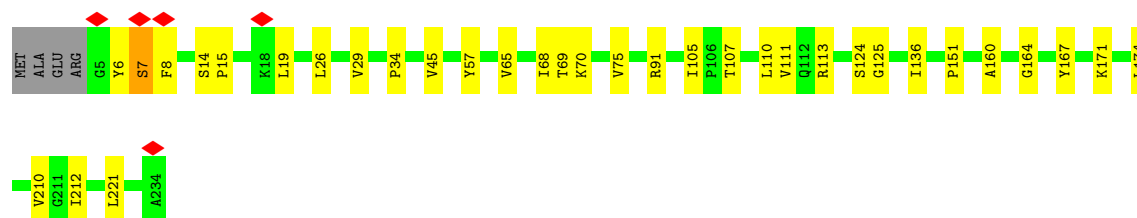
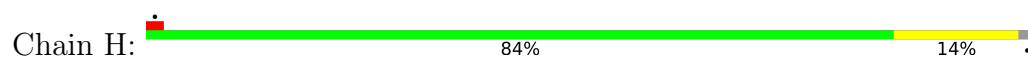
• Molecule 7: Proteasome subunit alpha type-6




• Molecule 7: Proteasome subunit alpha type-6

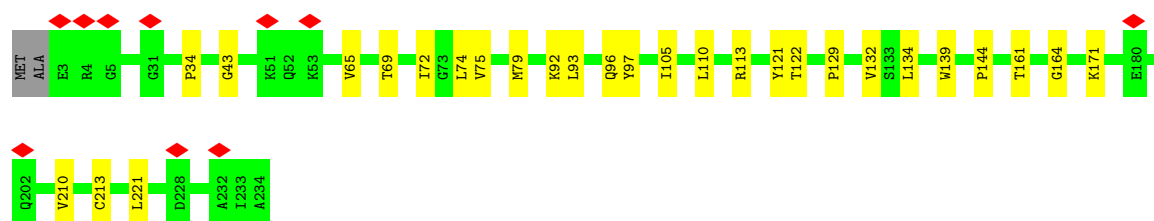


• Molecule 8: Proteasome subunit alpha type-2




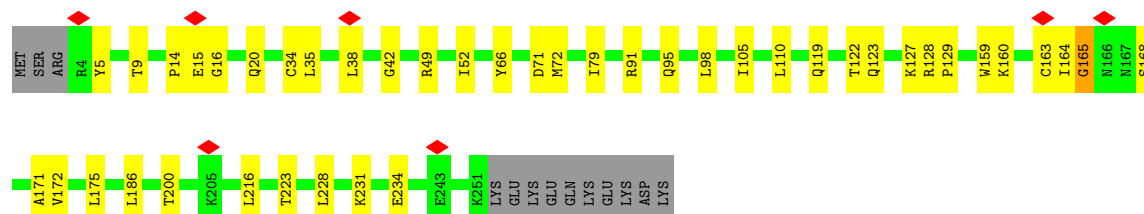
• Molecule 8: Proteasome subunit alpha type-2

Chain h:  87% 12%




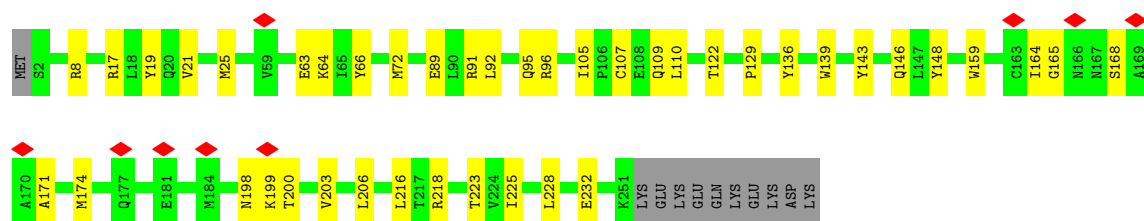
- Molecule 9: Proteasome subunit alpha type-4

Chain I:  79% 16% 5%




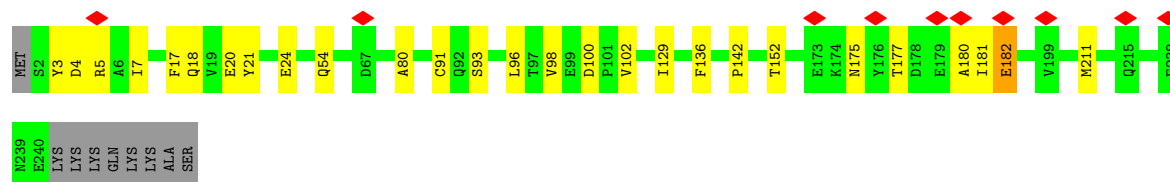
- Molecule 9: Proteasome subunit alpha type-4

Chain i:  80% 16%




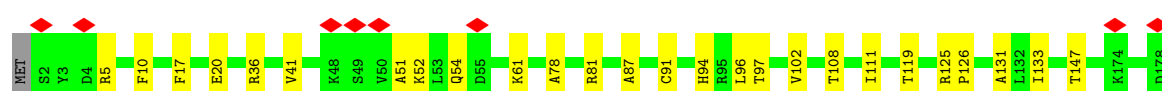
- Molecule 10: Proteasome subunit alpha type-7

Chain J:  85% 10%



- Molecule 10: Proteasome subunit alpha type-7

Chain j:  85% 12%



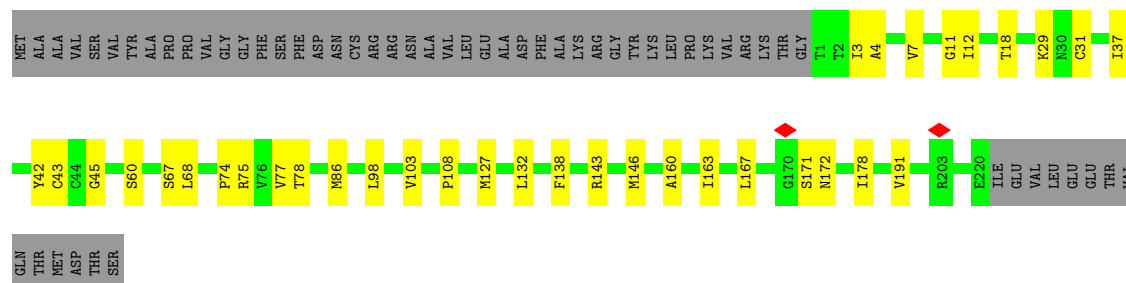




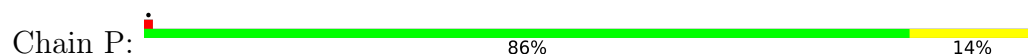




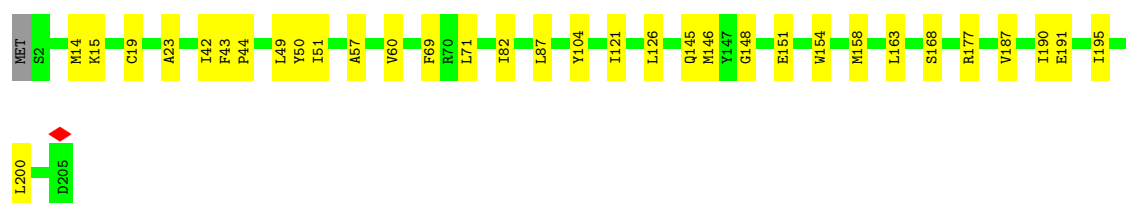
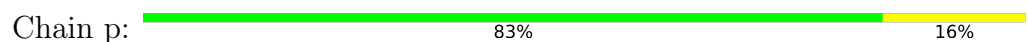
• Molecule 15: Proteasome subunit beta type-7



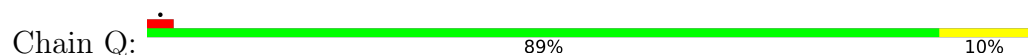
• Molecule 16: Proteasome subunit beta type-3



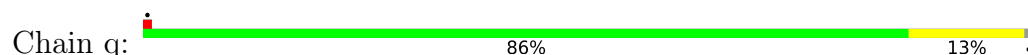
• Molecule 16: Proteasome subunit beta type-3



• Molecule 17: Proteasome subunit beta type-2

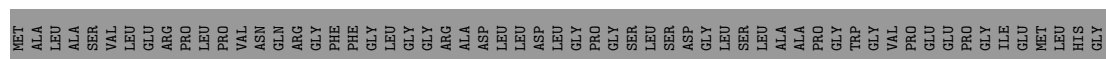


• Molecule 17: Proteasome subunit beta type-2

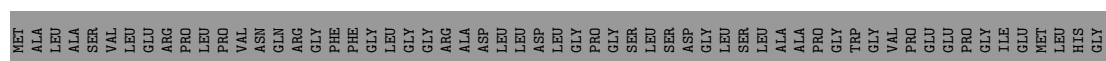




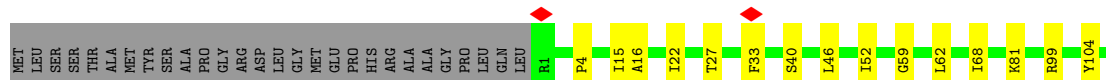
- Molecule 18: Proteasome subunit beta type-5



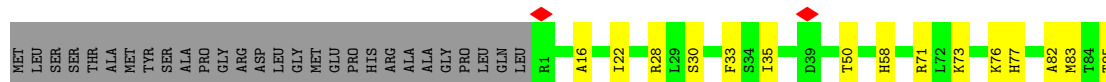
- Molecule 18: Proteasome subunit beta type-5



- Molecule 19: Proteasome subunit beta type-1

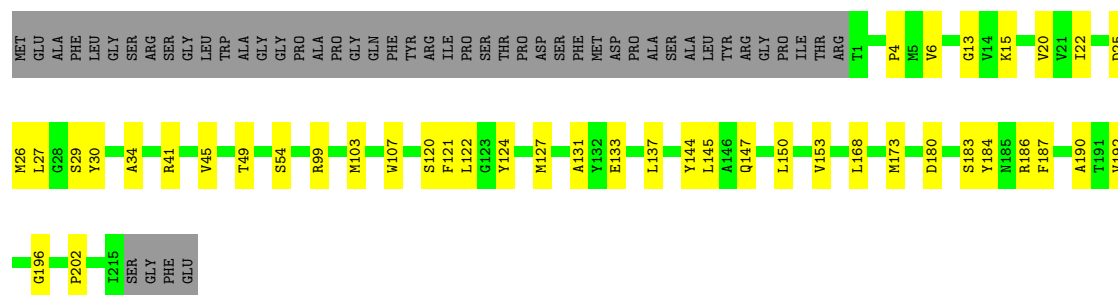


- Molecule 19: Proteasome subunit beta type-1

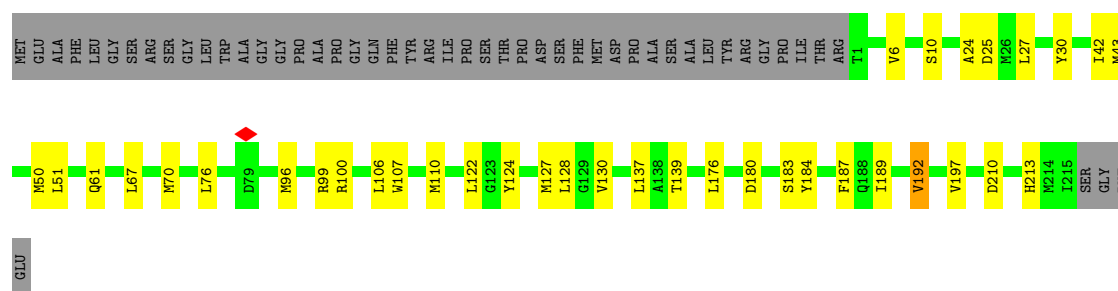


- Molecule 20: Proteasome subunit beta type-4

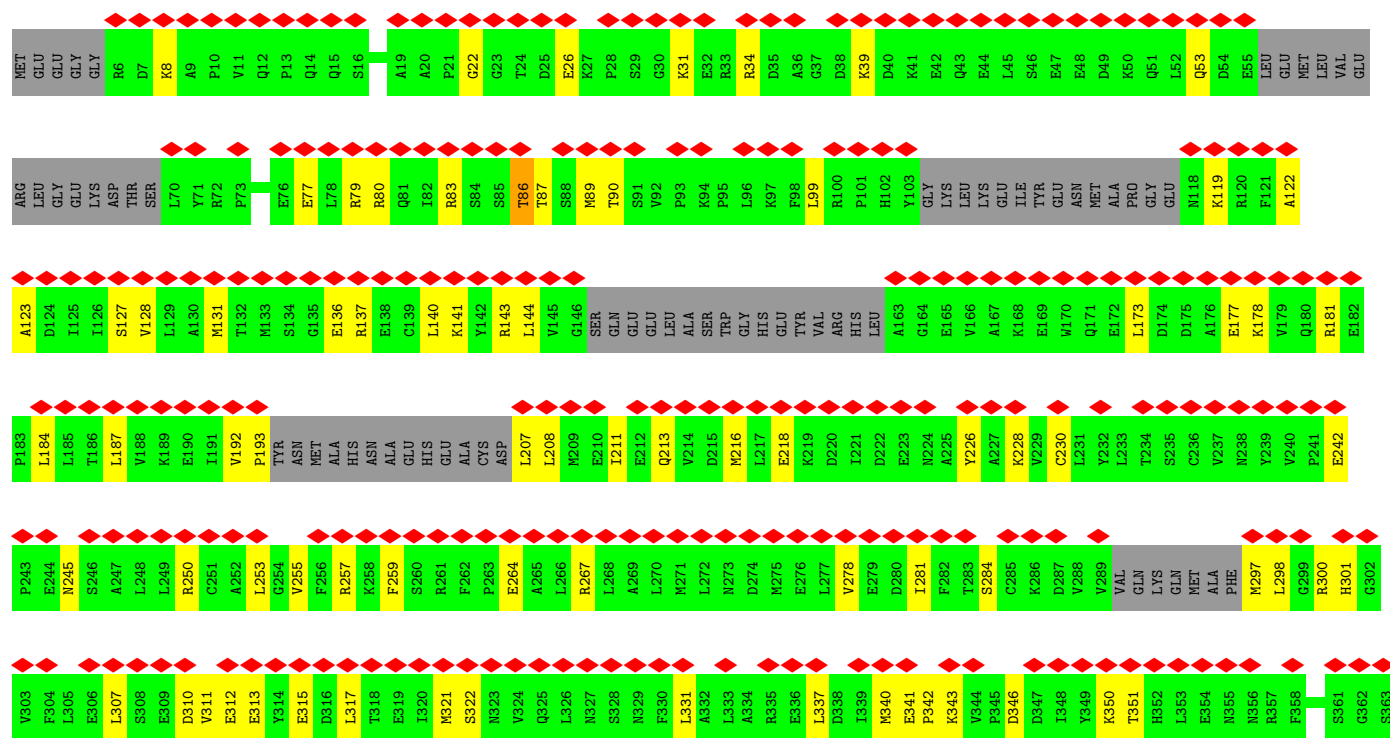




• Molecule 20: Proteasome subunit beta type-4



• Molecule 21: 26S proteasome non-ATPase regulatory subunit 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14101	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	0.119	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	369.59998, 369.59998, 369.59998	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.68, 1.68, 1.68	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	0.15	0/2939	0.44	0/3970
2	B	0.16	0/2844	0.46	0/3846
3	C	0.19	0/2522	0.53	4/3394 (0.1%)
4	D	0.20	0/2669	0.55	4/3606 (0.1%)
5	E	0.19	0/2695	0.53	1/3635 (0.0%)
6	F	0.16	0/2666	0.47	2/3597 (0.1%)
7	G	0.17	0/1853	0.48	0/2515
7	g	0.16	0/1859	0.42	0/2523
8	H	0.17	0/1723	0.39	2/2346 (0.1%)
8	h	0.16	0/1743	0.40	0/2372
9	I	0.18	0/1925	0.50	0/2606
9	i	0.16	0/1942	0.43	0/2628
10	J	0.18	0/1728	0.50	2/2358 (0.1%)
10	j	0.16	0/1728	0.41	0/2358
11	K	0.17	0/1755	0.47	2/2375 (0.1%)
11	k	0.15	0/1747	0.40	0/2364
12	L	0.17	0/1885	0.39	0/2552
12	l	0.17	0/1885	0.41	0/2552
13	M	0.18	0/1891	0.44	2/2552 (0.1%)
13	m	0.16	0/1891	0.39	0/2552
14	N	0.16	0/1454	0.40	0/1967
14	n	0.17	0/1454	0.45	2/1967 (0.1%)
15	O	0.16	0/1670	0.34	0/2265
15	o	0.17	0/1670	0.36	0/2265
16	P	0.16	0/1614	0.37	0/2177
16	p	0.17	0/1614	0.41	0/2177
17	Q	0.18	0/1603	0.42	0/2174
17	q	0.17	0/1603	0.43	0/2174
18	R	0.15	0/1579	0.37	0/2134
18	r	0.15	0/1579	0.35	0/2134
19	S	0.15	0/1671	0.36	0/2253
19	s	0.16	0/1671	0.38	0/2253

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.17	0/1700	0.42	0/2305
20	t	0.17	0/1700	0.38	0/2305
21	f	0.20	0/5393	0.53	1/7271 (0.0%)
All	All	0.17	0/69865	0.44	22/94522 (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
4	D	0	5
5	E	0	2
9	I	0	1
11	K	0	2
13	M	0	1
17	q	0	1
21	f	0	1
All	All	0	13

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	412	GLN	CA-C-N	7.28	134.80	121.70
4	D	412	GLN	C-N-CA	7.28	134.80	121.70
11	K	21	LEU	CA-C-N	6.92	134.15	121.70
11	K	21	LEU	C-N-CA	6.92	134.15	121.70
3	C	393	LYS	CA-C-N	6.27	132.98	121.70
3	C	393	LYS	C-N-CA	6.27	132.98	121.70
6	F	434	ASN	CA-C-N	6.26	132.96	121.70
6	F	434	ASN	C-N-CA	6.26	132.96	121.70
14	n	91	ARG	CA-C-N	6.06	133.12	121.54
14	n	91	ARG	C-N-CA	6.06	133.12	121.54
8	H	7	SER	CA-C-N	6.06	132.61	121.70
8	H	7	SER	C-N-CA	6.06	132.61	121.70
21	f	516	GLY	N-CA-C	6.04	127.50	113.18
3	C	287	LYS	CA-C-N	5.91	132.83	121.54
3	C	287	LYS	C-N-CA	5.91	132.83	121.54
10	J	182	GLU	CA-C-N	5.49	131.57	121.70
10	J	182	GLU	C-N-CA	5.49	131.57	121.70
13	M	6	GLY	CA-C-N	5.42	131.46	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	6	GLY	C-N-CA	5.42	131.46	121.70
5	E	181	THR	N-CA-C	-5.08	108.34	114.75
4	D	407	ILE	CA-C-N	5.01	130.73	121.70
4	D	407	ILE	C-N-CA	5.01	130.73	121.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	150	SER	Peptide
4	D	158	GLN	Peptide
4	D	299	PHE	Peptide
4	D	335	LEU	Peptide
4	D	410	ASP	Peptide
5	E	279	THR	Peptide
5	E	303	LEU	Peptide
9	I	165	GLY	Peptide
11	K	22	PHE	Peptide
11	K	9	ASP	Peptide
13	M	215	TRP	Peptide
21	f	558	LEU	Peptide
17	q	196	PHE	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	2893	0	2843	48	0
2	B	2806	0	2768	49	0
3	C	2486	0	2568	45	0
4	D	2625	0	2656	43	0
5	E	2651	0	2707	54	0
6	F	2628	0	2688	51	0
7	G	1820	0	1791	29	0
7	g	1826	0	1796	12	0
8	H	1688	0	1575	20	0
8	h	1708	0	1594	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1895	0	1833	29	0
9	i	1912	0	1851	24	0
10	J	1704	0	1517	21	0
10	j	1704	0	1517	18	0
11	K	1729	0	1680	20	0
11	k	1722	0	1673	17	0
12	L	1850	0	1822	19	0
12	l	1850	0	1822	29	0
13	M	1856	0	1814	29	0
13	m	1856	0	1814	33	0
14	N	1430	0	1398	20	0
14	n	1430	0	1398	15	0
15	O	1643	0	1644	27	0
15	o	1643	0	1644	25	0
16	P	1585	0	1598	18	0
16	p	1585	0	1598	20	0
17	Q	1570	0	1547	15	0
17	q	1570	0	1547	15	0
18	R	1548	0	1499	14	0
18	r	1548	0	1499	16	0
19	S	1641	0	1618	18	0
19	s	1641	0	1618	21	0
20	T	1667	0	1628	27	0
20	t	1667	0	1628	23	0
21	f	5319	0	5329	114	0
22	A	31	0	12	0	0
22	C	31	0	12	0	0
22	D	31	0	11	0	0
22	F	31	0	12	4	0
23	D	27	0	12	0	0
All	All	68847	0	67581	915	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (915) 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)
21:f:317:LEU:O	21:f:321:MET:HB3	1.75	0.86
21:f:137:ARG:O	21:f:141:LYS:HB2	1.74	0.86
15:o:11:GLY:HA3	15:o:178:ILE:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:226:TYR:O	21:f:230:CYS:HB2	1.81	0.80
5:E:280:ASN:HB3	5:E:387:LYS:H	1.46	0.80
4:D:106:THR:HG21	5:E:77:PRO:HB3	1.63	0.78
21:f:312:GLU:HB2	21:f:491:GLY:HA2	1.64	0.77
15:o:3:ILE:HB	15:o:127:MET:O	1.85	0.75
21:f:516:GLY:H	21:f:557:TRP:N	1.85	0.74
13:M:35:THR:HA	13:M:165:ILE:O	1.88	0.74
18:R:88:TYR:HA	18:R:91:LYS:HE3	1.70	0.72
13:m:53:VAL:HG13	13:m:58:TYR:HB3	1.72	0.72
3:C:113:ARG:HG2	3:C:130:LYS:HG2	1.72	0.71
9:i:198:ASN:HA	9:i:206:LEU:HD21	1.73	0.70
13:m:51:LYS:O	13:m:209:PHE:HA	1.91	0.70
21:f:691:PRO:HA	21:f:694:LEU:HB2	1.74	0.70
4:D:96:VAL:HG23	4:D:102:ILE:HD11	1.74	0.70
11:K:12:VAL:HG12	11:K:23:GLN:HG2	1.74	0.69
1:A:312:ARG:HB3	1:A:315:ILE:HB	1.73	0.69
2:B:123:VAL:HG11	2:B:152:LEU:HD11	1.75	0.69
3:C:231:VAL:HA	3:C:234:LEU:HB3	1.74	0.69
4:D:92:PHE:HA	4:D:103:VAL:HG12	1.74	0.69
7:G:73:THR:HG23	7:G:75:ASN:H	1.58	0.69
9:I:168:SER:O	9:I:171:ALA:HB3	1.93	0.69
14:N:115:PRO:HD2	14:N:119:MET:HB2	1.74	0.68
9:i:122:THR:HG22	9:i:129:PRO:HB3	1.76	0.68
6:F:191:LEU:HB3	6:F:194:GLN:HB2	1.77	0.67
15:o:37:ILE:HD11	15:o:43:CYS:HB2	1.75	0.67
5:E:60:VAL:HG11	5:E:92:LEU:HD22	1.77	0.67
20:T:145:LEU:HG	15:o:132:LEU:HD21	1.75	0.66
1:A:274:PHE:HB3	1:A:277:ILE:HD11	1.77	0.66
13:m:134:SER:HB2	13:m:153:PRO:HD3	1.76	0.66
13:M:39:ILE:HD11	13:M:181:MET:HG3	1.77	0.66
14:N:11:GLY:HA3	14:N:179:ILE:O	1.95	0.66
14:n:11:GLY:HA3	14:n:179:ILE:O	1.96	0.66
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.61	0.66
8:H:19:LEU:HD21	9:I:128:ARG:HE	1.60	0.65
9:I:105:ILE:HG12	9:I:110:LEU:HB2	1.77	0.65
1:A:119:ALA:HB1	6:F:87:PRO:HB3	1.78	0.65
6:F:341:ALA:HB2	6:F:344:ARG:HH21	1.62	0.65
18:r:59:LEU:HD21	18:r:83:LEU:HB2	1.78	0.65
13:M:52:LEU:HA	13:M:209:PHE:HA	1.78	0.65
3:C:307:ARG:HH21	3:C:310:ARG:HE	1.43	0.64
10:J:96:LEU:HG	17:Q:62:LYS:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:VAL:HG23	5:E:100:LEU:HD11	1.80	0.64
18:r:59:LEU:HD11	18:r:83:LEU:HD22	1.80	0.64
13:M:168:ALA:HB1	13:M:171:ALA:HB3	1.79	0.63
19:s:83:MET:HE1	19:s:91:MET:HE2	1.80	0.63
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.80	0.63
21:f:654:VAL:HA	21:f:657:ILE:HD12	1.80	0.63
13:m:48:GLY:HA2	13:m:212:GLU:O	1.98	0.63
13:m:67:PHE:HB2	13:m:75:MET:HB3	1.79	0.63
12:L:38:LEU:HB2	12:L:179:PHE:HZ	1.64	0.63
4:D:130:VAL:HG12	4:D:142:VAL:HG22	1.79	0.63
18:R:9:ARG:HE	18:R:146:ASP:HA	1.63	0.63
21:f:569:LYS:HE2	21:f:601:ALA:H	1.63	0.63
5:E:219:PHE:HB3	5:E:223:ARG:HE	1.62	0.63
17:q:117:TYR:HB3	17:q:125:ALA:HB3	1.81	0.63
6:F:235:LEU:HD11	22:F:501:ATP:H2'	1.81	0.62
13:m:35:THR:HA	13:m:165:ILE:O	1.98	0.62
21:f:541:THR:HA	21:f:544:GLU:HG2	1.80	0.62
11:K:36:THR:HA	11:K:170:ILE:O	1.98	0.62
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.81	0.62
11:k:36:THR:HG22	11:k:53:ARG:HH12	1.64	0.62
9:i:136:TYR:HB2	9:i:148:TYR:HB2	1.81	0.62
9:i:105:ILE:HG12	9:i:110:LEU:HG	1.81	0.62
2:B:176:VAL:HG11	2:B:249:ARG:HB2	1.81	0.62
10:J:93:SER:HA	10:J:96:LEU:HD12	1.82	0.62
18:r:100:MET:HE3	18:r:128:VAL:HG23	1.82	0.62
6:F:161:LEU:HD23	6:F:162:GLU:HG2	1.81	0.62
19:S:16:ALA:HB2	19:S:121:VAL:HG23	1.82	0.62
1:A:98:CYS:HB2	1:A:139:ARG:HB3	1.82	0.62
12:L:104:PRO:HG2	12:L:107:ARG:HH21	1.64	0.62
21:f:515:ALA:HB3	21:f:557:TRP:H	1.64	0.61
1:A:351:ARG:HH22	1:A:380:SER:H	1.48	0.61
18:R:173:ALA:HA	18:R:190:ASP:O	2.00	0.61
19:S:147:PRO:HG3	16:p:177:ARG:HG2	1.82	0.61
1:A:243:SER:HB2	2:B:268:ARG:HH21	1.66	0.61
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.81	0.61
8:h:122:THR:HG22	8:h:129:PRO:HB3	1.82	0.61
12:l:206:THR:HG23	12:l:208:LYS:H	1.65	0.61
21:f:794:ALA:HA	21:f:797:LEU:HD12	1.82	0.61
21:f:317:LEU:O	21:f:321:MET:CB	2.49	0.61
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.83	0.61
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:GLN:HB2	5:E:101:ASP:H	1.65	0.61
21:f:140:LEU:HD13	21:f:143:ARG:HB2	1.82	0.61
4:D:96:VAL:HB	4:D:100:THR:HG21	1.81	0.61
9:I:163:CYS:HB2	9:I:172:VAL:HG21	1.83	0.61
9:i:8:ARG:HH22	10:j:5:ARG:HH12	1.49	0.61
1:A:91:GLN:HG3	1:A:92:PRO:HD3	1.82	0.60
18:r:11:GLY:HA2	18:r:104:TRP:HZ3	1.66	0.60
6:F:205:PRO:HA	6:F:208:HIS:HB2	1.82	0.60
9:I:15:GLU:H	9:I:16:GLY:HA2	1.66	0.60
8:h:69:THR:HG22	8:h:72:ILE:HB	1.82	0.60
13:m:243:LEU:HD12	13:m:244:LYS:HG2	1.83	0.60
4:D:169:GLY:HA3	4:D:343:LEU:HD13	1.83	0.60
8:h:93:LEU:HD21	8:h:113:ARG:HD2	1.83	0.60
3:C:227:GLY:H	3:C:229:ARG:HH21	1.49	0.60
4:D:242:GLU:HG3	4:D:245:ARG:HB3	1.83	0.60
20:t:24:ALA:HB3	20:t:42:ILE:HD11	1.82	0.60
2:B:365:PHE:HD2	2:B:380:LEU:HB2	1.66	0.60
12:L:51:ARG:H	12:L:60:GLN:HE22	1.50	0.60
21:f:184:LEU:HD12	21:f:228:LYS:HZ1	1.66	0.60
1:A:172:VAL:HG21	1:A:227:ARG:HD3	1.84	0.60
21:f:136:GLU:O	21:f:140:LEU:HB2	2.02	0.60
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.83	0.59
20:T:144:TYR:HB3	15:o:132:LEU:HD22	1.84	0.59
4:D:391:ARG:HH12	4:D:395:LEU:H	1.50	0.59
6:F:246:ALA:HB1	6:F:280:PRO:HG2	1.84	0.59
6:F:313:LEU:HD23	6:F:317:LEU:HG	1.82	0.59
2:B:375:ALA:HB3	2:B:378:VAL:HG13	1.84	0.59
3:C:112:CYS:HA	3:C:130:LYS:HD3	1.83	0.59
14:n:133:SER:O	14:n:136:TYR:HB3	2.02	0.59
6:F:235:LEU:HD23	6:F:238:ARG:HH12	1.67	0.59
14:n:20:THR:HB	14:n:28:ASN:HB3	1.84	0.59
5:E:213:ARG:O	5:E:216:ARG:HB2	2.02	0.59
8:H:29:VAL:HG21	8:H:151:PRO:HG3	1.84	0.59
14:N:20:THR:HB	14:N:28:ASN:HB3	1.85	0.59
3:C:134:LEU:HD12	3:C:137:LEU:HD13	1.85	0.59
8:H:65:VAL:HG12	8:H:75:VAL:HG12	1.84	0.59
11:K:117:SER:HA	11:K:120:ALA:HB3	1.83	0.59
13:m:49:VAL:HG11	13:m:65:ARG:HB2	1.84	0.59
5:E:122:MET:HE1	5:E:202:SER:HB3	1.85	0.59
21:f:369:ARG:HB3	21:f:740:ARG:HH21	1.68	0.58
19:S:52:ILE:HG13	19:S:110:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:THR:HG22	1:A:323:ARG:H	1.68	0.58
6:F:363:ALA:HB2	6:F:385:ALA:HB2	1.85	0.58
20:t:25:ASP:HA	20:t:187:PHE:HA	1.85	0.58
15:O:203:ARG:HH22	16:P:162:HIS:CG	2.22	0.58
13:m:46:VAL:HG23	13:m:215:TRP:HB2	1.85	0.58
17:q:5:ILE:HG21	17:q:160:LEU:HD11	1.86	0.58
3:C:115:ALA:HB3	3:C:125:LYS:H	1.69	0.58
16:P:116:THR:HG23	16:P:118:LYS:H	1.68	0.58
20:T:6:VAL:HG22	20:T:30:TYR:HB2	1.85	0.58
21:f:620:PHE:HD2	21:f:623:LYS:HG3	1.69	0.58
15:o:18:THR:HB	15:o:31:CYS:H	1.67	0.58
16:p:71:LEU:HD11	16:p:82:ILE:HG21	1.85	0.58
11:k:85:ALA:HB2	11:k:139:VAL:HG21	1.86	0.58
3:C:268:GLU:HB2	4:D:287:ARG:HH12	1.69	0.57
7:G:174:GLU:HG3	7:G:205:VAL:HG22	1.86	0.57
12:L:182:CYS:HB2	12:L:186:GLU:HG3	1.86	0.57
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.85	0.57
9:i:228:LEU:HB2	9:i:232:GLU:HG3	1.85	0.57
17:Q:102:LEU:HB3	17:Q:118:MET:HB2	1.85	0.57
16:P:3:ILE:HG22	16:P:56:LEU:HD21	1.86	0.57
21:f:310:ASP:H	21:f:313:GLU:HB2	1.68	0.57
1:A:212:VAL:HG22	1:A:339:ARG:HB2	1.86	0.57
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.87	0.57
12:l:26:MET:HE1	12:l:148:CYS:HB2	1.86	0.57
13:m:168:ALA:HB2	13:m:200:VAL:HG21	1.86	0.57
17:q:49:GLU:HG3	17:q:52:ASP:HB2	1.87	0.57
2:B:103:ARG:HH11	2:B:107:MET:HE3	1.69	0.57
16:P:107:PRO:HG2	16:P:124:LEU:HB2	1.84	0.57
16:p:19:CYS:HB3	16:p:191:GLU:HG3	1.86	0.57
21:f:659:LEU:HD11	21:f:690:VAL:HA	1.87	0.57
10:j:36:ARG:HA	10:j:41:VAL:HG12	1.86	0.57
6:F:310:MET:HA	6:F:313:LEU:HD12	1.86	0.57
4:D:93:LEU:HD13	4:D:104:GLY:H	1.68	0.56
16:p:104:TYR:HA	16:p:126:LEU:HD11	1.86	0.56
21:f:675:PHE:HA	21:f:678:LEU:HB3	1.86	0.56
4:D:188:PHE:HA	4:D:191:TYR:HD2	1.70	0.56
10:J:80:ALA:HA	10:J:129:ILE:HD13	1.87	0.56
10:J:136:PHE:H	10:J:211:MET:HE1	1.70	0.56
19:S:27:THR:HB	19:S:40:SER:H	1.69	0.56
21:f:77:GLU:HB2	21:f:99:LEU:HD21	1.88	0.56
18:r:21:THR:HA	18:r:27:ALA:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:343:LYS:HA	21:f:346:ASP:HB2	1.85	0.56
5:E:185:ARG:HB3	5:E:189:SER:HB3	1.86	0.56
1:A:284:ARG:HH12	6:F:333:ASN:HB3	1.71	0.56
15:o:7:VAL:HG22	15:o:12:ILE:HG12	1.88	0.56
1:A:213:LEU:HB2	1:A:337:LEU:HD13	1.87	0.56
2:B:346:ARG:HG2	2:B:347:ILE:HG13	1.88	0.56
6:F:339:ASP:HB2	6:F:342:LEU:HG	1.87	0.56
14:n:40:ARG:HE	14:n:41:ILE:HG13	1.71	0.56
5:E:185:ARG:HA	5:E:188:ALA:HB3	1.87	0.56
6:F:233:LYS:HA	6:F:236:LEU:HD12	1.88	0.56
9:I:119:GLN:O	9:I:123:GLN:HB2	2.06	0.56
5:E:349:GLU:HB3	5:E:373:LYS:HZ2	1.71	0.55
7:G:206:LEU:HB3	7:G:208:ILE:HG12	1.88	0.55
2:B:222:VAL:HA	2:B:349:ARG:HB2	1.87	0.55
21:f:89:MET:HG3	21:f:90:THR:HG23	1.88	0.55
1:A:170:PRO:HG3	1:A:239:ARG:HH22	1.72	0.55
5:E:126:ASP:HB2	5:E:197:LYS:H	1.71	0.55
21:f:517:VAL:N	21:f:558:LEU:H	2.04	0.55
16:p:15:LYS:HD2	16:p:121:ILE:HG12	1.88	0.55
18:r:135:ALA:O	18:r:139:MET:HB3	2.05	0.55
12:l:13:TRP:HE1	13:m:130:PRO:HD2	1.71	0.55
1:A:375:ARG:HD2	11:K:173:ALA:HB2	1.89	0.55
13:M:77:VAL:HA	13:M:135:PHE:HB3	1.88	0.55
9:i:105:ILE:HD11	9:i:109:GLN:HB2	1.88	0.55
11:k:143:PHE:HB2	11:k:154:PHE:HB2	1.87	0.55
14:n:179:ILE:HG12	14:n:184:VAL:HG22	1.89	0.55
20:t:51:LEU:HD11	20:t:110:MET:HE3	1.89	0.55
2:B:322:ARG:HH21	2:B:325:VAL:HG21	1.71	0.55
5:E:57:VAL:HA	5:E:100:LEU:HD13	1.89	0.55
5:E:153:LEU:HB2	5:E:272:ARG:HD2	1.87	0.55
21:f:192:VAL:HG23	21:f:193:PRO:HD3	1.87	0.55
4:D:101:ALA:HB2	4:D:115:ILE:HB	1.88	0.55
4:D:207:PRO:HB2	4:D:335:LEU:HD21	1.89	0.55
1:A:244:GLU:HB3	2:B:268:ARG:HH22	1.72	0.55
2:B:224:LEU:HD13	2:B:232:LYS:HB3	1.87	0.55
3:C:311:ILE:HG23	3:C:314:LYS:HE2	1.89	0.55
15:O:152:LYS:HE2	15:O:177:VAL:HG21	1.89	0.55
7:g:80:MET:HE3	7:g:87:SER:HB3	1.89	0.55
11:k:104:ASN:HB3	18:r:57:ARG:HH22	1.70	0.55
7:G:43:ARG:HD3	7:G:149:PRO:HG2	1.89	0.55
13:M:42:LYS:HE2	13:M:185:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:21:THR:HG22	14:N:26:ILE:HG13	1.89	0.55
19:s:148:LEU:HD23	19:s:178:VAL:HG23	1.89	0.55
1:A:248:LYS:HA	2:B:260:LEU:HD12	1.89	0.54
3:C:287:LYS:HG3	3:C:288:ASN:H	1.72	0.54
14:N:164:MET:HG2	14:N:171:GLY:HA2	1.88	0.54
13:m:27:MET:HE1	13:m:153:PRO:HB2	1.89	0.54
15:o:37:ILE:HG23	15:o:60:SER:HA	1.89	0.54
3:C:76:VAL:O	3:C:111:ASN:HA	2.07	0.54
11:K:20:ARG:HB3	11:K:22:PHE:HD2	1.73	0.54
15:O:7:VAL:HG22	15:O:12:ILE:HG12	1.88	0.54
20:t:10:SER:HB2	20:t:176:LEU:HD21	1.89	0.54
18:R:39:PRO:HA	18:R:184:TRP:HE1	1.73	0.54
21:f:606:VAL:HA	21:f:609:VAL:HB	1.89	0.54
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.89	0.54
21:f:631:LYS:HA	21:f:634:LYS:HB2	1.89	0.54
9:i:199:LYS:HG3	9:i:200:THR:HG23	1.88	0.54
10:j:119:THR:HG22	10:j:126:PRO:HB3	1.88	0.54
6:F:338:LEU:HB3	6:F:342:LEU:HD12	1.88	0.54
9:i:92:LEU:HD13	9:i:96:ARG:HH21	1.72	0.54
3:C:201:ARG:HH22	3:C:213:ARG:HH22	1.56	0.54
15:O:163:ILE:HG23	15:O:169:SER:H	1.72	0.54
20:T:124:TYR:O	20:T:131:ALA:HA	2.07	0.54
1:A:365:GLU:HG2	1:A:367:ASP:H	1.72	0.54
9:I:42:GLY:HA2	9:I:216:LEU:O	2.07	0.54
11:K:19:GLY:HA3	11:K:20:ARG:HB2	1.90	0.54
4:D:149:SER:HB2	4:D:228:ILE:HG13	1.89	0.54
6:F:376:SER:HB3	6:F:414:GLU:HG3	1.90	0.54
21:f:119:LYS:HB3	21:f:122:ALA:H	1.73	0.54
2:B:174:MET:HB3	2:B:250:VAL:HG12	1.90	0.53
3:C:220:VAL:HG22	3:C:223:PHE:HB2	1.90	0.53
10:j:78:ALA:HA	10:j:81:ARG:HE	1.72	0.53
2:B:392:GLY:HA2	2:B:395:ILE:HD12	1.90	0.53
4:D:162:VAL:HG22	4:D:218:ALA:HB2	1.89	0.53
12:L:9:ASP:HB3	12:L:12:VAL:HG12	1.91	0.53
15:O:113:ILE:HG12	15:O:119:THR:HG22	1.90	0.53
17:q:22:ALA:HA	17:q:27:GLN:HA	1.89	0.53
14:N:58:ALA:HB3	14:N:86:MET:HE1	1.90	0.53
21:f:471:LEU:HD22	21:f:509:LYS:HZ3	1.74	0.53
4:D:191:TYR:HD1	4:D:196:ILE:HB	1.73	0.53
8:H:26:LEU:HD22	8:H:151:PRO:HG2	1.88	0.53
10:j:108:THR:HG22	10:j:133:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:45:VAL:HG22	8:H:212:ILE:HG22	1.89	0.53
15:o:143:ARG:HH12	15:o:146:MET:HA	1.74	0.53
21:f:519:ALA:H	21:f:558:LEU:HA	1.74	0.53
4:D:401:LYS:HA	4:D:404:LYS:HG2	1.91	0.53
21:f:31:LYS:HD2	21:f:34:ARG:HD2	1.90	0.53
21:f:187:LEU:HD11	21:f:216:MET:HE1	1.90	0.53
3:C:184:LYS:HB3	3:C:287:LYS:HE3	1.90	0.53
10:J:181:ILE:H	10:J:182:GLU:HA	1.74	0.53
7:g:80:MET:HG2	7:g:87:SER:HB2	1.91	0.53
1:A:396:ALA:HA	1:A:401:ARG:HH21	1.74	0.53
2:B:137:SER:HB2	2:B:141:LYS:HD3	1.91	0.53
8:h:43:GLY:CA	8:h:213:CYS:O	2.57	0.53
8:h:93:LEU:HD11	8:h:113:ARG:HB3	1.91	0.53
2:B:409:GLU:HG2	2:B:411:ARG:HH11	1.74	0.52
6:F:89:LEU:HD11	6:F:127:SER:H	1.73	0.52
15:O:172:ASN:HB3	15:O:191:VAL:HG22	1.91	0.52
14:n:127:ILE:HB	14:n:132:SER:HB2	1.91	0.52
19:s:28:ARG:HB2	19:s:191:ASP:HB2	1.90	0.52
2:B:115:ILE:HA	2:B:121:ALA:HA	1.91	0.52
7:g:224:ASN:HD21	7:g:228:ARG:HD3	1.74	0.52
4:D:211:GLY:HA3	4:D:214:MET:HE2	1.92	0.52
6:F:189:GLY:H	22:F:501:ATP:HN62	1.56	0.52
12:l:11:THR:HA	13:m:129:ARG:HB2	1.91	0.52
12:l:89:ARG:HG2	19:s:77:HIS:CE1	2.43	0.52
6:F:142:ALA:HA	6:F:145:LEU:HB2	1.91	0.52
14:n:40:ARG:HH12	14:n:105:PRO:HD3	1.73	0.52
15:o:42:TYR:HD2	15:o:178:ILE:HD11	1.75	0.52
3:C:144:PRO:HB3	3:C:201:ARG:HD2	1.92	0.52
12:L:109:VAL:HG21	12:L:145:PHE:HD2	1.75	0.52
21:f:517:VAL:H	21:f:557:TRP:HA	1.73	0.52
11:k:78:MET:HE1	11:k:82:ILE:HD13	1.90	0.52
13:m:21:PHE:HA	13:m:24:GLU:HG2	1.92	0.52
9:I:164:ILE:HG22	9:I:165:GLY:H	1.74	0.52
18:R:161:TYR:HB2	18:R:195:LEU:HD13	1.91	0.52
1:A:390:THR:HA	2:B:216:ILE:HD11	1.90	0.52
18:r:7:LYS:HD3	18:r:111:LEU:HB3	1.92	0.52
12:L:34:ALA:HA	12:L:161:ILE:O	2.10	0.51
21:f:475:ASN:O	21:f:478:ARG:HB2	2.10	0.51
16:p:190:ILE:HG22	16:p:195:ILE:HG23	1.92	0.51
7:G:67:THR:HG22	7:G:69:LEU:H	1.74	0.51
8:h:74:LEU:HD11	8:h:134:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:412:GLN:H	4:D:413:GLU:HB3	1.75	0.51
12:l:46:LEU:HD12	12:l:73:SER:HB2	1.93	0.51
13:m:82:ALA:HA	13:m:85:ARG:HD2	1.91	0.51
1:A:301:GLU:HB2	6:F:254:PRO:HB2	1.93	0.51
5:E:58:GLY:H	5:E:100:LEU:HD13	1.75	0.51
5:E:197:LYS:HA	5:E:231:PHE:HD2	1.75	0.51
18:R:38:ASN:HB3	18:R:41:LEU:HB3	1.92	0.51
21:f:140:LEU:HD12	21:f:144:LEU:HB2	1.91	0.51
4:D:86:PRO:HA	5:E:80:VAL:H	1.76	0.51
4:D:220:ALA:HA	4:D:223:THR:HB	1.92	0.51
19:S:145:LEU:HD21	19:S:182:ALA:HB2	1.93	0.51
21:f:79:ARG:HH21	21:f:83:ARG:HH22	1.58	0.51
16:P:12:MET:HG3	16:P:138:VAL:HG12	1.92	0.51
5:E:54:GLY:C	5:E:104:THR:H	2.19	0.51
7:G:212:PRO:HB3	7:G:239:LEU:HD23	1.93	0.51
21:f:560:LEU:HD22	21:f:594:LEU:HG	1.93	0.51
20:t:99:ARG:HD2	20:t:106:LEU:HB2	1.92	0.51
13:m:141:SER:HB3	13:m:144:ASP:HB2	1.93	0.51
2:B:191:ASP:HA	2:B:194:ILE:HB	1.91	0.50
5:E:57:VAL:HA	5:E:100:LEU:HB2	1.92	0.50
10:j:94:HIS:HA	10:j:97:THR:HG22	1.93	0.50
8:h:79:MET:H	8:h:132:VAL:HG22	1.76	0.50
11:k:195:ILE:HD11	11:k:217:LEU:HD13	1.92	0.50
17:q:29:LYS:HG2	17:q:31:ASP:H	1.76	0.50
2:B:365:PHE:CD2	2:B:380:LEU:HB2	2.46	0.50
3:C:219:LEU:HG	3:C:227:GLY:HA2	1.91	0.50
7:G:84:THR:HB	13:M:156:VAL:HG22	1.92	0.50
11:K:109:VAL:HG11	11:K:145:GLY:HA3	1.93	0.50
13:M:54:LEU:HD13	13:M:58:TYR:HB2	1.92	0.50
18:R:195:LEU:HD23	18:R:198:LYS:HE2	1.93	0.50
21:f:250:ARG:HH12	21:f:253:LEU:HD13	1.76	0.50
21:f:502:LEU:HD23	21:f:537:THR:HG23	1.93	0.50
15:o:4:ALA:HB1	15:o:138:PHE:HZ	1.77	0.50
3:C:86:LEU:HD11	3:C:94:LYS:HB2	1.94	0.50
14:N:12:VAL:HG21	14:N:101:ALA:HB1	1.94	0.50
21:f:574:GLU:O	21:f:577:LEU:HB2	2.11	0.50
5:E:62:LYS:HD3	5:E:70:ILE:HB	1.94	0.50
10:J:7:ILE:HG22	10:J:18:GLN:HB2	1.93	0.50
12:L:46:LEU:HD12	12:L:73:SER:HB2	1.92	0.50
20:T:153:VAL:HG21	20:T:168:LEU:HD11	1.92	0.50
20:t:192:VAL:HG12	20:t:197:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ALA:HB1	3:C:309:GLY:HA3	1.94	0.50
11:K:121:LEU:HD13	12:L:82:ARG:HD3	1.93	0.50
13:m:51:LYS:HZ1	13:m:64:LYS:HA	1.77	0.50
10:J:91:CYS:HB2	10:J:102:VAL:HG21	1.94	0.50
10:J:96:LEU:HD23	17:Q:58:GLU:HG3	1.94	0.50
17:q:64:VAL:HG23	17:q:75:LEU:HD12	1.94	0.50
11:K:43:SER:HA	11:K:151:PRO:HG3	1.93	0.50
19:s:71:ARG:HE	19:s:91:MET:HE1	1.77	0.50
7:G:208:ILE:HG22	7:G:210:PHE:HB3	1.92	0.50
9:I:14:PRO:HA	10:J:21:TYR:CE2	2.46	0.50
19:S:33:PHE:HE1	15:o:167:LEU:HB2	1.75	0.50
21:f:516:GLY:C	21:f:558:LEU:H	2.19	0.50
21:f:623:LYS:O	21:f:627:GLU:HB2	2.12	0.50
21:f:654:VAL:O	21:f:657:ILE:HB	2.12	0.50
3:C:376:VAL:HG12	4:D:193:GLN:HE22	1.77	0.49
5:E:159:PHE:HB3	5:E:164:ILE:HB	1.94	0.49
5:E:375:ALA:HA	5:E:378:LYS:HE2	1.93	0.49
7:G:37:LEU:HD23	7:G:81:THR:HG22	1.94	0.49
16:p:14:MET:HE3	16:p:154:TRP:HD1	1.75	0.49
1:A:386:ARG:HH21	2:B:345:GLY:HA2	1.77	0.49
3:C:114:VAL:HG21	3:C:123:LEU:HD22	1.93	0.49
5:E:304:PRO:HG3	5:E:338:PHE:HA	1.94	0.49
6:F:316:GLN:HG3	6:F:317:LEU:HD22	1.95	0.49
15:O:212:LEU:HB2	16:P:199:THR:HG23	1.93	0.49
21:f:446:LEU:HD11	21:f:483:PHE:HD2	1.77	0.49
21:f:626:GLU:HA	21:f:629:LYS:HB3	1.94	0.49
15:o:172:ASN:HB3	15:o:191:VAL:HG22	1.94	0.49
5:E:233:ASP:HA	5:E:278:ALA:HB3	1.94	0.49
21:f:340:MET:HA	21:f:343:LYS:HB2	1.94	0.49
8:h:34:PRO:HA	8:h:164:GLY:HA3	1.94	0.49
13:m:76:ALA:HB3	13:m:136:MET:HB2	1.95	0.49
1:A:186:LYS:HD3	6:F:409:ARG:HH22	1.77	0.49
3:C:140:VAL:HG13	3:C:211:PHE:H	1.77	0.49
6:F:249:LEU:HD23	6:F:283:ILE:HG12	1.93	0.49
7:G:60:LEU:HD21	13:M:177:GLU:HB3	1.95	0.49
17:Q:102:LEU:HD22	17:Q:118:MET:HG3	1.94	0.49
21:f:22:GLY:O	21:f:26:GLU:HB2	2.12	0.49
16:p:71:LEU:HD11	16:p:82:ILE:HD13	1.94	0.49
5:E:242:ARG:HD3	5:E:281:ARG:HE	1.78	0.49
21:f:520:LEU:HA	21:f:561:GLY:HA3	1.94	0.49
8:h:43:GLY:HA2	8:h:213:CYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:210:VAL:HG22	8:h:221:LEU:HD22	1.94	0.49
19:s:191:ASP:HA	19:s:212:LYS:HA	1.94	0.49
11:K:117:SER:HB3	11:K:121:LEU:HB2	1.93	0.49
15:o:67:SER:HB3	15:o:74:PRO:HG3	1.94	0.49
3:C:220:VAL:HG23	4:D:240:LEU:HD13	1.95	0.49
19:S:185:ARG:HH12	15:o:29:LYS:HG2	1.78	0.49
20:T:13:GLY:HA3	20:T:22:ILE:HD12	1.94	0.49
20:T:121:PHE:HE1	20:T:133:GLU:HG2	1.77	0.49
12:l:143:HIS:HB3	12:l:145:PHE:HE1	1.77	0.49
7:G:48:ALA:HB3	7:G:220:VAL:HG12	1.94	0.49
15:O:21:THR:HG22	15:O:26:VAL:HA	1.94	0.49
8:h:161:THR:HA	8:h:171:LYS:HE2	1.95	0.49
3:C:402:LYS:HD3	9:I:79:ILE:HG13	1.95	0.49
14:N:127:ILE:HB	14:N:132:SER:HB2	1.95	0.49
11:k:58:LEU:HB2	11:k:59:MET:HE2	1.93	0.49
16:p:23:ALA:HB2	16:p:187:VAL:HG13	1.95	0.49
4:D:194:ILE:HD12	4:D:196:ILE:HD11	1.94	0.48
7:G:100:ASN:O	7:G:103:TYR:HB2	2.11	0.48
8:H:160:ALA:HB3	8:H:174:LEU:HD21	1.94	0.48
9:i:216:LEU:HD12	9:i:225:ILE:HG22	1.95	0.48
10:J:152:THR:HG23	11:K:82:ILE:HD11	1.96	0.48
15:O:95:GLY:HA2	15:O:115:PRO:HB3	1.94	0.48
7:g:69:LEU:HD11	7:g:216:GLU:HB3	1.95	0.48
5:E:111:LEU:HD21	6:F:121:CYS:HB3	1.94	0.48
5:E:280:ASN:OD1	5:E:281:ARG:HD3	2.13	0.48
12:L:45:VAL:HG22	12:L:214:ILE:HG13	1.95	0.48
21:f:518:THR:H	21:f:558:LEU:N	2.11	0.48
21:f:625:LYS:HA	21:f:657:ILE:HD11	1.95	0.48
21:f:628:ASP:HB2	21:f:657:ILE:HD13	1.95	0.48
1:A:139:ARG:HB2	1:A:153:LEU:HB2	1.95	0.48
6:F:91:SER:HB2	6:F:124:ILE:HA	1.96	0.48
7:G:80:MET:HE1	7:G:91:VAL:HG23	1.94	0.48
7:G:189:TRP:HZ3	7:G:197:THR:HG21	1.78	0.48
12:L:125:ARG:HH21	12:L:128:TYR:HE1	1.60	0.48
13:M:215:TRP:O	13:M:224:HIS:HA	2.14	0.48
19:S:99:ARG:HH11	19:S:104:TYR:HE1	1.61	0.48
20:T:192:VAL:HA	20:T:196:GLY:O	2.13	0.48
21:f:513:GLU:HA	21:f:557:TRP:HB2	1.94	0.48
12:l:34:ALA:HA	12:l:162:GLY:HA3	1.96	0.48
15:o:29:LYS:HE2	15:o:171:SER:HB3	1.95	0.48
5:E:199:VAL:HG12	5:E:233:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:128:VAL:O	21:f:131:MET:HG2	2.14	0.48
13:m:77:VAL:HG11	13:m:84:ALA:HB1	1.95	0.48
13:M:134:SER:HB2	13:M:153:PRO:HD3	1.94	0.48
7:g:27:TYR:CZ	7:g:30:LYS:HD2	2.48	0.48
9:i:89:GLU:HA	9:i:92:LEU:HG	1.96	0.48
19:s:50:THR:HG21	19:s:88:ILE:HD13	1.96	0.48
3:C:188:LEU:HD21	3:C:199:LEU:HD23	1.95	0.48
12:L:185:ASN:O	12:L:189:LYS:HG2	2.12	0.48
20:T:147:GLN:HA	20:T:150:LEU:HD12	1.95	0.48
9:i:203:VAL:HG13	9:i:206:LEU:HD22	1.96	0.48
14:n:120:MET:H	20:t:61:GLN:HE22	1.61	0.48
1:A:190:VAL:HA	1:A:209:PRO:HG2	1.96	0.48
2:B:230:THR:HG21	2:B:353:PHE:HB3	1.95	0.48
17:Q:146:TYR:HE2	18:r:141:ARG:HG2	1.78	0.48
20:T:29:SER:HA	20:T:34:ALA:HA	1.96	0.48
21:f:242:GLU:HA	21:f:245:ASN:HB2	1.96	0.48
18:r:8:PHE:HE1	18:r:13:ILE:HG12	1.79	0.48
18:r:100:MET:HE2	18:r:126:PHE:HB3	1.96	0.48
20:t:96:MET:HB3	20:t:96:MET:HE2	1.72	0.48
3:C:344:LEU:HA	3:C:347:ILE:HD12	1.94	0.48
4:D:345:PHE:HE1	4:D:375:ILE:HD12	1.78	0.48
17:Q:5:ILE:HG21	17:Q:160:LEU:HD11	1.96	0.48
21:f:136:GLU:HA	21:f:140:LEU:HD23	1.96	0.48
21:f:505:MET:HG2	21:f:541:THR:HB	1.95	0.48
7:g:51:VAL:HG11	7:g:198:ALA:HB1	1.96	0.48
14:n:99:ILE:HG22	14:n:113:SER:HA	1.96	0.48
17:q:43:LEU:HD21	17:q:188:ILE:HG12	1.94	0.48
5:E:139:SER:O	5:E:143:ARG:HB2	2.14	0.48
7:G:80:MET:HG2	7:G:138:MET:HA	1.95	0.47
11:K:125:GLU:HA	11:K:134:SER:HA	1.96	0.47
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.95	0.47
15:o:127:MET:HB3	15:o:127:MET:HE3	1.75	0.47
16:p:49:LEU:HD21	16:p:87:LEU:HD22	1.96	0.47
20:t:50:MET:HE3	20:t:192:VAL:HG22	1.95	0.47
1:A:97:ARG:HB3	1:A:115:VAL:HG11	1.96	0.47
13:M:106:ILE:HG12	13:M:111:LEU:HB2	1.95	0.47
18:R:87:VAL:HG21	18:R:97:MET:HE2	1.95	0.47
21:f:213:GLN:HG2	21:f:255:VAL:HG13	1.96	0.47
13:m:77:VAL:HA	13:m:135:PHE:HB3	1.96	0.47
3:C:347:ILE:HG23	3:C:387:VAL:HG21	1.97	0.47
8:H:6:TYR:HE2	8:H:14:SER:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:68:ILE:HG23	8:H:91:ARG:HA	1.96	0.47
14:N:37:ILE:HG23	14:N:60:THR:HA	1.95	0.47
15:O:67:SER:HB3	15:O:74:PRO:HG3	1.96	0.47
14:n:119:MET:HE1	20:t:6:VAL:HB	1.95	0.47
1:A:211:GLY:HA3	1:A:337:LEU:HA	1.97	0.47
9:I:159:TRP:HA	10:J:54:GLN:HB2	1.96	0.47
21:f:660:ILE:HG12	21:f:692:LEU:HD23	1.95	0.47
7:g:105:TYR:HA	15:o:78:THR:HG23	1.97	0.47
6:F:365:ILE:HD11	22:F:501:ATP:C4	2.50	0.47
15:O:59:ILE:HD11	15:O:83:LEU:HD13	1.96	0.47
7:G:29:PHE:HE1	7:G:156:PRO:HD2	1.79	0.47
7:G:197:THR:HA	7:G:200:THR:HG22	1.97	0.47
9:I:14:PRO:HA	10:J:21:TYR:CZ	2.50	0.47
21:f:691:PRO:HB3	21:f:749:ALA:HA	1.96	0.47
2:B:283:PHE:HD1	2:B:328:ILE:HG23	1.79	0.47
2:B:363:ARG:HA	2:B:366:GLN:HB2	1.97	0.47
3:C:72:TYR:HB3	3:C:116:LEU:HB2	1.96	0.47
3:C:268:GLU:HG3	4:D:287:ARG:HH22	1.80	0.47
4:D:406:VAL:HG13	4:D:408:LYS:HE2	1.96	0.47
6:F:399:VAL:HG21	6:F:424:ILE:HD13	1.97	0.47
9:I:71:ASP:HB2	9:I:223:THR:HG21	1.97	0.47
9:I:72:MET:HE2	9:I:72:MET:HB2	1.75	0.47
13:M:66:LEU:HA	13:M:75:MET:O	2.15	0.47
9:i:95:GLN:HG3	16:p:69:PHE:CD1	2.49	0.47
12:l:104:PRO:HD2	12:l:107:ARG:HD2	1.96	0.47
13:m:239:ALA:O	13:m:243:LEU:HG	2.15	0.47
1:A:398:ARG:HE	2:B:199:GLU:HG2	1.80	0.47
13:M:192:GLU:HA	13:M:195:LYS:HE3	1.97	0.47
17:q:148:THR:HG22	17:q:150:THR:H	1.80	0.47
20:t:100:ARG:HH21	20:t:128:LEU:HD22	1.79	0.47
3:C:277:LEU:HA	3:C:280:LEU:HD13	1.97	0.47
4:D:238:LYS:HE2	4:D:273:LYS:HE2	1.96	0.47
5:E:60:VAL:HB	5:E:96:THR:HG23	1.97	0.47
8:H:210:VAL:HG23	8:H:221:LEU:HD12	1.97	0.47
9:I:122:THR:HG22	9:I:129:PRO:HB3	1.96	0.47
20:T:26:MET:HE1	20:T:202:PRO:HB3	1.96	0.47
16:p:168:SER:HB2	16:p:200:LEU:HG	1.97	0.47
12:l:47:VAL:HG13	12:l:212:ILE:HG13	1.96	0.47
14:N:138:TYR:HB2	14:n:138:TYR:CZ	2.50	0.46
19:S:113:LEU:HD23	19:S:119:GLY:HA2	1.97	0.46
21:f:382:ASN:HB3	21:f:417:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:593:THR:HG21	21:f:623:LYS:HA	1.96	0.46
3:C:277:LEU:HD21	3:C:305:LEU:HB3	1.96	0.46
5:E:191:LEU:HB3	5:E:195:PHE:CE2	2.50	0.46
9:I:42:GLY:HA3	9:I:186:LEU:HD21	1.97	0.46
9:I:49:ARG:HH22	9:I:52:ILE:HA	1.80	0.46
21:f:524:MET:HA	21:f:527:VAL:HB	1.97	0.46
3:C:272:THR:O	3:C:276:LEU:HB2	2.15	0.46
6:F:381:TYR:HA	6:F:384:LEU:HB2	1.95	0.46
9:I:175:LEU:HD23	9:I:175:LEU:HA	1.80	0.46
15:O:75:ARG:HB2	15:O:78:THR:HG22	1.95	0.46
19:s:58:HIS:HB3	20:t:130:VAL:HG13	1.97	0.46
20:t:124:TYR:HE1	20:t:139:THR:HG22	1.79	0.46
3:C:129:ASN:C	3:C:129:ASN:HD22	2.23	0.46
12:l:73:SER:HB3	12:l:133:LEU:HB2	1.96	0.46
18:r:12:VAL:HB	18:r:179:VAL:HB	1.97	0.46
2:B:171:VAL:HA	2:B:174:MET:HG2	1.96	0.46
6:F:223:VAL:HG22	6:F:350:ARG:HB3	1.98	0.46
9:I:38:LEU:HD23	9:I:160:LYS:HD2	1.97	0.46
10:J:175:ASN:HB3	10:J:177:THR:HG23	1.97	0.46
17:Q:3:TYR:CE2	17:Q:5:ILE:HB	2.50	0.46
21:f:593:THR:HB	21:f:623:LYS:HG2	1.97	0.46
17:q:13:VAL:HG11	17:q:105:ALA:HB1	1.96	0.46
2:B:361:LYS:HD3	2:B:384:ILE:HG23	1.97	0.46
6:F:92:ASN:HA	6:F:148:GLY:HA2	1.98	0.46
9:I:66:TYR:HB3	9:I:91:ARG:HH22	1.80	0.46
20:T:15:LYS:HE3	20:T:122:LEU:HB2	1.96	0.46
10:j:96:LEU:HG	17:q:62:LYS:HB2	1.96	0.46
5:E:138:LEU:HB3	5:E:142:ILE:HG12	1.97	0.46
16:P:88:MET:HE1	16:P:132:VAL:HG13	1.96	0.46
21:f:322:SER:HB2	21:f:331:LEU:HD11	1.98	0.46
21:f:509:LYS:HE3	21:f:511:SER:HB2	1.98	0.46
21:f:688:ARG:HH12	21:f:788:MET:HG3	1.81	0.46
9:i:105:ILE:HG13	9:i:107:CYS:H	1.81	0.46
1:A:368:ILE:HG22	1:A:406:GLU:HB3	1.97	0.46
2:B:400:THR:HG22	3:C:180:ILE:HB	1.98	0.46
15:O:216:ILE:HD13	16:P:196:THR:HG23	1.98	0.46
19:S:143:ALA:HB1	16:p:145:GLN:HG3	1.97	0.46
18:r:4:LEU:HD21	18:r:135:ALA:HB1	1.98	0.46
6:F:225:MET:HE3	6:F:233:LYS:HG2	1.98	0.46
9:I:9:THR:HB	9:I:20:GLN:HG3	1.98	0.46
12:L:192:LEU:HD13	12:L:236:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:45:VAL:HB	20:T:49:THR:HG23	1.98	0.46
21:f:337:LEU:HD22	21:f:420:TRP:HD1	1.81	0.46
2:B:372:MET:HE1	3:C:178:LEU:HG	1.97	0.46
19:S:15:ILE:HB	19:S:22:ILE:HG12	1.98	0.46
12:l:36:VAL:HG12	12:l:160:SER:HB3	1.97	0.46
12:l:41:LYS:HE2	12:l:181:GLU:HA	1.97	0.46
13:m:51:LYS:HZ1	13:m:64:LYS:HD3	1.81	0.46
19:s:22:ILE:HG12	19:s:197:ILE:HG13	1.97	0.46
20:T:26:MET:HE3	20:T:186:ARG:HG2	1.98	0.45
21:f:208:LEU:HD23	21:f:211:ILE:HG13	1.98	0.45
8:h:92:LYS:HA	8:h:92:LYS:HD3	1.80	0.45
12:l:72:ILE:HG22	12:l:134:ILE:HD13	1.97	0.45
12:l:215:VAL:HB	12:l:221:PHE:HD1	1.81	0.45
20:t:43:MET:HE2	20:t:43:MET:HB2	1.89	0.45
2:B:407:LEU:HD13	3:C:174:LEU:HD21	1.97	0.45
3:C:284:GLU:HG2	3:C:285:ALA:H	1.82	0.45
6:F:310:MET:O	6:F:314:LEU:HG	2.16	0.45
19:S:68:ILE:HD12	19:S:68:ILE:HA	1.88	0.45
21:f:506:GLY:HA2	21:f:540:GLN:HE22	1.81	0.45
20:t:6:VAL:HG22	20:t:30:TYR:HB2	1.97	0.45
5:E:55:GLN:HB2	5:E:100:LEU:HB3	1.98	0.45
7:G:191:PHE:HE2	7:G:221:THR:HG23	1.81	0.45
18:R:59:LEU:HD22	18:R:83:LEU:HB2	1.99	0.45
21:f:181:ARG:HH12	21:f:216:MET:HG3	1.80	0.45
21:f:297:MET:HG2	21:f:300:ARG:HG2	1.97	0.45
21:f:298:LEU:HA	21:f:301:HIS:CE1	2.51	0.45
21:f:350:LYS:HG2	21:f:351:THR:HG23	1.98	0.45
6:F:313:LEU:HA	6:F:317:LEU:HB2	1.98	0.45
21:f:517:VAL:HG22	21:f:556:ARG:O	2.16	0.45
17:q:7:ILE:HG21	17:q:160:LEU:HD21	1.98	0.45
2:B:424:GLU:HA	2:B:427:LEU:HD12	1.98	0.45
12:L:145:PHE:HD1	12:L:155:ASP:HA	1.82	0.45
13:M:57:LEU:HD23	13:M:57:LEU:H	1.81	0.45
14:N:138:TYR:HB2	14:n:138:TYR:CE1	2.51	0.45
15:O:54:MET:HG2	16:P:96:TYR:CZ	2.52	0.45
20:t:107:TRP:HA	20:t:127:MET:SD	2.56	0.45
6:F:93:VAL:HG23	6:F:147:PRO:HA	1.97	0.45
16:P:30:ILE:HG23	16:P:32:ALA:H	1.82	0.45
17:Q:13:VAL:HG11	17:Q:105:ALA:HB1	1.99	0.45
17:Q:19:ARG:HH21	17:Q:177:THR:HB	1.82	0.45
4:D:233:SER:HB3	4:D:269:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:407:ILE:N	4:D:408:LYS:HA	2.32	0.45
5:E:350:ALA:HA	5:E:353:PHE:HB2	1.99	0.45
14:N:45:ARG:HH21	14:N:53:GLN:HE21	1.65	0.45
21:f:311:VAL:HB	21:f:490:ALA:H	1.82	0.45
21:f:341:GLU:HG3	21:f:342:PRO:HD3	1.98	0.45
21:f:343:LYS:HA	21:f:343:LYS:HD2	1.78	0.45
11:k:67:ILE:HG21	11:k:218:ALA:HB2	1.98	0.45
2:B:253:SER:HA	2:B:290:ILE:HD11	1.99	0.45
4:D:398:ASP:HA	4:D:401:LYS:HB2	1.99	0.45
8:H:113:ARG:HA	8:H:113:ARG:HD3	1.82	0.45
20:T:173:MET:HE2	20:T:173:MET:HB3	1.65	0.45
5:E:261:LEU:HD23	5:E:294:ARG:HD3	1.99	0.45
10:J:21:TYR:CZ	10:J:24:GLU:HG2	2.52	0.45
13:M:175:GLU:HA	13:M:178:LYS:HE3	1.98	0.45
15:O:138:PHE:HZ	15:O:155:VAL:HG23	1.82	0.45
17:Q:182:ILE:HG23	17:Q:189:HIS:HB2	1.98	0.45
21:f:257:ARG:CZ	21:f:284:SER:HB3	2.47	0.45
9:i:218:ARG:HA	9:i:223:THR:HA	1.98	0.45
11:k:56:SER:HB3	11:k:59:MET:HE3	1.99	0.45
5:E:185:ARG:HH21	5:E:197:LYS:HE2	1.82	0.45
11:K:40:ILE:HD12	11:K:198:SER:HB3	1.97	0.45
13:M:90:ILE:HG12	13:M:118:TYR:CZ	2.52	0.45
13:M:231:ILE:O	13:M:232:ARG:HG2	2.17	0.45
20:T:15:LYS:HE2	20:T:20:VAL:HG13	1.99	0.45
15:O:42:TYR:HB2	15:O:178:ILE:HD11	1.99	0.44
21:f:123:ALA:HA	21:f:127:SER:HB3	1.98	0.44
21:f:411:ALA:HB3	21:f:443:GLY:HA3	1.99	0.44
21:f:780:PRO:HG2	21:f:802:SER:HA	1.98	0.44
13:m:161:TRP:HB3	13:m:181:MET:HE3	1.99	0.44
5:E:309:ARG:NH2	5:E:337:GLY:H	2.15	0.44
12:L:137:TYR:HA	12:L:141:GLY:O	2.17	0.44
13:M:38:GLY:O	13:M:162:GLY:HA2	2.17	0.44
21:f:8:LYS:HZ2	21:f:39:LYS:HE2	1.82	0.44
10:j:200:GLN:HG3	10:j:202:GLY:H	1.81	0.44
1:A:277:ILE:HG23	1:A:280:ILE:HD13	1.99	0.44
1:A:327:LEU:HD13	1:A:331:LEU:HD23	1.99	0.44
1:A:372:LEU:HD11	11:K:207:GLU:HB3	1.98	0.44
6:F:431:LYS:HA	6:F:431:LYS:HD3	1.80	0.44
10:J:5:ARG:HA	10:J:5:ARG:HD3	1.86	0.44
15:o:86:MET:HE3	15:o:86:MET:HB3	1.87	0.44
1:A:284:ARG:HH11	6:F:334:ARG:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:253:ILE:HA	5:E:256:THR:HB	2.00	0.44
7:G:11:ARG:HG3	7:G:27:TYR:HE2	1.82	0.44
11:K:27:ALA:O	11:K:31:ILE:HG12	2.17	0.44
12:L:193:ARG:HA	12:L:196:ARG:HD2	1.98	0.44
21:f:470:VAL:HG12	21:f:471:LEU:HG	1.98	0.44
14:n:19:ARG:HD2	14:n:171:GLY:N	2.32	0.44
19:s:175:VAL:HA	19:s:178:VAL:HG12	2.00	0.44
6:F:364:ARG:HH11	6:F:368:ILE:HD12	1.82	0.44
9:I:5:TYR:HE2	10:J:4:ASP:HB3	1.81	0.44
11:K:81:LEU:HD23	11:K:83:ALA:H	1.83	0.44
14:N:14:LEU:HD11	14:N:101:ALA:HB3	1.99	0.44
15:O:159:ILE:O	15:O:163:ILE:HG12	2.16	0.44
12:l:137:TYR:CZ	12:l:215:VAL:HG13	2.52	0.44
13:m:70:ASP:HA	20:t:76:LEU:HD11	2.00	0.44
16:p:57:ALA:HA	16:p:60:VAL:HB	2.00	0.44
19:s:30:SER:HB3	19:s:35:ILE:HD13	1.99	0.44
5:E:116:ASP:HA	5:E:117:PRO:HD3	1.92	0.44
21:f:119:LYS:N	21:f:122:ALA:HB3	2.32	0.44
21:f:399:LEU:HD21	21:f:440:ILE:HG12	1.99	0.44
11:k:167:ALA:HB1	11:k:181:LEU:HD21	1.99	0.44
13:m:195:LYS:O	13:m:199:ILE:HG12	2.17	0.44
3:C:117:ARG:HG3	3:C:122:THR:HG22	1.99	0.44
3:C:165:ILE:HG23	3:C:166:GLU:HG3	1.99	0.44
15:O:200:GLY:HA2	19:s:173:ARG:HD3	1.99	0.44
19:S:4:PRO:HB3	20:T:103:MET:HE1	2.00	0.44
19:S:193:LEU:HB3	19:S:210:LEU:HD23	1.98	0.44
10:j:61:LYS:HE2	10:j:61:LYS:HB2	1.85	0.44
10:j:131:ALA:H	10:j:147:THR:HG22	1.82	0.44
13:m:66:LEU:HD12	13:m:212:GLU:HB3	2.00	0.44
13:m:119:VAL:HG13	13:m:131:PHE:HD2	1.82	0.44
16:p:44:PRO:HB3	16:p:50:TYR:CZ	2.53	0.44
5:E:100:LEU:HD21	5:E:107:ILE:HG12	2.00	0.44
5:E:337:GLY:HA2	5:E:378:LYS:HE3	1.98	0.44
15:O:17:ASP:HB2	15:O:169:SER:HB3	1.99	0.44
16:P:49:LEU:HD21	16:P:87:LEU:HD22	1.99	0.44
21:f:53:GLN:H	21:f:53:GLN:HG3	1.67	0.44
12:l:229:VAL:HG12	12:l:233:LEU:HG	2.00	0.44
15:o:103:VAL:HG22	15:o:108:PRO:HB3	2.00	0.44
17:q:85:ARG:HA	17:q:118:MET:HE1	1.99	0.44
19:s:85:THR:HA	19:s:88:ILE:HD12	2.00	0.44
3:C:328:ILE:HA	3:C:331:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:7:SER:N	8:H:8:PHE:HB2	2.32	0.44
9:I:95:GLN:HE22	9:I:98:LEU:HD23	1.83	0.44
13:M:120:HIS:HA	13:M:123:THR:HG22	2.00	0.44
14:N:51:ASP:HB2	14:N:94:LEU:HD22	2.00	0.44
12:I:189:LYS:HZ3	12:I:237:GLU:H	1.65	0.44
19:S:46:LEU:HD11	19:S:52:ILE:HB	2.00	0.43
21:f:250:ARG:HH22	21:f:253:LEU:HD22	1.83	0.43
7:G:99:ALA:HB1	14:N:61:TYR:CE1	2.53	0.43
13:M:68:ASN:HB3	13:M:224:HIS:CE1	2.53	0.43
11:k:206:MET:HE1	11:k:210:LEU:HD13	2.00	0.43
1:A:302:LEU:O	1:A:306:LEU:HB2	2.18	0.43
3:C:238:ALA:HB1	3:C:289:ILE:HD13	2.00	0.43
3:C:313:ARG:HD2	3:C:313:ARG:HA	1.75	0.43
6:F:256:LEU:HD21	6:F:309:THR:HG21	1.98	0.43
21:f:637:LYS:HE2	21:f:637:LYS:HB2	1.90	0.43
7:g:189:TRP:HZ3	7:g:197:THR:HG21	1.83	0.43
14:n:7:GLN:HA	14:n:12:VAL:HG12	2.01	0.43
15:O:112:SER:HB3	15:O:125:VAL:HG11	2.00	0.43
18:R:68:LEU:HD23	18:R:68:LEU:HA	1.91	0.43
21:f:515:ALA:HA	21:f:554:TYR:HB2	2.00	0.43
2:B:123:VAL:HG21	2:B:152:LEU:HD21	2.01	0.43
5:E:203:ILE:HG21	5:E:256:THR:HG23	1.99	0.43
8:H:124:SER:HA	8:H:125:GLY:HA2	1.71	0.43
13:M:175:GLU:HB3	13:M:196:ILE:HD12	2.01	0.43
16:P:104:TYR:HA	16:P:126:LEU:HD11	2.00	0.43
12:I:120:THR:HG22	12:I:127:PRO:HB3	1.99	0.43
20:t:180:ASP:HB3	20:t:183:SER:HB3	1.99	0.43
3:C:127:LEU:HD22	4:D:112:TYR:CZ	2.53	0.43
21:f:724:ASN:HA	21:f:728:ALA:HB3	1.99	0.43
9:i:164:ILE:HG22	9:i:165:GLY:H	1.84	0.43
11:k:203:LYS:HA	11:k:206:MET:HE3	2.00	0.43
19:s:16:ALA:HB2	19:s:121:VAL:HG23	2.00	0.43
8:H:6:TYR:HE2	8:H:15:PRO:HD3	1.84	0.43
12:L:50:LYS:HE2	12:L:50:LYS:HB2	1.77	0.43
17:Q:12:TYR:HB2	17:Q:182:ILE:HD11	2.01	0.43
10:j:17:PHE:HA	10:j:20:GLU:HG2	1.99	0.43
15:o:45:GLY:HA2	15:o:98:LEU:HD13	2.00	0.43
4:D:181:VAL:HG23	4:D:306:LYS:HD2	2.01	0.43
6:F:121:CYS:HA	6:F:133:PHE:HE1	1.84	0.43
11:K:113:THR:HA	11:K:116:VAL:HG12	2.01	0.43
21:f:463:LEU:HD13	21:f:500:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:659:LEU:HD12	21:f:693:ALA:HB3	2.01	0.43
12:l:70:ILE:HD11	12:l:105:VAL:HG22	1.99	0.43
1:A:101:ILE:HB	1:A:136:GLU:HA	2.01	0.43
15:O:37:ILE:HD11	15:O:43:CYS:HB2	2.01	0.43
20:T:99:ARG:HA	20:T:99:ARG:HD3	1.80	0.43
21:f:173:LEU:O	21:f:177:GLU:HG2	2.19	0.43
10:j:91:CYS:HB2	10:j:102:VAL:HG21	2.01	0.43
11:k:149:LYS:HE3	11:k:149:LYS:HB2	1.91	0.43
1:A:250:VAL:HG22	1:A:294:GLU:HG2	2.00	0.43
4:D:152:MET:HG3	4:D:153:MET:HG3	2.00	0.43
21:f:307:LEU:HD23	21:f:307:LEU:HA	1.91	0.43
9:i:17:ARG:NH1	9:i:19:TYR:HA	2.33	0.43
13:m:231:ILE:O	13:m:232:ARG:HD3	2.19	0.43
1:A:242:GLY:HA2	1:A:245:LEU:HD23	2.00	0.42
4:D:317:LEU:HG	4:D:321:LEU:HD23	2.01	0.42
6:F:394:ALA:HB2	22:F:501:ATP:H4'	2.00	0.42
8:H:34:PRO:HA	8:H:164:GLY:HA3	2.00	0.42
12:L:41:LYS:HD3	12:L:180:MET:HG3	2.01	0.42
13:M:191:LYS:HG2	13:M:195:LYS:HE2	2.00	0.42
21:f:687:ARG:HH21	21:f:745:LEU:HD21	1.84	0.42
8:h:97:TYR:CD1	8:h:105:ILE:HB	2.53	0.42
2:B:111:THR:H	2:B:123:VAL:HG13	1.84	0.42
4:D:413:GLU:N	4:D:414:HIS:HA	2.34	0.42
15:O:111:TYR:CZ	15:O:121:LYS:HD3	2.54	0.42
16:P:12:MET:HE3	16:P:171:MET:HG2	2.01	0.42
1:A:138:MET:HB3	1:A:138:MET:HE3	1.69	0.42
9:I:35:LEU:HD23	9:I:35:LEU:HA	1.90	0.42
12:L:74:ILE:HD12	12:L:74:ILE:HA	1.94	0.42
17:Q:45:LEU:HD12	17:Q:103:LEU:HD11	2.00	0.42
20:T:4:PRO:HG3	20:T:107:TRP:CE2	2.54	0.42
21:f:510:SER:HB3	21:f:550:LEU:HD11	2.01	0.42
11:k:202:LEU:HD23	11:k:202:LEU:HA	1.92	0.42
12:l:118:ILE:HG23	12:l:122:ARG:HH12	1.83	0.42
4:D:192:LYS:HA	4:D:192:LYS:HD2	1.85	0.42
6:F:315:ASN:HA	6:F:320:PHE:HD2	1.84	0.42
8:H:167:TYR:O	8:H:171:LYS:HG2	2.19	0.42
21:f:625:LYS:HE3	21:f:653:ALA:HB1	2.01	0.42
9:i:72:MET:HE1	9:i:139:TRP:H	1.85	0.42
9:i:159:TRP:CE3	10:j:54:GLN:HB3	2.54	0.42
2:B:153:ASN:HD21	2:B:160:ILE:HD11	1.85	0.42
2:B:224:LEU:HB2	2:B:353:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:153:LEU:HD23	5:E:274:LYS:HE2	2.01	0.42
7:G:51:VAL:HG23	7:G:217:VAL:HG22	2.01	0.42
10:J:3:TYR:HD2	10:J:5:ARG:HE	1.67	0.42
11:K:221:GLN:HB2	11:K:224:GLN:HB3	2.02	0.42
21:f:566:HIS:HB2	21:f:598:CYS:SG	2.59	0.42
3:C:326:LEU:HD11	3:C:330:LYS:HE3	2.00	0.42
7:G:170:VAL:HB	7:G:171:LYS:HD2	2.00	0.42
21:f:207:LEU:O	21:f:211:ILE:HG12	2.19	0.42
16:p:42:ILE:HD13	16:p:42:ILE:HA	1.91	0.42
18:r:195:LEU:HD23	18:r:195:LEU:HA	1.86	0.42
4:D:115:ILE:HA	4:D:139:LEU:HD23	2.01	0.42
18:R:83:LEU:HA	18:R:86:MET:HE2	2.01	0.42
18:R:148:GLU:HG3	18:R:151:GLN:HG2	2.01	0.42
1:A:261:PHE:O	1:A:265:ARG:HD3	2.19	0.42
5:E:325:GLU:HB3	5:E:363:VAL:HG23	2.02	0.42
10:J:180:ALA:HA	10:J:181:ILE:HA	1.77	0.42
21:f:681:TYR:CE2	21:f:683:GLU:HB2	2.55	0.42
8:h:65:VAL:HG13	8:h:75:VAL:HG22	2.02	0.42
10:j:10:PHE:HB2	11:k:23:GLN:HG3	2.00	0.42
19:s:71:ARG:NE	19:s:91:MET:HE1	2.35	0.42
19:s:76:LYS:HG2	19:s:82:ALA:HA	2.02	0.42
7:G:47:CYS:HB3	7:G:191:PHE:CD2	2.55	0.42
10:J:136:PHE:HA	10:J:142:PRO:HA	2.01	0.42
15:O:54:MET:HE3	16:P:96:TYR:HE2	1.85	0.42
16:P:190:ILE:HG22	16:P:195:ILE:HG12	2.02	0.42
8:h:139:TRP:HA	8:h:144:PRO:HA	2.02	0.42
13:m:108:LEU:HD12	13:m:108:LEU:HA	1.91	0.42
13:m:228:PRO:HB2	13:m:231:ILE:HB	2.01	0.42
15:o:143:ARG:H	15:o:146:MET:HE2	1.84	0.42
2:B:109:VAL:HG23	3:C:94:LYS:HE2	2.02	0.42
11:K:21:LEU:HA	11:K:22:PHE:HB2	2.01	0.42
13:M:56:LYS:HD2	13:M:56:LYS:HA	1.76	0.42
15:O:112:SER:HB2	15:O:127:MET:HE3	2.02	0.42
21:f:429:ILE:HA	21:f:432:TYR:HD2	1.85	0.42
7:g:114:LEU:HD23	7:g:114:LEU:HA	1.90	0.42
10:j:200:GLN:HG2	10:j:205:ASN:HD21	1.85	0.42
13:m:81:LEU:H	13:m:81:LEU:HD23	1.85	0.42
2:B:432:GLU:HA	2:B:433:GLY:HA3	1.69	0.41
5:E:55:GLN:HB2	5:E:101:ASP:N	2.31	0.41
7:G:21:ARG:HA	7:G:21:ARG:HD2	1.91	0.41
13:M:36:ALA:O	13:M:164:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:81:LYS:HD2	19:S:81:LYS:HA	1.81	0.41
10:j:125:ARG:HA	10:j:126:PRO:HD3	1.95	0.41
12:l:61:LYS:HB2	12:l:61:LYS:HE3	1.77	0.41
13:m:197:ILE:HD13	13:m:197:ILE:HA	1.93	0.41
15:o:68:LEU:HD23	15:o:68:LEU:HA	1.93	0.41
19:s:211:ARG:H	19:s:211:ARG:HG2	1.63	0.41
1:A:157:ILE:HD12	2:B:114:GLU:HG3	2.01	0.41
1:A:244:GLU:HB3	2:B:268:ARG:HH12	1.84	0.41
5:E:176:PRO:HG3	5:E:385:ASP:HB3	2.01	0.41
6:F:362:ARG:O	6:F:365:ILE:HG22	2.19	0.41
11:K:199:LEU:HD23	11:K:199:LEU:HA	1.84	0.41
12:l:13:TRP:HB3	13:m:25:TYR:CE2	2.55	0.41
14:n:167:ASP:HB3	14:n:170:SER:HB2	2.02	0.41
1:A:415:LYS:O	1:A:419:SER:HB3	2.20	0.41
16:P:125:ASP:HB2	16:P:129:CYS:HB3	2.02	0.41
20:T:22:ILE:HG22	20:T:190:ALA:HB3	2.01	0.41
21:f:687:ARG:NH2	21:f:745:LEU:HD21	2.35	0.41
1:A:112:ILE:HG12	1:A:120:LYS:HD3	2.02	0.41
2:B:312:LEU:HD13	2:B:315:GLN:HE21	1.86	0.41
6:F:97:LEU:H	6:F:120:LYS:N	2.18	0.41
6:F:284:PHE:HA	6:F:329:ILE:HG23	2.02	0.41
8:H:69:THR:HG22	8:H:70:LYS:H	1.86	0.41
16:P:34:MET:HE3	16:P:34:MET:HB3	1.82	0.41
17:Q:21:ALA:HB2	17:Q:32:HIS:CG	2.55	0.41
20:T:107:TRP:HA	20:T:127:MET:SD	2.60	0.41
16:p:158:MET:HG2	16:p:163:LEU:HB2	2.01	0.41
1:A:114:ASN:HB2	1:A:120:LYS:HG2	2.03	0.41
4:D:144:PRO:HA	4:D:145:PRO:HD3	1.92	0.41
7:G:185:LYS:HE2	7:G:185:LYS:HB2	1.82	0.41
9:I:127:LYS:HE2	9:I:127:LYS:HB2	1.95	0.41
7:g:123:GLN:HA	7:g:126:THR:HG22	2.02	0.41
9:i:168:SER:HA	9:i:171:ALA:HB3	2.02	0.41
12:l:39:LYS:HD2	12:l:142:PRO:HG2	2.01	0.41
12:l:50:LYS:HG2	12:l:59:HIS:HB3	2.03	0.41
12:l:85:CYS:O	12:l:89:ARG:HG3	2.21	0.41
12:l:189:LYS:HZ3	12:l:236:LEU:HA	1.85	0.41
16:p:146:MET:HE3	16:p:146:MET:HB3	1.91	0.41
9:I:231:LYS:O	9:I:234:GLU:HG3	2.21	0.41
13:M:160:TYR:HD2	13:M:163:CYS:HB3	1.85	0.41
16:P:88:MET:HE2	16:P:130:PRO:HB3	2.03	0.41
21:f:264:GLU:O	21:f:267:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:623:LYS:O	21:f:627:GLU:CB	2.69	0.41
9:i:66:TYR:HB3	9:i:91:ARG:HH21	1.85	0.41
11:k:104:ASN:ND2	19:s:90:ALA:HB2	2.36	0.41
15:o:160:ALA:O	15:o:163:ILE:HG22	2.20	0.41
9:I:172:VAL:HA	9:I:175:LEU:HB2	2.02	0.41
14:N:33:LYS:HD2	14:N:33:LYS:HA	1.76	0.41
15:O:167:LEU:HD13	19:s:33:PHE:HZ	1.86	0.41
17:Q:38:MET:HE2	17:Q:38:MET:HB2	1.85	0.41
21:f:218:GLU:HA	21:f:259:PHE:HZ	1.85	0.41
21:f:471:LEU:HA	21:f:509:LYS:HD2	2.02	0.41
8:h:93:LEU:O	8:h:96:GLN:HG3	2.20	0.41
15:o:75:ARG:HG2	15:o:77:VAL:HG22	2.02	0.41
5:E:169:GLY:HA2	5:E:275:MET:SD	2.61	0.41
5:E:308:ALA:O	5:E:312:ILE:HG12	2.19	0.41
18:R:166:ARG:HD2	18:R:166:ARG:HA	1.82	0.41
21:f:278:VAL:HA	21:f:281:ILE:HG22	2.03	0.41
11:k:236:GLU:HA	11:k:239:LYS:HG2	2.03	0.41
1:A:147:TYR:OH	6:F:86:LEU:HG	2.21	0.41
4:D:283:ARG:HA	4:D:283:ARG:HD2	1.87	0.41
5:E:171:LEU:HD21	5:E:389:VAL:HB	2.03	0.41
5:E:219:PHE:O	5:E:223:ARG:HG2	2.21	0.41
6:F:124:ILE:HB	6:F:132:TYR:HB3	2.03	0.41
6:F:391:PHE:CD2	6:F:395:GLN:HB3	2.56	0.41
10:J:17:PHE:O	10:J:20:GLU:HG2	2.21	0.41
19:S:135:PHE:O	19:S:136:LYS:HE2	2.21	0.41
20:T:25:ASP:HA	20:T:187:PHE:HA	2.02	0.41
20:T:41:ARG:NH2	20:T:54:SER:HA	2.36	0.41
7:g:101:TRP:CG	7:g:109:ILE:HB	2.56	0.41
18:r:157:ARG:HD3	18:r:195:LEU:HD21	2.02	0.41
19:s:73:LYS:HE2	19:s:73:LYS:HB2	1.81	0.41
20:t:67:LEU:HA	20:t:70:MET:HG2	2.03	0.41
20:t:187:PHE:HE2	20:t:189:ILE:HD11	1.86	0.41
1:A:94:GLN:HG2	2:B:131:HIS:CD2	2.56	0.41
4:D:263:PHE:HD1	4:D:308:ILE:HB	1.87	0.41
9:I:171:ALA:HB2	9:I:200:THR:HG21	2.03	0.41
13:M:41:CYS:HB3	13:M:189:ILE:HG13	2.01	0.41
14:N:18:SER:HB2	14:N:31:THR:H	1.85	0.41
21:f:77:GLU:O	21:f:80:ARG:HG3	2.21	0.41
21:f:628:ASP:HB3	21:f:631:LYS:HE3	2.02	0.41
2:B:149:SER:HB3	2:B:163:LEU:HD22	2.03	0.40
2:B:435:PRO:HA	2:B:436:GLU:HA	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:ILE:HA	3:C:164:VAL:HG12	2.02	0.40
5:E:84:ARG:HG2	5:E:85:ARG:H	1.86	0.40
6:F:191:LEU:HD21	6:F:354:PHE:CE1	2.56	0.40
7:G:163:PHE:HB3	8:H:57:TYR:HA	2.02	0.40
10:j:51:ALA:O	10:j:52:LYS:HG3	2.22	0.40
10:j:87:ALA:HB2	10:j:111:ILE:HD11	2.03	0.40
16:p:148:GLY:O	16:p:151:GLU:HG3	2.21	0.40
2:B:329:MET:HE3	2:B:329:MET:HB3	1.95	0.40
5:E:191:LEU:HB3	5:E:195:PHE:HE2	1.86	0.40
6:F:247:THR:HB	6:F:280:PRO:HB2	2.04	0.40
13:M:228:PRO:HB3	13:M:231:ILE:HD13	2.03	0.40
14:N:19:ARG:HD3	14:N:170:SER:C	2.47	0.40
21:f:86:THR:HG23	21:f:87:THR:H	1.87	0.40
1:A:284:ARG:HH22	6:F:333:ASN:HD22	1.70	0.40
2:B:309:MET:HE3	2:B:309:MET:HB3	1.83	0.40
6:F:384:LEU:HG	6:F:417:HIS:CE1	2.56	0.40
8:H:107:THR:HA	8:H:110:LEU:HD13	2.03	0.40
14:N:104:ASP:OD2	14:N:106:GLN:HG3	2.21	0.40
15:O:103:VAL:HA	15:O:108:PRO:HA	2.03	0.40
19:S:59:GLY:HA2	19:S:62:LEU:HD12	2.04	0.40
21:f:655:LEU:HD23	21:f:655:LEU:HA	1.91	0.40
8:h:121:TYR:HD1	8:h:121:TYR:HA	1.77	0.40
9:i:21:VAL:HG13	9:i:25:MET:HE3	2.02	0.40
9:i:63:GLU:OE1	9:i:64:LYS:HG3	2.21	0.40
20:t:210:ASP:HA	20:t:213:HIS:ND1	2.37	0.40
2:B:273:VAL:HG13	2:B:277:HIS:CE1	2.56	0.40
2:B:411:ARG:H	2:B:411:ARG:HG2	1.80	0.40
4:D:342:ARG:HG2	4:D:364:VAL:HG21	2.03	0.40
7:G:43:ARG:HH11	7:G:149:PRO:HG2	1.86	0.40
10:J:98:VAL:HG12	10:J:100:ASP:H	1.87	0.40
15:O:20:ALA:HB3	15:O:28:ASP:HB3	2.03	0.40
17:Q:26:VAL:HG12	17:q:138:LEU:HD21	2.02	0.40
18:R:141:ARG:HB2	17:q:142:ILE:HD11	2.03	0.40
20:T:180:ASP:HB3	20:T:183:SER:HB3	2.03	0.40
21:f:311:VAL:O	21:f:315:GLU:HB2	2.21	0.40
17:q:103:LEU:HD23	17:q:132:HIS:HD2	1.86	0.40
1:A:332:MET:HE3	1:A:332:MET:HB3	1.82	0.40
4:D:392:TYR:CG	4:D:393:ILE:HD12	2.57	0.40
5:E:207:TYR:CE2	5:E:210:GLU:HB2	2.56	0.40
5:E:216:ARG:HA	5:E:219:PHE:HB2	2.03	0.40
7:G:22:LEU:O	7:G:25:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:105:ILE:HG12	8:H:110:LEU:HD12	2.04	0.40
9:I:34:CYS:H	9:I:164:ILE:HG13	1.86	0.40
14:N:138:TYR:HA	14:N:141:ALA:HB3	2.02	0.40
20:T:20:VAL:HG22	20:T:120:SER:HB3	2.03	0.40
21:f:178:LYS:NZ	21:f:216:MET:HB2	2.37	0.40
21:f:486:GLY:HA3	21:f:525:ILE:HG12	2.03	0.40
12:l:6:TYR:HB3	12:l:13:TRP:O	2.22	0.40
12:l:146:GLN:HE21	12:l:154:PHE:HD2	1.70	0.40
16:p:43:PHE:HB2	16:p:51:ILE:HG23	2.03	0.40
18:r:97:MET:HE3	18:r:97:MET:HB3	1.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/433 (87%)	330 (88%)	46 (12%)	0	100	100
2	B	366/440 (83%)	320 (87%)	46 (13%)	0	100	100
3	C	315/406 (78%)	266 (84%)	49 (16%)	0	100	100
4	D	331/418 (79%)	271 (82%)	59 (18%)	1 (0%)	36	70
5	E	334/389 (86%)	272 (81%)	62 (19%)	0	100	100
6	F	333/439 (76%)	298 (90%)	35 (10%)	0	100	100
7	G	237/246 (96%)	217 (92%)	20 (8%)	0	100	100
7	g	238/246 (97%)	217 (91%)	21 (9%)	0	100	100
8	H	228/234 (97%)	216 (95%)	12 (5%)	0	100	100
8	h	230/234 (98%)	224 (97%)	6 (3%)	0	100	100
9	I	246/261 (94%)	223 (91%)	23 (9%)	0	100	100
9	i	248/261 (95%)	227 (92%)	21 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	237/248 (96%)	222 (94%)	15 (6%)	0	100	100
10	j	237/248 (96%)	222 (94%)	15 (6%)	0	100	100
11	K	224/241 (93%)	208 (93%)	16 (7%)	0	100	100
11	k	224/241 (93%)	212 (95%)	12 (5%)	0	100	100
12	L	236/269 (88%)	224 (95%)	12 (5%)	0	100	100
12	l	236/269 (88%)	226 (96%)	10 (4%)	0	100	100
13	M	238/255 (93%)	219 (92%)	19 (8%)	0	100	100
13	m	238/255 (93%)	223 (94%)	15 (6%)	0	100	100
14	N	189/239 (79%)	176 (93%)	13 (7%)	0	100	100
14	n	189/239 (79%)	176 (93%)	11 (6%)	2 (1%)	11	44
15	O	218/277 (79%)	200 (92%)	18 (8%)	0	100	100
15	o	218/277 (79%)	204 (94%)	14 (6%)	0	100	100
16	P	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
16	p	202/205 (98%)	187 (93%)	15 (7%)	0	100	100
17	Q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
17	q	197/201 (98%)	185 (94%)	12 (6%)	0	100	100
18	R	199/263 (76%)	187 (94%)	12 (6%)	0	100	100
18	r	199/263 (76%)	189 (95%)	10 (5%)	0	100	100
19	S	211/241 (88%)	196 (93%)	15 (7%)	0	100	100
19	s	211/241 (88%)	200 (95%)	11 (5%)	0	100	100
20	T	213/264 (81%)	201 (94%)	12 (6%)	0	100	100
20	t	213/264 (81%)	199 (93%)	14 (7%)	0	100	100
21	f	669/908 (74%)	563 (84%)	104 (16%)	2 (0%)	36	70
All	All	8879/10321 (86%)	8072 (91%)	802 (9%)	5 (0%)	49	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	f	365	VAL
21	f	558	LEU
14	n	92	GLU
14	n	91	ARG
4	D	411	GLU

### 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	297/372 (80%)	296 (100%)	1 (0%)	86	85
2	B	300/385 (78%)	299 (100%)	1 (0%)	86	85
3	C	273/352 (78%)	267 (98%)	6 (2%)	45	64
4	D	287/366 (78%)	286 (100%)	1 (0%)	86	85
5	E	292/341 (86%)	285 (98%)	7 (2%)	43	63
6	F	285/379 (75%)	284 (100%)	1 (0%)	84	83
7	G	192/210 (91%)	192 (100%)	0	100	100
7	g	193/210 (92%)	193 (100%)	0	100	100
8	H	162/191 (85%)	162 (100%)	0	100	100
8	h	164/191 (86%)	163 (99%)	1 (1%)	78	80
9	I	191/221 (86%)	190 (100%)	1 (0%)	81	82
9	i	193/221 (87%)	192 (100%)	1 (0%)	81	82
10	J	152/211 (72%)	152 (100%)	0	100	100
10	j	152/211 (72%)	152 (100%)	0	100	100
11	K	187/203 (92%)	187 (100%)	0	100	100
11	k	186/203 (92%)	186 (100%)	0	100	100
12	L	198/230 (86%)	198 (100%)	0	100	100
12	l	198/230 (86%)	196 (99%)	2 (1%)	68	76
13	M	192/212 (91%)	191 (100%)	1 (0%)	81	82
13	m	192/212 (91%)	191 (100%)	1 (0%)	81	82
14	N	148/181 (82%)	148 (100%)	0	100	100
14	n	148/181 (82%)	147 (99%)	1 (1%)	76	79
15	O	177/228 (78%)	177 (100%)	0	100	100
15	o	177/228 (78%)	177 (100%)	0	100	100
16	P	172/174 (99%)	171 (99%)	1 (1%)	78	80
16	p	172/174 (99%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	152 (99%)	1 (1%)	76	79
18	r	153/202 (76%)	153 (100%)	0	100	100
19	S	174/199 (87%)	174 (100%)	0	100	100
19	s	174/199 (87%)	174 (100%)	0	100	100
20	T	175/215 (81%)	175 (100%)	0	100	100
20	t	175/215 (81%)	174 (99%)	1 (1%)	78	80
21	f	580/763 (76%)	579 (100%)	1 (0%)	87	87
All	All	7192/8654 (83%)	7163 (100%)	29 (0%)	81	83

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ILE
2	B	282	VAL
3	C	109	THR
3	C	129	ASN
3	C	210	THR
3	C	214	VAL
3	C	219	LEU
3	C	371	LEU
4	D	393	ILE
5	E	56	ILE
5	E	104	THR
5	E	172	LEU
5	E	215	ILE
5	E	247	THR
5	E	276	ILE
5	E	326	ILE
6	F	416	THR
9	I	228	LEU
13	M	31	GLU
16	P	58	THR
18	R	197	GLU
21	f	86	THR
8	h	110	LEU
9	i	174	MET
12	l	173	GLU

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Mol	Chain	Res	Type
12	l	211	SER
13	m	232	ARG
14	n	114	VAL
20	t	192	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	ASN
1	A	353	HIS
2	B	195	GLN
2	B	241	ASN
2	B	277	HIS
2	B	306	GLN
2	B	368	HIS
3	C	111	ASN
4	D	98	GLN
4	D	257	ASN
4	D	301	GLN
4	D	353	ASN
4	D	412	GLN
5	E	190	GLN
5	E	262	ASN
5	E	263	GLN
5	E	300	HIS
6	F	380	ASN
6	F	417	HIS
7	G	100	ASN
7	G	127	GLN
7	G	128	ASN
8	H	109	GLN
8	H	166	ASN
9	I	100	GLN
9	I	167	ASN
11	K	152	GLN
12	L	68	ASN
12	L	175	HIS
14	N	53	GLN
15	O	30	ASN
15	O	193	ASN
16	P	18	ASN
16	P	169	GLN

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Mol	Chain	Res	Type
17	Q	168	GLN
20	T	2	GLN
21	f	102	HIS
21	f	382	ASN
21	f	428	GLN
7	g	68	HIS
7	g	90	GLN
7	g	92	GLN
7	g	224	ASN
8	h	21	GLN
8	h	112	GLN
9	i	40	ASN
9	i	53	HIS
10	j	200	GLN
12	l	60	GLN
12	l	90	GLN
12	l	146	GLN
14	n	123	GLN
15	o	62	ASN
16	p	93	ASN
17	q	101	ASN
17	q	132	HIS
18	r	162	GLN
20	t	81	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 ⓘ

5 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	$\# Z  > 2$
22	ATP	D	501	-	29,33,33	0.28	0	44,52,52	0.52	1 (2%)
22	ATP	F	501	-	29,33,33	0.29	0	44,52,52	0.49	0
22	ATP	C	501	-	29,33,33	0.30	0	44,52,52	0.54	1 (2%)
23	ADP	D	502	-	27,29,29	1.35	4 (14%)	42,45,45	1.98	9 (21%)
22	ATP	A	501	-	29,33,33	0.31	0	44,52,52	0.52	1 (2%)

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
22	ATP	D	501	-	-	6/22/38/38	0/3/3/3
22	ATP	F	501	-	-	3/22/38/38	0/3/3/3
22	ATP	C	501	-	-	3/22/38/38	0/3/3/3
23	ADP	D	502	-	-	3/16/32/32	0/3/3/3
22	ATP	A	501	-	-	4/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	502	ADP	C5-C4	4.56	1.47	1.39
23	D	502	ADP	C5-C6	2.55	1.48	1.41
23	D	502	ADP	C5-N7	-2.31	1.34	1.39
23	D	502	ADP	C8-N7	2.22	1.35	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	502	ADP	C5-C4-N3	-6.06	118.84	126.75
23	D	502	ADP	N3-C4-N9	4.91	135.17	127.08
23	D	502	ADP	PA-O3A-PB	-3.97	119.21	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	502	ADP	C2-N3-C4	3.80	120.73	111.75
23	D	502	ADP	N3-C2-N1	-3.26	123.50	128.60
23	D	502	ADP	C4-C5-N7	-2.91	107.07	110.62
23	D	502	ADP	C3'-C2'-C1'	2.64	106.44	101.43
23	D	502	ADP	C5-N7-C8	2.44	106.97	103.51
23	D	502	ADP	C4-N9-C8	2.43	108.36	105.73
22	D	501	ATP	PB-O3B-PG	2.08	139.97	132.83
22	C	501	ATP	PB-O3B-PG	2.02	139.76	132.83
22	A	501	ATP	PB-O3B-PG	2.02	139.75	132.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	501	ATP	PB-O3B-PG-O2G
22	F	501	ATP	PB-O3B-PG-O2G
22	C	501	ATP	O4'-C4'-C5'-O5'
23	D	502	ADP	O4'-C4'-C5'-O5'
23	D	502	ADP	C3'-C4'-C5'-O5'
22	C	501	ATP	C3'-C4'-C5'-O5'
22	F	501	ATP	PB-O3B-PG-O1G
22	A	501	ATP	PA-O3A-PB-O1B
22	D	501	ATP	C4'-C5'-O5'-PA
22	D	501	ATP	PG-O3B-PB-O1B
22	D	501	ATP	PG-O3B-PB-O2B
22	D	501	ATP	PA-O3A-PB-O2B
22	F	501	ATP	O4'-C4'-C5'-O5'
22	A	501	ATP	PB-O3B-PG-O1G
22	D	501	ATP	O4'-C4'-C5'-O5'
22	C	501	ATP	PB-O3B-PG-O2G
23	D	502	ADP	PA-O3A-PB-O2B
22	A	501	ATP	C3'-C4'-C5'-O5'
22	D	501	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

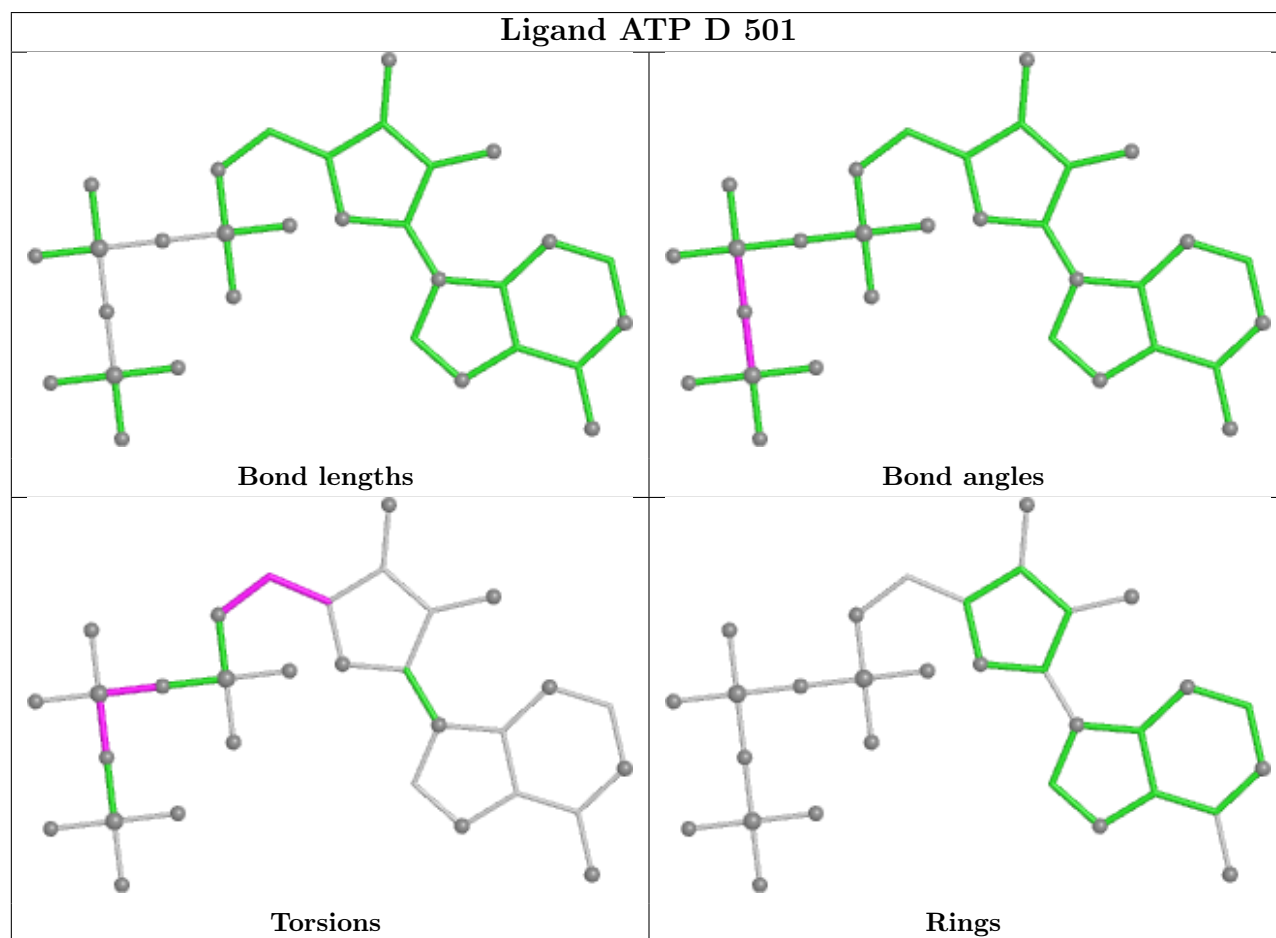
1 monomer is involved in 4 short contacts:

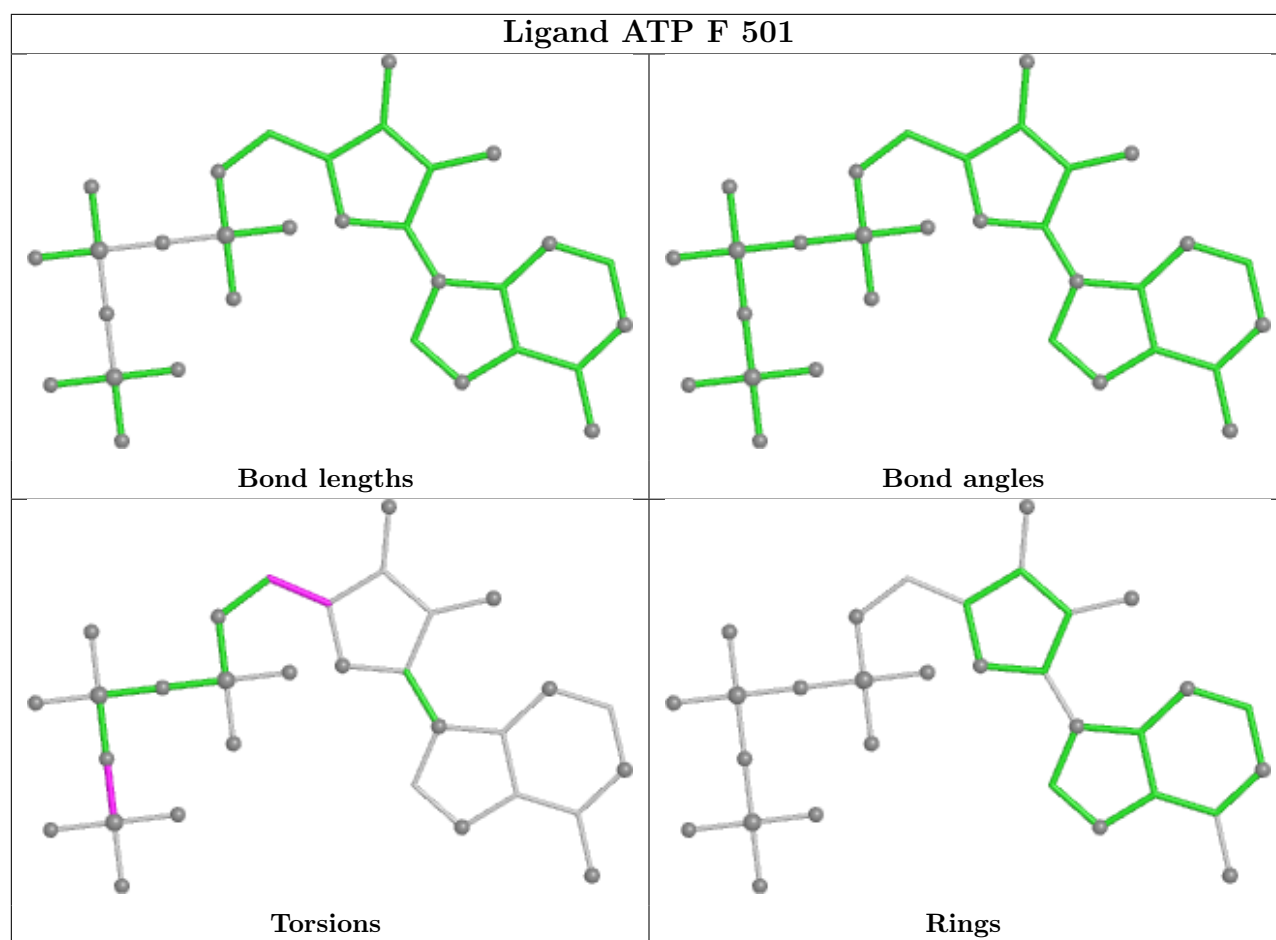
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	501	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

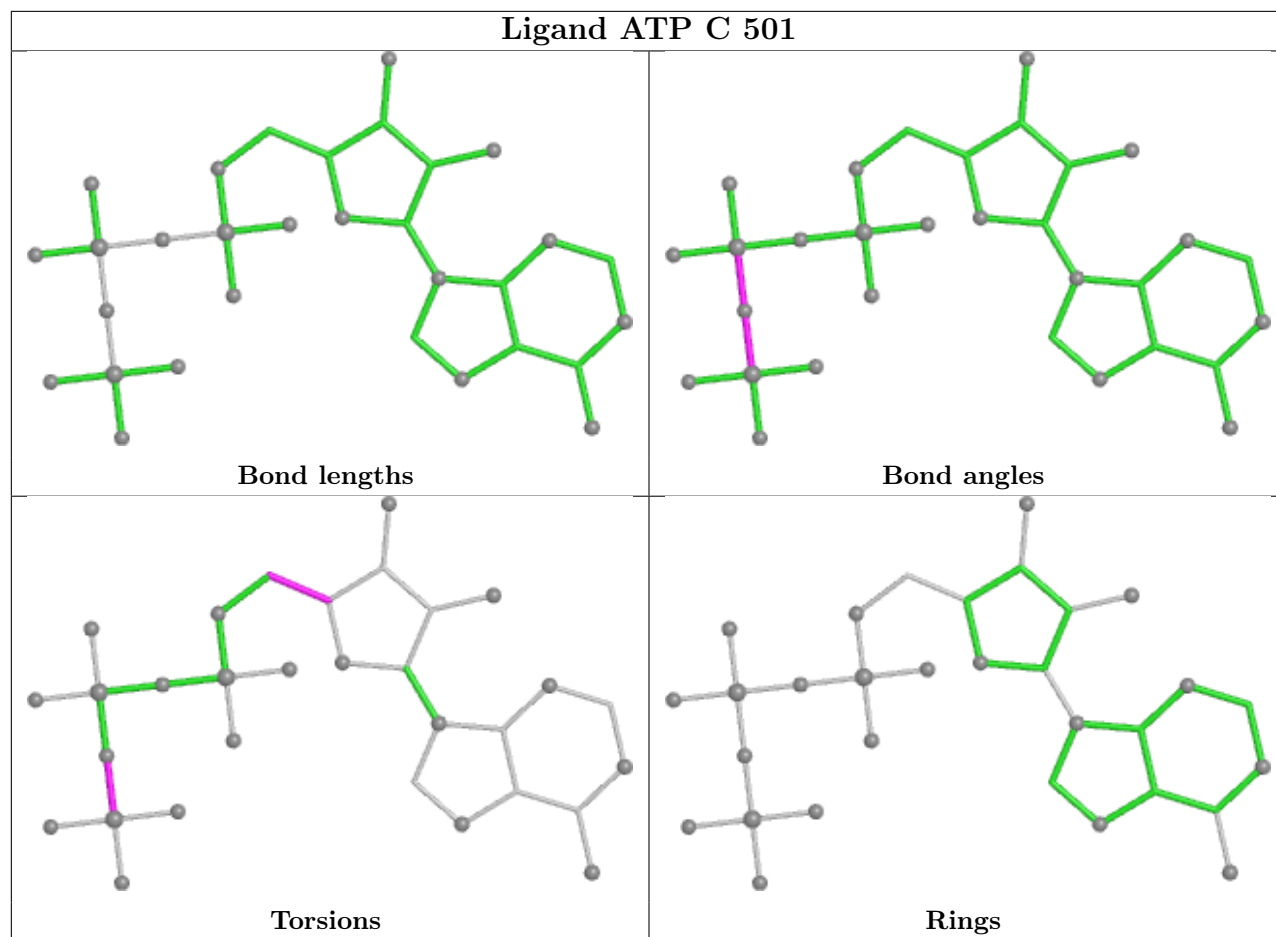


bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

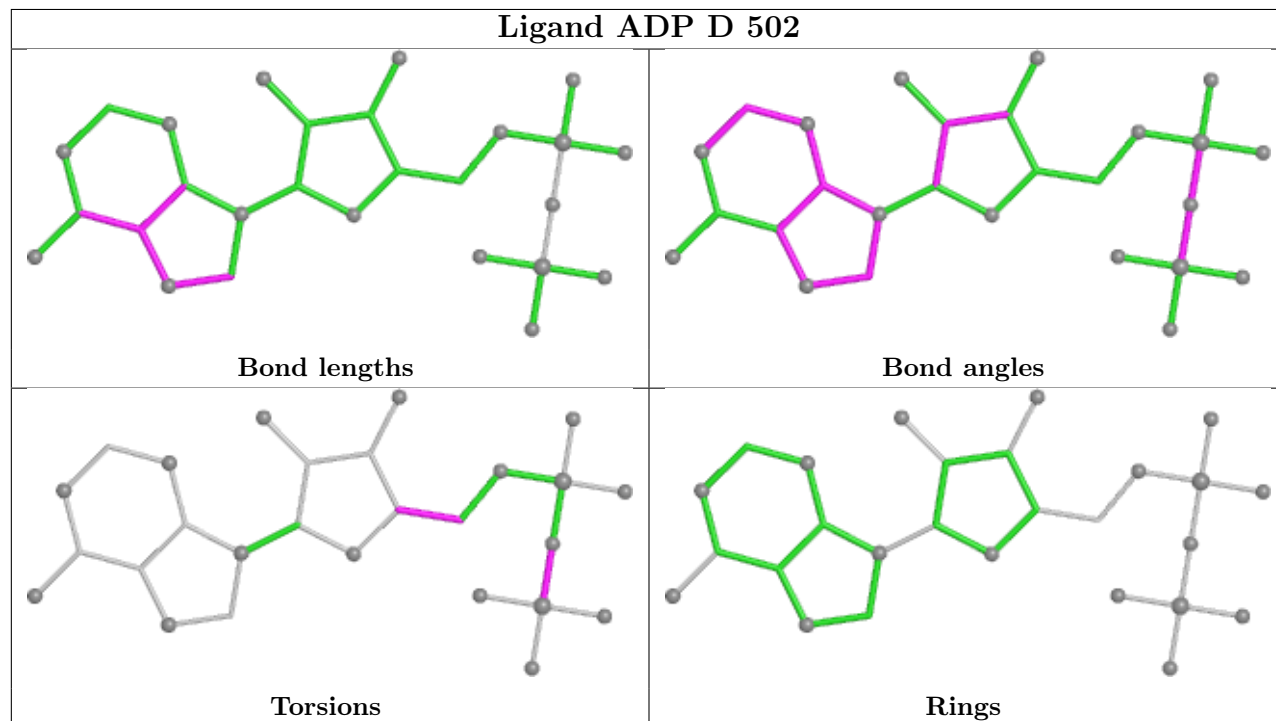


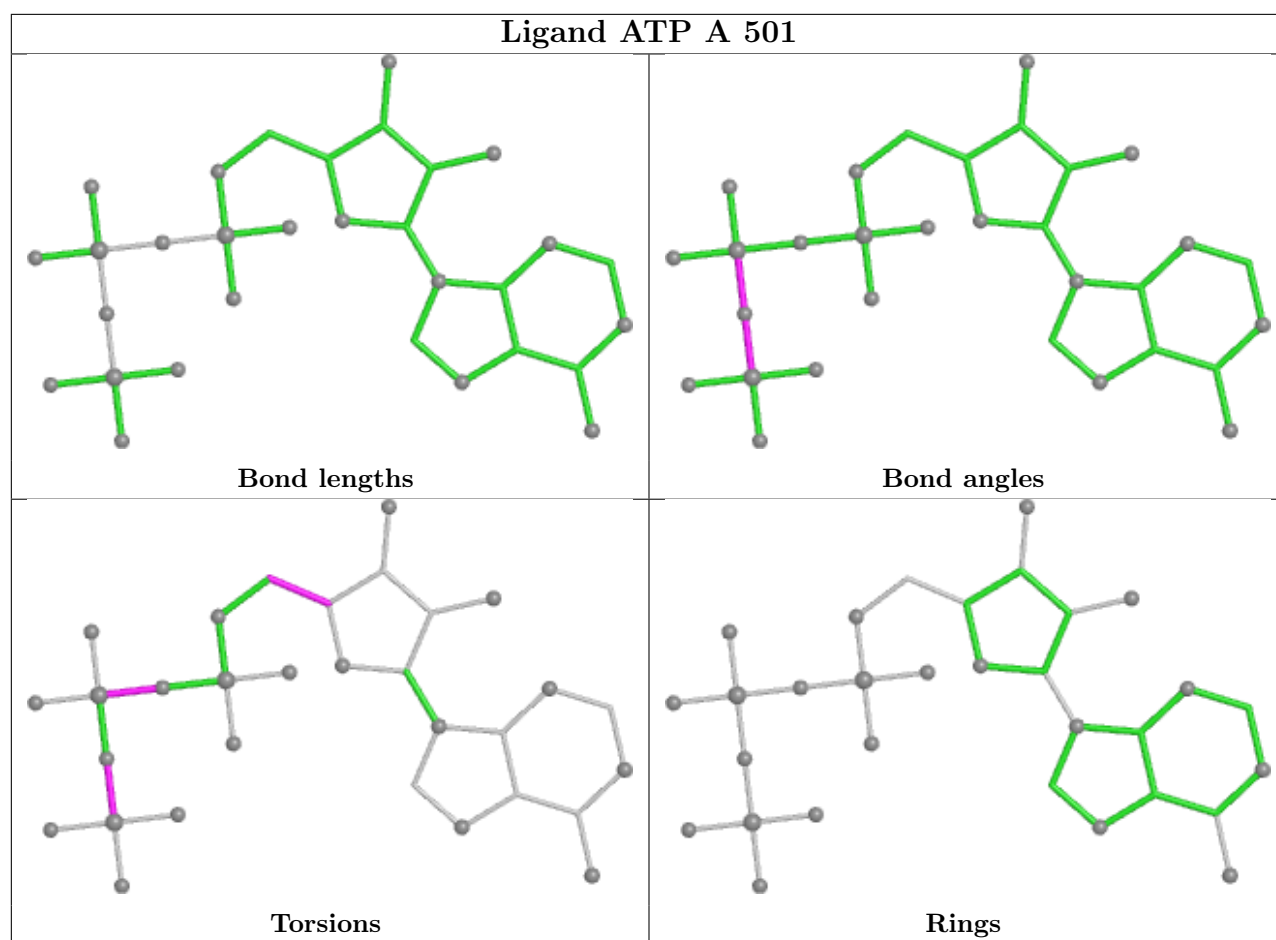


## Ligand ATP C 501



## Ligand ADP D 502





## 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.

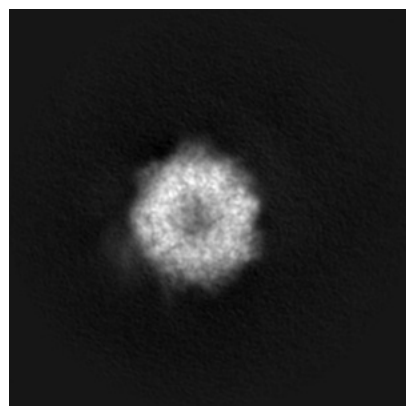
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65362. These allow visual inspection of the internal detail of the map and identification of artifacts.

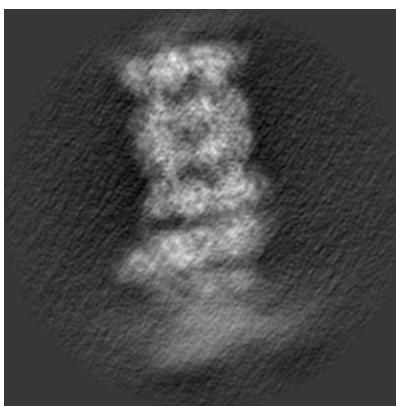
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

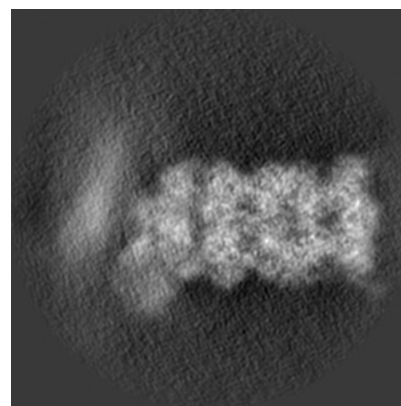
#### 6.1.1 Primary map



X

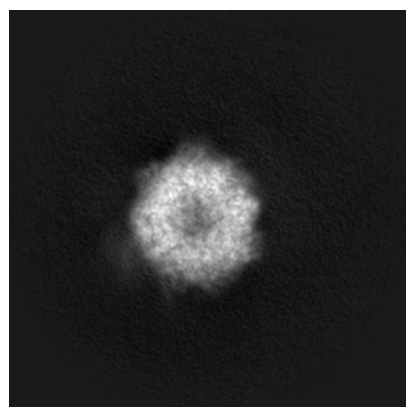


Y

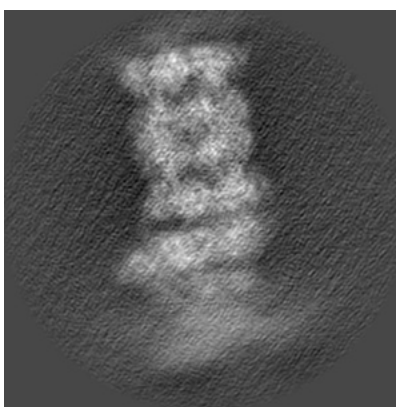


Z

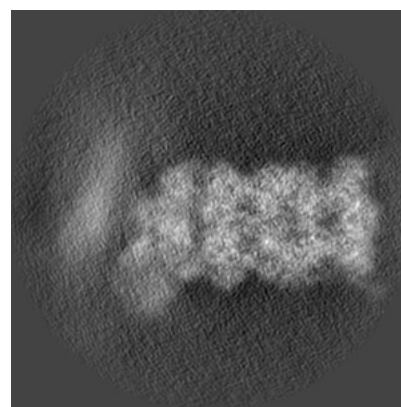
#### 6.1.2 Raw map



X



Y

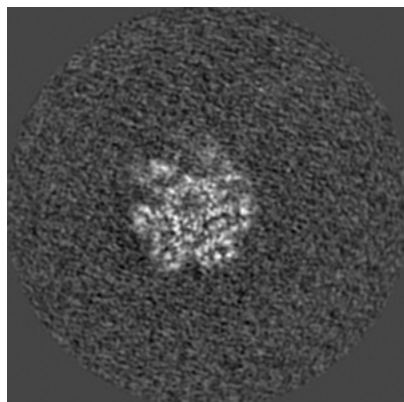


Z

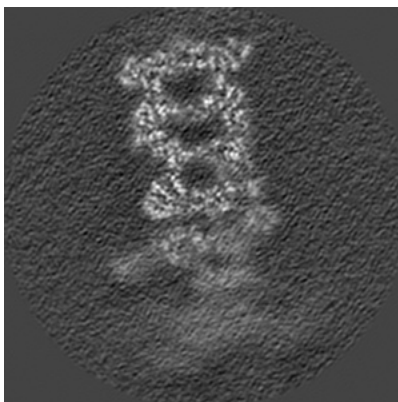
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 110

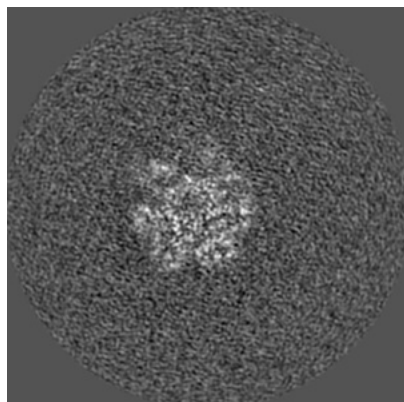


Y Index: 110

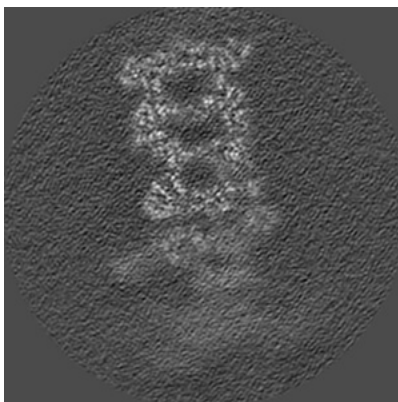


Z Index: 110

### 6.2.2 Raw map



X Index: 110



Y Index: 110



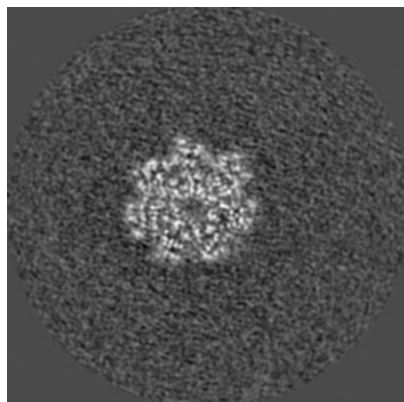
Z Index: 110

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

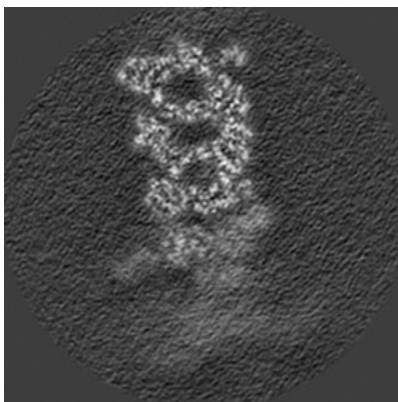


## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 118

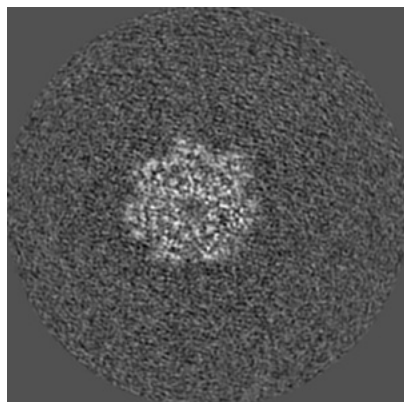


Y Index: 113

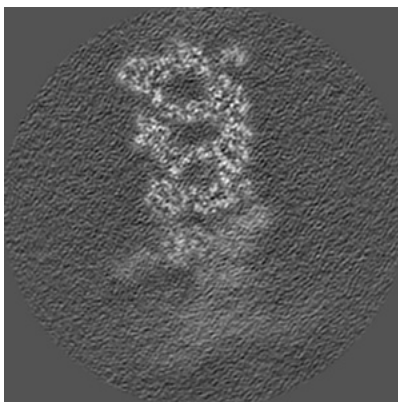


Z Index: 109

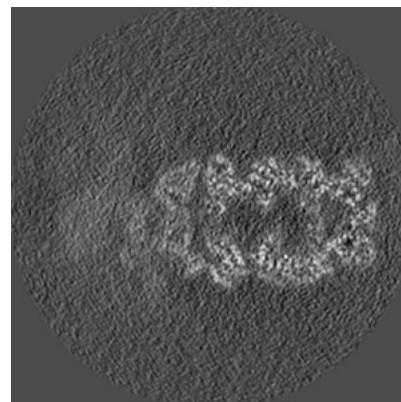
### 6.3.2 Raw map



X Index: 118



Y Index: 113

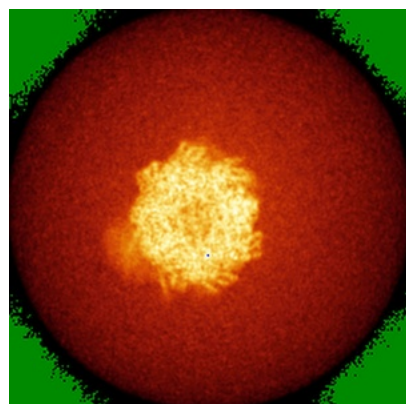


Z Index: 109

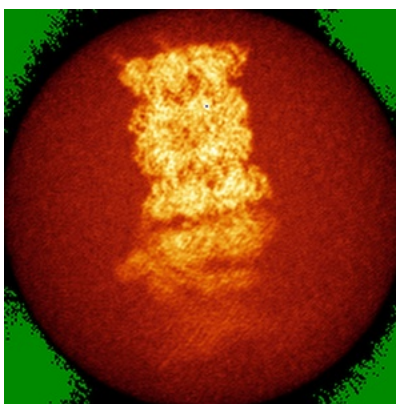
The images above show the largest variance slices of the map in three orthogonal directions.

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

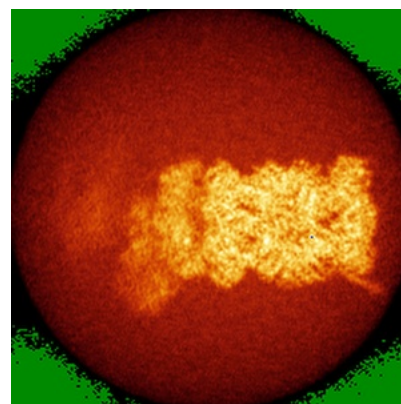
### 6.4.1 Primary map



X

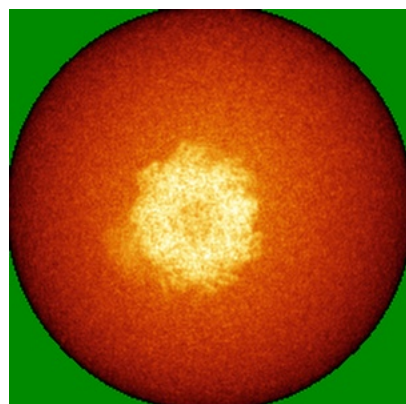


Y

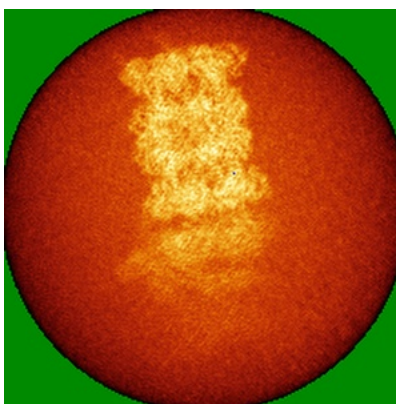


Z

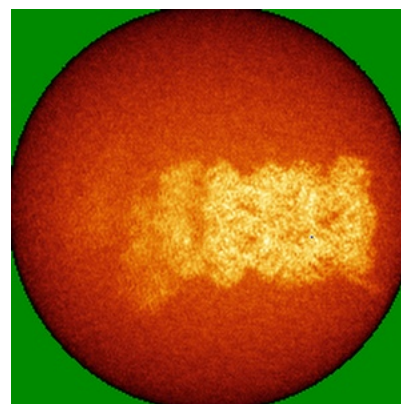
### 6.4.2 Raw map



X



Y



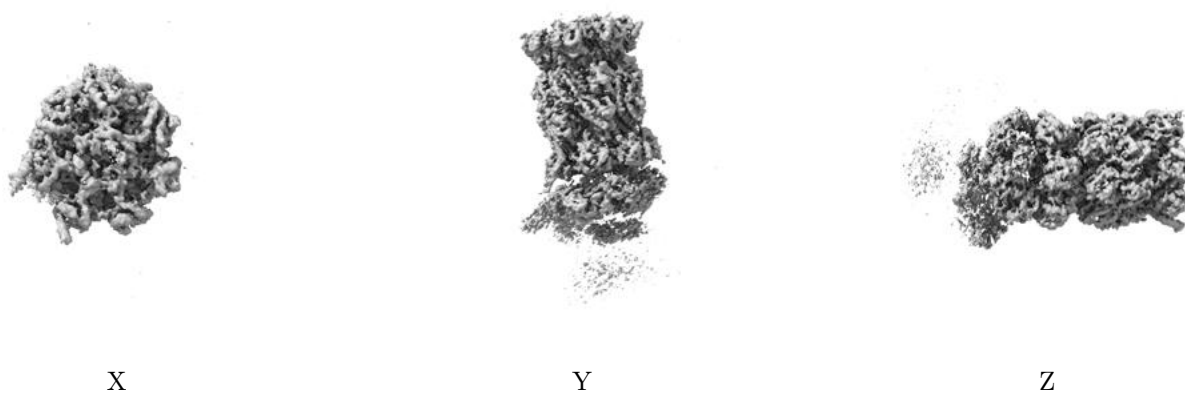
Z

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.



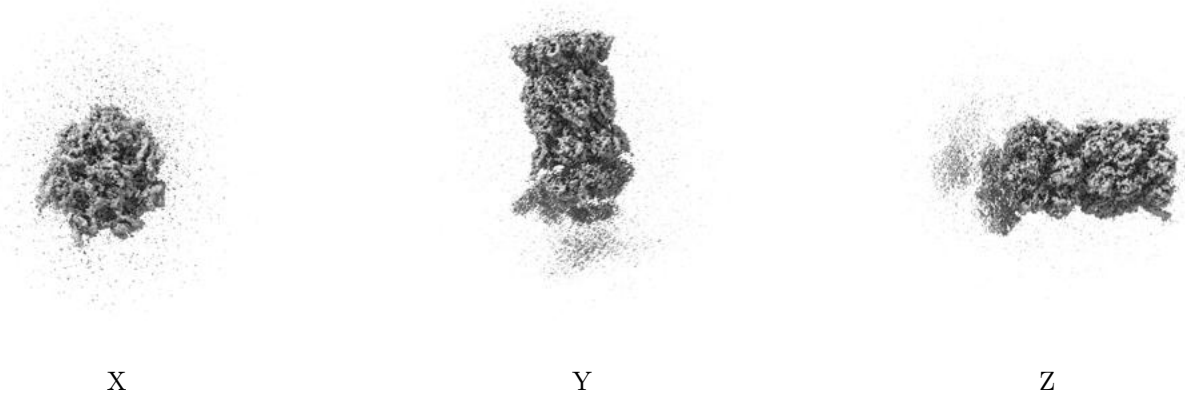
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.033. 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.

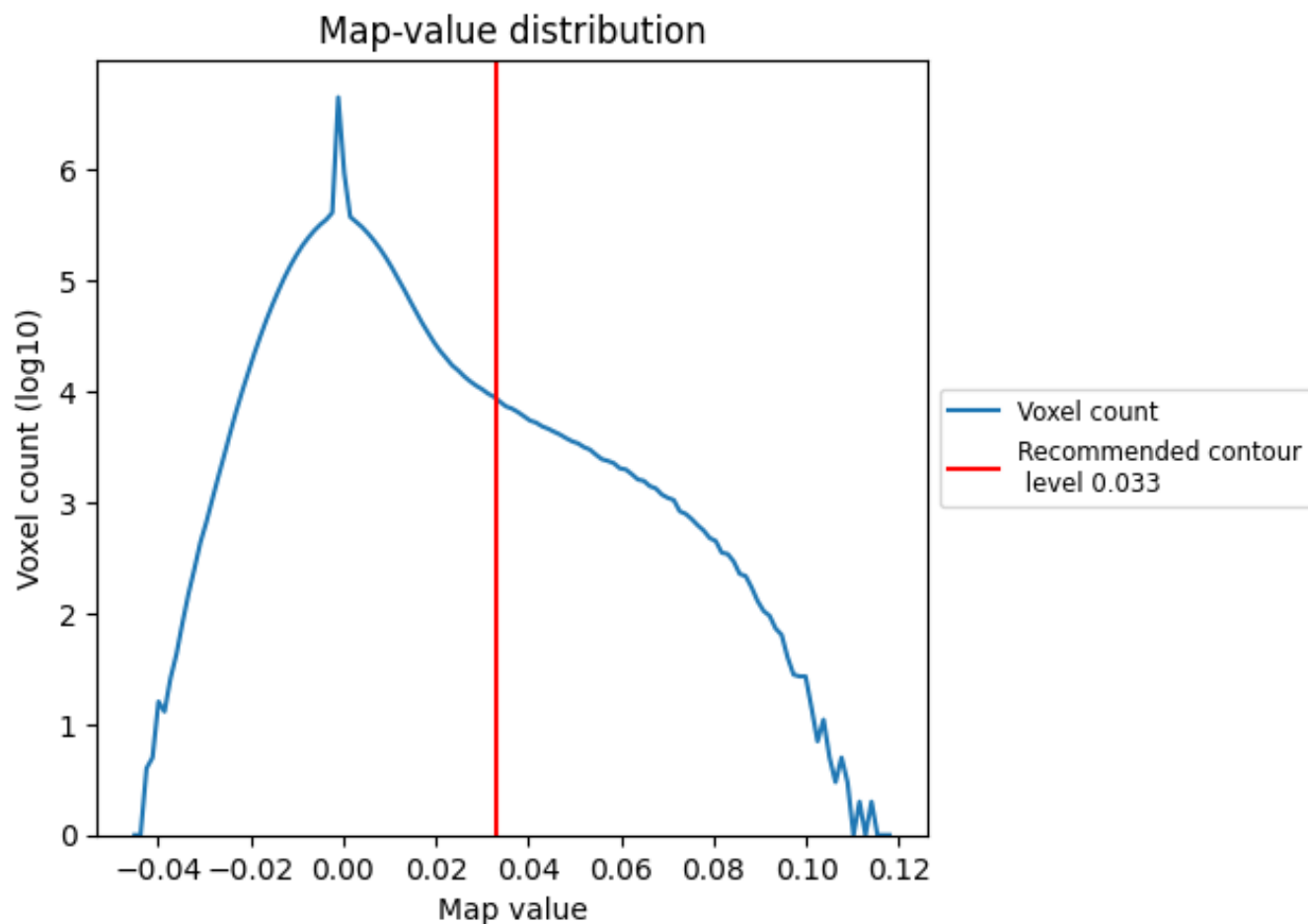
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

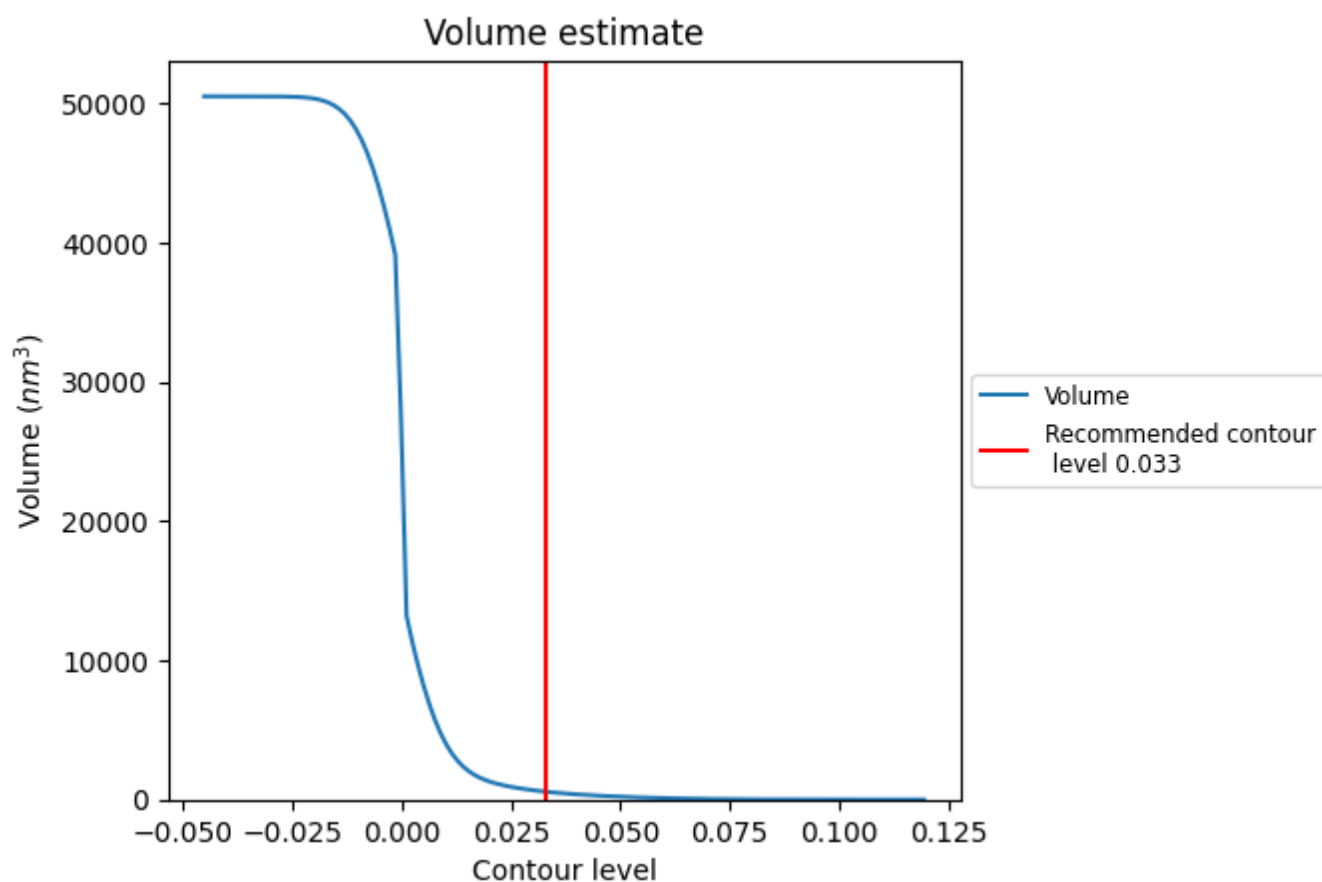
This section contains the results of statistical analysis of the map.

### 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.

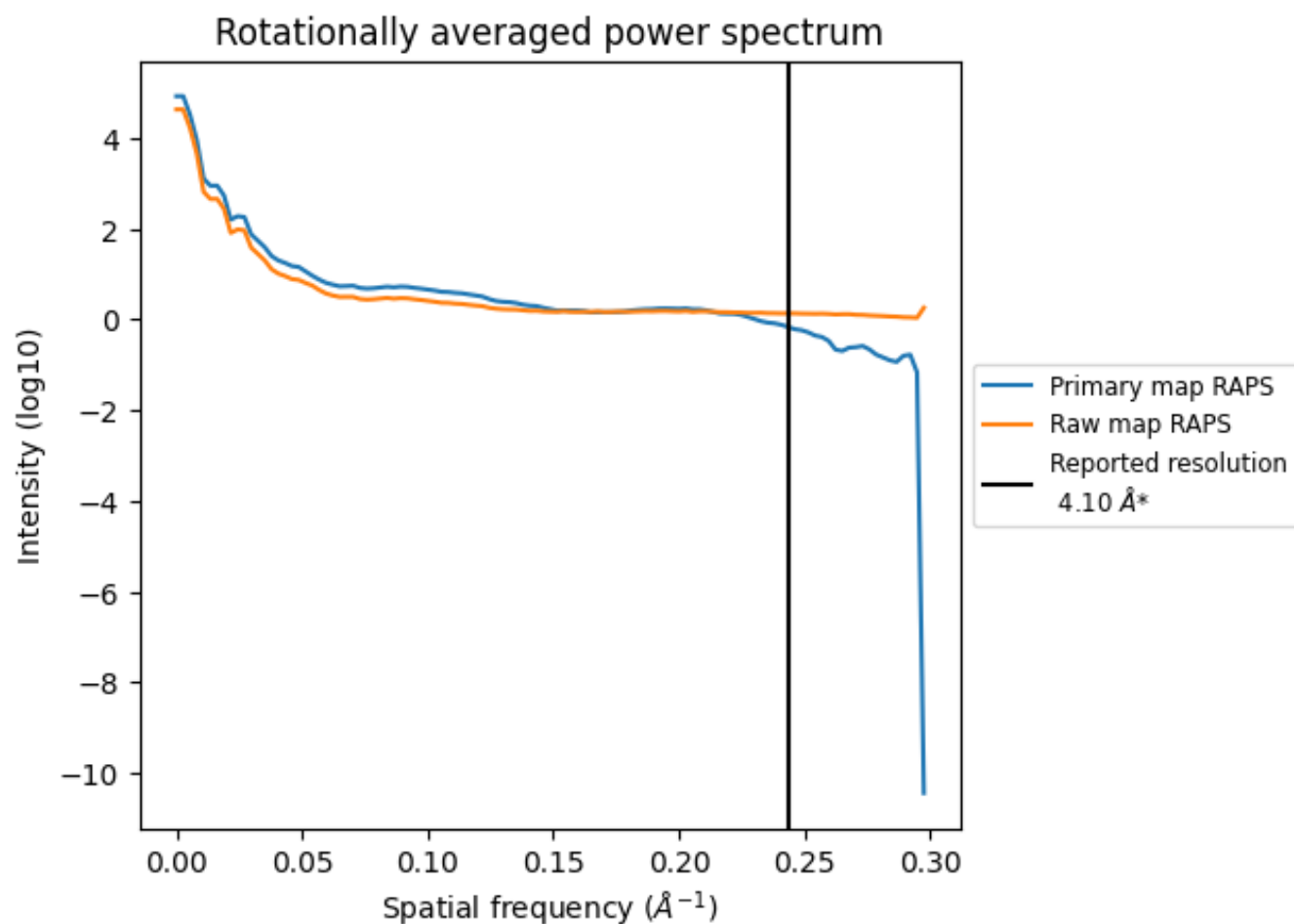
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 561 nm<sup>3</sup>; this corresponds to an approximate mass of 507 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 ⓘ

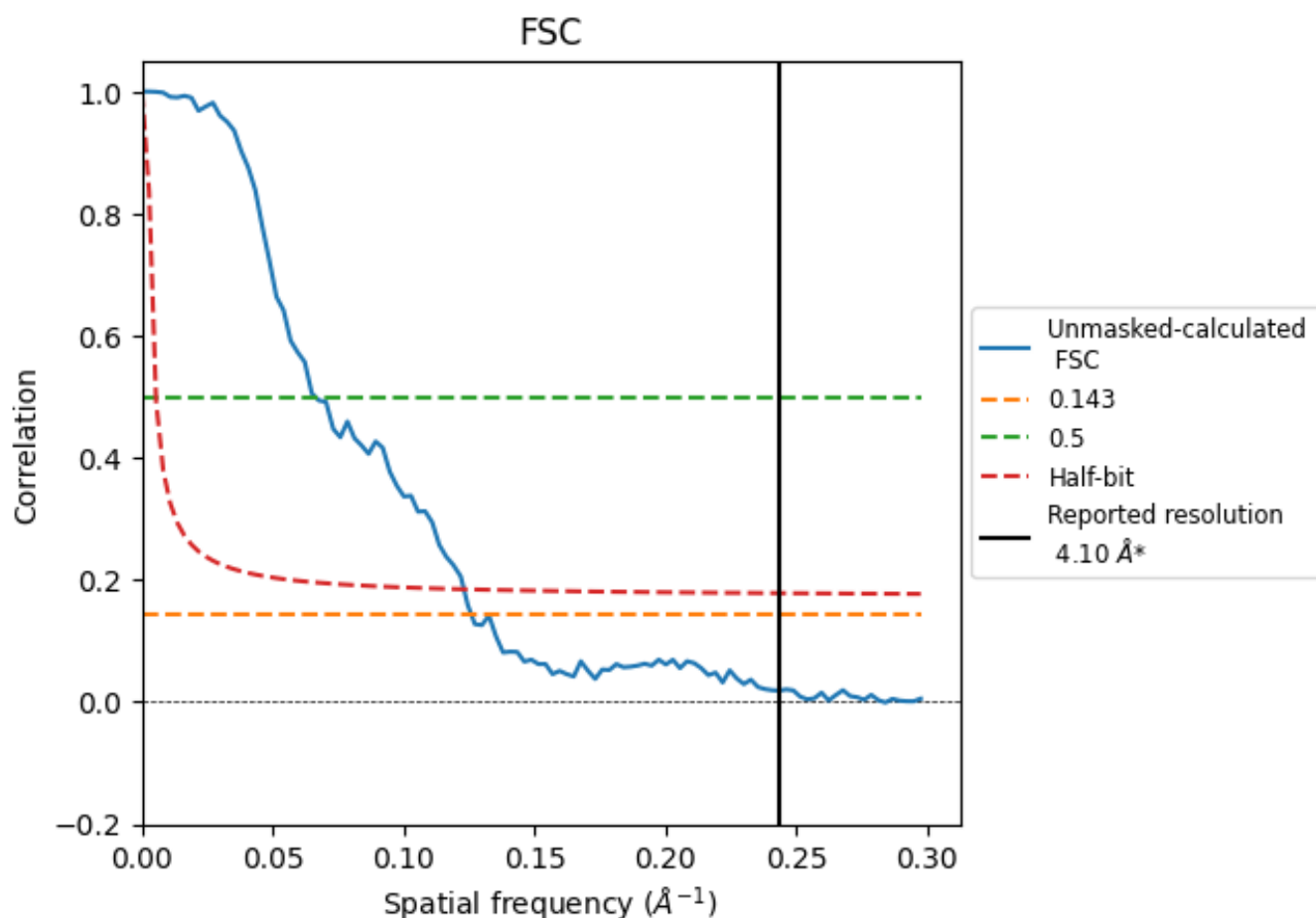


\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 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 0.244 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

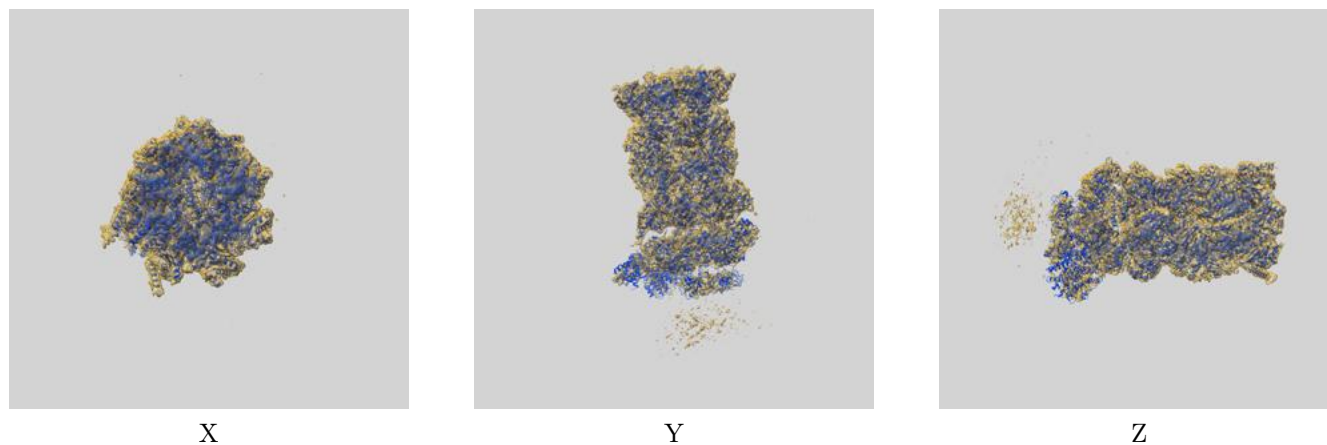
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.95	15.11	8.13

\*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 7.95 differs from the reported value 4.1 by more than 10 %

## 9 Map-model fit [i](#)

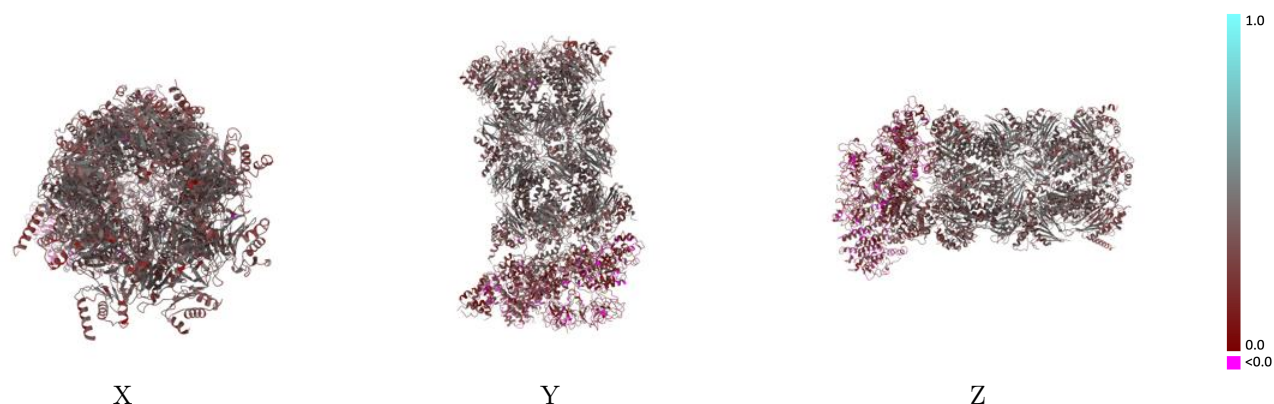
This section contains information regarding the fit between EMDB map EMD-65362 and PDB model 9VUG. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

### 9.1 Map-model overlay [i](#)



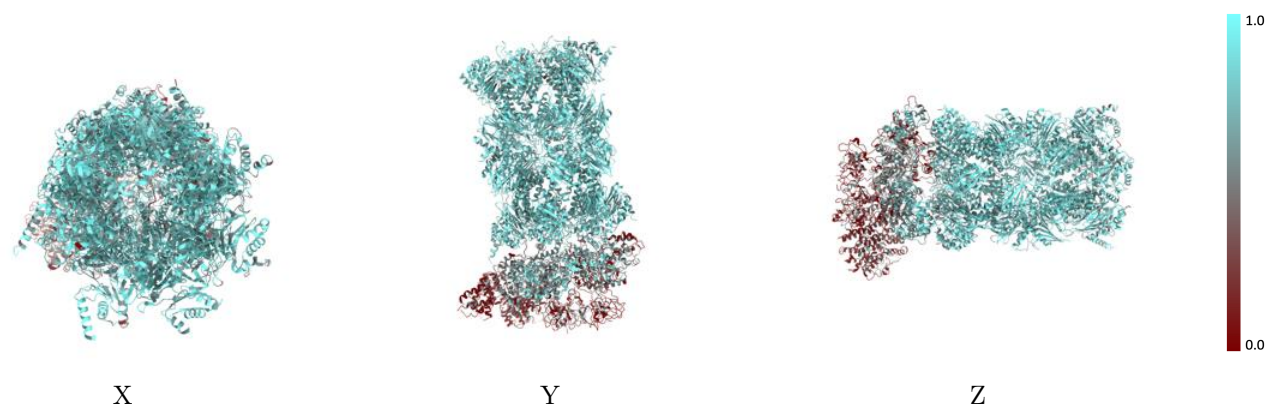
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

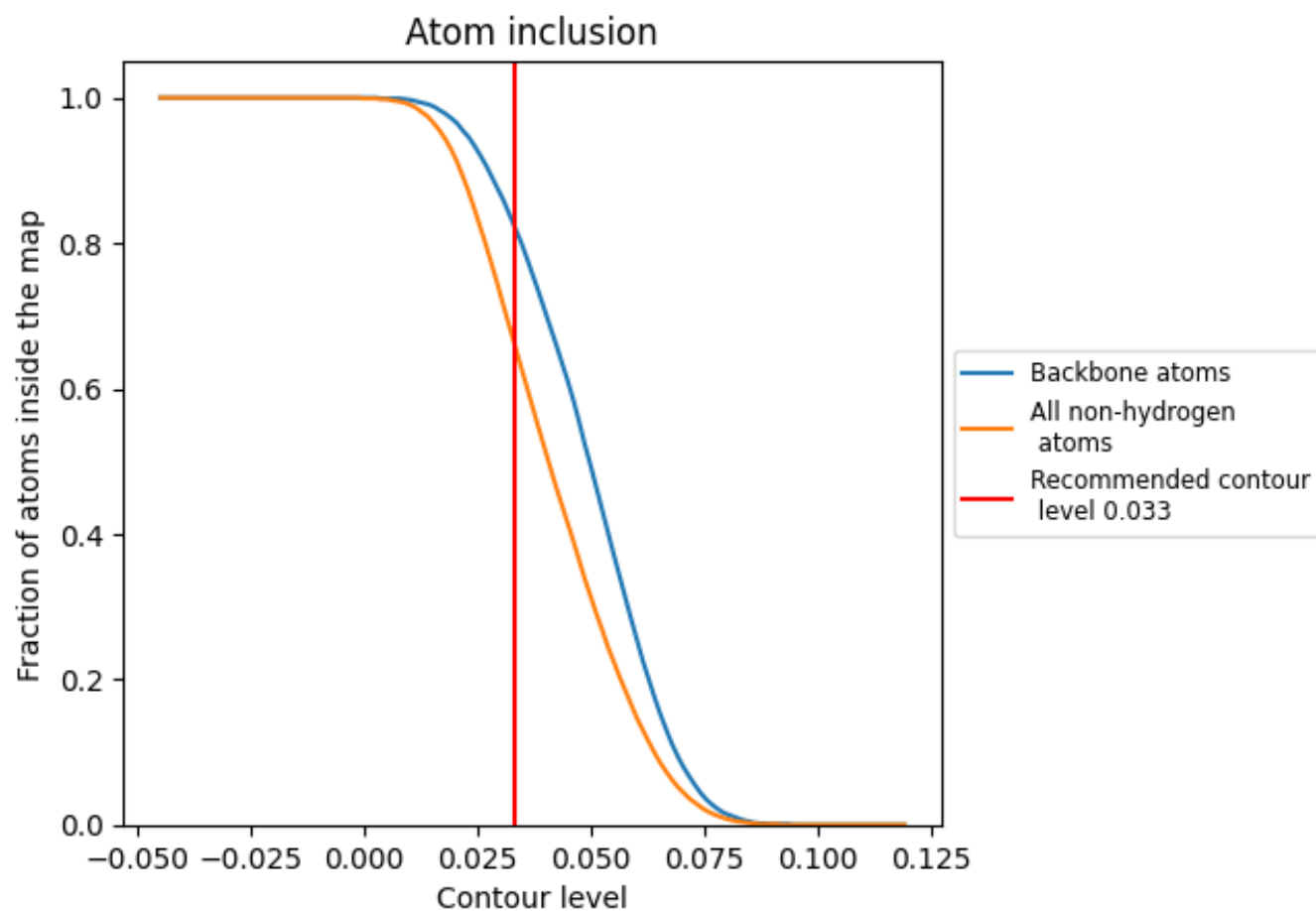
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.033).











































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.3240
A	 0.4680	 0.2580
B	 0.4450	 0.2520
C	 0.5040	 0.2430
D	 0.4800	 0.2070
E	 0.2760	 0.1650
F	 0.5010	 0.2340
G	 0.7780	 0.3570
H	 0.8080	 0.3870
I	 0.7560	 0.3470
J	 0.7550	 0.3580
K	 0.7500	 0.3650
L	 0.8170	 0.3850
M	 0.7940	 0.3660
N	 0.8510	 0.3970
O	 0.8490	 0.4010
P	 0.8160	 0.4040
Q	 0.7950	 0.3690
R	 0.8330	 0.4020
S	 0.8160	 0.3910
T	 0.8420	 0.3970
f	 0.1530	 0.1690
g	 0.7450	 0.3550
h	 0.7750	 0.3620
i	 0.7480	 0.3340
j	 0.7840	 0.3510
k	 0.7570	 0.3520
l	 0.7760	 0.3500
m	 0.7530	 0.3500
n	 0.8280	 0.3900
o	 0.8190	 0.3910
p	 0.8220	 0.3950
q	 0.8100	 0.3830
r	 0.8430	 0.3850
s	 0.8000	 0.3930
t	 0.8400	 0.4000

