



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 02:44 PM EDT

PDB ID : 9PMJ / pdb_00009pmj
EMDB ID : EMD-71737
Title : Human 19S proteasome bound to TXNL1 PITH domain without C-terminus
Authors : Chen, X.; Negi, H.; Walters, K.J.
Deposited on : 2025-07-17
Resolution : 4.22 Å(reported)
Based on initial models : 7WSI, 1WWY

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

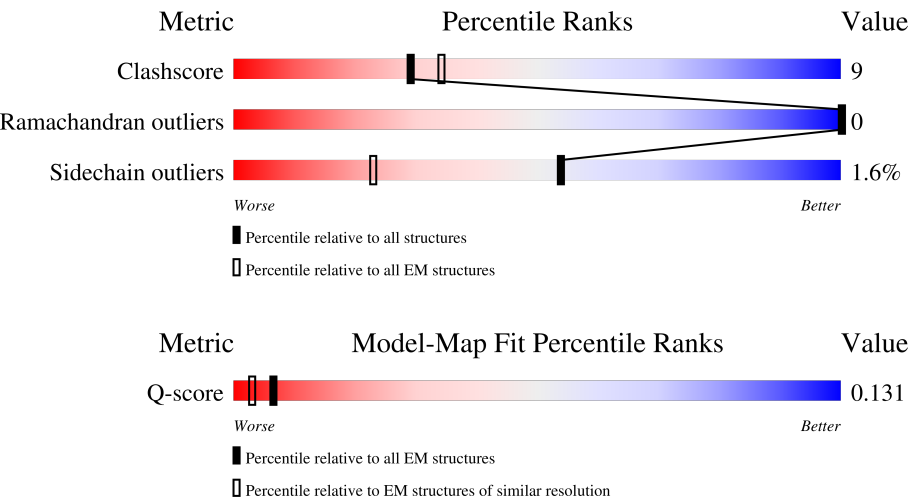
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.22 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	4772 (3.72 - 4.72)

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

Mol	Chain	Length	Quality of chain
1	A	433	<div><div></div><div>71%21%7%</div></div>
2	B	440	<div><div></div><div>63%24%12%</div></div>
3	C	406	<div><div></div><div>72%21%7%</div></div>
4	D	418	<div><div></div><div>71%18%11%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	U	953	
8	V	534	
9	W	456	
10	X	422	
11	Y	389	
12	Z	324	
13	a	376	
14	b	377	
15	c	310	
16	d	350	
17	e	70	
18	f	908	
19	g	289	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 54955 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	403	Total	C	N	O	S	0	0
			3170	1995	556	601	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	387	Total	C	N	O	S	0	0
			3038	1915	522	586	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	379	Total	C	N	O	S	0	0
			2985	1876	535	557	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	372	Total	C	N	O	S	0	0
			2961	1873	512	563	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	385	Total	C	N	O	S	0	0
			3070	1930	548	576	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	360	Total	C	N	O	S	0	0
			2808	1769	486	537	16		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	806	Total	C	N	O	S	0	0
			6288	3988	1071	1185	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	437	Total	C	N	O	S	0	0
			3564	2258	609	674	23		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	105	Total	C	N	O	S	0	0
			844	542	140	160	2		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	377	Total	C	N	O	S	0	0
			3106	1982	532	576	16		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	274	Total	C	N	O	S	0	0
			2191	1402	376	408	5		

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 17 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	e	49	Total	C	N	O	0	0
			417	256	64	97		

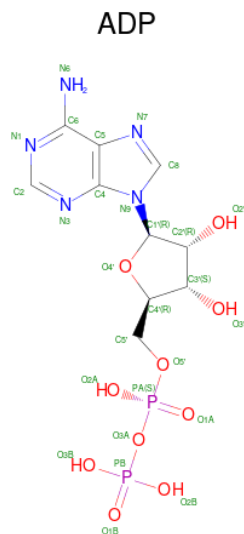
- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	885	Total	C	N	O	S	0	0
			6830	4295	1167	1323	45		

- Molecule 19 is a protein called Thioredoxin-like protein 1.

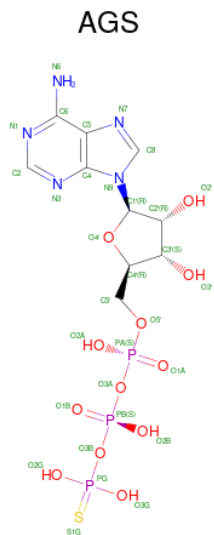
Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	132	Total	C	N	O	S	0	0
			1065	671	172	218	4		

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 27	C 10	N 5	O 10	P 2	0
20	B	1	Total 27	C 10	N 5	O 10	P 2	0
20	C	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 21 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3\text{S}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
21	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
21	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
21	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
22	D	1	Total	Mg	0
			1	1	
22	E	1	Total	Mg	0
			1	1	

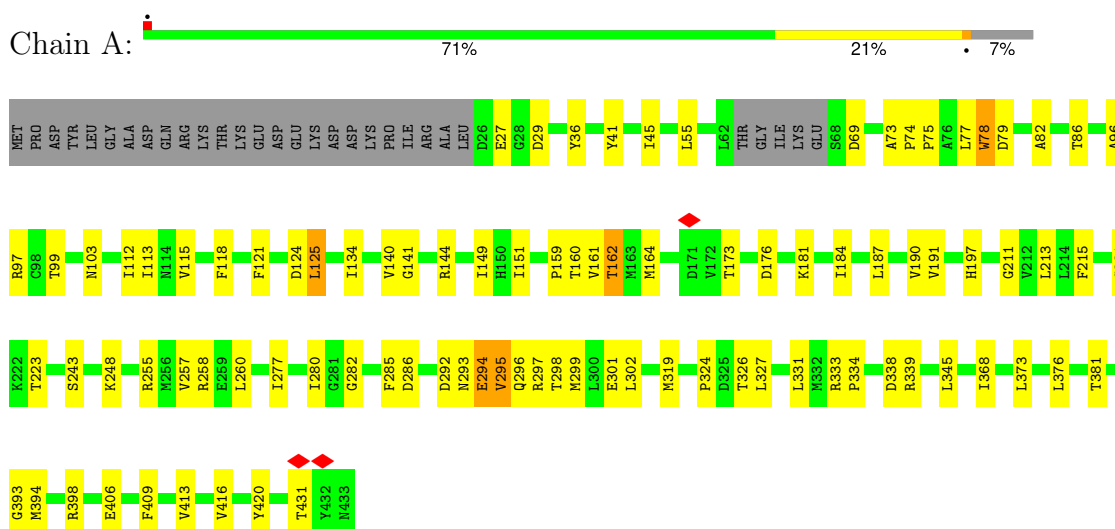
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
23	c	1	Total	Zn	0
			1	1	

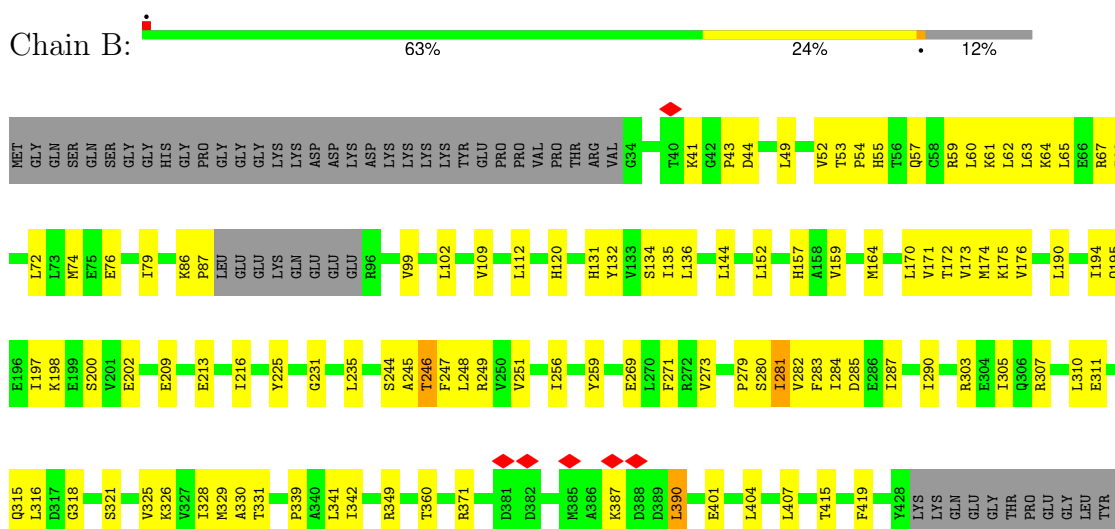
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 26S proteasome regulatory subunit 7

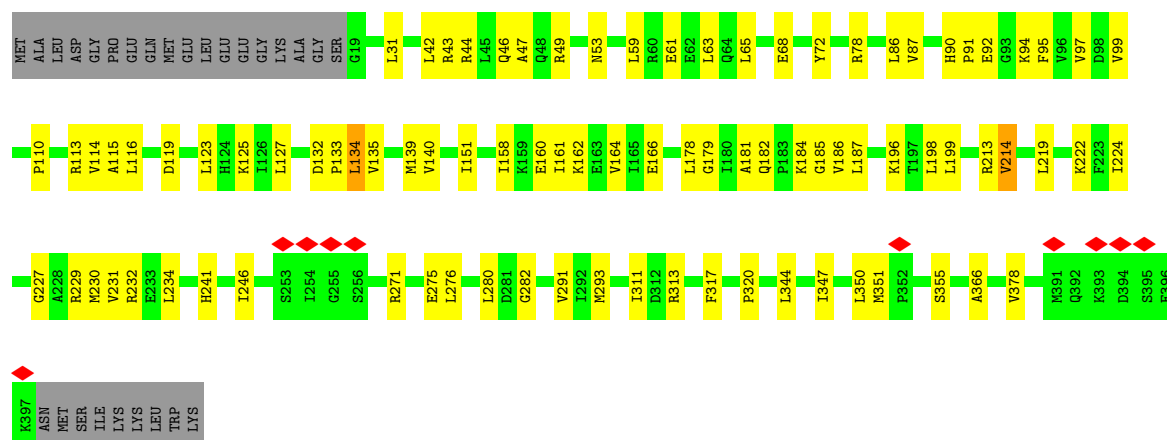


- Molecule 2: 26S proteasome regulatory subunit 4



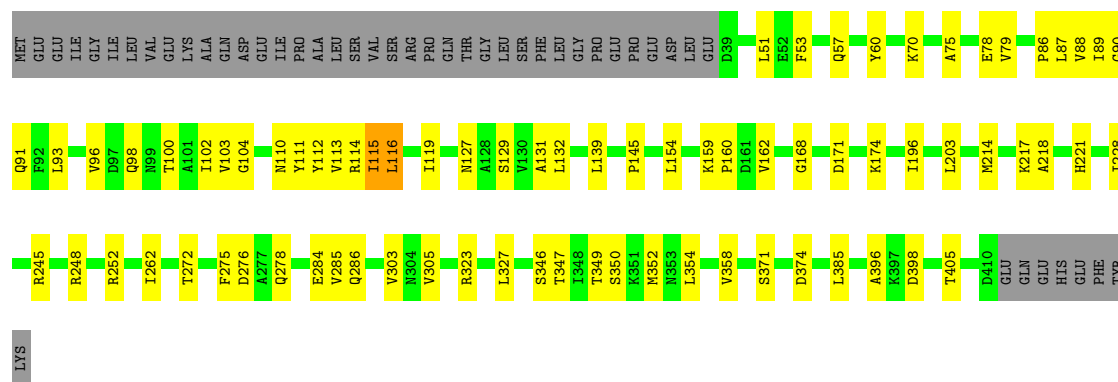
- Molecule 3: 26S protease regulatory subunit 8

Chain C: 



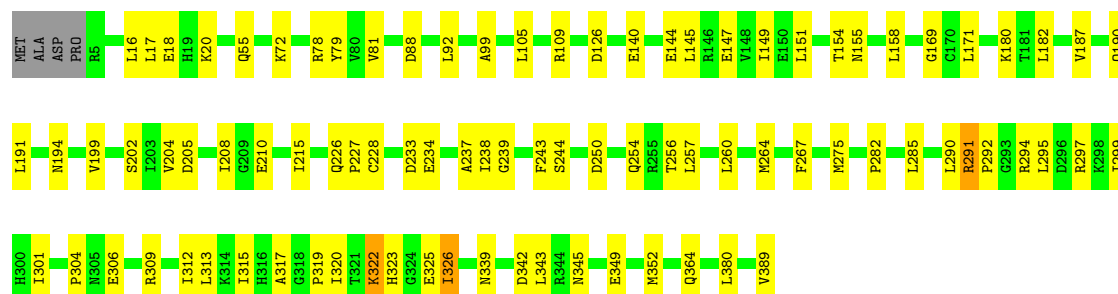
- Molecule 4: 26S proteasome regulatory subunit 6B

Chain D: 



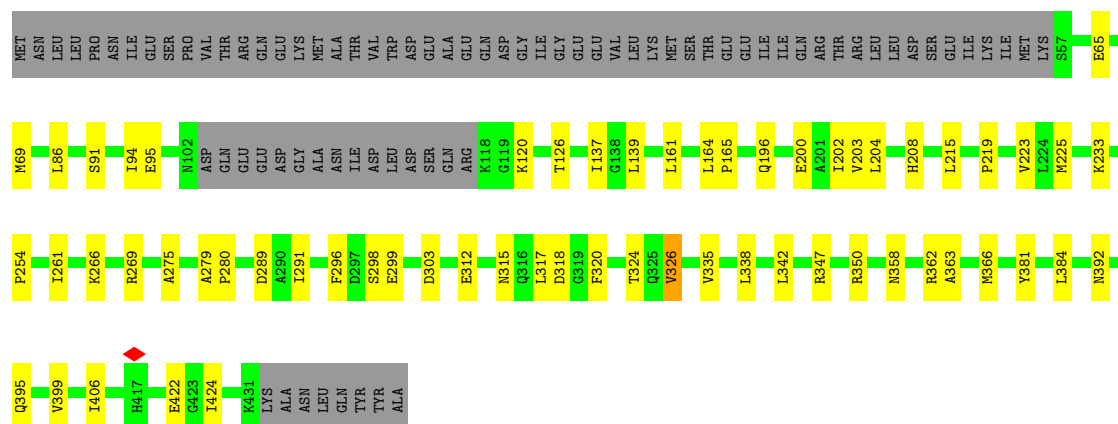
- Molecule 5: 26S protease regulatory subunit 10B

Chain E: 



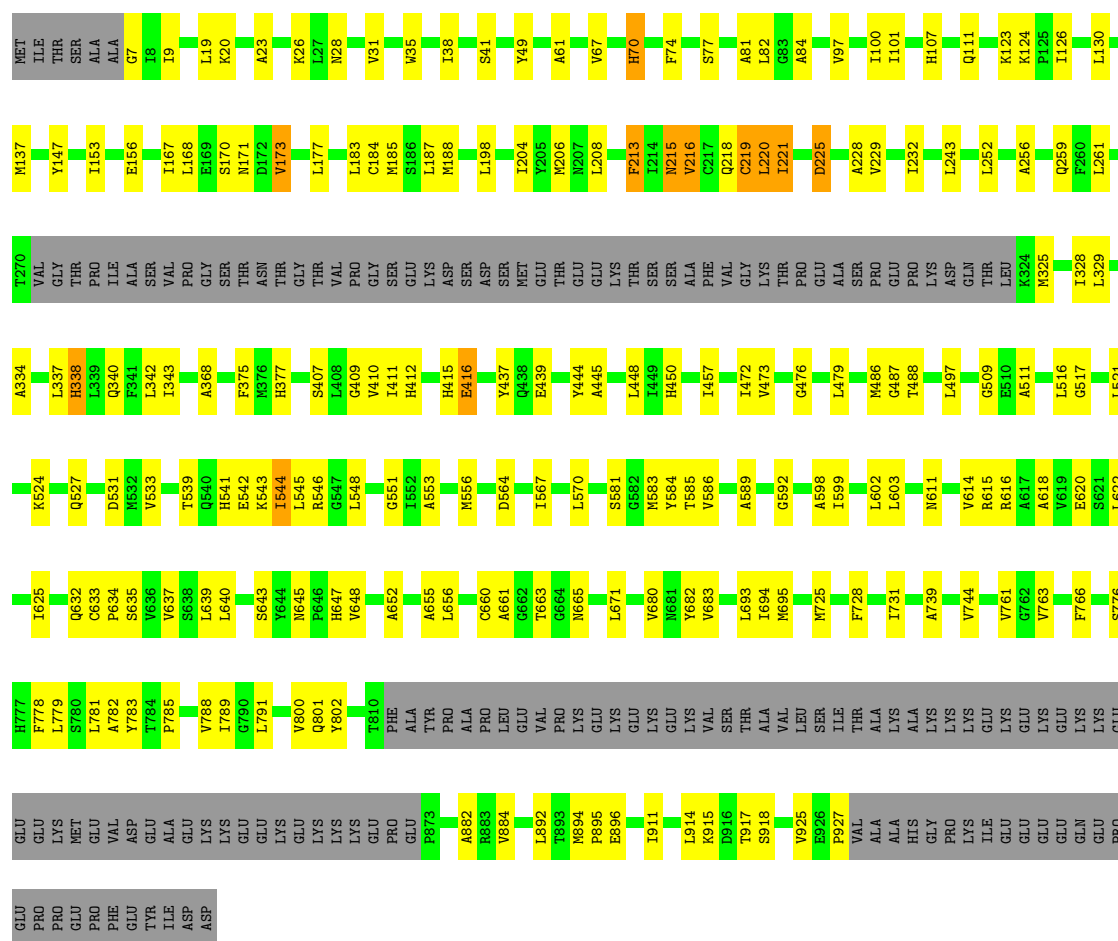
- Molecule 6: 26S proteasome regulatory subunit 6A

Chain F: 



• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1

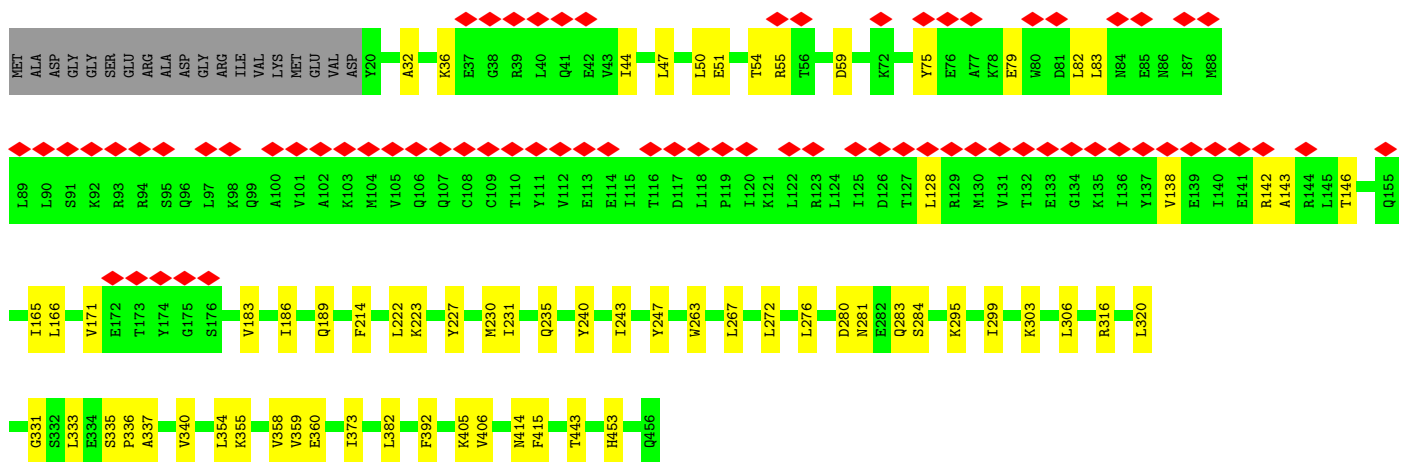
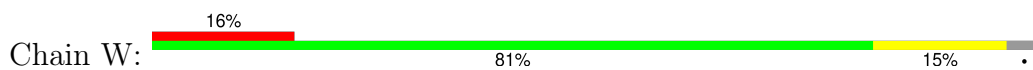
Chain U: 64% 20% 15%



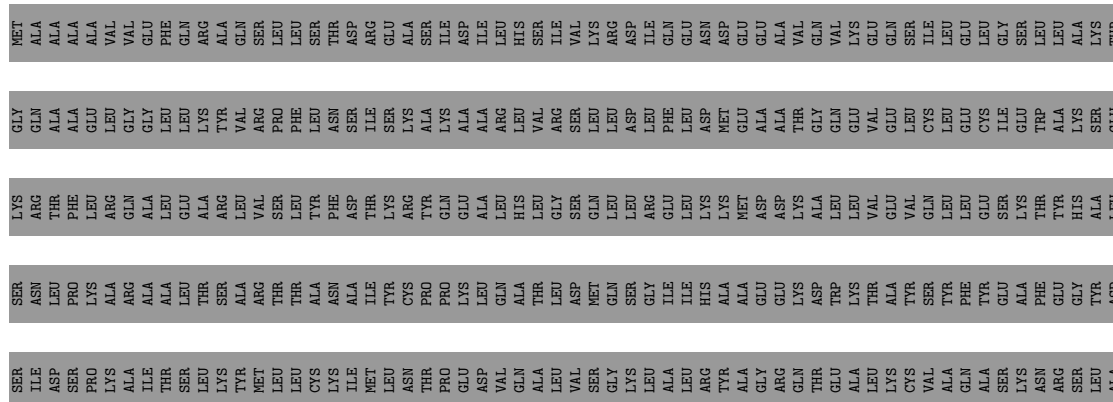
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 3

Chain V: 68% 14% 17%

- Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

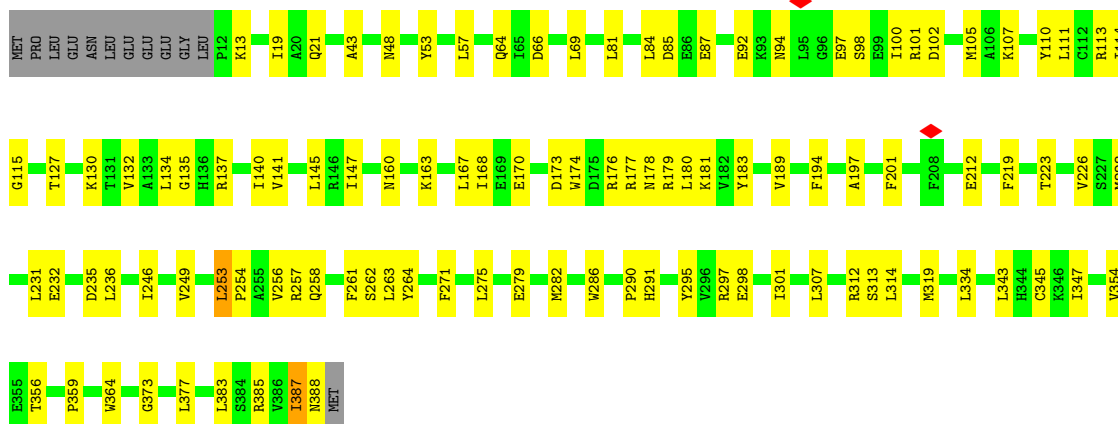


- Molecule 10: 26S proteasome non-ATPase regulatory subunit 11



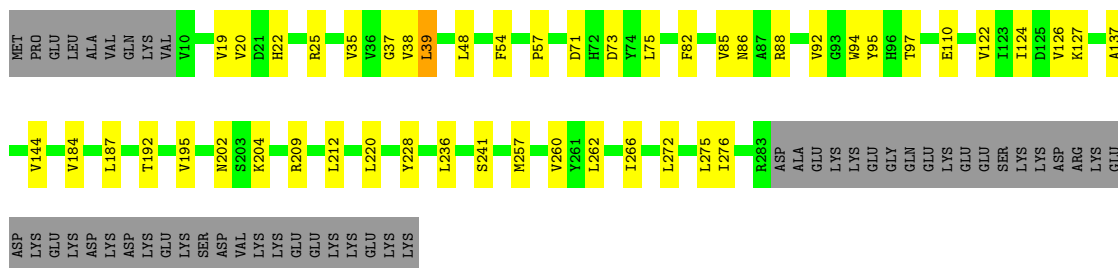
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 70% 27% ..



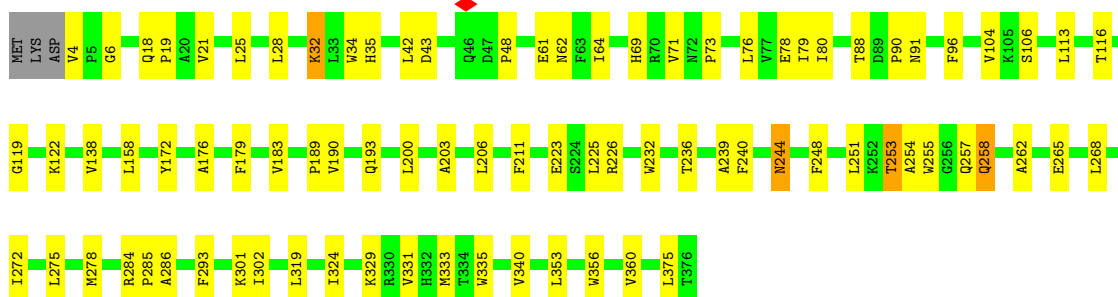
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 70% 15% 15%

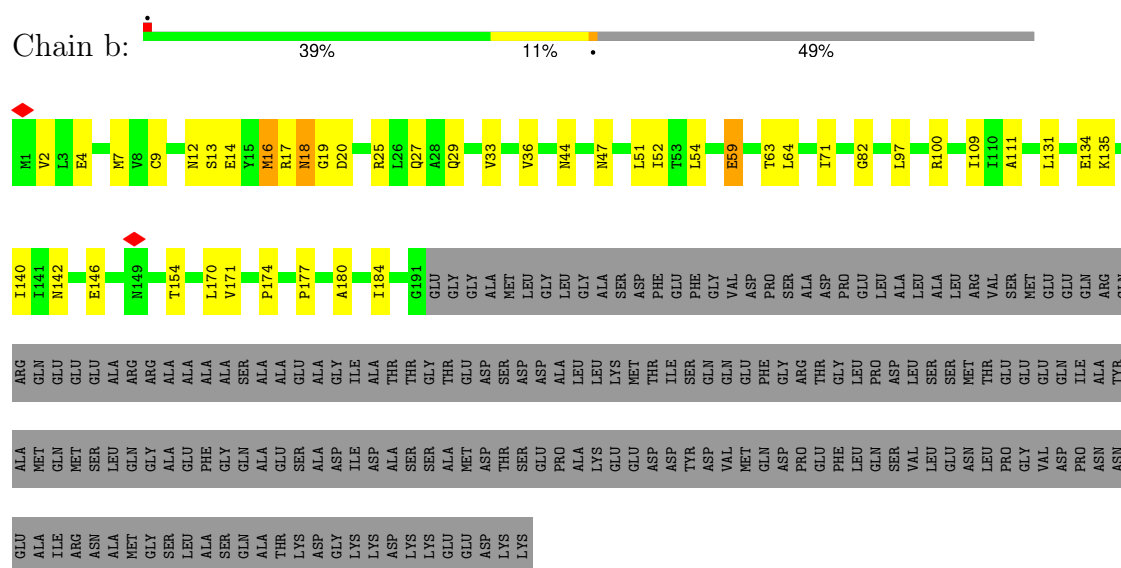


- Molecule 13: 26S proteasome non-ATPase regulatory subunit 13

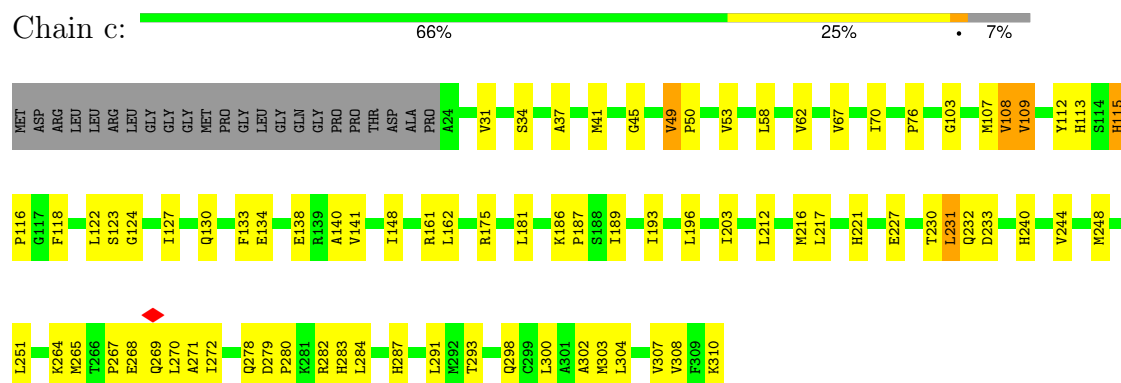
Chain a: 77% 21%



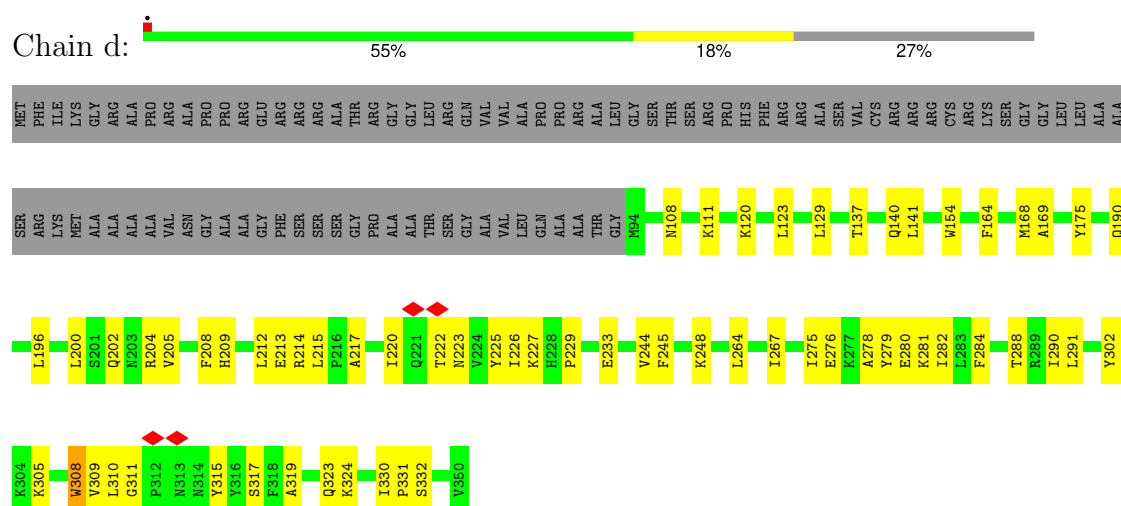
- Molecule 14: 26S proteasome non-ATPase regulatory subunit 4



- Molecule 15: 26S proteasome non-ATPase regulatory subunit 14

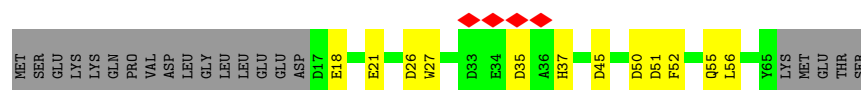


- Molecule 16: 26S proteasome non-ATPase regulatory subunit 8



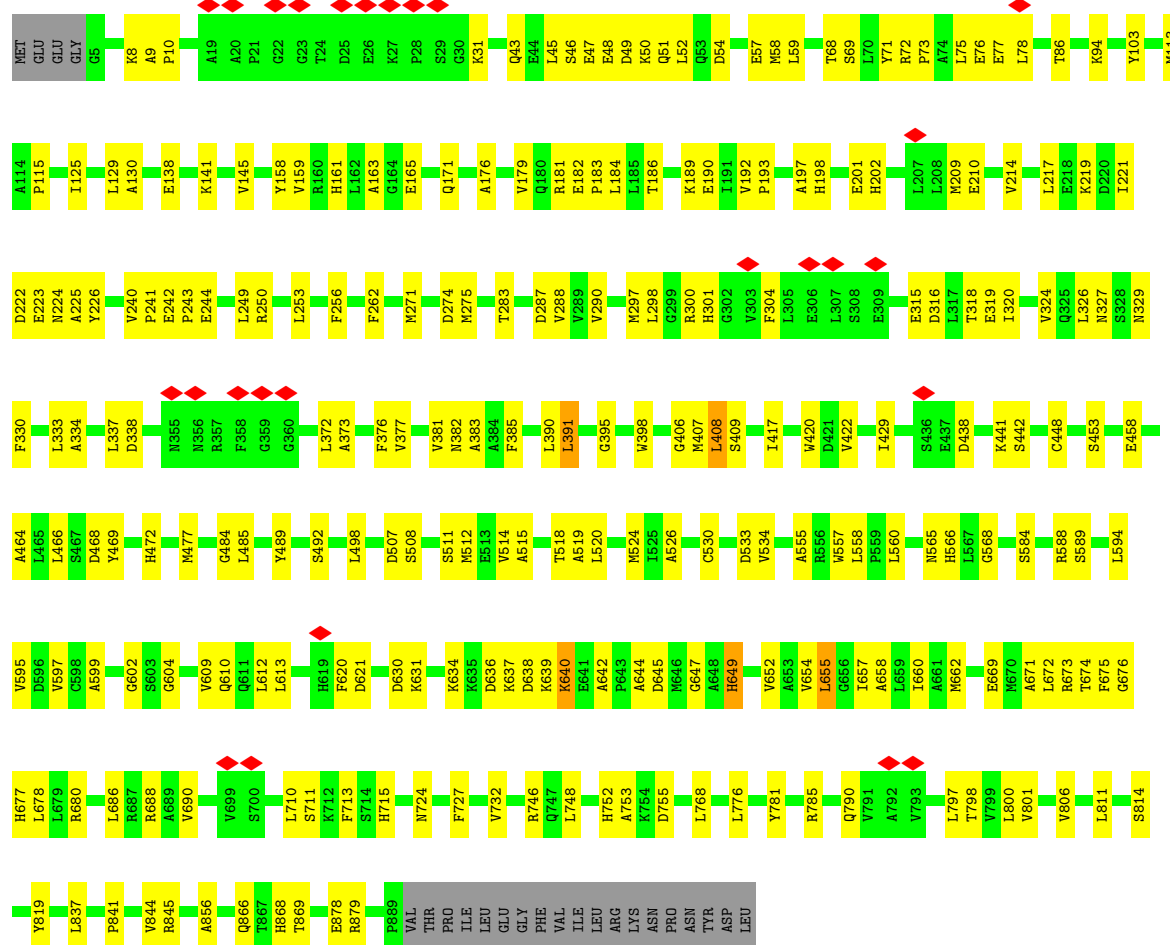
- Molecule 17: 26S proteasome complex subunit SEM1





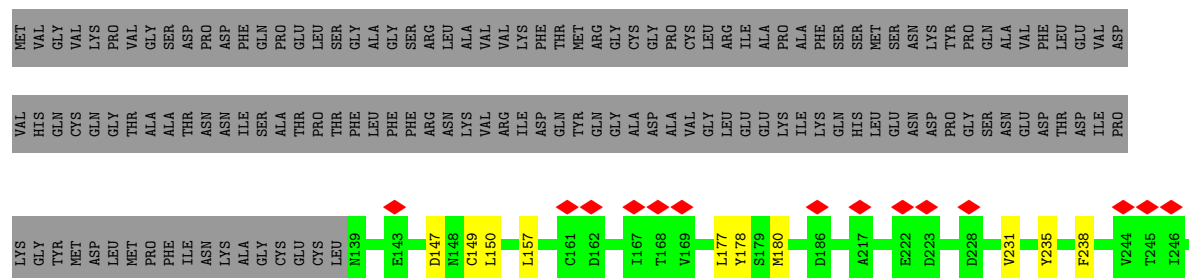
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 2

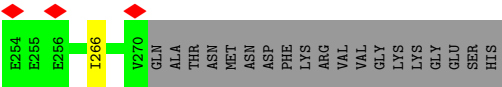
Chain f: 70% 27%



• Molecule 19: Thioredoxin-like protein 1

Chain g: 6% 42% 54%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39459	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	100000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.467	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.510	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	349.92, 349.92, 349.92	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, ZN, 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	0.53	0/3222	0.88	0/4348
2	B	0.53	0/3082	0.90	0/4154
3	C	0.48	0/3024	0.85	0/4067
4	D	0.51	0/3008	0.86	0/4060
5	E	0.55	0/3117	0.87	0/4193
6	F	0.47	0/2846	0.83	0/3837
7	U	0.54	0/6398	0.90	0/8655
8	V	0.42	0/3681	0.78	0/4969
9	W	0.51	0/3612	0.81	0/4858
10	X	0.59	0/855	0.98	0/1150
11	Y	0.58	0/3164	0.90	0/4263
12	Z	0.57	0/2234	0.89	0/3031
13	a	0.62	0/3053	0.90	0/4133
14	b	0.65	0/1478	0.92	0/2001
15	c	0.67	0/2302	0.96	0/3110
16	d	0.51	0/2162	0.87	0/2919
17	e	0.67	0/429	0.94	0/584
18	f	0.51	0/6944	0.89	0/9387
19	g	0.22	0/1086	0.49	0/1470
All	All	0.53	0/55697	0.87	0/75189

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3170	0	3214	65	0
2	B	3038	0	3127	84	0
3	C	2985	0	3097	75	0
4	D	2961	0	3012	65	0
5	E	3070	0	3146	68	0
6	F	2808	0	2888	44	0
7	U	6288	0	6317	130	0
8	V	3612	0	3682	58	0
9	W	3564	0	3685	43	0
10	X	844	0	886	17	0
11	Y	3106	0	3111	71	0
12	Z	2191	0	2218	41	0
13	a	2995	0	3012	58	0
14	b	1458	0	1505	28	0
15	c	2260	0	2276	58	0
16	d	2116	0	2143	44	0
17	e	417	0	324	9	0
18	f	6830	0	6828	186	0
19	g	1065	0	1015	6	0
20	A	27	0	12	1	0
20	B	27	0	12	1	0
20	C	27	0	12	1	0
21	D	31	0	12	1	0
21	E	31	0	12	1	0
21	F	31	0	12	2	0
22	D	1	0	0	0	0
22	E	1	0	0	0	0
23	c	1	0	0	0	0
All	All	54955	0	55558	1022	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 9.

All (1022) 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)
15:c:45:GLY:HA2	15:c:53:VAL:HG21	1.57	0.85
11:Y:94:ASN:HB2	11:Y:98:SER:HB3	1.63	0.79
18:f:171:GLN:HB3	18:f:179:VAL:HG22	1.65	0.79
7:U:409:GLY:HA3	7:U:445:ALA:HB1	1.65	0.77
2:B:60:LEU:HD11	18:f:222:ASP:HB2	1.67	0.77
7:U:183:LEU:HA	7:U:187:LEU:HD13	1.68	0.76
7:U:665:ASN:HB3	7:U:694:ILE:HD11	1.68	0.75
1:A:221:GLY:HA2	20:A:501:ADP:H5'1	1.69	0.75
13:a:232:TRP:HB2	13:a:253:THR:HA	1.69	0.74
3:C:68:GLU:HG2	15:c:189:ILE:CD1	2.16	0.74
13:a:284:ARG:HG2	13:a:333:MET:HE2	1.70	0.73
16:d:190:GLN:HB3	16:d:225:TYR:HD1	1.54	0.73
15:c:278:GLN:HG3	15:c:280:PRO:HD2	1.71	0.72
18:f:141:LYS:HG2	18:f:159:VAL:HG22	1.72	0.72
1:A:333:ARG:HH21	21:F:501:AGS:H8	1.55	0.71
4:D:100:THR:HA	4:D:114:ARG:HA	1.72	0.71
16:d:303:ALA:HB1	16:d:308:TRP:HB3	1.71	0.71
2:B:387:LYS:HB2	2:B:390:LEU:HD22	1.70	0.71
9:W:331:GLY:HA2	9:W:336:PRO:HG3	1.71	0.71
13:a:25:LEU:HA	13:a:28:LEU:HB3	1.72	0.71
2:B:245:ALA:HB1	2:B:280:SER:HB3	1.72	0.71
18:f:652:VAL:HB	18:f:675:PHE:HA	1.73	0.71
3:C:113:ARG:HB3	3:C:127:LEU:HD22	1.73	0.71
4:D:371:SER:HB3	5:E:291:ARG:HH21	1.56	0.71
12:Z:82:PHE:O	12:Z:86:ASN:HB3	1.91	0.71
13:a:71:VAL:HG11	14:b:17:ARG:HD3	1.73	0.70
1:A:301:GLU:HB3	6:F:254:PRO:HG2	1.73	0.70
18:f:176:ALA:HA	18:f:179:VAL:HB	1.74	0.70
18:f:634:LYS:HB3	18:f:785:ARG:HH12	1.55	0.70
18:f:680:ARG:HA	18:f:688:ARG:HH22	1.56	0.70
15:c:116:PRO:HA	15:c:148:ILE:HD13	1.73	0.69
5:E:297:ARG:HG3	5:E:299:ILE:HG13	1.74	0.69
15:c:134:GLU:HG3	15:c:162:LEU:HD23	1.75	0.69
4:D:371:SER:CB	5:E:291:ARG:HH21	2.05	0.69
13:a:206:LEU:HD23	13:a:268:LEU:HD11	1.75	0.69
18:f:198:HIS:O	18:f:202:HIS:HB2	1.92	0.69
6:F:318:ASP:HB3	6:F:347:ARG:HD3	1.72	0.68
15:c:134:GLU:HA	15:c:138:GLU:HA	1.76	0.68
15:c:141:VAL:HG22	15:c:161:ARG:HD3	1.74	0.68
18:f:673:ARG:NH2	18:f:781:TYR:O	2.26	0.68
3:C:132:ASP:HB2	3:C:135:VAL:HB	1.75	0.68
8:V:259:LEU:HA	8:V:264:TYR:HE1	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:189:PRO:HA	13:a:193:GLN:HB2	1.74	0.68
15:c:49:VAL:HG13	15:c:50:PRO:HD3	1.74	0.68
16:d:281:LYS:HG3	16:d:282:ILE:HG12	1.75	0.68
2:B:44:ASP:HA	18:f:686:LEU:HB2	1.74	0.68
8:V:315:LYS:HG2	11:Y:385:ARG:HB3	1.75	0.68
13:a:62:ASN:HD21	13:a:96:PHE:HZ	1.39	0.68
14:b:154:THR:HG23	14:b:170:LEU:HD11	1.76	0.67
6:F:196:GLN:O	6:F:200:GLU:HB2	1.95	0.67
8:V:256:ARG:NH2	17:e:21:GLU:HG3	2.09	0.67
6:F:219:PRO:HG3	6:F:324:THR:HG23	1.76	0.67
3:C:86:LEU:HD11	3:C:94:LYS:HB3	1.76	0.67
9:W:79:GLU:O	9:W:83:LEU:HB2	1.95	0.67
9:W:280:ASP:OD1	9:W:281:ASN:N	2.26	0.67
7:U:412:HIS:HB3	7:U:415:HIS:HB2	1.77	0.67
15:c:115:HIS:HB3	15:c:118:PHE:HB2	1.75	0.67
2:B:256:ILE:HD11	2:B:290:ILE:HG23	1.76	0.67
18:f:190:GLU:HB2	18:f:193:PRO:HD2	1.77	0.67
18:f:485:LEU:O	18:f:489:TYR:HB2	1.95	0.67
2:B:79:ILE:HD11	18:f:658:ALA:HB1	1.77	0.66
16:d:309:VAL:HB	16:d:317:SER:HA	1.77	0.66
1:A:333:ARG:NH2	21:F:501:AGS:H8	2.09	0.66
15:c:127:ILE:HA	15:c:130:GLN:HB3	1.77	0.66
9:W:47:LEU:HD23	9:W:50:LEU:HD21	1.76	0.66
16:d:200:LEU:HD21	16:d:233:GLU:HB2	1.77	0.66
4:D:127:ASN:HB3	4:D:248:ARG:HE	1.59	0.66
1:A:97:ARG:HG2	2:B:131:HIS:CD2	2.30	0.66
3:C:87:VAL:HB	3:C:95:PHE:HB2	1.77	0.66
5:E:180:LYS:HG2	5:E:301:ILE:HD13	1.75	0.66
11:Y:231:LEU:HB3	11:Y:235:ASP:HB2	1.77	0.66
18:f:283:THR:O	18:f:287:ASP:CB	2.45	0.65
18:f:372:LEU:HD21	18:f:409:SER:HB2	1.78	0.65
2:B:284:ILE:HB	2:B:329:MET:HG3	1.78	0.65
5:E:126:ASP:HB3	6:F:320:PHE:CE2	2.32	0.65
13:a:254:ALA:HA	13:a:258:GLN:HG2	1.79	0.65
4:D:272:THR:OG1	4:D:276:ASP:HB3	1.95	0.65
3:C:160:GLU:HB3	3:C:313:ARG:NH2	2.12	0.65
9:W:406:VAL:H	10:X:342:PHE:HA	1.61	0.65
18:f:377:VAL:HA	18:f:752:HIS:HB3	1.79	0.65
1:A:333:ARG:HH12	6:F:392:ASN:HD21	1.45	0.65
7:U:74:PHE:HA	7:U:77:SER:HB2	1.77	0.65
1:A:173:THR:HB	1:A:176:ASP:HB3	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:222:LYS:HB3	4:D:278:GLN:HB3	1.78	0.64
11:Y:258:GLN:O	11:Y:262:SER:HB2	1.97	0.64
6:F:139:LEU:HD12	6:F:161:LEU:HD21	1.80	0.64
16:d:244:VAL:HG12	16:d:248:LYS:HE3	1.79	0.64
7:U:622:LEU:HA	7:U:625:ILE:HG22	1.79	0.64
18:f:171:GLN:HE21	18:f:182:GLU:HG2	1.62	0.64
1:A:86:THR:HG22	2:B:136:LEU:HD12	1.80	0.64
7:U:766:PHE:HE1	7:U:782:ALA:HB2	1.62	0.64
8:V:224:LEU:HB2	8:V:261:TYR:HE1	1.63	0.64
12:Z:19:VAL:HG21	12:Z:124:ILE:HG13	1.79	0.64
18:f:31:LYS:HG2	18:f:77:GLU:HG3	1.78	0.64
8:V:141:THR:HB	8:V:144:ASP:HB3	1.80	0.63
8:V:262:SER:HB3	16:d:213:GLU:HG3	1.80	0.63
2:B:74:MET:HE2	18:f:613:LEU:HB2	1.79	0.63
4:D:358:VAL:HA	4:D:396:ALA:HB2	1.80	0.63
18:f:334:ALA:HA	18:f:338:ASP:HB2	1.81	0.63
7:U:243:LEU:HD21	7:U:915:LYS:HA	1.80	0.63
12:Z:257:MET:HA	12:Z:260:VAL:HG22	1.81	0.63
18:f:637:LYS:HE2	18:f:674:THR:HB	1.81	0.63
2:B:109:VAL:HB	3:C:94:LYS:HB2	1.79	0.63
11:Y:314:LEU:HB3	11:Y:354:VAL:HG22	1.80	0.63
18:f:710:LEU:HA	18:f:713:PHE:HD2	1.63	0.63
5:E:81:VAL:HG12	5:E:105:LEU:HG	1.81	0.63
8:V:302:TYR:HB3	8:V:339:LEU:CD1	2.28	0.63
18:f:713:PHE:CE1	18:f:748:LEU:HG	2.33	0.63
1:A:255:ARG:HA	1:A:258:ARG:HD2	1.81	0.62
3:C:78:ARG:HG3	3:C:110:PRO:HG3	1.80	0.62
3:C:139:MET:HE3	3:C:140:VAL:H	1.63	0.62
18:f:660:ILE:HG23	18:f:669:GLU:HG2	1.82	0.62
12:Z:127:LYS:HA	15:c:212:LEU:HD11	1.81	0.62
1:A:213:LEU:HA	1:A:319:MET:HB3	1.80	0.62
2:B:74:MET:HE1	18:f:610:GLN:HA	1.80	0.62
13:a:35:HIS:HB3	14:b:17:ARG:HH21	1.63	0.62
13:a:232:TRP:O	13:a:236:THR:HB	1.99	0.62
5:E:194:ASN:HB2	5:E:228:CYS:HA	1.82	0.62
16:d:209:HIS:HA	16:d:212:LEU:HD23	1.81	0.62
15:c:267:PRO:HA	15:c:271:ALA:H	1.64	0.62
18:f:713:PHE:HE1	18:f:748:LEU:HG	1.65	0.62
2:B:371:ARG:HB3	3:C:179:GLY:HA3	1.81	0.61
5:E:239:GLY:HA3	5:E:257:LEU:HD22	1.82	0.61
7:U:524:LYS:HG3	7:U:556:MET:HE1	1.80	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:240:TYR:HA	9:W:243:ILE:HD12	1.82	0.61
14:b:146:GLU:HB3	14:b:174:PRO:HG2	1.82	0.61
16:d:248:LYS:NZ	16:d:264:LEU:HD11	2.14	0.61
16:d:290:ILE:HG13	16:d:291:LEU:HG	1.82	0.61
18:f:790:GLN:HB3	18:f:800:LEU:HD11	1.82	0.61
2:B:135:ILE:HA	2:B:159:VAL:HB	1.81	0.61
2:B:249:ARG:HH22	3:C:282:GLY:HA2	1.65	0.61
18:f:43:GLN:HG3	18:f:47:GLU:HG3	1.81	0.61
18:f:145:VAL:HG21	18:f:159:VAL:HG11	1.83	0.61
18:f:597:VAL:HA	18:f:639:LYS:HD2	1.82	0.61
3:C:59:LEU:HD11	15:c:282:ARG:NH1	2.15	0.61
7:U:337:LEU:HD13	7:U:789:ILE:HG21	1.82	0.61
1:A:394:MET:O	1:A:398:ARG:HB2	2.00	0.61
4:D:346:SER:O	4:D:350:SER:HB3	2.00	0.61
8:V:321:ALA:HB1	8:V:324:PHE:HB3	1.81	0.61
13:a:119:GLY:HA2	13:a:122:LYS:HG2	1.82	0.61
4:D:90:GLY:HA2	4:D:245:ARG:HH12	1.65	0.61
8:V:102:PRO:HB2	17:e:18:GLU:HB2	1.83	0.61
12:Z:39:LEU:H	12:Z:94:TRP:HA	1.66	0.61
2:B:67:ARG:NE	18:f:642:ALA:HB2	2.16	0.61
11:Y:145:LEU:HD13	11:Y:183:TYR:HA	1.83	0.61
2:B:43:PRO:HD3	2:B:244:SER:HA	1.82	0.60
7:U:637:VAL:HG11	7:U:656:LEU:HB2	1.83	0.60
15:c:268:GLU:HG2	15:c:269:GLN:HG3	1.82	0.60
18:f:298:LEU:HB2	18:f:492:SER:HB3	1.81	0.60
3:C:113:ARG:HB2	3:C:127:LEU:HB2	1.82	0.60
9:W:75:TYR:HA	9:W:79:GLU:HB3	1.84	0.60
18:f:198:HIS:HA	18:f:201:GLU:HB3	1.84	0.60
5:E:290:LEU:HD13	5:E:389:VAL:HA	1.84	0.60
3:C:31:LEU:HD11	4:D:51:LEU:HD22	1.83	0.60
4:D:116:LEU:H	4:D:119:ILE:CD1	2.15	0.60
13:a:4:VAL:HG22	13:a:6:GLY:H	1.66	0.60
18:f:324:VAL:HG13	18:f:422:VAL:HG11	1.83	0.60
7:U:368:ALA:HB2	7:U:728:PHE:HD1	1.66	0.60
7:U:744:VAL:HB	7:U:783:TYR:HB2	1.84	0.60
14:b:14:GLU:O	14:b:17:ARG:NH1	2.35	0.60
1:A:393:GLY:HA3	2:B:216:ILE:HG21	1.84	0.59
12:Z:73:ASP:HB3	14:b:63:THR:HB	1.82	0.59
7:U:661:ALA:HA	7:U:693:LEU:HG	1.84	0.59
18:f:324:VAL:HG22	18:f:422:VAL:HG21	1.84	0.59
1:A:55:LEU:HB3	2:B:76:GLU:HG3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:9:ILE:HG12	7:U:41:SER:HB2	1.84	0.59
18:f:54:ASP:H	18:f:57:GLU:HB2	1.67	0.59
2:B:60:LEU:HD22	18:f:219:LYS:HE3	1.85	0.59
9:W:280:ASP:H	9:W:283:GLN:HB3	1.66	0.59
5:E:282:PRO:HA	5:E:285:LEU:HD13	1.85	0.59
11:Y:194:PHE:H	11:Y:197:ALA:HB3	1.67	0.59
11:Y:201:PHE:HD2	11:Y:226:VAL:HG11	1.67	0.59
14:b:7:MET:HE3	14:b:97:LEU:HD13	1.83	0.59
18:f:161:HIS:O	18:f:165:GLU:HG2	2.03	0.59
18:f:226:TYR:HB2	18:f:604:GLY:HA2	1.84	0.59
2:B:271:PHE:CZ	2:B:321:SER:HB3	2.37	0.59
2:B:401:GLU:HA	2:B:404:LEU:HB2	1.83	0.59
5:E:149:ILE:HG21	5:E:190:GLN:HB3	1.84	0.59
7:U:615:ARG:HH11	7:U:645:ASN:HD22	1.50	0.59
3:C:99:VAL:HG22	3:C:123:LEU:HD13	1.85	0.59
9:W:231:ILE:HG23	9:W:243:ILE:HG23	1.83	0.59
8:V:299:GLN:HB3	8:V:301:GLU:HG2	1.83	0.59
3:C:114:VAL:HG11	3:C:123:LEU:HD11	1.83	0.59
2:B:198:LYS:O	2:B:202:GLU:HB3	2.03	0.58
5:E:99:ALA:HB3	5:E:109:ARG:HG3	1.84	0.58
14:b:52:ILE:HD11	14:b:59:GLU:HA	1.84	0.58
7:U:375:PHE:HB3	7:U:739:ALA:HA	1.84	0.58
1:A:79:ASP:HB3	1:A:82:ALA:HB2	1.86	0.58
14:b:7:MET:HB2	14:b:109:ILE:HG12	1.85	0.58
7:U:925:VAL:HG23	7:U:927:PRO:HD3	1.85	0.58
13:a:34:TRP:HB2	14:b:17:ARG:HD2	1.84	0.58
3:C:119:ASP:HB3	15:c:193:ILE:HD13	1.84	0.58
5:E:126:ASP:HB3	6:F:320:PHE:HE2	1.66	0.58
5:E:243:PHE:HA	6:F:299:GLU:HB3	1.85	0.58
7:U:252:LEU:O	7:U:256:ALA:HB3	2.04	0.58
4:D:89:ILE:HB	5:E:78:ARG:HB2	1.86	0.58
7:U:167:ILE:HD12	7:U:177:LEU:HD21	1.86	0.58
11:Y:253:LEU:HB2	11:Y:256:VAL:HB	1.86	0.58
8:V:264:TYR:HD2	8:V:298:ILE:HD13	1.69	0.58
11:Y:297:ARG:HH12	17:e:45:ASP:HA	1.69	0.58
18:f:43:GLN:HA	18:f:46:SER:HB3	1.84	0.58
1:A:257:VAL:HA	1:A:260:LEU:HB2	1.86	0.58
2:B:209:GLU:HG2	2:B:213:GLU:HB2	1.85	0.58
5:E:17:LEU:HG	5:E:20:LYS:HB2	1.86	0.57
5:E:202:SER:O	6:F:269:ARG:HD2	2.04	0.57
7:U:583:MET:HE1	7:U:602:LEU:HG	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:175:ARG:HB3	15:c:181:LEU:HD22	1.86	0.57
7:U:776:SER:HA	7:U:779:LEU:HD23	1.85	0.57
17:e:35:ASP:HB3	17:e:37:HIS:HD2	1.68	0.57
3:C:186:VAL:HA	3:C:313:ARG:HB3	1.85	0.57
2:B:194:ILE:O	2:B:198:LYS:HB2	2.03	0.57
11:Y:279:GLU:HA	11:Y:282:MET:HB3	1.87	0.57
18:f:560:LEU:HD23	18:f:594:LEU:HD21	1.86	0.57
18:f:566:HIS:HD2	18:f:599:ALA:HB1	1.70	0.57
1:A:416:VAL:HA	1:A:420:TYR:HB2	1.86	0.57
2:B:303:ARG:O	2:B:307:ARG:HD3	2.04	0.57
13:a:116:THR:HG23	13:a:138:VAL:HG21	1.87	0.57
18:f:453:SER:HB2	18:f:484:GLY:HA2	1.86	0.57
8:V:157:THR:N	8:V:158:PRO:HD2	2.20	0.57
4:D:104:GLY:HA2	4:D:110:ASN:HA	1.86	0.56
6:F:204:LEU:HG	6:F:208:HIS:HB2	1.86	0.56
10:X:365:LEU:HB3	10:X:378:LEU:HD21	1.87	0.56
13:a:69:HIS:HB3	13:a:73:PRO:HB3	1.87	0.56
1:A:211:GLY:HA3	1:A:338:ASP:H	1.70	0.56
4:D:275:PHE:O	4:D:276:ASP:C	2.46	0.56
7:U:342:LEU:HD21	7:U:785:PRO:HG3	1.86	0.56
7:U:407:SER:HA	7:U:410:VAL:HG12	1.87	0.56
15:c:244:VAL:HG22	15:c:291:LEU:HD22	1.87	0.56
18:f:288:VAL:HG11	18:f:879:ARG:HB2	1.87	0.56
7:U:216:VAL:HA	7:U:220:LEU:HD23	1.87	0.56
7:U:259:GLN:HG3	7:U:488:THR:HA	1.86	0.56
7:U:640:LEU:HD22	7:U:652:ALA:HB2	1.86	0.56
11:Y:254:PRO:O	11:Y:257:ARG:HB2	2.06	0.56
15:c:141:VAL:HG11	15:c:203:ILE:HD11	1.88	0.56
16:d:202:GLN:HB3	16:d:204:ARG:HG2	1.86	0.56
18:f:595:VAL:O	18:f:599:ALA:HB2	2.04	0.56
4:D:272:THR:O	4:D:276:ASP:N	2.39	0.56
5:E:147:GLU:HA	5:E:151:LEU:HD12	1.88	0.56
7:U:766:PHE:CE1	7:U:782:ALA:HB2	2.39	0.56
18:f:674:THR:HA	18:f:677:HIS:HB3	1.87	0.56
2:B:197:ILE:HG13	2:B:235:LEU:HD21	1.87	0.56
5:E:191:LEU:HD13	5:E:194:ASN:HD21	1.70	0.56
3:C:49:ARG:HH22	7:U:643:SER:HB3	1.70	0.56
5:E:349:GLU:HA	5:E:352:MET:HB2	1.88	0.56
9:W:453:HIS:HB2	12:Z:220:LEU:HD12	1.88	0.56
7:U:541:HIS:CD2	15:c:62:VAL:HG12	2.39	0.56
18:f:442:SER:HB3	18:f:477:MET:HG2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:296:LYS:HA	8:V:299:GLN:HB2	1.87	0.56
13:a:211:PHE:CZ	13:a:275:LEU:HD23	2.40	0.56
5:E:208:ILE:HA	6:F:261:ILE:HD11	1.88	0.56
8:V:160:LEU:HB2	8:V:162:GLU:HG2	1.88	0.56
8:V:337:LEU:HD13	8:V:367:VAL:HG21	1.88	0.56
18:f:283:THR:O	18:f:287:ASP:HB3	2.05	0.56
1:A:324:PRO:HG2	1:A:431:THR:HG22	1.88	0.56
4:D:214:MET:SD	4:D:217:LYS:HD2	2.46	0.56
5:E:243:PHE:HD1	6:F:299:GLU:HA	1.70	0.56
7:U:261:LEU:HD12	7:U:329:LEU:HD11	1.88	0.56
7:U:592:GLY:H	7:U:625:ILE:HA	1.70	0.56
11:Y:334:LEU:HD13	11:Y:343:LEU:HD21	1.89	0.56
12:Z:25:ARG:HD3	15:c:103:GLY:HA3	1.88	0.56
1:A:27:GLU:C	1:A:29:ASP:H	2.14	0.55
5:E:171:LEU:HB2	5:E:295:LEU:HD13	1.87	0.55
11:Y:85:ASP:HB2	11:Y:100:ILE:HG13	1.89	0.55
13:a:62:ASN:OD1	13:a:80:ILE:HD12	2.05	0.55
15:c:41:MET:HE1	15:c:112:TYR:CD1	2.41	0.55
19:g:178:TYR:HB3	19:g:266:ILE:HG23	1.87	0.55
1:A:36:TYR:CD2	18:f:52:LEU:HG	2.40	0.55
2:B:63:LEU:HD12	18:f:223:GLU:HG2	1.89	0.55
3:C:49:ARG:O	3:C:53:ASN:HB2	2.07	0.55
9:W:183:VAL:HA	9:W:186:ILE:HG12	1.88	0.55
1:A:223:THR:HG21	2:B:318:GLY:HA2	1.87	0.55
3:C:181:ALA:HB1	3:C:182:GLN:HE21	1.71	0.55
8:V:470:ARG:HG3	8:V:471:GLU:N	2.22	0.55
1:A:103:ASN:HB3	1:A:112:ILE:HB	1.89	0.55
1:A:373:LEU:HD13	1:A:376:LEU:HD12	1.88	0.55
2:B:112:LEU:HD21	2:B:144:LEU:HD13	1.89	0.55
4:D:171:ASP:HA	4:D:174:LYS:HD3	1.88	0.55
9:W:128:LEU:HB3	9:W:142:ARG:HH12	1.71	0.55
1:A:124:ASP:HB3	6:F:86:LEU:HD22	1.88	0.55
3:C:46:GLN:HG3	7:U:639:LEU:HD13	1.88	0.55
19:g:177:LEU:HD21	19:g:235:TYR:HA	1.88	0.55
7:U:368:ALA:HB1	7:U:731:ILE:HB	1.88	0.55
7:U:487:GLY:HA2	7:U:521:LEU:HB3	1.89	0.55
16:d:196:LEU:HD11	16:d:208:PHE:HD1	1.72	0.55
18:f:52:LEU:H	18:f:52:LEU:HD22	1.72	0.55
3:C:222:LYS:HB3	4:D:278:GLN:CB	2.37	0.55
4:D:168:GLY:H	4:D:347:THR:HG21	1.71	0.55
2:B:281:ILE:HA	2:B:325:VAL:HG13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:442:ILE:HD13	8:V:451:ILE:HG22	1.88	0.54
18:f:512:MET:C	18:f:514:VAL:H	2.15	0.54
2:B:120:HIS:HA	2:B:134:SER:HA	1.89	0.54
18:f:68:THR:HA	18:f:71:TYR:HB2	1.89	0.54
18:f:283:THR:O	18:f:287:ASP:HB2	2.08	0.54
7:U:539:THR:HG23	7:U:545:LEU:HD11	1.88	0.54
10:X:379:ASP:HA	11:Y:313:SER:HB3	1.88	0.54
2:B:246:THR:O	2:B:280:SER:HB2	2.07	0.54
13:a:62:ASN:ND2	13:a:96:PHE:HZ	2.05	0.54
13:a:76:LEU:HA	13:a:79:ILE:HD12	1.89	0.54
1:A:125:LEU:HA	1:A:149:ILE:H	1.72	0.54
3:C:246:ILE:HD12	3:C:276:LEU:HD11	1.89	0.54
7:U:215:ASN:HA	7:U:219:CYS:HB3	1.90	0.54
7:U:325:MET:HA	7:U:328:ILE:HG12	1.89	0.54
8:V:284:GLU:HA	8:V:287:ARG:HD2	1.90	0.54
14:b:131:LEU:O	14:b:134:GLU:O	2.25	0.54
3:C:158:ILE:HG12	3:C:199:LEU:HD11	1.90	0.54
18:f:186:THR:HG23	18:f:197:ALA:HB3	1.89	0.54
8:V:470:ARG:HG3	8:V:471:GLU:H	1.72	0.54
18:f:179:VAL:HG11	18:f:209:MET:HE1	1.90	0.54
18:f:214:VAL:HA	18:f:217:LEU:HB3	1.90	0.54
18:f:814:SER:HA	18:f:819:TYR:HA	1.88	0.54
12:Z:37:GLY:HA3	12:Z:95:TYR:CZ	2.43	0.53
17:e:50:ASP:HB2	17:e:55:GLN:HB3	1.90	0.53
18:f:125:ILE:HG12	18:f:129:LEU:HB3	1.89	0.53
1:A:97:ARG:HG2	2:B:131:HIS:HD2	1.73	0.53
18:f:163:ALA:HB1	18:f:197:ALA:HB2	1.90	0.53
8:V:256:ARG:CZ	17:e:21:GLU:HG3	2.39	0.53
18:f:429:ILE:HG21	18:f:448:CYS:HB2	1.89	0.53
5:E:204:VAL:HG13	6:F:269:ARG:HD3	1.91	0.53
6:F:225:MET:HE3	6:F:233:LYS:HB3	1.90	0.53
7:U:28:ASN:HA	7:U:31:VAL:HB	1.90	0.53
7:U:38:ILE:HA	7:U:41:SER:HB3	1.91	0.53
11:Y:111:LEU:HD23	11:Y:115:GLY:HA3	1.91	0.53
13:a:189:PRO:HA	13:a:193:GLN:HE21	1.73	0.53
13:a:189:PRO:HB2	13:a:225:LEU:HD11	1.91	0.53
18:f:171:GLN:HE22	18:f:201:GLU:HG3	1.73	0.53
19:g:180:MET:HB2	19:g:231:VAL:HB	1.89	0.53
4:D:349:THR:HA	4:D:352:MET:HG3	1.90	0.53
12:Z:110:GLU:CD	12:Z:110:GLU:O	2.51	0.53
15:c:227:GLU:HA	15:c:230:THR:HG23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:VAL:HA	3:C:123:LEU:HB3	1.91	0.53
5:E:234:GLU:HB3	5:E:237:ALA:HB3	1.90	0.53
12:Z:228:TYR:HE2	13:a:340:VAL:HA	1.73	0.53
11:Y:307:LEU:HD11	11:Y:319:MET:HE1	1.90	0.53
11:Y:177:ARG:HA	11:Y:180:LEU:HD13	1.91	0.53
18:f:48:GLU:HA	18:f:125:ILE:HA	1.91	0.53
1:A:113:ILE:HD11	1:A:121:PHE:HD2	1.74	0.52
2:B:190:LEU:HD23	2:B:360:THR:HG21	1.90	0.52
7:U:882:ALA:O	7:U:884:VAL:N	2.42	0.52
18:f:242:GLU:HB3	18:f:243:PRO:HD3	1.91	0.52
5:E:297:ARG:CG	5:E:299:ILE:HG13	2.38	0.52
18:f:710:LEU:HA	18:f:713:PHE:CD2	2.43	0.52
3:C:61:GLU:O	3:C:65:LEU:HG	2.10	0.52
3:C:344:LEU:HD23	3:C:347:ILE:HD12	1.91	0.52
5:E:323:HIS:N	5:E:326:ILE:HD11	2.24	0.52
18:f:636:ASP:O	18:f:640:LYS:HB2	2.09	0.52
3:C:133:PRO:HG2	3:C:134:LEU:HD23	1.91	0.52
12:Z:202:ASN:HD21	13:a:360:VAL:HG12	1.74	0.52
13:a:43:ASP:HB2	13:a:48:PRO:HB3	1.90	0.52
18:f:327:ASN:HD21	18:f:422:VAL:HB	1.75	0.52
2:B:59:ARG:HA	2:B:62:LEU:HB3	1.92	0.52
9:W:44:ILE:HD13	9:W:47:LEU:HD12	1.91	0.52
15:c:34:SER:H	15:c:70:ILE:HD11	1.74	0.52
2:B:65:LEU:HA	2:B:68:ILE:HD12	1.91	0.52
10:X:351:SER:O	10:X:355:LYS:HA	2.09	0.52
10:X:415:TYR:HB2	11:Y:383:LEU:HD12	1.92	0.52
11:Y:81:LEU:HD13	11:Y:107:LYS:HA	1.90	0.52
11:Y:373:GLY:O	11:Y:377:LEU:HB2	2.10	0.52
1:A:115:VAL:HG11	1:A:118:PHE:HB2	1.92	0.52
5:E:380:LEU:HD13	6:F:335:VAL:HG11	1.91	0.52
9:W:267:LEU:HD22	9:W:299:ILE:HG13	1.92	0.52
18:f:48:GLU:HG2	18:f:49:ASP:H	1.75	0.52
15:c:31:VAL:HG23	15:c:67:VAL:HG13	1.92	0.52
1:A:161:VAL:HA	1:A:164:MET:HB2	1.91	0.52
2:B:283:PHE:HD1	2:B:328:ILE:HG23	1.75	0.52
4:D:91:GLN:HA	4:D:129:SER:HA	1.91	0.52
16:d:175:TYR:HB3	16:d:214:ARG:HH21	1.74	0.52
18:f:31:LYS:NZ	18:f:76:GLU:HB2	2.25	0.52
18:f:192:VAL:HG23	18:f:193:PRO:HD3	1.92	0.52
18:f:673:ARG:O	18:f:674:THR:C	2.52	0.52
2:B:152:LEU:HD23	2:B:157:HIS:HB3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:214:MET:HA	4:D:217:LYS:HG2	1.92	0.51
6:F:223:VAL:HG22	6:F:350:ARG:HB2	1.93	0.51
18:f:373:ALA:HB1	18:f:748:LEU:HB2	1.92	0.51
3:C:366:ALA:HB1	3:C:378:VAL:HG11	1.93	0.51
5:E:16:LEU:HG	5:E:18:GLU:H	1.75	0.51
11:Y:246:ILE:HA	11:Y:249:VAL:HG22	1.91	0.51
18:f:262:PHE:HB3	18:f:568:GLY:HA2	1.91	0.51
18:f:811:LEU:HD23	18:f:878:GLU:HA	1.92	0.51
2:B:200:SER:HB3	2:B:349:ARG:HH21	1.75	0.51
5:E:204:VAL:HA	6:F:266:LYS:HB2	1.91	0.51
18:f:381:VAL:HA	18:f:755:ASP:HB2	1.93	0.51
6:F:65:GLU:O	6:F:69:MET:HB2	2.10	0.51
7:U:252:LEU:O	7:U:256:ALA:CB	2.58	0.51
18:f:221:ILE:HA	18:f:224:ASN:HB2	1.92	0.51
2:B:283:PHE:CE2	2:B:285:ASP:HB2	2.46	0.51
4:D:115:ILE:HB	4:D:119:ILE:HD11	1.92	0.51
4:D:203:LEU:HD22	4:D:327:LEU:HD13	1.93	0.51
5:E:149:ILE:HG12	5:E:187:VAL:HG22	1.92	0.51
7:U:509:GLY:HA3	7:U:544:ILE:HG13	1.92	0.51
12:Z:22:HIS:HA	12:Z:25:ARG:HD2	1.93	0.51
18:f:602:GLY:HA2	18:f:639:LYS:O	2.11	0.51
3:C:44:ARG:HE	8:V:491:VAL:HG23	1.74	0.51
5:E:309:ARG:HD3	5:E:339:ASN:HB3	1.93	0.51
9:W:142:ARG:O	9:W:143:ALA:C	2.54	0.51
18:f:711:SER:HA	18:f:781:TYR:OH	2.11	0.51
19:g:147:ASP:HA	19:g:150:LEU:HB2	1.92	0.51
1:A:75:PRO:HA	1:A:79:ASP:HB2	1.92	0.51
7:U:620:GLU:HA	7:U:655:ALA:HB2	1.93	0.51
2:B:74:MET:HG2	18:f:613:LEU:HD12	1.92	0.51
8:V:156:SER:C	8:V:158:PRO:HD2	2.36	0.51
8:V:224:LEU:HB2	8:V:261:TYR:CE1	2.44	0.51
9:W:183:VAL:HG11	9:W:222:LEU:HD13	1.92	0.51
15:c:231:LEU:O	15:c:232:GLN:C	2.53	0.51
1:A:373:LEU:HD11	1:A:409:PHE:HB3	1.93	0.51
5:E:304:PRO:HG2	5:E:339:ASN:HB2	1.93	0.51
7:U:656:LEU:HD23	7:U:671:LEU:HD11	1.93	0.51
9:W:359:VAL:HB	9:W:382:LEU:HD22	1.91	0.51
18:f:524:MET:HB2	18:f:776:LEU:HD13	1.92	0.51
4:D:103:VAL:HG21	4:D:132:LEU:HD21	1.93	0.51
7:U:479:LEU:HB2	7:U:511:ALA:HB1	1.93	0.51
8:V:113:LEU:HD13	8:V:171:VAL:HG23	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:337:LEU:HD22	8:V:367:VAL:HG11	1.92	0.51
12:Z:20:VAL:HG22	12:Z:126:VAL:HG23	1.92	0.51
12:Z:88:ARG:O	12:Z:88:ARG:HG2	2.11	0.51
15:c:130:GLN:HE22	15:c:133:PHE:HD2	1.58	0.51
5:E:233:ASP:HB3	5:E:234:GLU:HG2	1.92	0.50
6:F:254:PRO:HG3	6:F:291:ILE:HD11	1.93	0.50
16:d:196:LEU:HD23	16:d:229:PRO:HB2	1.94	0.50
19:g:177:LEU:HD22	19:g:238:PHE:HB3	1.93	0.50
1:A:74:PRO:HB2	1:A:77:LEU:HB2	1.93	0.50
7:U:126:ILE:CG1	7:U:130:LEU:HD22	2.41	0.50
8:V:117:VAL:HA	8:V:121:PHE:CD2	2.45	0.50
8:V:258:TYR:HD1	8:V:263:LEU:HB2	1.76	0.50
11:Y:232:GLU:O	11:Y:236:LEU:HB2	2.12	0.50
13:a:301:LYS:HG2	13:a:301:LYS:O	2.11	0.50
15:c:217:LEU:O	15:c:221:HIS:HB2	2.12	0.50
1:A:285:PHE:CZ	1:A:326:THR:HB	2.46	0.50
2:B:316:LEU:HD12	2:B:341:LEU:HD11	1.94	0.50
18:f:732:VAL:HA	18:f:746:ARG:HG3	1.93	0.50
4:D:75:ALA:HA	4:D:78:GLU:HB2	1.93	0.50
11:Y:105:MET:HE3	11:Y:140:ILE:HD12	1.93	0.50
18:f:469:TYR:HA	18:f:472:HIS:HB2	1.93	0.50
18:f:645:ASP:C	18:f:647:GLY:N	2.66	0.50
18:f:688:ARG:CZ	18:f:715:HIS:HE1	2.25	0.50
1:A:295:VAL:HG21	2:B:307:ARG:HH21	1.75	0.50
3:C:63:LEU:HD21	4:D:79:VAL:HG12	1.94	0.50
7:U:26:LYS:HD3	16:d:129:LEU:H	1.76	0.50
9:W:146:THR:HG23	9:W:165:ILE:HG22	1.92	0.50
18:f:297:MET:HA	18:f:300:ARG:HH21	1.77	0.50
4:D:98:GLN:C	4:D:115:ILE:HD11	2.37	0.50
8:V:479:ARG:HA	8:V:482:PHE:HB3	1.93	0.50
18:f:298:LEU:HD11	18:f:458:GLU:HG3	1.94	0.50
18:f:621:ASP:HA	18:f:630:ASP:HB2	1.92	0.50
2:B:174:MET:O	2:B:175:LYS:C	2.54	0.50
2:B:415:THR:O	2:B:419:PHE:HB2	2.12	0.50
7:U:567:ILE:HD12	7:U:586:VAL:HG22	1.94	0.50
9:W:55:ARG:HA	9:W:59:ASP:CB	2.42	0.50
9:W:373:ILE:HG22	9:W:415:PHE:HE1	1.77	0.50
16:d:137:THR:HA	16:d:140:GLN:HG3	1.93	0.50
18:f:9:ALA:HB3	18:f:10:PRO:HD3	1.94	0.50
18:f:241:PRO:HB3	18:f:253:LEU:HD22	1.92	0.50
18:f:327:ASN:HB3	18:f:420:TRP:HE3	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:329:ASN:O	18:f:333:LEU:HB2	2.12	0.50
18:f:620:PHE:HZ	18:f:631:LYS:HE3	1.76	0.50
18:f:673:ARG:O	18:f:676:GLY:N	2.45	0.50
6:F:202:ILE:HG13	6:F:203:VAL:HG23	1.94	0.50
8:V:76:LYS:HA	8:V:79:VAL:HG22	1.94	0.50
9:W:44:ILE:HD11	9:W:82:LEU:HD23	1.93	0.50
18:f:466:LEU:HB3	18:f:485:LEU:HD12	1.94	0.50
18:f:595:VAL:O	18:f:599:ALA:CB	2.60	0.50
3:C:134:LEU:HD11	3:C:241:HIS:CD2	2.47	0.49
3:C:162:LYS:O	3:C:166:GLU:HB2	2.12	0.49
7:U:788:VAL:HG13	7:U:884:VAL:HG11	1.93	0.49
15:c:122:LEU:H	15:c:196:LEU:HD13	1.76	0.49
6:F:381:TYR:HA	6:F:384:LEU:HD12	1.93	0.49
11:Y:387:ILE:O	11:Y:388:ASN:C	2.54	0.49
18:f:221:ILE:HB	18:f:768:LEU:HD11	1.94	0.49
7:U:334:ALA:O	7:U:338:HIS:HB2	2.12	0.49
8:V:302:TYR:HB3	8:V:339:LEU:HD11	1.94	0.49
7:U:215:ASN:H	7:U:215:ASN:HD22	1.61	0.49
18:f:141:LYS:HE3	18:f:159:VAL:HA	1.93	0.49
5:E:323:HIS:H	5:E:326:ILE:HD11	1.77	0.49
18:f:671:ALA:HB1	18:f:674:THR:HG23	1.94	0.49
12:Z:122:VAL:HA	12:Z:137:ALA:HA	1.94	0.49
3:C:92:GLU:HB3	3:C:95:PHE:CE1	2.48	0.49
7:U:220:LEU:HG	7:U:229:VAL:HB	1.93	0.49
9:W:166:LEU:HD13	9:W:189:GLN:HA	1.94	0.49
16:d:223:ASN:HD22	16:d:227:LYS:HB2	1.77	0.49
1:A:215:PHE:HB2	1:A:324:PRO:HG3	1.94	0.49
12:Z:192:THR:HG22	13:a:375:LEU:HD23	1.95	0.49
13:a:104:VAL:HG12	13:a:106:SER:H	1.77	0.49
7:U:218:GLN:O	7:U:221:ILE:HG23	2.13	0.49
7:U:682:TYR:HB3	7:U:725:MET:HE1	1.95	0.49
16:d:302:TYR:O	16:d:305:LYS:HG3	2.13	0.49
18:f:189:LYS:HG3	18:f:190:GLU:HG2	1.94	0.49
18:f:438:ASP:HA	18:f:441:LYS:HB3	1.94	0.49
6:F:312:GLU:HA	6:F:315:ASN:HD21	1.78	0.49
14:b:20:ASP:HA	14:b:177:PRO:HA	1.94	0.49
18:f:181:ARG:O	18:f:184:LEU:HG	2.13	0.49
18:f:301:HIS:HB3	18:f:304:PHE:HB3	1.95	0.49
18:f:382:ASN:HA	18:f:385:PHE:HB2	1.94	0.49
4:D:160:PRO:HD2	4:D:221:HIS:HB2	1.94	0.48
5:E:306:GLU:HA	5:E:309:ARG:HH21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:92:ARG:HA	8:V:95:LEU:HG	1.95	0.48
16:d:275:ILE:HG23	16:d:280:GLU:HB3	1.95	0.48
7:U:19:LEU:HD21	16:d:120:LYS:HA	1.95	0.48
7:U:97:VAL:HA	7:U:100:ILE:HG22	1.94	0.48
12:Z:38:VAL:HB	12:Z:54:PHE:CE2	2.48	0.48
13:a:232:TRP:CZ2	13:a:257:GLN:HB3	2.48	0.48
2:B:55:HIS:HA	18:f:837:LEU:HA	1.95	0.48
2:B:287:ILE:HB	2:B:331:THR:HG22	1.94	0.48
5:E:244:SER:H	6:F:299:GLU:HB3	1.78	0.48
18:f:407:MET:HE3	18:f:408:LEU:HD22	1.95	0.48
18:f:512:MET:O	18:f:514:VAL:N	2.41	0.48
1:A:339:ARG:HA	1:A:339:ARG:HD3	1.68	0.48
2:B:67:ARG:HE	18:f:642:ALA:HB2	1.79	0.48
3:C:185:GLY:HA3	3:C:311:ILE:HA	1.96	0.48
7:U:126:ILE:HG13	7:U:130:LEU:HD22	1.95	0.48
7:U:153:ILE:HA	7:U:156:GLU:HG2	1.96	0.48
7:U:184:CYS:SG	7:U:198:LEU:HD21	2.53	0.48
8:V:110:HIS:CG	8:V:136:GLU:HB3	2.48	0.48
8:V:299:GLN:HA	16:d:209:HIS:CE1	2.49	0.48
9:W:263:TRP:CZ3	9:W:295:LYS:HB3	2.48	0.48
3:C:42:LEU:HD13	4:D:57:GLN:HG2	1.96	0.48
6:F:312:GLU:HA	6:F:315:ASN:ND2	2.27	0.48
11:Y:176:ARG:HD2	11:Y:183:TYR:OH	2.13	0.48
16:d:164:PHE:O	16:d:168:MET:HB2	2.13	0.48
18:f:271:MET:HE3	18:f:274:ASP:HB3	1.94	0.48
5:E:290:LEU:HB3	5:E:389:VAL:HG22	1.95	0.48
5:E:312:ILE:HB	5:E:343:LEU:HD13	1.96	0.48
7:U:213:PHE:N	7:U:213:PHE:CD2	2.82	0.48
11:Y:84:LEU:O	11:Y:87:GLU:HG3	2.14	0.48
16:d:248:LYS:HZ3	16:d:264:LEU:HD11	1.78	0.48
18:f:507:ASP:O	18:f:511:SER:HB2	2.14	0.48
7:U:611:ASN:HB3	7:U:614:VAL:HG12	1.94	0.48
9:W:32:ALA:O	9:W:36:LYS:HB3	2.14	0.48
11:Y:137:ARG:O	11:Y:141:VAL:HG23	2.14	0.48
18:f:72:ARG:HB3	18:f:73:PRO:HD3	1.96	0.48
18:f:271:MET:HG3	18:f:275:MET:HE2	1.95	0.48
2:B:99:VAL:HG23	2:B:102:LEU:HD23	1.95	0.48
4:D:174:LYS:HD2	21:D:501:AGS:HN62	1.78	0.48
5:E:312:ILE:HA	5:E:315:ILE:HG12	1.96	0.48
11:Y:167:LEU:O	11:Y:170:GLU:HG2	2.14	0.48
1:A:327:LEU:HD21	1:A:331:LEU:HD23	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:363:ALA:HA	6:F:366:MET:HE2	1.96	0.47
7:U:791:LEU:HB3	7:U:911:ILE:HD11	1.96	0.47
11:Y:64:GLN:HG3	11:Y:66:ASP:H	1.79	0.47
1:A:345:LEU:HA	1:A:381:THR:HG23	1.95	0.47
14:b:142:ASN:ND2	14:b:171:VAL:O	2.46	0.47
18:f:158:TYR:HA	18:f:161:HIS:CE1	2.49	0.47
2:B:251:VAL:HA	2:B:285:ASP:HB3	1.95	0.47
7:U:533:VAL:HG21	7:U:570:LEU:HD21	1.94	0.47
11:Y:21:GLN:HB2	11:Y:286:TRP:HZ3	1.79	0.47
1:A:285:PHE:HZ	1:A:326:THR:HB	1.79	0.47
16:d:284:PHE:O	16:d:288:THR:HB	2.15	0.47
18:f:125:ILE:HD13	18:f:130:ALA:HB2	1.96	0.47
18:f:138:GLU:HA	18:f:141:LYS:HB2	1.96	0.47
1:A:45:ILE:HD13	2:B:57:GLN:HB3	1.95	0.47
2:B:52:VAL:C	2:B:54:PRO:HD3	2.38	0.47
3:C:43:ARG:O	8:V:494:MET:HE2	2.15	0.47
15:c:240:HIS:O	15:c:244:VAL:HG23	2.14	0.47
18:f:645:ASP:C	18:f:647:GLY:H	2.21	0.47
3:C:280:LEU:HD12	3:C:291:VAL:HB	1.97	0.47
13:a:176:ALA:HB3	13:a:200:LEU:HD13	1.97	0.47
14:b:142:ASN:HB3	14:b:174:PRO:HG3	1.95	0.47
18:f:125:ILE:HG21	18:f:130:ALA:H	1.78	0.47
18:f:287:ASP:HA	18:f:290:VAL:HG12	1.95	0.47
3:C:72:TYR:HA	4:D:111:TYR:HA	1.97	0.47
7:U:67:VAL:HA	7:U:70:HIS:HD2	1.80	0.47
7:U:107:HIS:CE1	7:U:111:GLN:HE22	2.33	0.47
7:U:645:ASN:HB3	7:U:648:VAL:HG12	1.97	0.47
9:W:280:ASP:O	9:W:284:SER:N	2.46	0.47
11:Y:291:HIS:HB3	11:Y:295:TYR:HB2	1.97	0.47
14:b:64:LEU:HD22	14:b:100:ARG:HB2	1.96	0.47
16:d:330:ILE:HG13	16:d:331:PRO:HD3	1.96	0.47
18:f:326:LEU:O	18:f:330:PHE:HB2	2.15	0.47
1:A:96:ALA:HB3	2:B:132:TYR:HB3	1.96	0.47
5:E:291:ARG:HD2	5:E:291:ARG:HA	1.51	0.47
7:U:167:ILE:HD11	7:U:204:ILE:HD13	1.97	0.47
7:U:206:MET:SD	7:U:232:ILE:HG12	2.55	0.47
9:W:443:THR:HG21	12:Z:204:LYS:HB3	1.96	0.47
11:Y:53:TYR:HD2	11:Y:57:LEU:HD12	1.80	0.47
3:C:140:VAL:HG22	4:D:323:ARG:HG2	1.96	0.47
4:D:385:LEU:HD23	4:D:398:ASP:HA	1.96	0.47
7:U:101:ILE:HD13	7:U:137:MET:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:377:HIS:HB3	7:U:411:ILE:HD11	1.95	0.47
7:U:894:MET:HE2	7:U:896:GLU:HA	1.97	0.47
14:b:4:GLU:HB3	14:b:44:ASN:OD1	2.14	0.47
15:c:134:GLU:HA	15:c:138:GLU:CA	2.42	0.47
18:f:609:VAL:HG22	18:f:612:LEU:HD12	1.96	0.47
2:B:53:THR:N	2:B:54:PRO:HD3	2.29	0.47
7:U:599:ILE:HA	7:U:602:LEU:HB3	1.96	0.47
10:X:351:SER:O	10:X:355:LYS:CA	2.63	0.47
11:Y:160:ASN:HA	11:Y:163:LYS:HB2	1.97	0.47
11:Y:174:TRP:O	11:Y:177:ARG:HB2	2.15	0.47
17:e:52:PHE:CE2	17:e:56:LEU:HD11	2.50	0.47
18:f:372:LEU:HG	18:f:406:GLY:HA2	1.96	0.47
3:C:151:ILE:HG12	3:C:199:LEU:HD22	1.97	0.46
4:D:371:SER:HB2	5:E:291:ARG:HH21	1.79	0.46
5:E:342:ASP:HA	5:E:345:ASN:HB2	1.97	0.46
7:U:564:ASP:HA	7:U:567:ILE:HG12	1.96	0.46
11:Y:135:GLY:C	11:Y:137:ARG:N	2.72	0.46
12:Z:57:PRO:HB2	12:Z:71:ASP:HB2	1.97	0.46
15:c:58:LEU:HD12	15:c:108:VAL:HA	1.97	0.46
15:c:303:MET:HB2	16:d:332:SER:HB2	1.97	0.46
18:f:69:SER:HA	18:f:72:ARG:HH21	1.79	0.46
18:f:72:ARG:NH1	18:f:94:LYS:HE2	2.30	0.46
3:C:280:LEU:HD23	3:C:280:LEU:HA	1.78	0.46
7:U:497:LEU:HG	7:U:516:LEU:HG	1.98	0.46
9:W:276:LEU:HD23	9:W:354:LEU:HB2	1.97	0.46
9:W:360:GLU:HB3	9:W:392:PHE:HZ	1.81	0.46
2:B:61:LYS:HG3	2:B:64:LYS:NZ	2.30	0.46
3:C:97:VAL:HG11	3:C:116:LEU:HD11	1.96	0.46
3:C:229:ARG:HH21	3:C:232:ARG:HB2	1.80	0.46
4:D:113:VAL:HG21	4:D:132:LEU:HD11	1.97	0.46
7:U:527:GLN:O	7:U:531:ASP:HB2	2.16	0.46
7:U:801:GLN:HG2	7:U:895:PRO:HG3	1.97	0.46
18:f:113:MET:HG2	18:f:115:PRO:HD3	1.96	0.46
18:f:519:ALA:HB2	18:f:558:LEU:HD23	1.96	0.46
13:a:278:MET:HB2	13:a:319:LEU:HD11	1.98	0.46
15:c:264:LYS:HD2	15:c:270:LEU:HB3	1.97	0.46
4:D:87:LEU:HD13	4:D:131:ALA:HB1	1.98	0.46
4:D:374:ASP:OD1	5:E:292:PRO:HG3	2.15	0.46
11:Y:282:MET:HE1	11:Y:291:HIS:ND1	2.31	0.46
12:Z:82:PHE:O	12:Z:86:ASN:CB	2.61	0.46
18:f:391:LEU:HD11	18:f:417:ILE:HG13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ARG:NH2	3:C:282:GLY:HA2	2.31	0.46
3:C:184:LYS:HD3	3:C:280:LEU:HB3	1.96	0.46
6:F:358:ASN:HA	6:F:362:ARG:HG2	1.97	0.46
7:U:206:MET:O	7:U:206:MET:HG2	2.15	0.46
15:c:282:ARG:O	15:c:284:LEU:N	2.46	0.46
18:f:319:GLU:HG2	18:f:458:GLU:HB2	1.98	0.46
18:f:688:ARG:HH21	18:f:711:SER:HB2	1.81	0.46
2:B:170:LEU:HG	2:B:269:GLU:HB3	1.97	0.46
2:B:281:ILE:HG22	2:B:326:LYS:H	1.81	0.46
8:V:176:MET:HE3	8:V:217:VAL:HG22	1.98	0.46
9:W:55:ARG:HA	9:W:59:ASP:HB2	1.98	0.46
2:B:245:ALA:HB1	2:B:280:SER:CB	2.42	0.46
3:C:219:LEU:HD13	3:C:224:ILE:CG1	2.46	0.46
11:Y:66:ASP:O	11:Y:69:LEU:HG	2.16	0.46
11:Y:101:ARG:HG3	11:Y:102:ASP:N	2.31	0.46
16:d:310:LEU:HG	16:d:311:GLY:N	2.31	0.46
18:f:202:HIS:NE2	18:f:242:GLU:HB3	2.31	0.46
1:A:243:SER:HB3	2:B:311:GLU:HG3	1.98	0.46
2:B:60:LEU:HD13	18:f:219:LYS:HG3	1.98	0.46
2:B:256:ILE:HD12	2:B:305:ILE:HD12	1.98	0.46
2:B:310:LEU:HA	2:B:310:LEU:HD23	1.83	0.46
3:C:115:ALA:HB3	3:C:125:LYS:HB3	1.98	0.46
7:U:225:ASP:HB3	7:U:228:ALA:HB3	1.97	0.46
3:C:31:LEU:HD12	3:C:31:LEU:HA	1.79	0.45
4:D:116:LEU:H	4:D:119:ILE:HD13	1.81	0.45
8:V:121:PHE:HB3	8:V:128:ARG:HB2	1.97	0.45
8:V:395:ILE:HA	8:V:398:LEU:HD12	1.97	0.45
13:a:61:GLU:HA	13:a:64:ILE:HD12	1.98	0.45
13:a:119:GLY:HA3	13:a:158:LEU:HD21	1.97	0.45
16:d:310:LEU:HG	16:d:311:GLY:H	1.81	0.45
18:f:72:ARG:HD2	18:f:103:TYR:HD2	1.81	0.45
18:f:391:LEU:HD23	18:f:391:LEU:H	1.81	0.45
1:A:181:LYS:HA	1:A:184:ILE:HD12	1.99	0.45
7:U:598:ALA:O	7:U:602:LEU:HB2	2.16	0.45
15:c:233:ASP:HA	15:c:298:GLN:NE2	2.32	0.45
1:A:41:TYR:OH	18:f:184:LEU:HD13	2.17	0.45
2:B:171:VAL:HG23	2:B:172:THR:HG23	1.99	0.45
5:E:260:LEU:O	5:E:264:MET:HG2	2.16	0.45
13:a:211:PHE:HZ	13:a:275:LEU:HA	1.81	0.45
14:b:18:ASN:HD22	14:b:19:GLY:H	1.65	0.45
15:c:130:GLN:NE2	15:c:134:GLU:OE2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:54:ASP:O	18:f:58:MET:HG2	2.16	0.45
4:D:86:PRO:HB3	5:E:105:LEU:HB3	1.99	0.45
4:D:228:ILE:HD11	4:D:262:ILE:HG22	1.98	0.45
7:U:168:LEU:C	7:U:170:SER:H	2.24	0.45
7:U:340:GLN:HA	7:U:343:ILE:HD12	1.99	0.45
7:U:542:GLU:HG3	7:U:546:ARG:HE	1.82	0.45
8:V:110:HIS:CD2	8:V:136:GLU:HB3	2.52	0.45
9:W:337:ALA:HB1	9:W:340:VAL:HB	1.99	0.45
15:c:107:MET:HE3	15:c:107:MET:HB3	1.75	0.45
5:E:313:LEU:HG	5:E:343:LEU:HD22	1.98	0.45
15:c:282:ARG:HG3	15:c:283:HIS:H	1.81	0.45
1:A:190:VAL:HG13	1:A:191:VAL:HG23	1.99	0.45
2:B:79:ILE:HG23	18:f:662:MET:HE3	1.97	0.45
2:B:225:TYR:HB3	2:B:330:ALA:HA	1.99	0.45
4:D:102:ILE:HG12	4:D:112:TYR:HA	1.98	0.45
11:Y:19:ILE:HD13	11:Y:43:ALA:HB2	1.99	0.45
18:f:515:ALA:HA	18:f:518:THR:HG22	1.98	0.45
7:U:660:CYS:HB3	7:U:694:ILE:HG13	1.99	0.45
13:a:240:PHE:CD1	13:a:272:ILE:HD12	2.51	0.45
15:c:251:LEU:HD11	15:c:287:HIS:CE1	2.51	0.45
18:f:845:ARG:HD2	18:f:845:ARG:HA	1.77	0.45
1:A:187:LEU:HA	1:A:190:VAL:HG12	1.98	0.45
2:B:195:GLN:HB2	18:f:845:ARG:HE	1.82	0.45
11:Y:13:LYS:HE2	11:Y:147:ILE:HD13	1.98	0.45
13:a:268:LEU:O	13:a:272:ILE:HG12	2.16	0.45
18:f:244:GLU:HB3	18:f:250:ARG:O	2.17	0.45
19:g:149:CYS:HB3	19:g:157:LEU:HD23	1.98	0.45
3:C:222:LYS:CB	4:D:278:GLN:HB3	2.46	0.45
6:F:289:ASP:HA	6:F:338:LEU:HD13	1.99	0.45
8:V:117:VAL:HA	8:V:121:PHE:HD2	1.82	0.45
9:W:272:LEU:HB3	9:W:340:VAL:HG11	1.97	0.45
11:Y:387:ILE:HD13	11:Y:387:ILE:H	1.80	0.45
18:f:210:GLU:HB3	18:f:249:LEU:HG	1.99	0.45
1:A:27:GLU:C	1:A:29:ASP:N	2.75	0.45
6:F:296:PHE:HD2	6:F:298:SER:H	1.64	0.45
7:U:416:GLU:HB2	7:U:450:HIS:NE2	2.32	0.45
8:V:97:ALA:HA	8:V:100:MET:HE3	1.98	0.45
10:X:377:ILE:HB	10:X:386:ILE:HB	1.99	0.45
12:Z:241:SER:H	15:c:310:LYS:HB2	1.82	0.45
1:A:282:GLY:HA3	1:A:285:PHE:CE2	2.52	0.44
3:C:198:LEU:HD11	20:C:501:ADP:H2'	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:ASP:HB3	5:E:92:LEU:HD23	1.98	0.44
8:V:357:LEU:O	8:V:361:PHE:HB2	2.17	0.44
11:Y:261:PHE:HA	11:Y:264:TYR:HD1	1.80	0.44
12:Z:20:VAL:HG21	15:c:216:MET:HE1	1.99	0.44
18:f:72:ARG:HH11	18:f:94:LYS:HE2	1.82	0.44
18:f:526:ALA:HB3	18:f:565:ASN:HB2	1.99	0.44
18:f:594:LEU:HA	18:f:597:VAL:HG12	1.98	0.44
1:A:69:ASP:HB3	2:B:164:MET:HB2	1.99	0.44
4:D:53:PHE:CE2	7:U:632:GLN:HB3	2.52	0.44
8:V:453:HIS:HB2	16:d:279:TYR:O	2.17	0.44
18:f:315:GLU:HA	18:f:318:THR:HG22	1.99	0.44
18:f:507:ASP:O	18:f:508:SER:C	2.60	0.44
2:B:248:LEU:HB2	2:B:282:VAL:HG12	1.99	0.44
5:E:72:LYS:HA	5:E:78:ARG:HE	1.83	0.44
7:U:444:TYR:HB2	7:U:476:GLY:HA2	1.99	0.44
13:a:90:PRO:O	13:a:91:ASN:C	2.60	0.44
13:a:254:ALA:HA	13:a:258:GLN:CG	2.46	0.44
18:f:524:MET:HE2	18:f:776:LEU:HD13	1.99	0.44
2:B:176:VAL:HG22	2:B:247:PHE:H	1.82	0.44
7:U:147:TYR:OH	7:U:173:VAL:HG11	2.18	0.44
8:V:483:CYS:HA	8:V:486:ILE:HD12	1.98	0.44
11:Y:181:LYS:HE3	11:Y:219:PHE:HB2	2.00	0.44
12:Z:82:PHE:HA	12:Z:85:VAL:HG12	1.99	0.44
1:A:99:THR:HG21	1:A:113:ILE:HD12	1.99	0.44
2:B:171:VAL:HA	2:B:273:VAL:HG22	1.99	0.44
3:C:213:ARG:O	3:C:214:VAL:C	2.59	0.44
3:C:219:LEU:HD13	3:C:224:ILE:HG13	1.99	0.44
5:E:140:GLU:O	5:E:144:GLU:HG2	2.18	0.44
15:c:300:LEU:O	15:c:304:LEU:HB2	2.18	0.44
4:D:349:THR:HG21	4:D:354:LEU:HD13	1.99	0.44
4:D:405:THR:HB	5:E:297:ARG:NH1	2.33	0.44
6:F:91:SER:HB2	6:F:126:THR:HA	1.99	0.44
18:f:240:VAL:N	18:f:241:PRO:HD2	2.33	0.44
7:U:185:MET:HA	7:U:188:MET:HE3	1.99	0.44
9:W:316:ARG:O	9:W:320:LEU:HG	2.17	0.44
11:Y:258:GLN:O	11:Y:262:SER:CB	2.66	0.44
3:C:44:ARG:HB2	8:V:491:VAL:HA	1.99	0.44
6:F:275:ALA:HB1	6:F:326:VAL:HG11	2.00	0.44
7:U:123:LYS:O	7:U:124:LYS:C	2.60	0.44
8:V:465:ASP:HB3	8:V:467:TYR:HD1	1.83	0.44
11:Y:359:PRO:HG2	11:Y:364:TRP:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:285:PRO:O	13:a:286:ALA:C	2.61	0.44
2:B:41:LYS:HD2	2:B:279:PRO:HD2	2.00	0.44
4:D:100:THR:HG22	4:D:114:ARG:HG2	2.00	0.44
5:E:226:GLN:HB2	5:E:227:PRO:HD3	2.00	0.44
13:a:239:ALA:HB1	13:a:244:ASN:CB	2.48	0.44
14:b:13:SER:HB2	14:b:82:GLY:C	2.42	0.44
14:b:180:ALA:O	14:b:184:ILE:HG12	2.17	0.44
1:A:141:GLY:H	1:A:151:ILE:HG21	1.83	0.43
5:E:319:PRO:HG2	5:E:320:ILE:HD12	2.00	0.43
6:F:120:LYS:HB3	6:F:137:ILE:HD13	2.00	0.43
7:U:171:ASN:O	7:U:208:LEU:HD22	2.18	0.43
9:W:166:LEU:HD22	9:W:189:GLN:HG2	2.00	0.43
13:a:28:LEU:O	13:a:32:LYS:N	2.51	0.43
18:f:8:LYS:H	18:f:59:LEU:HD21	1.83	0.43
1:A:334:PRO:HG3	6:F:395:GLN:HG3	2.00	0.43
3:C:219:LEU:HB3	3:C:224:ILE:HB	2.00	0.43
4:D:116:LEU:H	4:D:119:ILE:HD11	1.81	0.43
12:Z:187:LEU:HB2	15:c:293:THR:HB	1.99	0.43
16:d:205:VAL:HA	16:d:208:PHE:HB3	1.99	0.43
18:f:256:PHE:HE2	18:f:271:MET:HG2	1.83	0.43
18:f:520:LEU:HD12	18:f:557:TRP:HD1	1.83	0.43
1:A:296:GLN:HA	1:A:299:MET:HG2	2.00	0.43
2:B:407:LEU:HD21	3:C:178:LEU:HD11	2.00	0.43
3:C:227:GLY:HA2	3:C:230:MET:HE2	2.01	0.43
7:U:26:LYS:HG3	16:d:129:LEU:HD12	2.00	0.43
9:W:303:LYS:HA	9:W:306:LEU:HD12	2.01	0.43
10:X:344:ARG:HA	10:X:385:LEU:O	2.19	0.43
11:Y:48:ASN:O	11:Y:114:ILE:HG23	2.18	0.43
13:a:262:ALA:HA	13:a:265:GLU:HB2	1.99	0.43
14:b:9:CYS:HB3	14:b:54:LEU:HD23	1.99	0.43
18:f:464:ALA:O	18:f:468:ASP:HB2	2.18	0.43
2:B:72:LEU:HD22	18:f:654:VAL:HG21	2.00	0.43
7:U:19:LEU:HD22	16:d:123:LEU:HB3	1.99	0.43
7:U:81:ALA:HA	7:U:84:ALA:HB3	2.01	0.43
7:U:802:TYR:HB3	7:U:892:LEU:HD11	2.00	0.43
9:W:227:TYR:O	9:W:230:MET:HG2	2.18	0.43
11:Y:135:GLY:C	11:Y:137:ARG:H	2.25	0.43
12:Z:35:VAL:H	12:Z:97:THR:HG22	1.83	0.43
14:b:111:ALA:HB3	14:b:140:ILE:HD12	1.99	0.43
4:D:60:TYR:CZ	7:U:603:LEU:HD23	2.54	0.43
4:D:154:LEU:HD11	4:D:159:LYS:HD3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:205:ASP:H	6:F:266:LYS:HB2	1.84	0.43
6:F:196:GLN:O	6:F:200:GLU:CB	2.65	0.43
7:U:543:LYS:HA	7:U:546:ARG:HD2	2.01	0.43
13:a:179:PHE:O	13:a:183:VAL:HB	2.19	0.43
3:C:231:VAL:O	3:C:234:LEU:HB2	2.19	0.43
5:E:17:LEU:O	5:E:18:GLU:C	2.61	0.43
7:U:220:LEU:HD13	7:U:220:LEU:HA	1.90	0.43
7:U:437:TYR:HA	7:U:472:ILE:HG21	2.00	0.43
7:U:660:CYS:O	7:U:663:THR:HG23	2.17	0.43
11:Y:298:GLU:HA	11:Y:301:ILE:HG12	2.01	0.43
11:Y:314:LEU:HD11	11:Y:319:MET:HE2	2.00	0.43
2:B:173:VAL:HG22	3:C:231:VAL:HB	2.01	0.43
3:C:320:PRO:HD2	3:C:355:SER:HA	2.00	0.43
4:D:88:VAL:HG12	5:E:79:TYR:HE1	1.84	0.43
5:E:325:GLU:HG2	5:E:364:GLN:HE22	1.83	0.43
7:U:581:SER:O	7:U:585:THR:HG23	2.19	0.43
14:b:12:ASN:HA	14:b:16:MET:HB3	2.01	0.43
16:d:245:PHE:HA	16:d:248:LYS:HD2	2.00	0.43
1:A:73:ALA:HA	1:A:78:TRP:HE1	1.82	0.43
3:C:113:ARG:CB	3:C:127:LEU:HB2	2.47	0.43
3:C:161:ILE:HA	3:C:164:VAL:HG12	2.00	0.43
11:Y:127:THR:HA	11:Y:130:LYS:HE2	2.01	0.43
13:a:172:TYR:HD2	13:a:203:ALA:HB2	1.83	0.43
13:a:189:PRO:O	13:a:225:LEU:HD13	2.18	0.43
4:D:160:PRO:HA	5:E:267:PHE:O	2.19	0.43
8:V:159:LEU:HD13	8:V:159:LEU:HA	1.80	0.43
11:Y:179:ARG:HA	11:Y:212:GLU:HB2	1.99	0.43
13:a:223:GLU:HA	13:a:226:ARG:HB2	2.00	0.43
13:a:248:PHE:O	13:a:251:LEU:HG	2.18	0.43
16:d:217:ALA:O	16:d:220:ILE:HG22	2.19	0.43
18:f:669:GLU:O	18:f:672:LEU:HB2	2.19	0.43
4:D:284:GLU:O	4:D:285:VAL:C	2.62	0.43
7:U:553:ALA:HB2	7:U:584:TYR:HB3	2.00	0.43
7:U:680:VAL:HB	7:U:683:VAL:HG22	2.00	0.43
11:Y:307:LEU:HD11	11:Y:319:MET:CE	2.49	0.43
12:Z:236:LEU:HD23	13:a:335:TRP:HB3	2.01	0.43
15:c:267:PRO:C	15:c:269:GLN:N	2.74	0.43
16:d:278:ALA:H	16:d:319:ALA:HA	1.83	0.43
18:f:171:GLN:NE2	18:f:201:GLU:HG3	2.33	0.43
18:f:724:ASN:HA	18:f:727:PHE:HB3	2.00	0.43
6:F:399:VAL:HG21	6:F:424:ILE:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:616:ARG:HD3	7:U:647:HIS:CD2	2.54	0.42
8:V:313:LEU:HD11	8:V:329:HIS:CE1	2.55	0.42
8:V:355:ARG:HA	8:V:358:MET:HE1	2.01	0.42
11:Y:132:VAL:C	11:Y:134:LEU:H	2.26	0.42
11:Y:347:ILE:HA	11:Y:354:VAL:HG12	2.00	0.42
18:f:512:MET:C	18:f:514:VAL:N	2.77	0.42
18:f:657:ILE:HD13	18:f:690:VAL:HG11	2.01	0.42
18:f:72:ARG:HD2	18:f:103:TYR:CD2	2.54	0.42
18:f:202:HIS:NE2	18:f:243:PRO:HD3	2.33	0.42
18:f:715:HIS:HB2	18:f:753:ALA:HB1	2.01	0.42
2:B:176:VAL:HG13	2:B:247:PHE:O	2.19	0.42
7:U:439:GLU:HG3	7:U:473:VAL:HG22	2.00	0.42
10:X:380:GLN:HE22	11:Y:314:LEU:HA	1.83	0.42
11:Y:345:CYS:HA	11:Y:356:THR:HA	2.02	0.42
13:a:324:ILE:HD13	13:a:331:VAL:HG22	2.01	0.42
14:b:131:LEU:O	14:b:135:LYS:HA	2.19	0.42
17:e:26:ASP:O	17:e:27:TRP:C	2.61	0.42
18:f:584:SER:HB2	18:f:588:ARG:HD3	2.01	0.42
18:f:798:THR:HA	18:f:801:VAL:HG22	2.01	0.42
1:A:113:ILE:HD11	1:A:121:PHE:CD2	2.53	0.42
2:B:173:VAL:CG2	3:C:231:VAL:HB	2.49	0.42
4:D:70:LYS:HB2	12:Z:184:VAL:HG21	2.01	0.42
5:E:55:GLN:HB3	5:E:99:ALA:HB1	2.01	0.42
5:E:182:LEU:HD22	21:E:501:AGS:H2'	2.01	0.42
6:F:279:ALA:HB3	6:F:280:PRO:HD3	2.01	0.42
7:U:603:LEU:HA	7:U:603:LEU:HD12	1.77	0.42
7:U:800:VAL:HG21	7:U:914:LEU:HD21	2.00	0.42
11:Y:173:ASP:HA	11:Y:176:ARG:NH1	2.33	0.42
11:Y:228:MET:HB2	11:Y:263:LEU:HD22	2.01	0.42
14:b:27:GLN:C	14:b:29:GLN:N	2.77	0.42
15:c:37:ALA:O	15:c:41:MET:HB2	2.19	0.42
18:f:655:LEU:HD21	18:f:674:THR:HB	2.00	0.42
18:f:811:LEU:HG	18:f:856:ALA:HB2	2.00	0.42
3:C:196:LYS:HA	3:C:317:PHE:HE2	1.84	0.42
4:D:145:PRO:HG2	4:D:252:ARG:HG2	2.01	0.42
5:E:317:ALA:HB1	5:E:322:LYS:HE3	2.01	0.42
7:U:20:LYS:HA	7:U:23:ALA:HB3	2.01	0.42
10:X:377:ILE:HG13	10:X:388:PHE:HE1	1.84	0.42
13:a:211:PHE:CE1	13:a:275:LEU:HD23	2.54	0.42
13:a:293:PHE:HB2	13:a:329:LYS:HB3	2.01	0.42
14:b:52:ILE:CD1	14:b:59:GLU:HA	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:GLU:HG2	15:c:189:ILE:HD13	1.95	0.42
3:C:113:ARG:HE	3:C:127:LEU:HD23	1.84	0.42
8:V:489:MET:HG3	12:Z:275:LEU:HD11	2.00	0.42
10:X:407:MET:HE1	15:c:248:MET:SD	2.59	0.42
13:a:353:LEU:HD12	13:a:353:LEU:HA	1.75	0.42
14:b:51:LEU:CD2	14:b:71:ILE:HG23	2.50	0.42
15:c:267:PRO:C	15:c:269:GLN:H	2.27	0.42
1:A:277:ILE:HA	1:A:280:ILE:HG12	2.01	0.42
1:A:376:LEU:HB3	1:A:413:VAL:HG11	2.00	0.42
6:F:318:ASP:HB3	6:F:347:ARG:CD	2.47	0.42
7:U:82:LEU:HD21	7:U:130:LEU:HD12	2.01	0.42
7:U:517:GLY:HA3	7:U:551:GLY:HA2	2.01	0.42
9:W:214:PHE:HB3	9:W:223:LYS:HE2	2.00	0.42
10:X:377:ILE:HG23	11:Y:312:ARG:H	1.84	0.42
11:Y:387:ILE:HG13	12:Z:276:ILE:HD11	2.01	0.42
16:d:141:LEU:HD23	16:d:141:LEU:HA	1.84	0.42
18:f:225:ALA:HB3	18:f:644:ALA:HB2	2.01	0.42
2:B:57:GLN:HG2	2:B:61:LYS:HD3	2.01	0.42
5:E:250:ASP:O	5:E:254:GLN:HB2	2.19	0.42
5:E:264:MET:HB2	5:E:275:MET:HE2	2.02	0.42
7:U:198:LEU:HB3	7:U:219:CYS:SG	2.60	0.42
7:U:448:LEU:HD11	7:U:778:PHE:HA	2.02	0.42
18:f:333:LEU:HG	18:f:337:LEU:HB2	2.01	0.42
18:f:383:ALA:HB1	18:f:806:VAL:HG21	2.02	0.42
5:E:169:GLY:HA3	5:E:294:ARG:O	2.20	0.42
7:U:486:MET:HE3	7:U:761:VAL:HG11	2.02	0.42
7:U:763:VAL:HA	7:U:766:PHE:CD1	2.54	0.42
8:V:97:ALA:O	8:V:101:LEU:HG	2.20	0.42
10:X:365:LEU:O	10:X:369:ILE:HG12	2.20	0.42
11:Y:100:ILE:O	11:Y:101:ARG:C	2.62	0.42
1:A:297:ARG:HH22	6:F:303:ASP:HB2	1.85	0.42
3:C:187:LEU:HA	3:C:293:MET:HB2	2.02	0.42
3:C:350:LEU:HB3	3:C:351:MET:HE2	2.02	0.42
7:U:49:TYR:HE1	7:U:61:ALA:HB2	1.85	0.42
10:X:361:VAL:O	10:X:365:LEU:HB2	2.20	0.42
18:f:589:SER:HB3	18:f:631:LYS:HE3	2.02	0.42
18:f:655:LEU:HD21	18:f:674:THR:CB	2.50	0.42
18:f:841:PRO:HB2	18:f:844:VAL:HA	2.01	0.42
7:U:614:VAL:O	7:U:618:ALA:CB	2.68	0.41
9:W:355:LYS:HA	9:W:358:VAL:HG22	2.02	0.41
13:a:356:TRP:HH2	15:c:310:LYS:HA	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:78:LEU:HG	18:f:78:LEU:O	2.20	0.41
18:f:498:LEU:HD21	18:f:533:ASP:HB2	2.02	0.41
1:A:160:THR:HG23	1:A:161:VAL:HG23	2.02	0.41
3:C:90:HIS:N	3:C:91:PRO:HD2	2.34	0.41
4:D:60:TYR:CE2	7:U:603:LEU:HD23	2.56	0.41
7:U:338:HIS:CE1	7:U:785:PRO:HD2	2.55	0.41
7:U:725:MET:O	7:U:728:PHE:HB3	2.20	0.41
8:V:329:HIS:CD2	8:V:347:GLN:HB3	2.55	0.41
9:W:231:ILE:HD13	9:W:247:TYR:CE1	2.55	0.41
14:b:19:GLY:O	14:b:177:PRO:HG3	2.19	0.41
18:f:186:THR:HA	18:f:189:LYS:HG2	2.01	0.41
2:B:231:GLY:HA2	20:B:501:ADP:H5'2	2.01	0.41
8:V:85:ALA:HB2	8:V:93:PHE:HB2	2.02	0.41
9:W:280:ASP:CG	9:W:281:ASN:H	2.21	0.41
9:W:405:LYS:HB2	9:W:414:ASN:HD21	1.84	0.41
12:Z:38:VAL:HG21	12:Z:75:LEU:HD13	2.02	0.41
13:a:78:GLU:HG2	13:a:113:LEU:HD21	2.03	0.41
13:a:360:VAL:HG13	15:c:308:VAL:HG22	2.02	0.41
16:d:190:GLN:HB3	16:d:225:TYR:CD1	2.44	0.41
16:d:323:GLN:O	16:d:324:LYS:C	2.63	0.41
18:f:555:ALA:HB1	18:f:558:LEU:HD12	2.03	0.41
1:A:368:ILE:HA	1:A:406:GLU:HB3	2.01	0.41
6:F:406:ILE:HD13	6:F:422:GLU:HB3	2.02	0.41
11:Y:57:LEU:HD23	11:Y:57:LEU:HA	1.95	0.41
12:Z:209:ARG:O	12:Z:212:LEU:HG	2.20	0.41
12:Z:228:TYR:CE2	13:a:340:VAL:HA	2.55	0.41
12:Z:262:LEU:HD22	12:Z:262:LEU:H	1.85	0.41
16:d:208:PHE:CZ	16:d:233:GLU:HG2	2.55	0.41
5:E:145:LEU:O	5:E:149:ILE:HG13	2.21	0.41
12:Z:39:LEU:N	12:Z:94:TRP:HA	2.34	0.41
12:Z:272:LEU:HD12	12:Z:275:LEU:HD23	2.03	0.41
16:d:108:ASN:O	16:d:111:LYS:HG2	2.21	0.41
18:f:75:LEU:HD13	18:f:86:THR:HG21	2.03	0.41
18:f:530:CYS:SG	18:f:534:VAL:HG23	2.60	0.41
18:f:649:HIS:HA	18:f:652:VAL:HG22	2.03	0.41
2:B:283:PHE:CD1	2:B:328:ILE:HG23	2.55	0.41
3:C:47:ALA:HB2	8:V:494:MET:HE1	2.02	0.41
6:F:94:ILE:HG22	6:F:95:GLU:H	1.86	0.41
6:F:164:LEU:HA	6:F:165:PRO:HD3	1.91	0.41
7:U:183:LEU:O	7:U:187:LEU:HB2	2.20	0.41
12:Z:192:THR:HA	12:Z:195:VAL:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:634:PRO:O	7:U:635:SER:C	2.64	0.41
11:Y:178:ASN:HB3	11:Y:212:GLU:HG3	2.03	0.41
13:a:18:GLN:O	13:a:19:PRO:C	2.63	0.41
14:b:33:VAL:HA	14:b:36:VAL:HG22	2.02	0.41
15:c:123:SER:HA	15:c:127:ILE:HG23	2.03	0.41
15:c:134:GLU:HA	15:c:138:GLU:N	2.36	0.41
18:f:638:ASP:C	18:f:640:LYS:H	2.28	0.41
2:B:339:PRO:HA	2:B:342:ILE:HB	2.03	0.41
6:F:338:LEU:HD21	6:F:342:LEU:HD22	2.02	0.41
7:U:368:ALA:HB2	7:U:728:PHE:CD1	2.52	0.41
7:U:917:THR:O	7:U:918:SER:C	2.64	0.41
10:X:345:VAL:HB	10:X:385:LEU:HB3	2.03	0.41
11:Y:223:THR:HA	11:Y:226:VAL:HG12	2.01	0.41
15:c:303:MET:O	15:c:307:VAL:HG23	2.21	0.41
1:A:140:VAL:HB	1:A:151:ILE:HG23	2.02	0.41
3:C:219:LEU:HD21	4:D:286:GLN:HE21	1.85	0.41
4:D:162:VAL:HB	4:D:218:ALA:HA	2.03	0.41
4:D:272:THR:O	4:D:276:ASP:HB3	2.20	0.41
4:D:354:LEU:HD11	4:D:358:VAL:HG11	2.01	0.41
7:U:126:ILE:HD12	7:U:126:ILE:HA	1.93	0.41
8:V:333:ILE:HD13	8:V:360:TYR:HB3	2.03	0.41
11:Y:111:LEU:HA	11:Y:115:GLY:HA3	2.02	0.41
12:Z:48:LEU:HD11	12:Z:92:VAL:HG11	2.03	0.41
13:a:18:GLN:HA	13:a:21:VAL:HG12	2.02	0.41
16:d:310:LEU:HD12	16:d:315:TYR:HA	2.03	0.41
18:f:376:PHE:HE2	18:f:797:LEU:HG	1.85	0.41
4:D:132:LEU:HD13	4:D:139:LEU:HA	2.02	0.41
9:W:47:LEU:HA	9:W:50:LEU:HG	2.03	0.41
11:Y:271:PHE:O	11:Y:275:LEU:HG	2.21	0.41
12:Z:85:VAL:HA	15:c:76:PRO:HG3	2.02	0.41
15:c:109:VAL:HG12	15:c:140:ALA:HB2	2.03	0.41
1:A:159:PRO:O	1:A:162:THR:HG22	2.21	0.40
1:A:299:MET:HA	1:A:302:LEU:HD12	2.03	0.40
3:C:125:LYS:HG2	4:D:96:VAL:HG21	2.02	0.40
3:C:271:ARG:O	3:C:275:GLU:HG3	2.21	0.40
7:U:539:THR:HG23	7:U:545:LEU:CD1	2.52	0.40
9:W:333:LEU:HB3	9:W:335:SER:H	1.85	0.40
10:X:407:MET:HA	10:X:410:VAL:HB	2.03	0.40
17:e:50:ASP:O	17:e:51:ASP:C	2.63	0.40
18:f:72:ARG:CZ	18:f:103:TYR:HD2	2.34	0.40
18:f:316:ASP:HA	18:f:320:ILE:HD13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLU:O	1:A:298:THR:HG23	2.21	0.40
4:D:93:LEU:HB2	4:D:102:ILE:HG22	2.02	0.40
4:D:303:VAL:HG12	4:D:305:VAL:HG23	2.03	0.40
5:E:155:ASN:HB2	5:E:158:LEU:HG	2.04	0.40
7:U:7:GLY:HA3	16:d:169:ALA:HB1	2.03	0.40
7:U:694:ILE:HG23	7:U:695:MET:HG2	2.03	0.40
10:X:407:MET:HE3	12:Z:266:ILE:CD1	2.50	0.40
15:c:124:GLY:O	15:c:127:ILE:HG12	2.21	0.40
15:c:231:LEU:HD11	15:c:302:ALA:HB2	2.03	0.40
16:d:111:LYS:HD3	16:d:154:TRP:CE2	2.56	0.40
16:d:264:LEU:HA	16:d:267:ILE:HG12	2.03	0.40
18:f:637:LYS:HD2	18:f:678:LEU:HB2	2.02	0.40
18:f:642:ALA:HB3	18:f:647:GLY:C	2.45	0.40
2:B:86:LYS:HA	2:B:87:PRO:HD3	1.88	0.40
5:E:215:ILE:HD11	5:E:256:THR:HG23	2.03	0.40
7:U:35:TRP:HB3	7:U:70:HIS:CE1	2.56	0.40
7:U:585:THR:O	7:U:589:ALA:HB2	2.21	0.40
8:V:168:GLN:HB3	8:V:191:LEU:HD22	2.02	0.40
8:V:488:ASN:O	8:V:491:VAL:HB	2.21	0.40
13:a:232:TRP:O	13:a:236:THR:CB	2.67	0.40
1:A:125:LEU:HD13	1:A:134:ILE:HG21	2.03	0.40
5:E:234:GLU:O	5:E:238:ILE:HG12	2.21	0.40
8:V:98:LEU:HD23	8:V:98:LEU:HA	1.95	0.40
8:V:157:THR:N	8:V:158:PRO:CD	2.85	0.40
11:Y:189:VAL:C	11:Y:290:PRO:HG3	2.46	0.40
15:c:186:LYS:HA	15:c:187:PRO:HD3	1.97	0.40
18:f:45:LEU:HG	18:f:50:LYS:HD2	2.02	0.40
18:f:395:GLY:HA2	18:f:398:TRP:HB3	2.02	0.40
18:f:868:HIS:O	18:f:869:THR:C	2.64	0.40
2:B:259:TYR:CE1	4:D:275:PHE:HD1	2.39	0.40
7:U:457:ILE:HD12	7:U:457:ILE:HA	1.89	0.40
9:W:54:THR:O	9:W:59:ASP:N	2.50	0.40
11:Y:97:GLU:HA	11:Y:130:LYS:O	2.22	0.40
11:Y:110:TYR:HD1	11:Y:114:ILE:HD12	1.86	0.40
11:Y:113:ARG:HG3	11:Y:114:ILE:HG13	2.03	0.40
12:Z:37:GLY:HA3	12:Z:95:TYR:CE1	2.56	0.40
18:f:182:GLU:O	18:f:183:PRO:C	2.64	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	399/433 (92%)	356 (89%)	43 (11%)	0	100	100
2	B	383/440 (87%)	327 (85%)	56 (15%)	0	100	100
3	C	377/406 (93%)	345 (92%)	32 (8%)	0	100	100
4	D	370/418 (88%)	338 (91%)	32 (9%)	0	100	100
5	E	383/389 (98%)	339 (88%)	44 (12%)	0	100	100
6	F	356/439 (81%)	315 (88%)	41 (12%)	0	100	100
7	U	800/953 (84%)	732 (92%)	68 (8%)	0	100	100
8	V	442/534 (83%)	419 (95%)	23 (5%)	0	100	100
9	W	435/456 (95%)	402 (92%)	33 (8%)	0	100	100
10	X	103/422 (24%)	93 (90%)	10 (10%)	0	100	100
11	Y	375/389 (96%)	340 (91%)	35 (9%)	0	100	100
12	Z	272/324 (84%)	240 (88%)	32 (12%)	0	100	100
13	a	371/376 (99%)	335 (90%)	36 (10%)	0	100	100
14	b	189/377 (50%)	171 (90%)	18 (10%)	0	100	100
15	c	285/310 (92%)	253 (89%)	32 (11%)	0	100	100
16	d	255/350 (73%)	223 (88%)	32 (12%)	0	100	100
17	e	47/70 (67%)	39 (83%)	8 (17%)	0	100	100
18	f	883/908 (97%)	733 (83%)	150 (17%)	0	100	100
19	g	130/289 (45%)	123 (95%)	7 (5%)	0	100	100
All	All	6855/8283 (83%)	6123 (89%)	732 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	346/372 (93%)	335 (97%)	11 (3%)	34	55
2	B	341/385 (89%)	336 (98%)	5 (2%)	57	70
3	C	330/352 (94%)	328 (99%)	2 (1%)	78	80
4	D	325/366 (89%)	322 (99%)	3 (1%)	70	76
5	E	338/341 (99%)	332 (98%)	6 (2%)	51	66
6	F	308/379 (81%)	305 (99%)	3 (1%)	68	75
7	U	688/816 (84%)	673 (98%)	15 (2%)	45	64
8	V	390/460 (85%)	385 (99%)	5 (1%)	61	71
9	W	402/416 (97%)	398 (99%)	4 (1%)	68	75
10	X	97/362 (27%)	97 (100%)	0	100	100
11	Y	333/344 (97%)	329 (99%)	4 (1%)	63	73
12	Z	248/295 (84%)	246 (99%)	2 (1%)	73	77
13	a	333/336 (99%)	324 (97%)	9 (3%)	39	60
14	b	167/312 (54%)	161 (96%)	6 (4%)	31	52
15	c	252/268 (94%)	243 (96%)	9 (4%)	31	52
16	d	231/294 (79%)	226 (98%)	5 (2%)	45	64
17	e	43/63 (68%)	43 (100%)	0	100	100
18	f	741/763 (97%)	733 (99%)	8 (1%)	65	73
19	g	122/253 (48%)	122 (100%)	0	100	100
All	All	6035/7177 (84%)	5938 (98%)	97 (2%)	54	69

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TRP
1	A	125	LEU
1	A	144	ARG
1	A	162	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	HIS
1	A	248	LYS
1	A	286	ASP
1	A	292	ASP
1	A	293	ASN
1	A	294	GLU
1	A	295	VAL
2	B	49	LEU
2	B	246	THR
2	B	281	ILE
2	B	315	GLN
2	B	390	LEU
3	C	134	LEU
3	C	214	VAL
4	D	115	ILE
4	D	116	LEU
4	D	196	ILE
5	E	154	THR
5	E	199	VAL
5	E	210	GLU
5	E	291	ARG
5	E	322	LYS
5	E	326	ILE
6	F	215	LEU
6	F	317	LEU
6	F	326	VAL
7	U	70	HIS
7	U	173	VAL
7	U	213	PHE
7	U	215	ASN
7	U	216	VAL
7	U	219	CYS
7	U	220	LEU
7	U	221	ILE
7	U	225	ASP
7	U	338	HIS
7	U	416	GLU
7	U	544	ILE
7	U	548	LEU
7	U	633	CYS
7	U	781	LEU
8	V	139	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	157	THR
8	V	159	LEU
8	V	160	LEU
8	V	212	TYR
9	W	51	GLU
9	W	138	VAL
9	W	171	VAL
9	W	235	GLN
11	Y	92	GLU
11	Y	168	ILE
11	Y	253	LEU
11	Y	387	ILE
12	Z	39	LEU
12	Z	144	VAL
13	a	32	LYS
13	a	42	LEU
13	a	88	THR
13	a	190	VAL
13	a	244	ASN
13	a	253	THR
13	a	255	TRP
13	a	258	GLN
13	a	302	ILE
14	b	2	VAL
14	b	16	MET
14	b	18	ASN
14	b	25	ARG
14	b	47	ASN
14	b	59	GLU
15	c	49	VAL
15	c	108	VAL
15	c	109	VAL
15	c	113	HIS
15	c	115	HIS
15	c	231	LEU
15	c	265	MET
15	c	272	ILE
15	c	279	ASP
16	d	215	LEU
16	d	222	THR
16	d	226	ILE
16	d	276	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	d	308	TRP
18	f	51	GLN
18	f	390	LEU
18	f	391	LEU
18	f	408	LEU
18	f	640	LYS
18	f	649	HIS
18	f	655	LEU
18	f	866	GLN

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

Mol	Chain	Res	Type
1	A	293	ASN
2	B	55	HIS
2	B	131	HIS
2	B	241	ASN
2	B	242	GLN
2	B	277	HIS
2	B	368	HIS
3	C	157	GLN
3	C	279	GLN
4	D	49	GLN
4	D	57	GLN
4	D	173	GLN
4	D	278	GLN
4	D	286	GLN
5	E	86	GLN
5	E	141	GLN
5	E	194	ASN
5	E	220	ASN
6	F	214	ASN
6	F	315	ASN
6	F	316	GLN
6	F	392	ASN
7	U	18	GLN
7	U	70	HIS
7	U	91	ASN
7	U	107	HIS
7	U	111	GLN
7	U	139	GLN
7	U	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	345	ASN
7	U	453	HIS
7	U	464	GLN
7	U	632	GLN
7	U	645	ASN
7	U	874	ASN
7	U	888	GLN
8	V	78	HIS
8	V	110	HIS
8	V	283	ASN
8	V	347	GLN
8	V	350	GLN
8	V	401	ASN
8	V	487	HIS
9	W	107	GLN
9	W	414	ASN
11	Y	136	HIS
11	Y	178	ASN
11	Y	363	ASN
11	Y	367	GLN
11	Y	381	GLN
11	Y	388	ASN
12	Z	109	ASN
12	Z	193	ASN
12	Z	224	HIS
13	a	18	GLN
13	a	193	GLN
13	a	219	HIS
14	b	18	ASN
14	b	29	GLN
14	b	142	ASN
15	c	30	GLN
15	c	44	HIS
15	c	149	GLN
15	c	206	ASN
15	c	269	GLN
15	c	274	ASN
15	c	287	HIS
16	d	103	ASN
16	d	195	ASN
16	d	223	ASN
17	e	37	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	f	14	GLN
18	f	171	GLN
18	f	180	GLN
18	f	531	ASN
18	f	705	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	AGS	F	501	-	32,33,33	0.68	1 (3%)	45,52,52	0.57	0
20	ADP	C	501	-	28,29,29	1.47	5 (17%)	43,45,45	1.87	7 (16%)
20	ADP	A	501	-	28,29,29	1.37	4 (14%)	43,45,45	1.91	9 (20%)
21	AGS	D	501	22	32,33,33	0.67	1 (3%)	45,52,52	0.55	0
21	AGS	E	501	22	32,33,33	0.67	1 (3%)	45,52,52	0.50	0
20	ADP	B	501	-	28,29,29	1.32	3 (10%)	43,45,45	2.08	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	AGS	F	501	-	-	8/21/38/38	0/3/3/3
20	ADP	C	501	-	-	5/16/32/32	0/3/3/3
20	ADP	A	501	-	-	0/16/32/32	0/3/3/3
21	AGS	D	501	22	-	8/21/38/38	0/3/3/3
21	AGS	E	501	22	-	0/21/38/38	0/3/3/3
20	ADP	B	501	-	-	5/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	501	ADP	C5-C4	4.79	1.47	1.39
20	A	501	ADP	C5-C4	4.52	1.47	1.39
20	B	501	ADP	C5-C4	4.40	1.46	1.39
20	C	501	ADP	C5-C6	2.72	1.48	1.41
20	A	501	ADP	C5-N7	-2.66	1.34	1.39
20	B	501	ADP	C5-N7	-2.64	1.34	1.39
20	C	501	ADP	C5-N7	-2.53	1.34	1.39
20	C	501	ADP	PA-O3A	2.48	1.62	1.59
20	B	501	ADP	C5-C6	2.38	1.47	1.41
20	A	501	ADP	C5-C6	2.23	1.47	1.41
20	C	501	ADP	C8-N7	2.21	1.35	1.31
21	F	501	AGS	PG-S1G	2.17	1.95	1.90
21	E	501	AGS	PG-S1G	2.13	1.95	1.90
21	D	501	AGS	PG-S1G	2.13	1.95	1.90
20	A	501	ADP	C8-N9	-2.04	1.34	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	501	ADP	C5-C4-N3	-6.50	117.77	126.72
20	C	501	ADP	C5-C4-N3	-6.48	117.79	126.72
20	A	501	ADP	C5-C4-N3	-6.29	118.06	126.72
20	B	501	ADP	N3-C4-N9	5.80	137.04	127.17
20	A	501	ADP	N3-C4-N9	5.65	136.78	127.17
20	C	501	ADP	N3-C4-N9	4.93	135.56	127.17
20	B	501	ADP	C2-N3-C4	4.00	121.61	111.83
20	C	501	ADP	C2-N3-C4	3.82	121.17	111.83
20	A	501	ADP	C2-N3-C4	3.78	121.06	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	501	ADP	C4-C5-N7	-3.73	106.31	110.58
20	B	501	ADP	N3-C2-N1	-3.51	123.27	128.58
20	B	501	ADP	C3'-C2'-C1'	3.29	107.68	101.46
20	A	501	ADP	N3-C2-N1	-3.22	123.71	128.58
20	B	501	ADP	C4-N9-C8	3.15	109.05	105.74
20	B	501	ADP	C2'-C1'-N9	-3.11	105.58	113.30
20	C	501	ADP	N3-C2-N1	-2.82	124.32	128.58
20	C	501	ADP	C3'-C2'-C1'	2.77	106.70	101.46
20	B	501	ADP	C4-C5-N7	-2.71	107.49	110.58
20	C	501	ADP	C5-N7-C8	2.63	107.58	103.45
20	A	501	ADP	C4-N9-C8	2.63	108.50	105.74
20	A	501	ADP	C3'-C2'-C1'	2.53	106.26	101.46
20	B	501	ADP	C5-N7-C8	2.52	107.41	103.45
20	A	501	ADP	C4-C5-N7	-2.41	107.83	110.58
20	A	501	ADP	N6-C6-N1	2.30	123.50	118.38
20	B	501	ADP	N9-C8-N7	-2.17	110.85	113.94
20	A	501	ADP	C5-C6-N6	-2.07	118.16	123.29

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	B	501	ADP	C5'-O5'-PA-O1A
20	B	501	ADP	C5'-O5'-PA-O2A
20	B	501	ADP	C5'-O5'-PA-O3A
20	C	501	ADP	C5'-O5'-PA-O1A
20	C	501	ADP	C5'-O5'-PA-O2A
21	D	501	AGS	C5'-O5'-PA-O1A
21	D	501	AGS	C5'-O5'-PA-O3A
21	D	501	AGS	C4'-C5'-O5'-PA
21	F	501	AGS	C5'-O5'-PA-O1A
21	F	501	AGS	C5'-O5'-PA-O2A
21	F	501	AGS	C5'-O5'-PA-O3A
21	F	501	AGS	O4'-C4'-C5'-O5'
21	D	501	AGS	C3'-C4'-C5'-O5'
21	F	501	AGS	C3'-C4'-C5'-O5'
21	D	501	AGS	O4'-C4'-C5'-O5'
20	B	501	ADP	O4'-C4'-C5'-O5'
20	B	501	ADP	C3'-C4'-C5'-O5'
21	D	501	AGS	O4'-C1'-N9-C4
21	D	501	AGS	O4'-C1'-N9-C8
20	C	501	ADP	PB-O3A-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	C	501	ADP	C5'-O5'-PA-O3A
21	F	501	AGS	C4'-C5'-O5'-PA
20	C	501	ADP	PB-O3A-PA-O2A
21	F	501	AGS	C2'-C1'-N9-C8
21	F	501	AGS	C2'-C1'-N9-C4
21	D	501	AGS	C2'-C1'-N9-C8

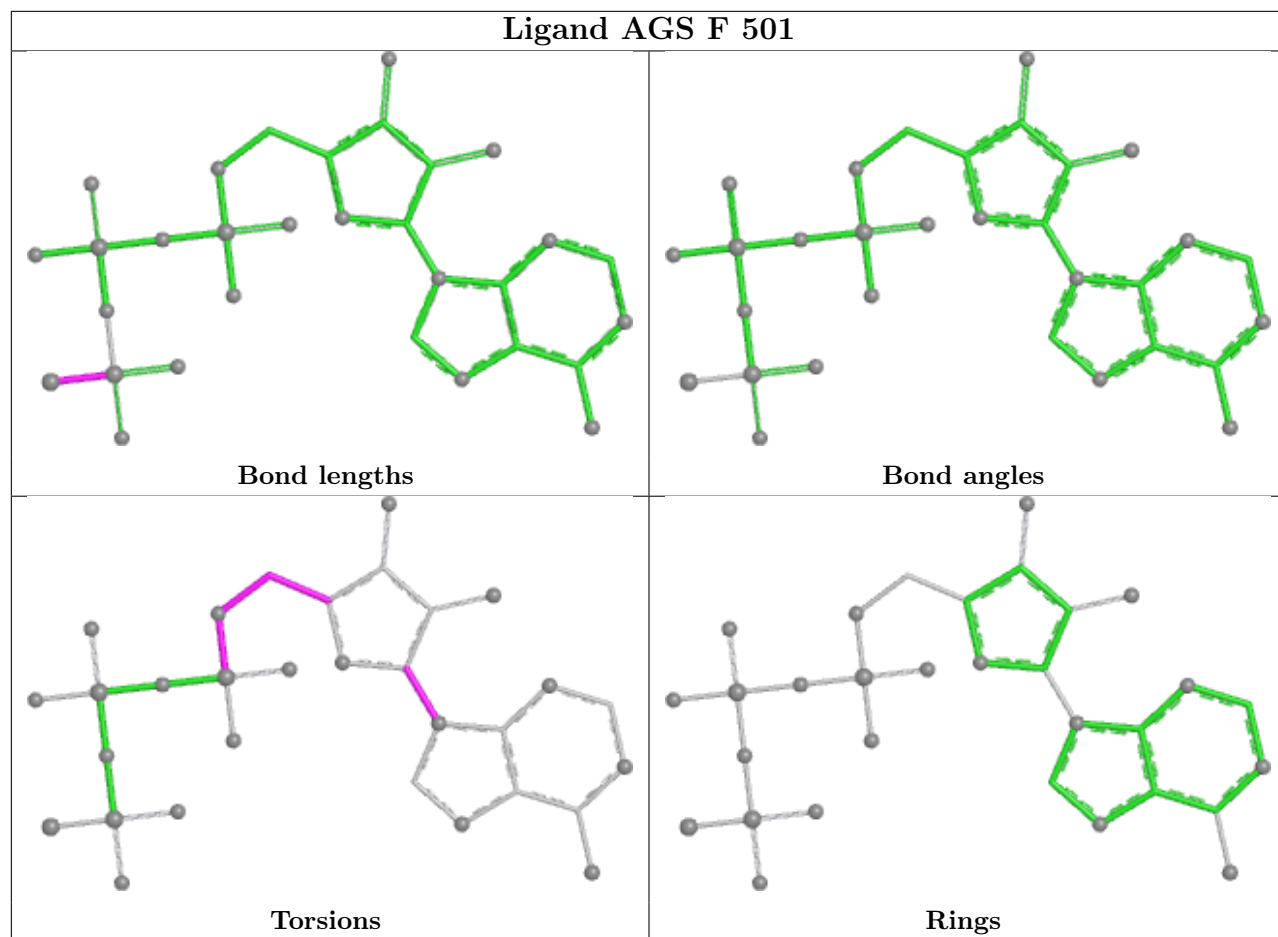
There are no ring outliers.

6 monomers are involved in 7 short contacts:

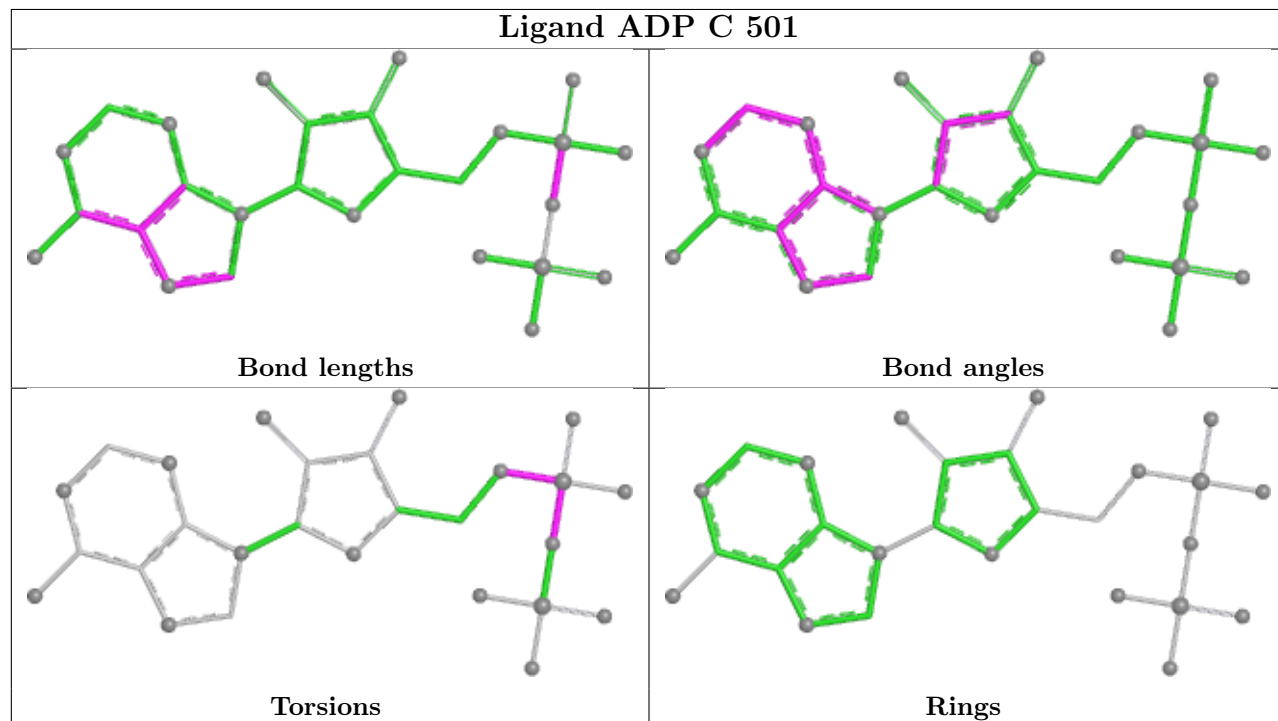
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	501	AGS	2	0
20	C	501	ADP	1	0
20	A	501	ADP	1	0
21	D	501	AGS	1	0
21	E	501	AGS	1	0
20	B	501	ADP	1	0

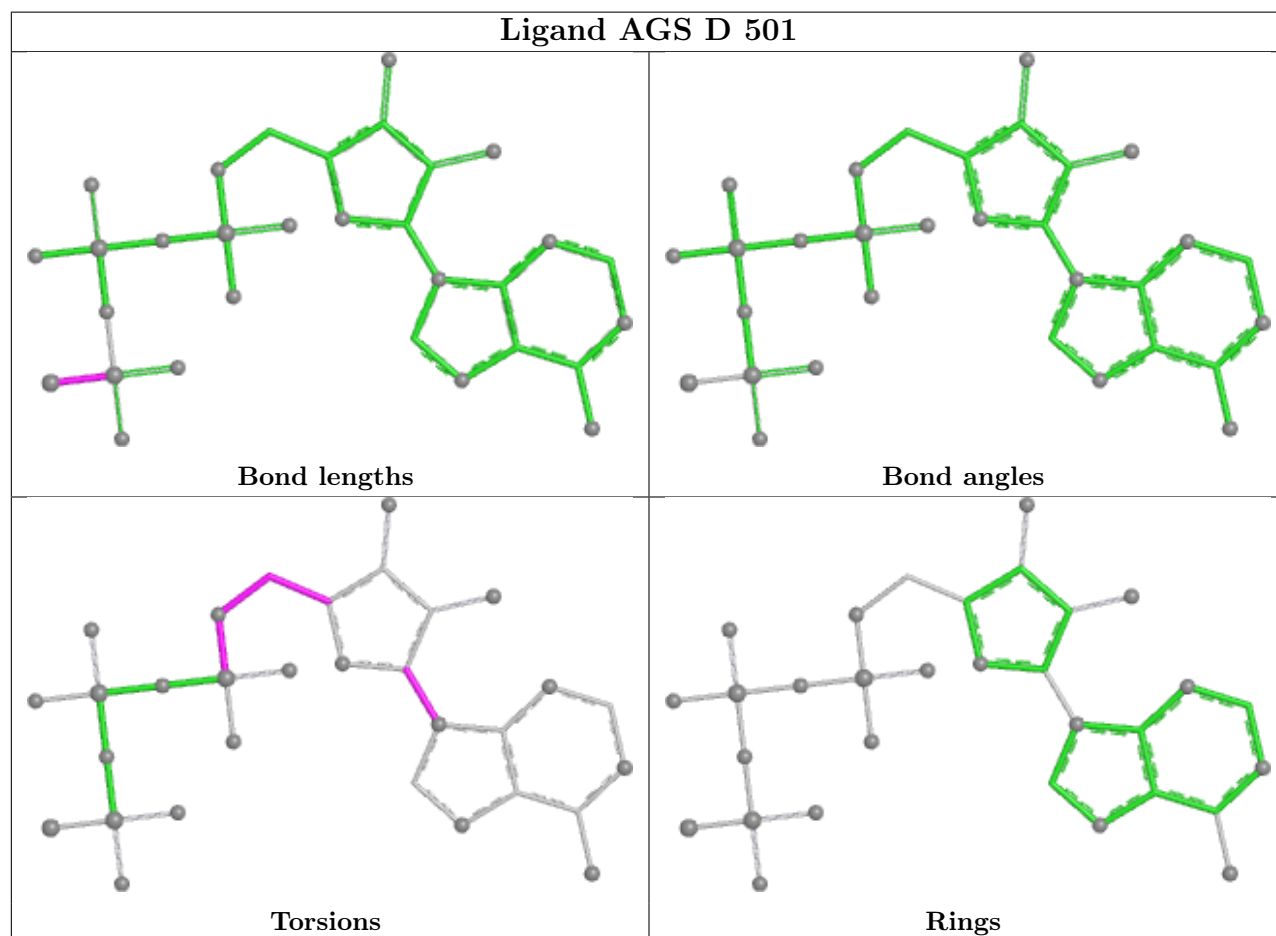
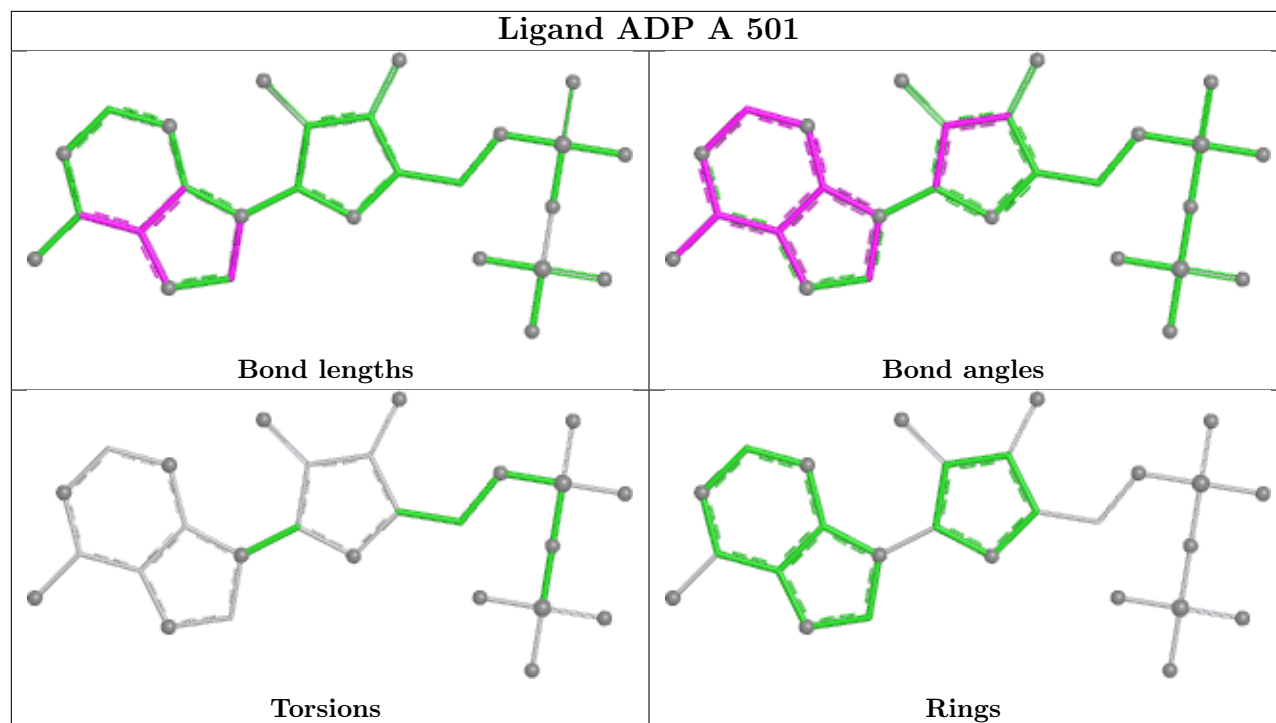
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand AGS F 501

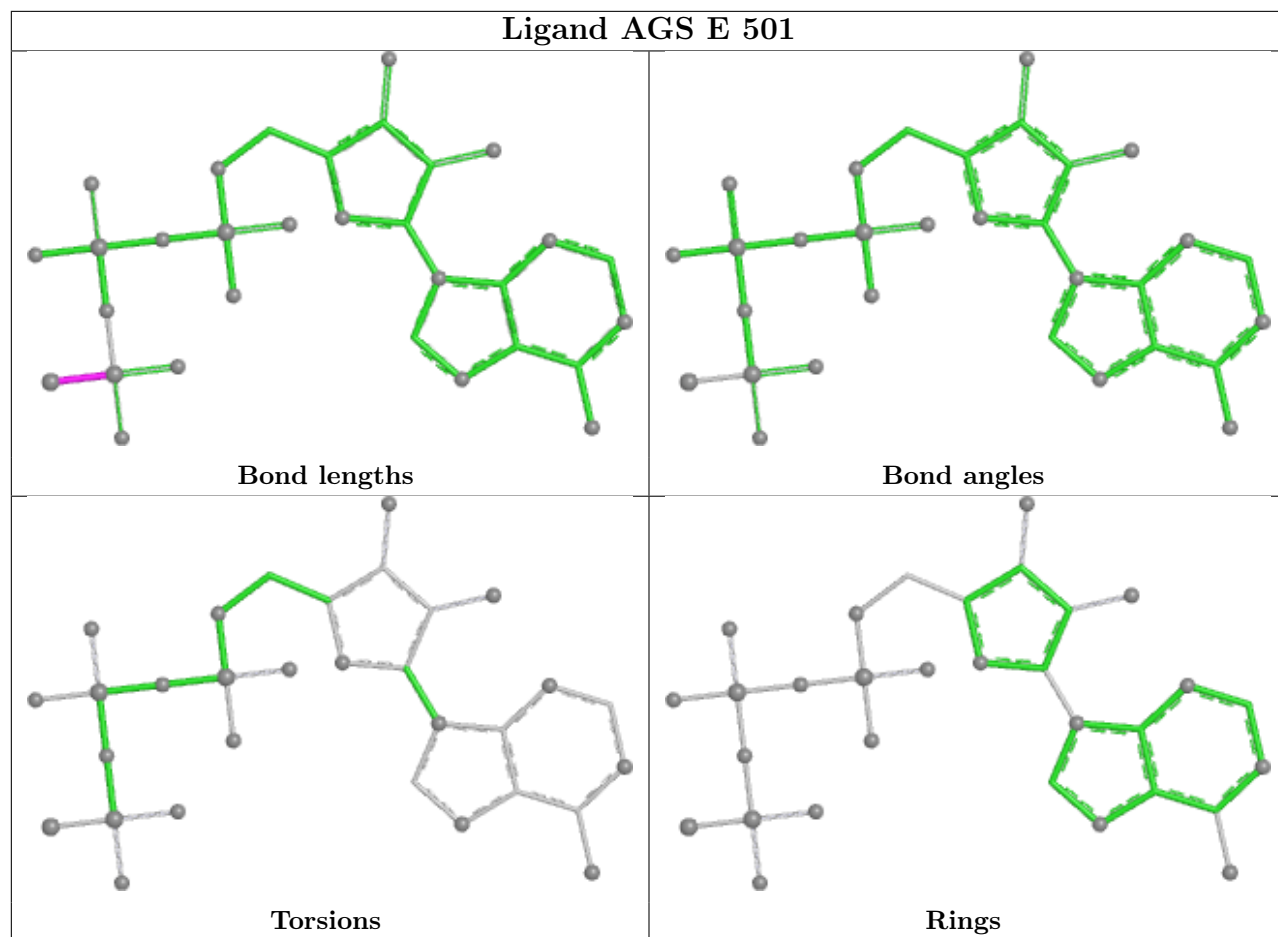


Ligand ADP C 501

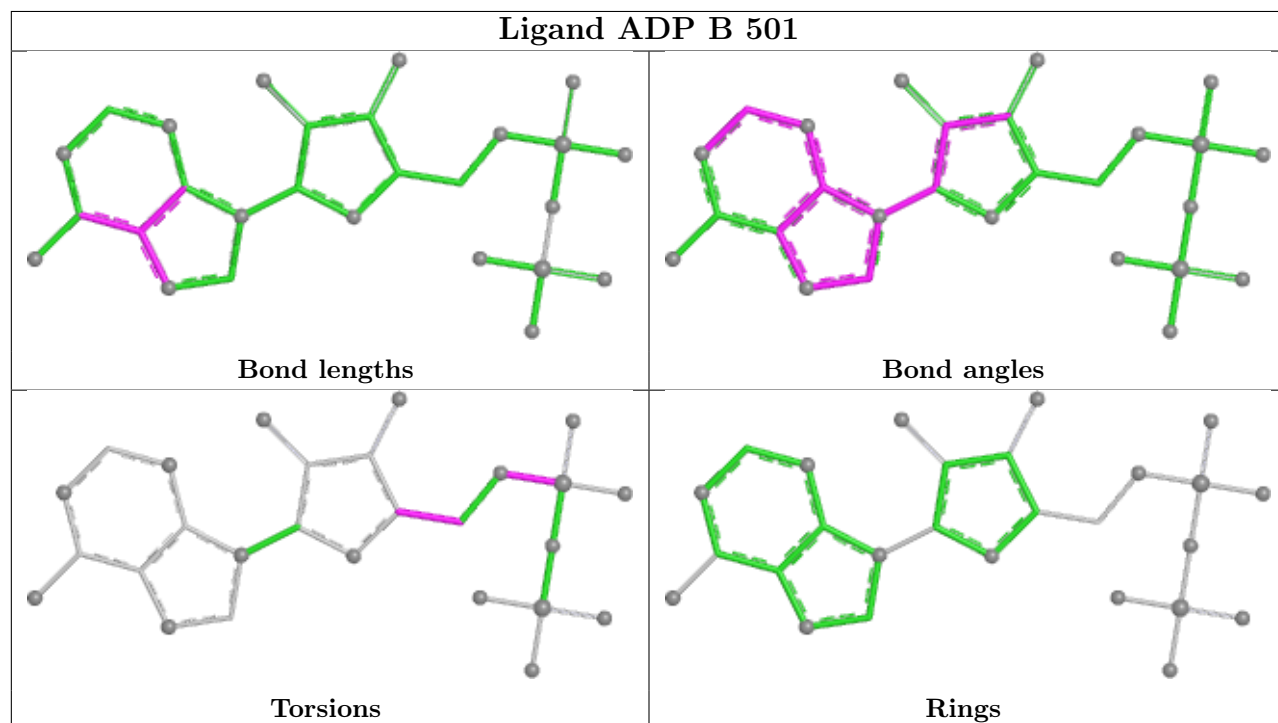




Ligand AGS E 501



Ligand ADP B 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

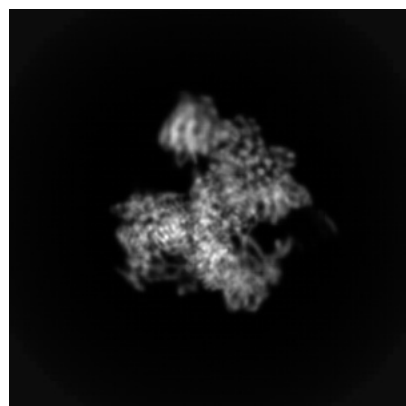
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71737. These allow visual inspection of the internal detail of the map and identification of artifacts.

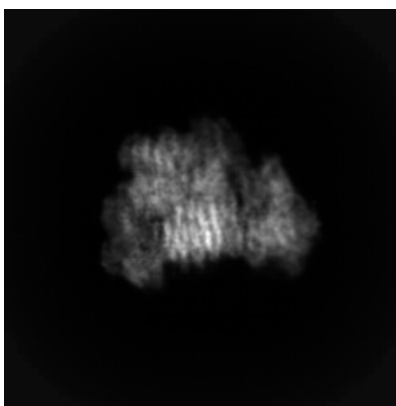
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

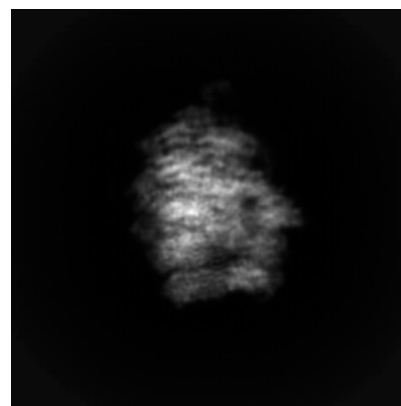
6.1.1 Primary map



X

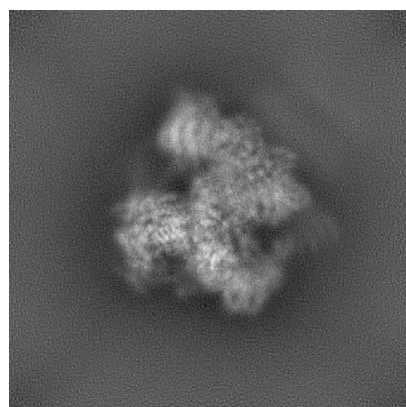


Y

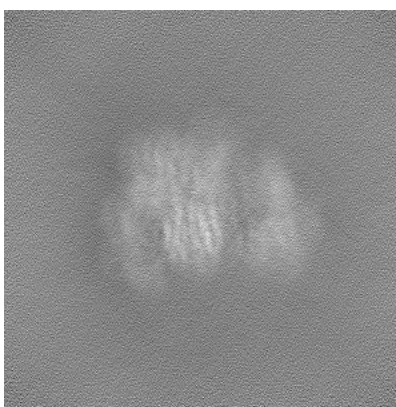


Z

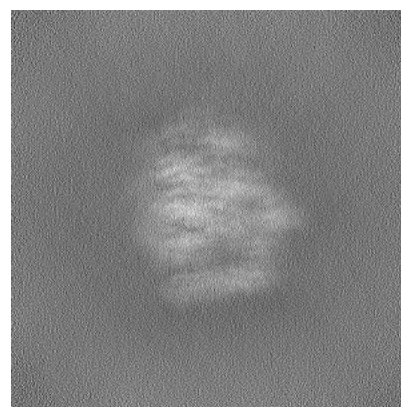
6.1.2 Raw map



X



Y



Z

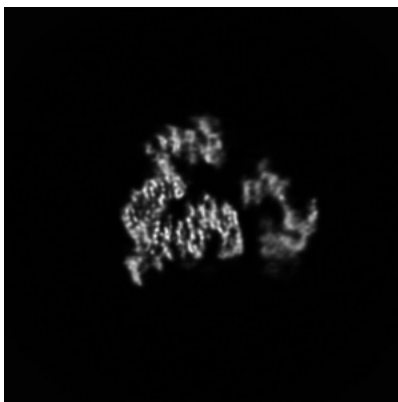
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 216

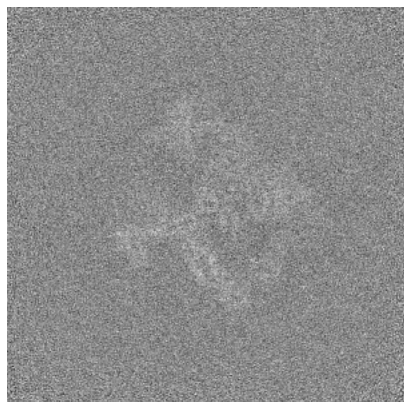


Y Index: 216

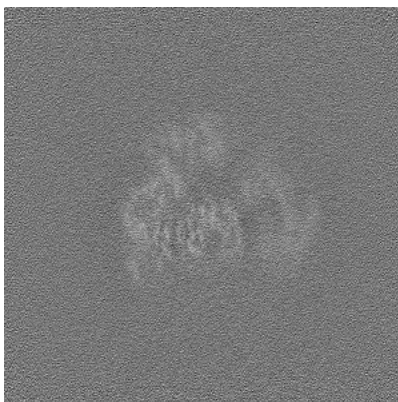


Z Index: 216

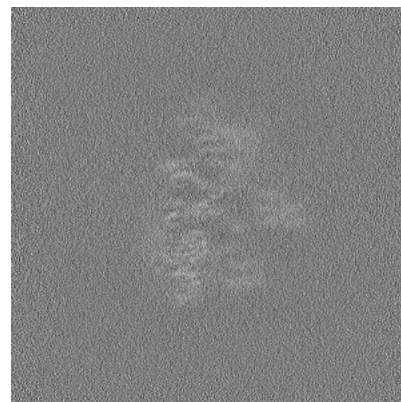
6.2.2 Raw map



X Index: 216



Y Index: 216

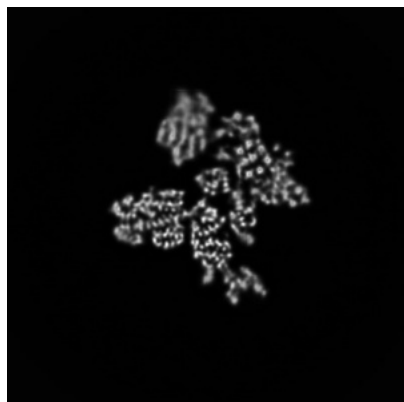


Z Index: 216

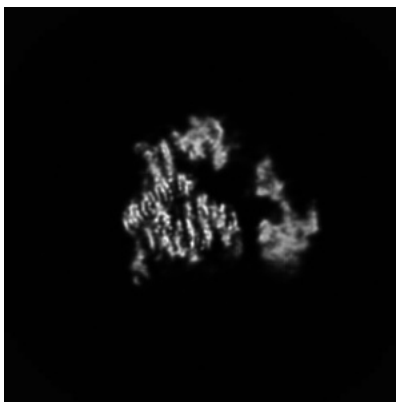
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

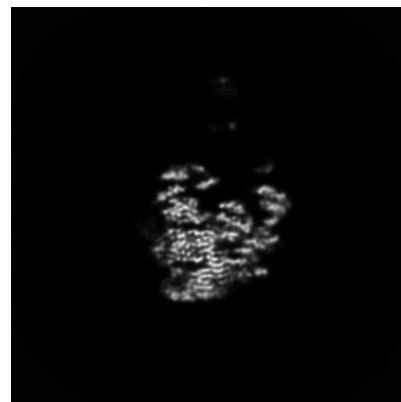
6.3.1 Primary map



X Index: 189

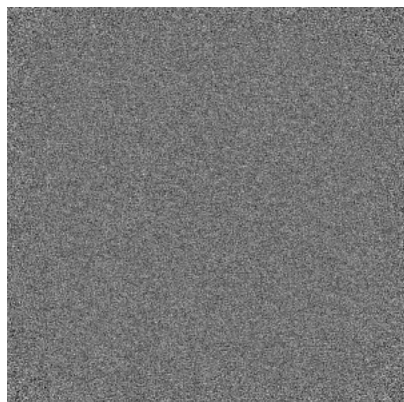


Y Index: 211

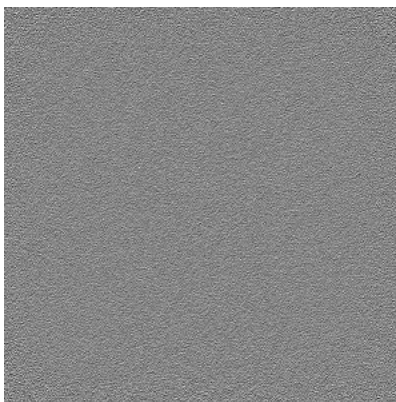


Z Index: 188

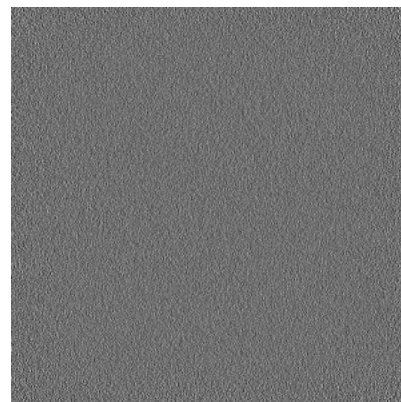
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

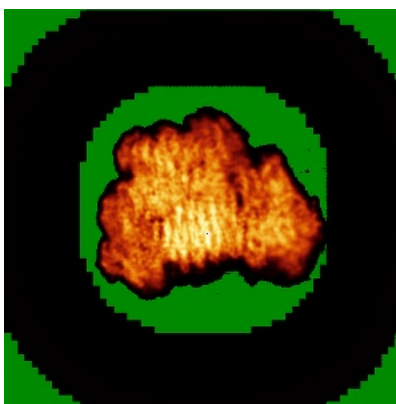
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

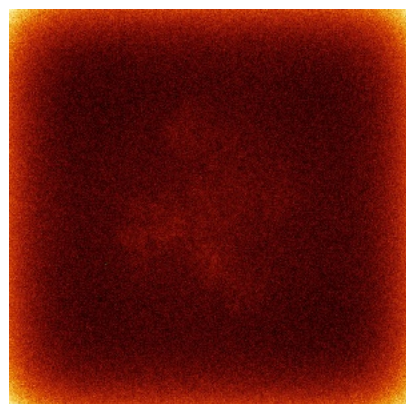


Y

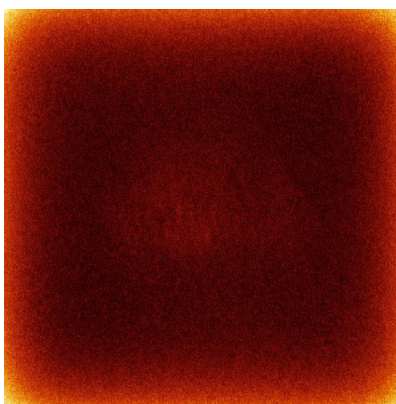


Z

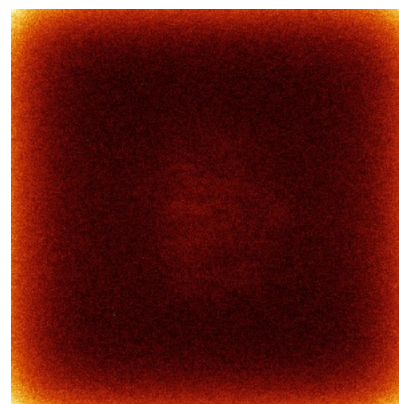
6.4.2 Raw map



X



Y

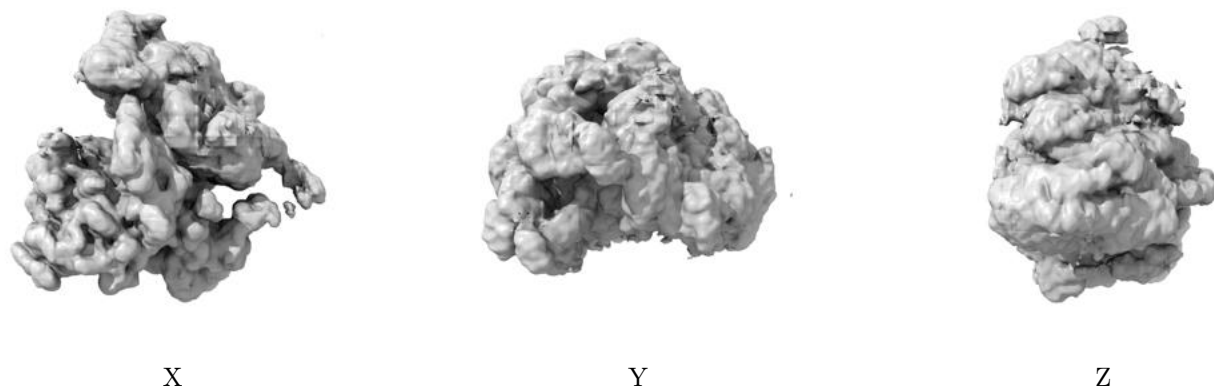


Z

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.

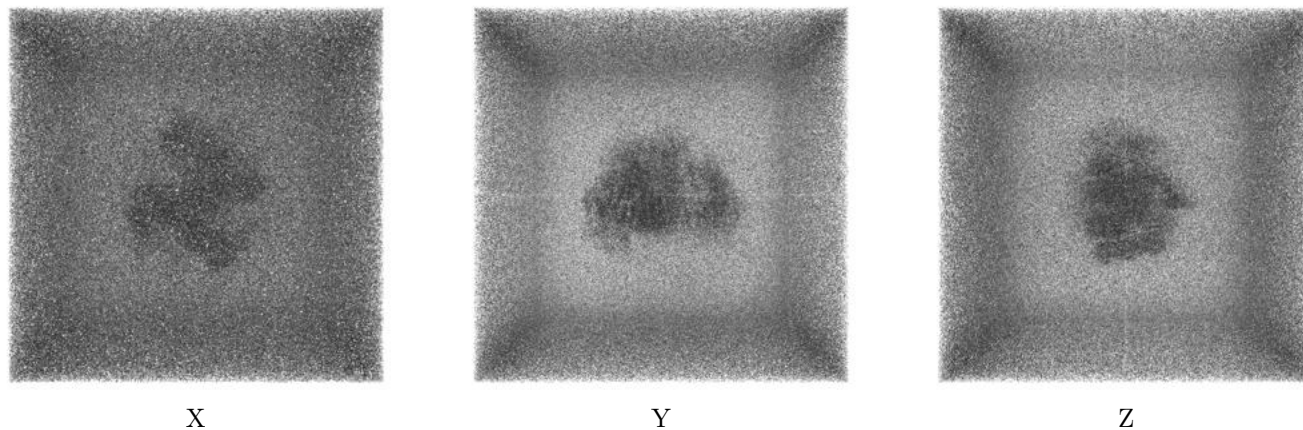
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

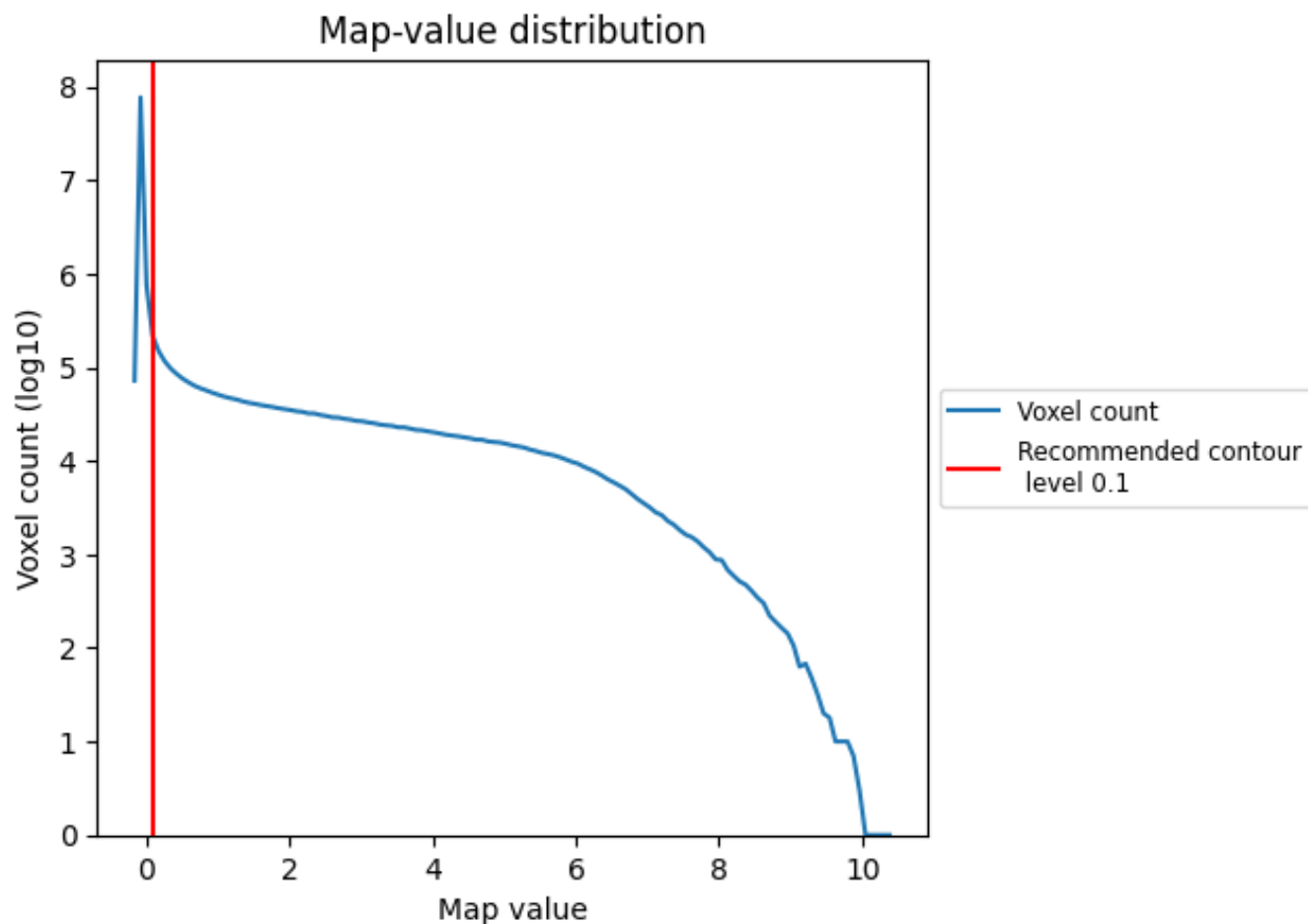
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

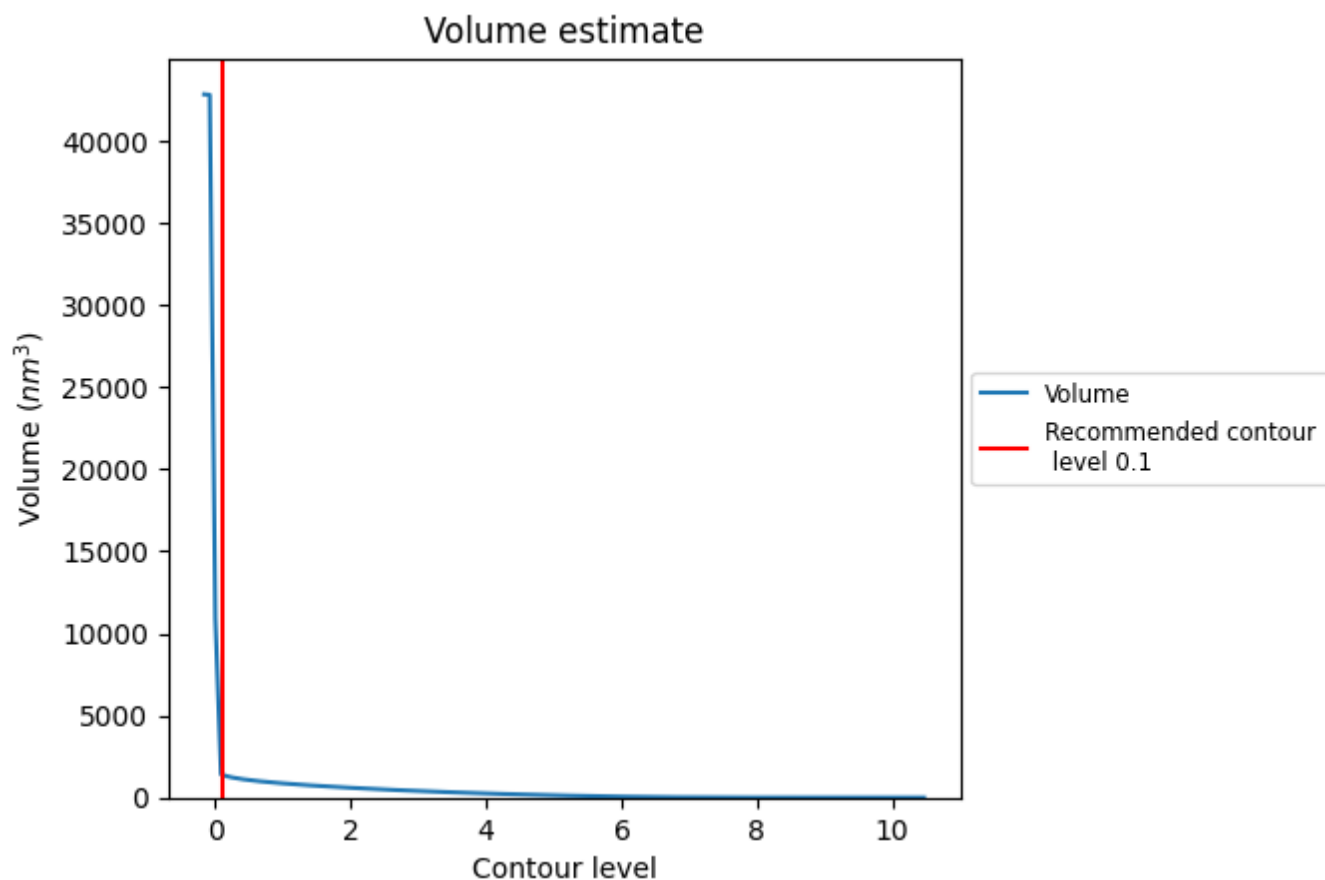
This section contains the results of statistical analysis of the map.

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.

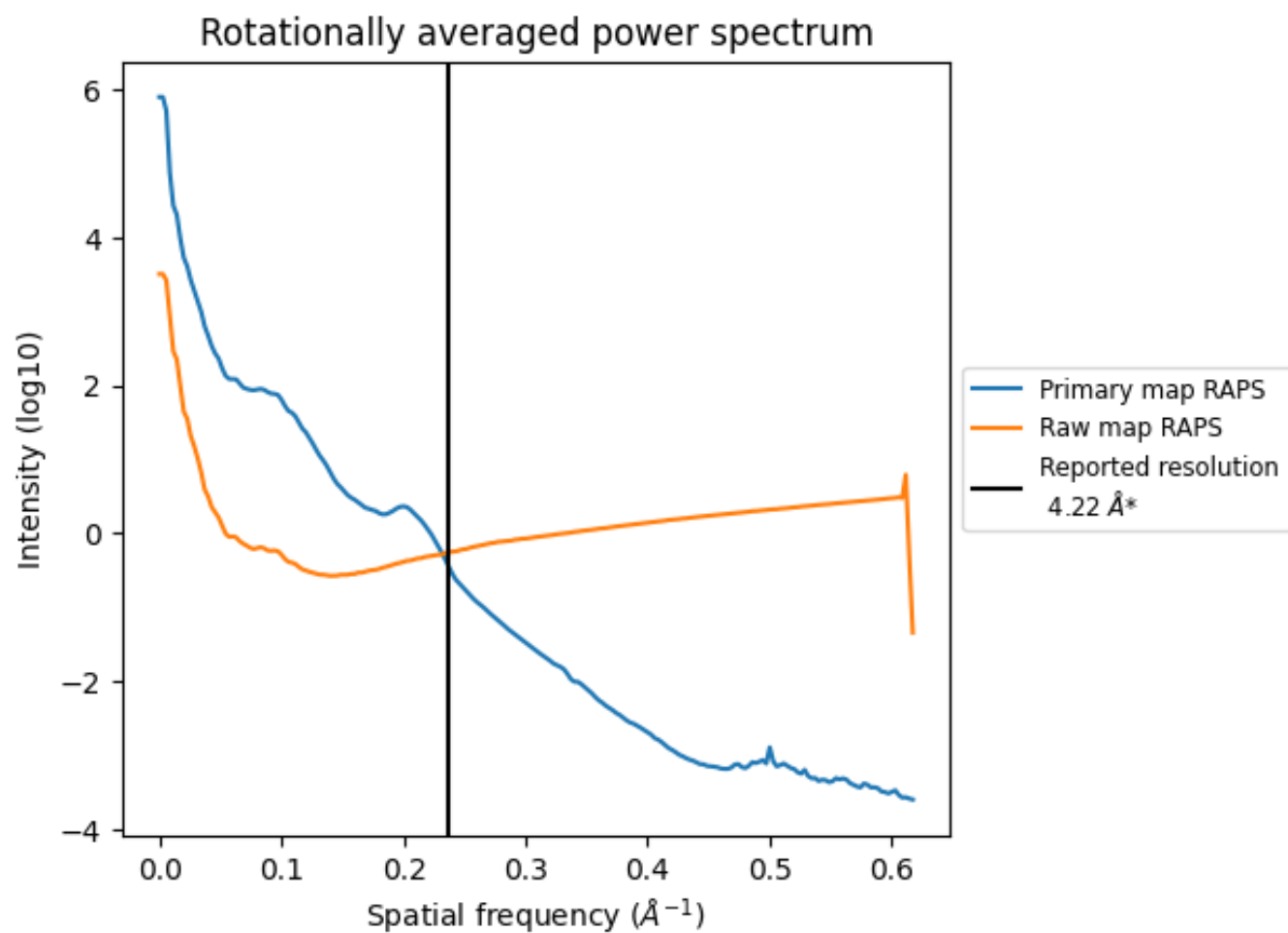
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1397 nm^3 ; this corresponds to an approximate mass of 1262 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

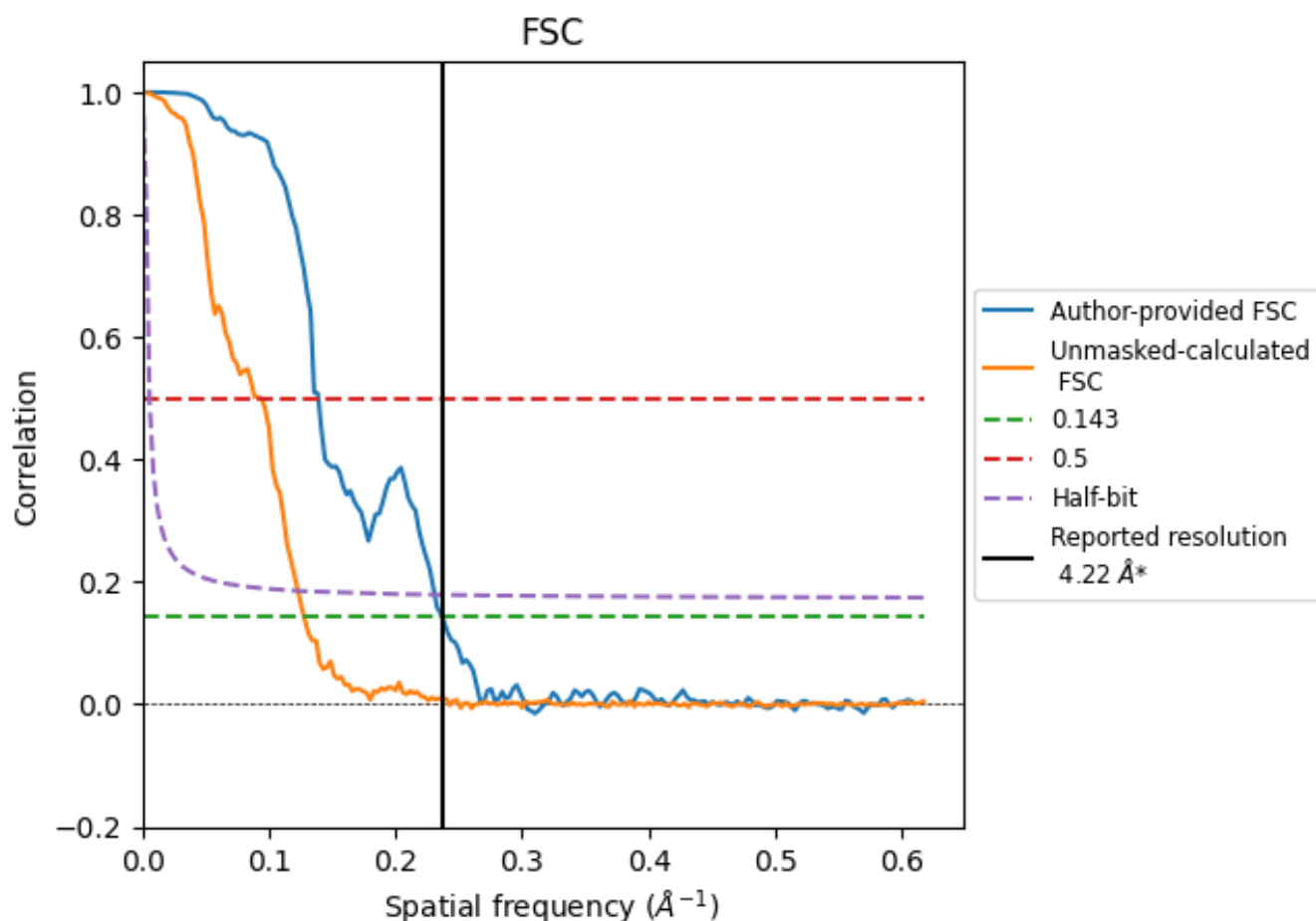


*Reported resolution corresponds to spatial frequency of 0.237 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.237 Å⁻¹

8.2 Resolution estimates [i](#)

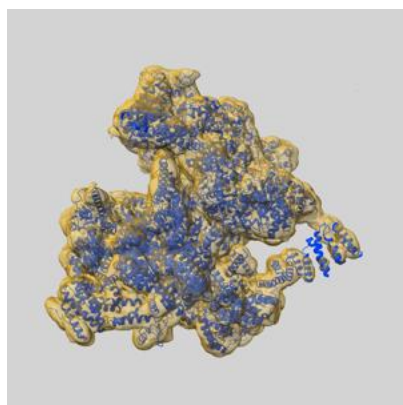
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.22	-	-
Author-provided FSC curve	4.22	7.19	4.33
Unmasked-calculated*	7.83	10.66	8.14

*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 7.83 differs from the reported value 4.22 by more than 10 %

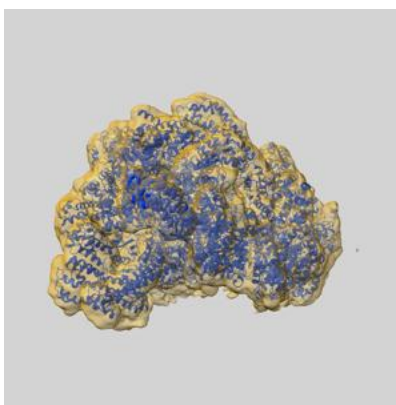
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71737 and PDB model 9PMJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

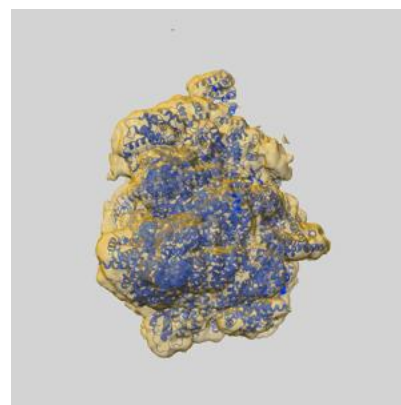
9.1 Map-model overlay [i](#)



X



Y



Z

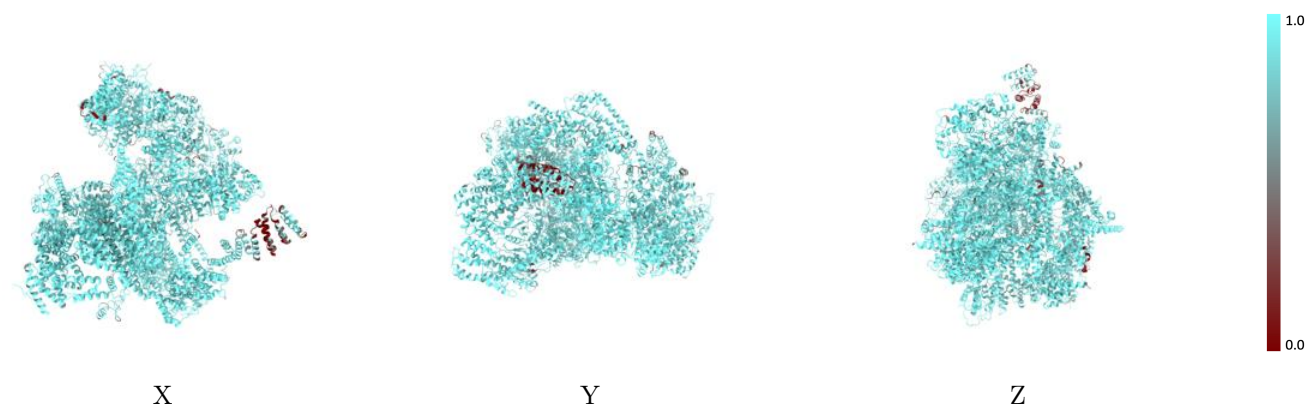
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



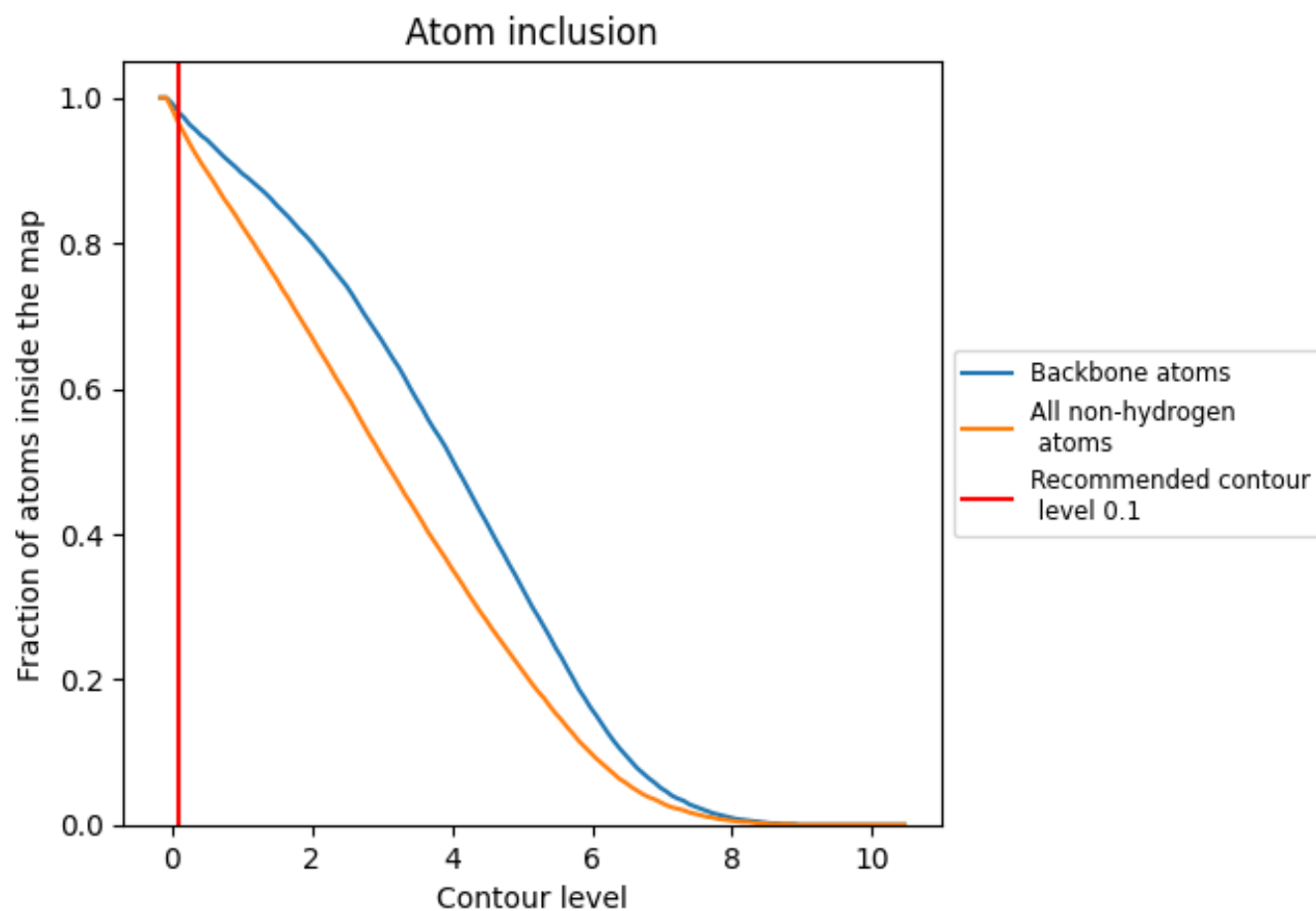
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.1310
A	 0.9770	 0.1440
B	 0.9680	 0.1220
C	 0.9590	 0.1220
D	 0.9950	 0.1360
E	 0.9850	 0.1390
F	 0.9870	 0.1600
U	 0.9920	 0.1740
V	 0.9820	 0.1370
W	 0.7990	 0.1020
X	 0.9770	 0.1390
Y	 0.9810	 0.1180
Z	 0.9970	 0.2200
a	 0.9850	 0.1410
b	 0.9690	 0.1340
c	 0.9840	 0.1870
d	 0.9600	 0.0950
e	 0.8880	 0.0960
f	 0.9610	 0.0630
g	 0.8280	 0.0480

