Full wwPDB EM Validation Report (i)

Aug 8, 2026 – 01:25 PM EDT

PDB ID	:	9PMQ / pdb_00009pmq
EMDB ID	:	EMD-71741
Title	:	Human 26S proteasome bound to TXNL1 with closed gate of core particle
Authors	:	Chen, X.; Negi, H.; Walters, K.J.
Deposited on	:	2025-07-18
Resolution	:	4.00 Å(reported)
Based on initial models	:	1WWY, 7WSI

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 (i) 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 (i)) were used in the production of this report:

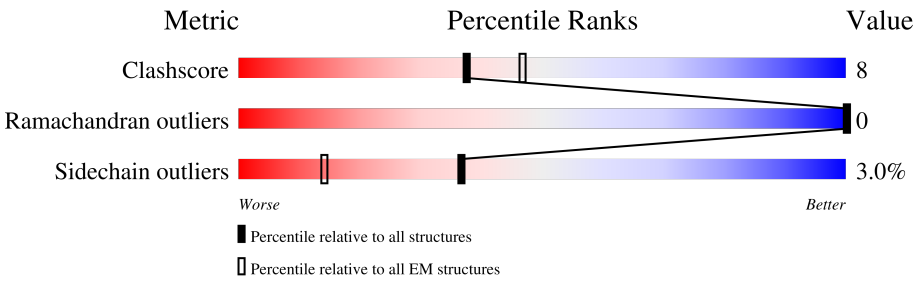
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

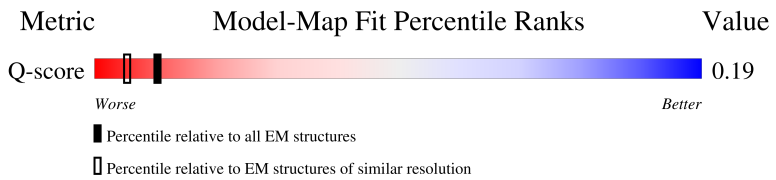
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	A	433	7%, 79%, 15%, • 5%
2	B	440	5%, 65%, 18%, •, 15%
3	C	398	•, 70%, 23%, •, •
4	D	418	•, 69%, 20%, •, 9%

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Mol	Chain	Length	Quality of chain
5	E	403	79% 18%
6	F	439	5% 72% 18% 10%
7	G	246	32% 87% 11%
8	H	234	17% 90% 9%
9	I	261	17% 83% 13%
10	J	248	25% 79% 15%
11	K	241	23% 81% 15%
12	L	269	13% 78% 10% 12%
13	M	255	21% 83% 11% 6%
14	U	953	71% 17% 10%
15	V	534	71% 12% 17%
16	W	456	25% 81% 15%
17	X	422	6% 20% 9% 70%
18	Y	389	74% 22%
19	Z	324	63% 24% 12%
20	a	376	77% 20%
21	b	377	38% 11% 49%
22	c	310	61% 27% 5% 7%
23	d	350	61% 13% 27%
24	e	70	63% 9% 29%
25	f	908	22% 82% 16%
26	g	289	7% 45% 13% 40%

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 69506 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
			Total	C	N	O	S		
1	A	412	3237	2038	569	612	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	375	2960	1861	504	580	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	381	2988	1876	536	559	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3039	1923	524	579	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	389	3097	1947	552	581	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	397	3112	1960	535	599	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	244	1903	1206	320	364	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	232	1813	1158	307	342	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	250	1971	1245	339	377	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	239	1887	1183	334	365	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	233	1778	1116	294	357	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	238	1873	1172	337	353	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	239	1874	1189	320	354	11	0	0

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	U	853	6671	4235	1133	1259	44	0	0

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	V	442	3594	2287	643	651	13	0	0

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	W	446	3635	2302	622	687	24	0	0

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	X	125	1007	643	167	195	2	0	0

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Y	378	3115	1987	533	578	17	0	0

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	286	2281	1457	392	427	5	0	0

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	a	372	2987	1907	509	556	15	0	0

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 24 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	e	50	425	260	65	100	0	0

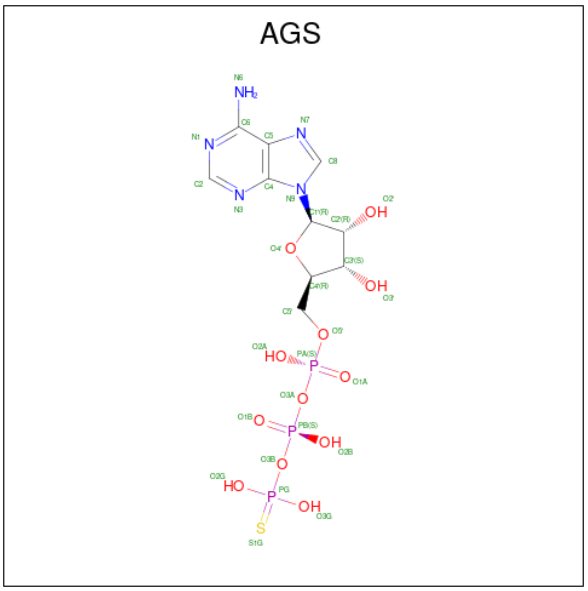
- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	f	889	6866	4315	1174	1331	46	0	0

- Molecule 26 is a protein called Thioredoxin-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	g	172	1376	865	226	276	9	0	0

- Molecule 27 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).

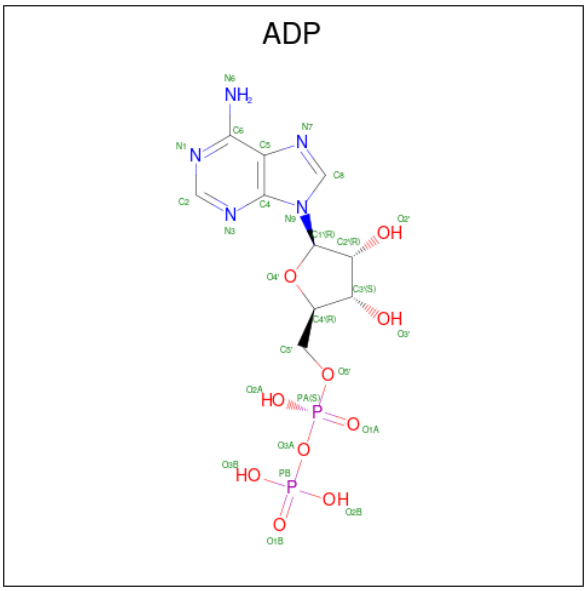


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
27	A	1	31	10	5	12	3	1	0
27	D	1	31	10	5	12	3	1	0
27	E	1	31	10	5	12	3	1	0
27	F	1	31	10	5	12	3	1	0

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
28	A	1	1	1	0
28	D	1	1	1	0
28	E	1	1	1	0
28	F	1	1	1	0

- Molecule 29 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

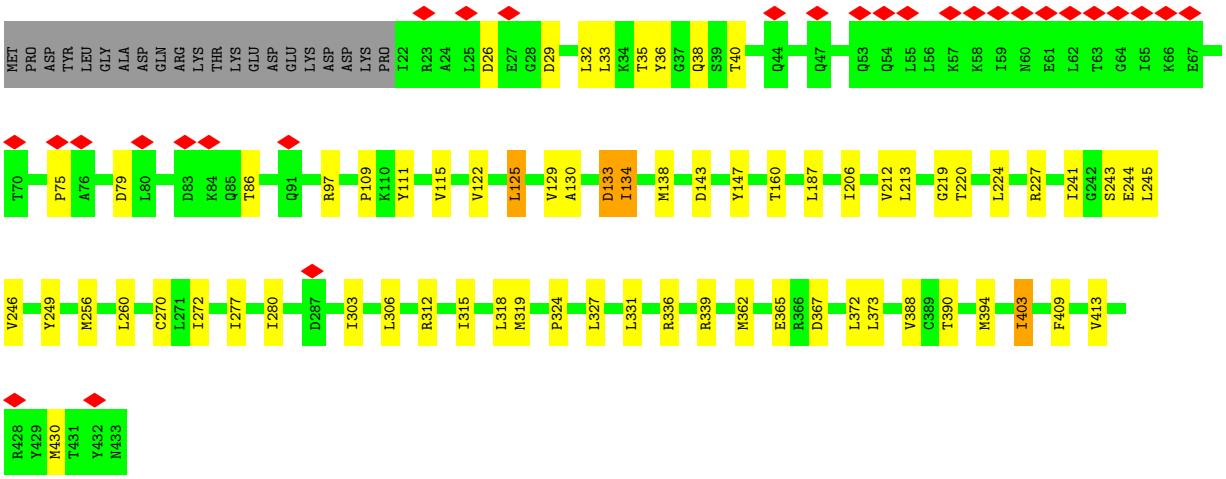
Mol	Chain	Residues	Atoms		AltConf
30	c	1	Total	Zn	0
			1	1	

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.

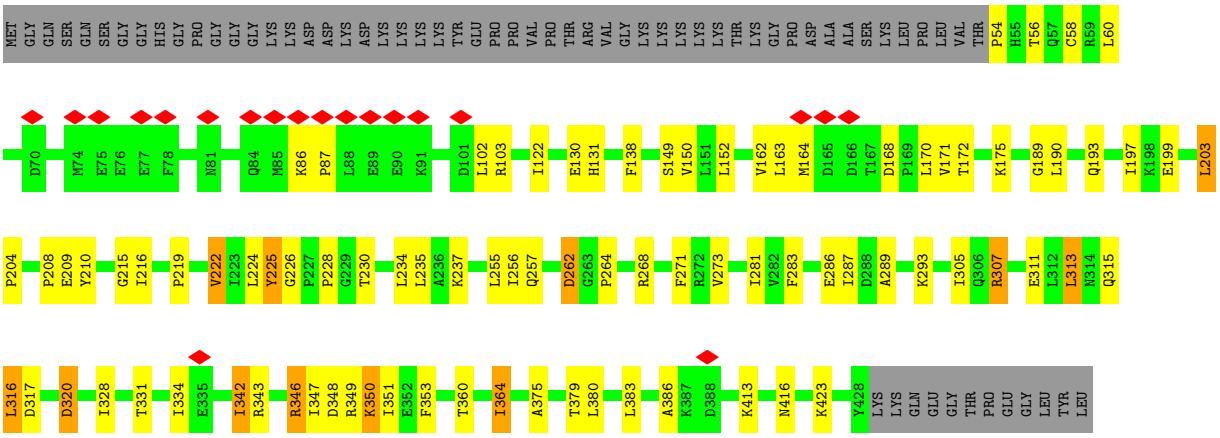
- Molecule 1: 26S proteasome regulatory subunit 7

Chain A:



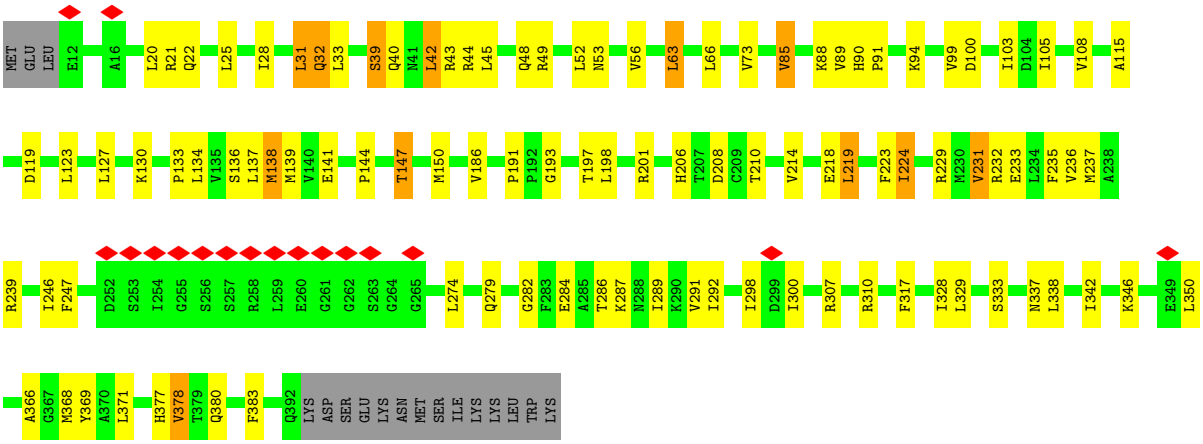
- Molecule 2: 26S proteasome regulatory subunit 4

Chain B:



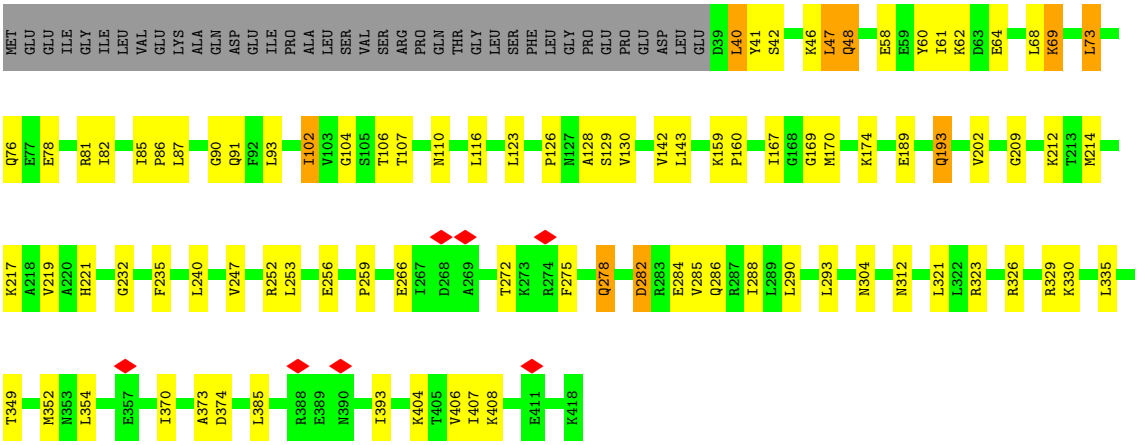
- Molecule 3: 26S proteasome regulatory subunit 8

Chain C:



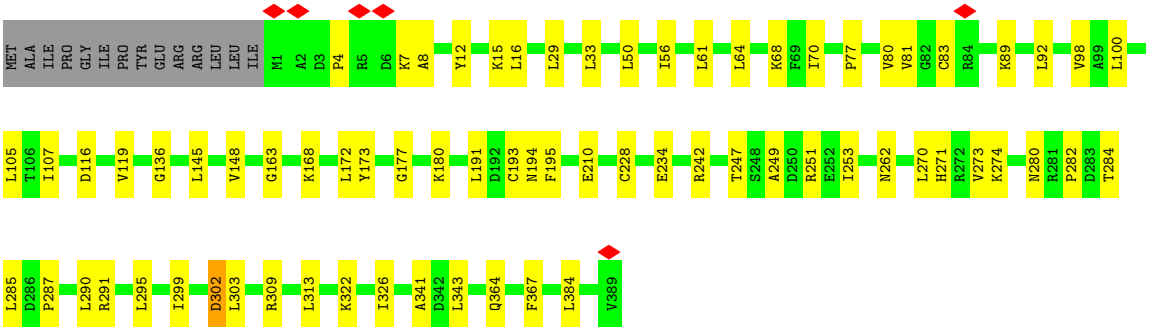
- Molecule 4: 26S proteasome regulatory subunit 6B

Chain D:



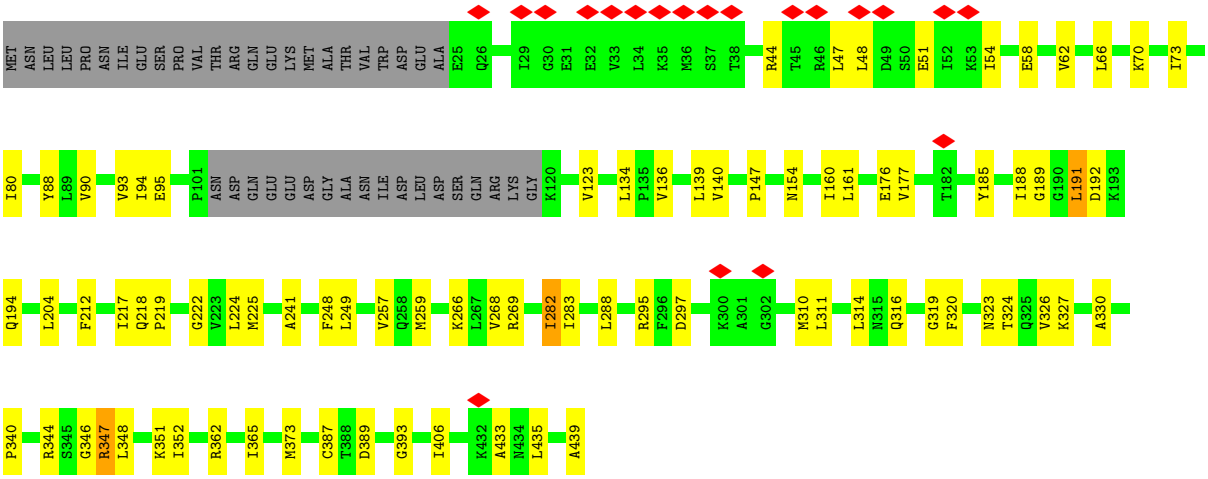
- Molecule 5: 26S proteasome regulatory subunit 10B

Chain E:



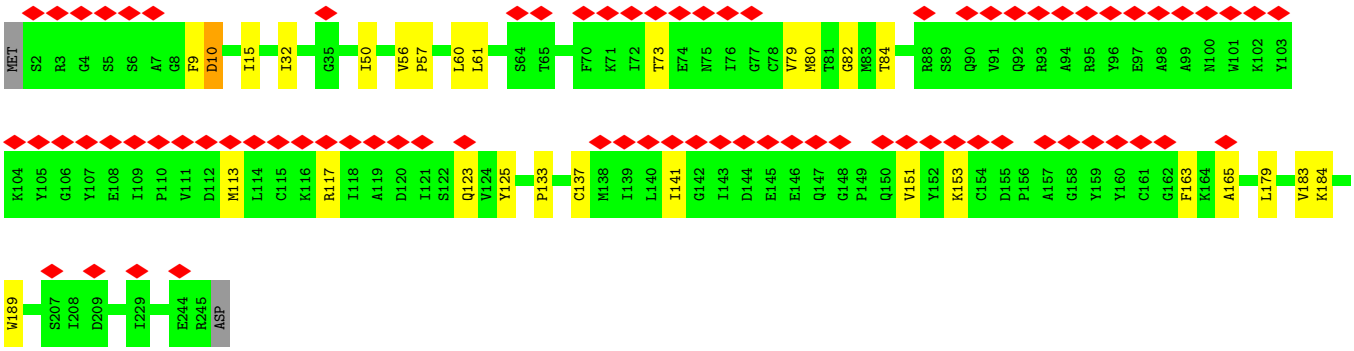
- Molecule 6: 26S proteasome regulatory subunit 6A

Chain F:



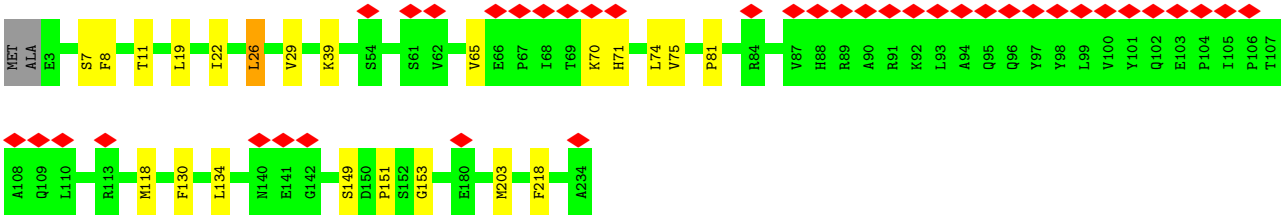
- Molecule 7: Proteasome subunit alpha type-6

Chain G:



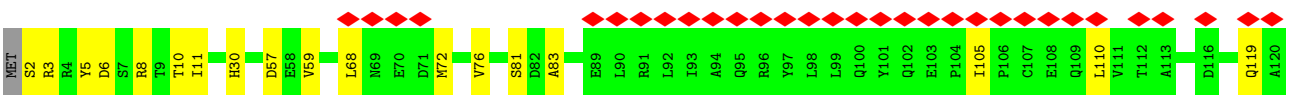
- Molecule 8: Proteasome subunit alpha type-2

Chain H:



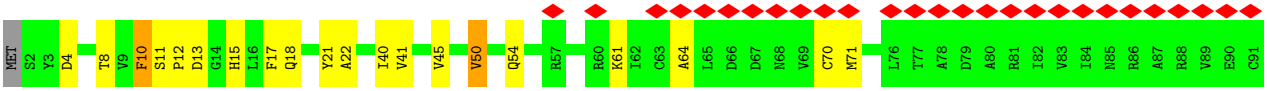
- Molecule 9: Proteasome subunit alpha type-4

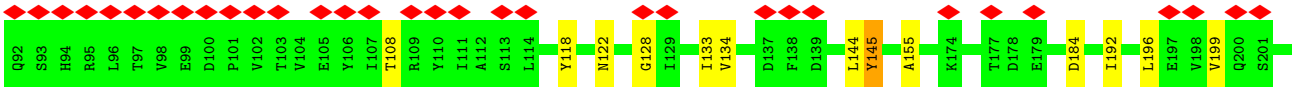
Chain I:

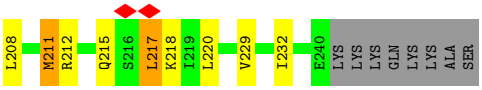


- Molecule 10: Proteasome subunit alpha type-7

Chain J:

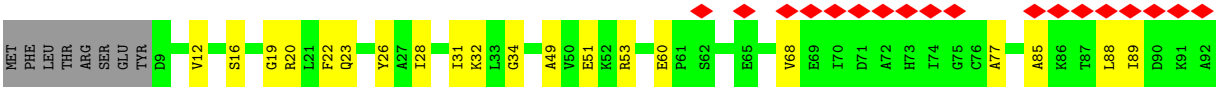


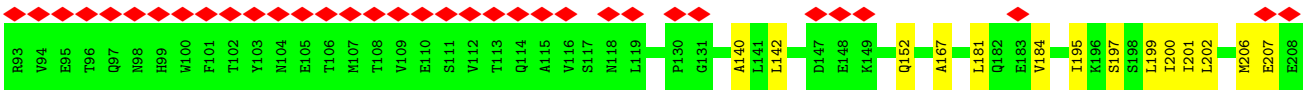


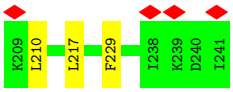


- Molecule 11: Proteasome subunit alpha type-5

Chain K:

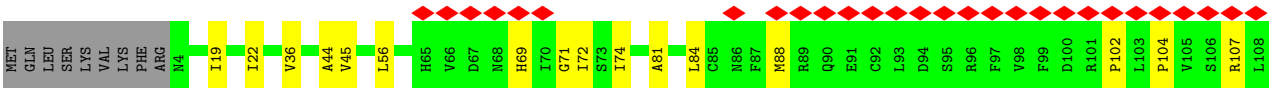


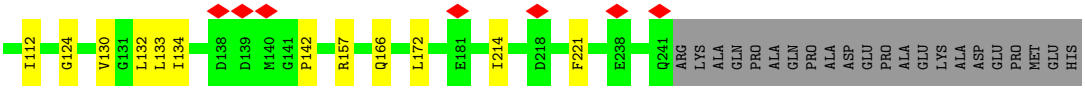




- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

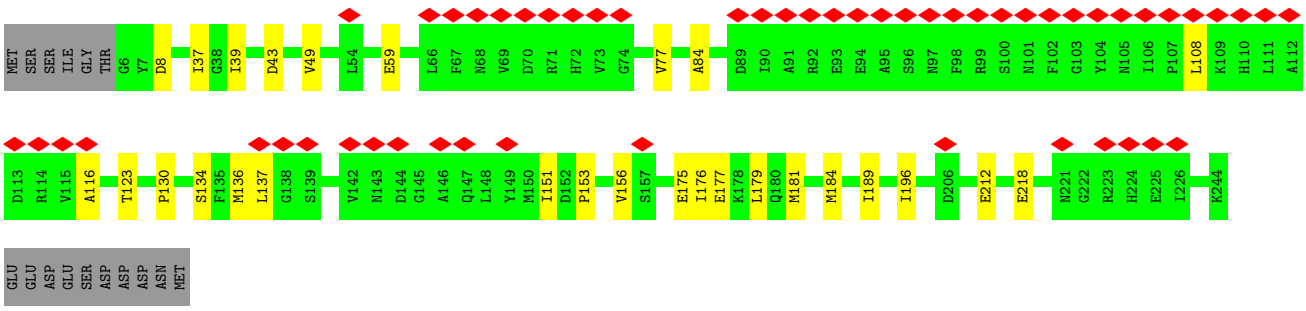
Chain L:





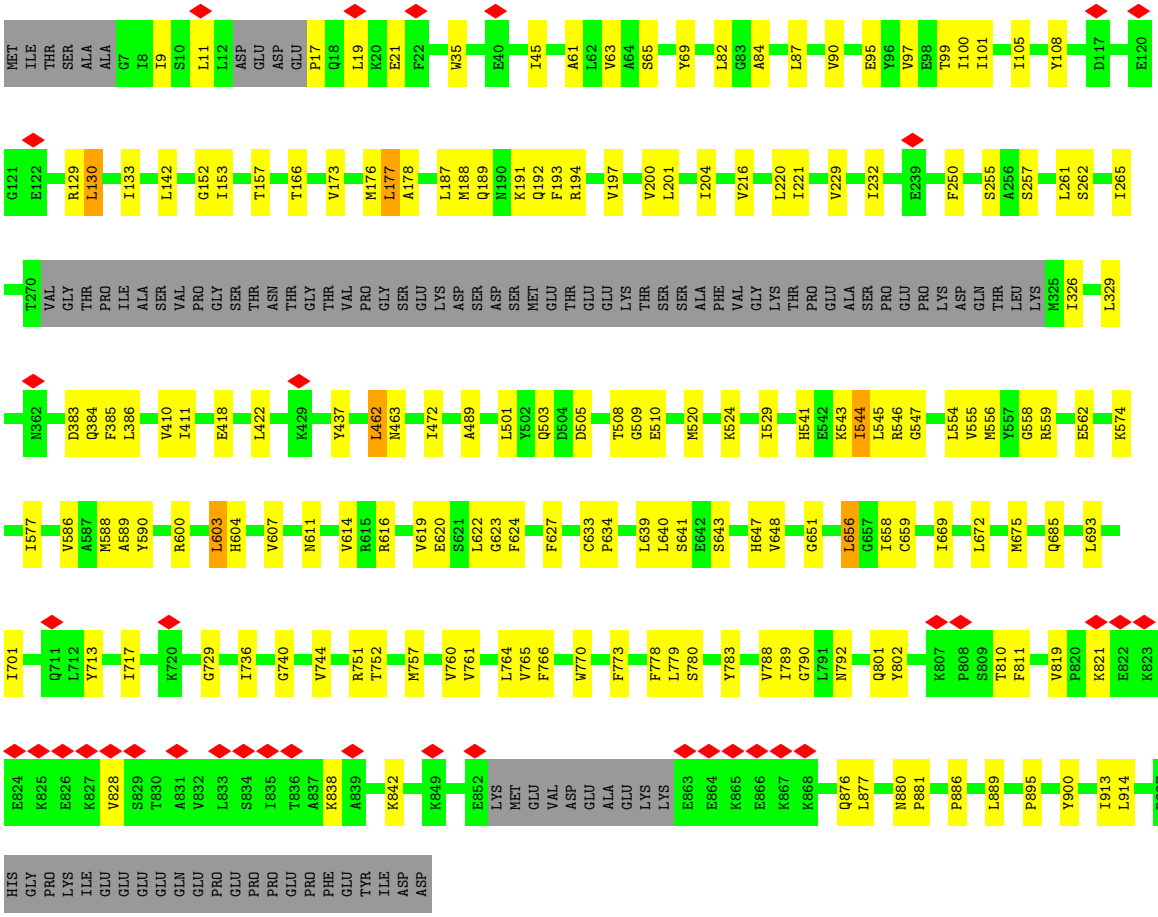
- Molecule 13: Proteasome subunit alpha type-3

Chain M:



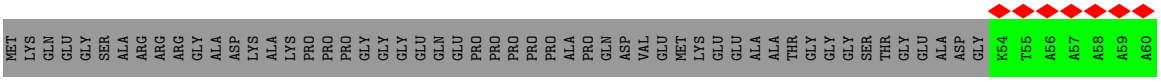
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 1

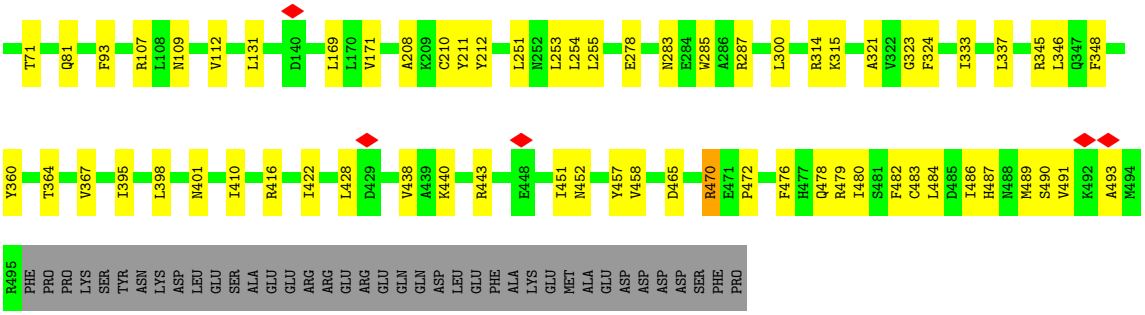
Chain U:



• Molecule 15: 26S proteasome non-ATPase regulatory subunit 3

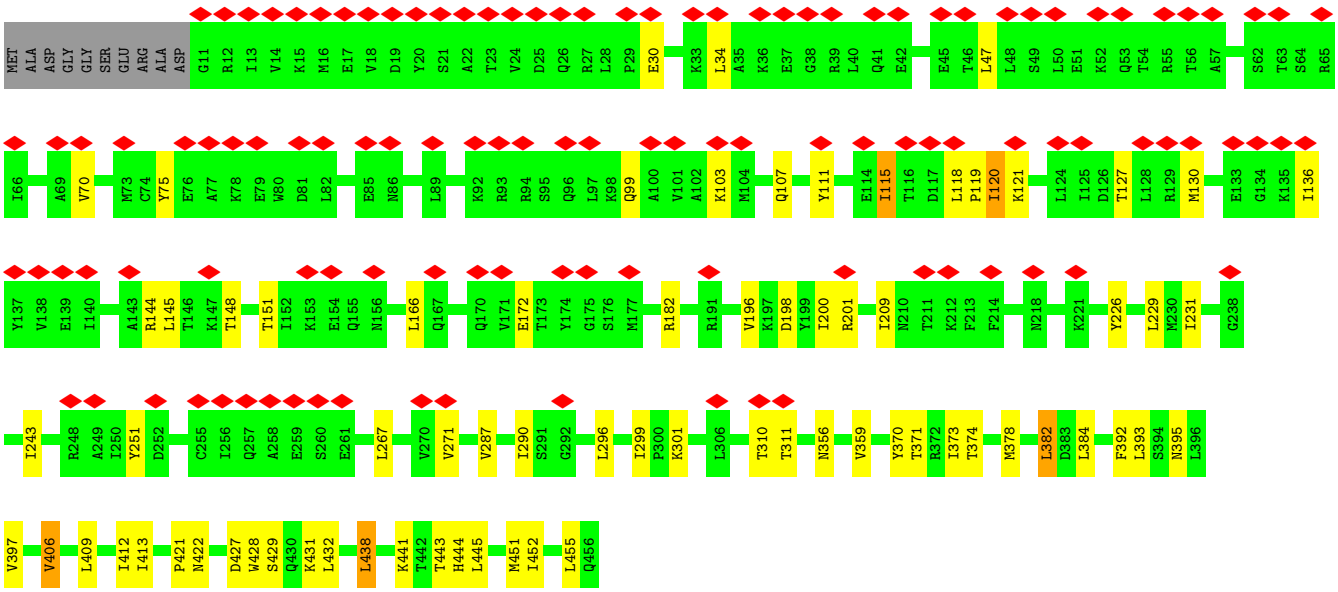
Chain V:





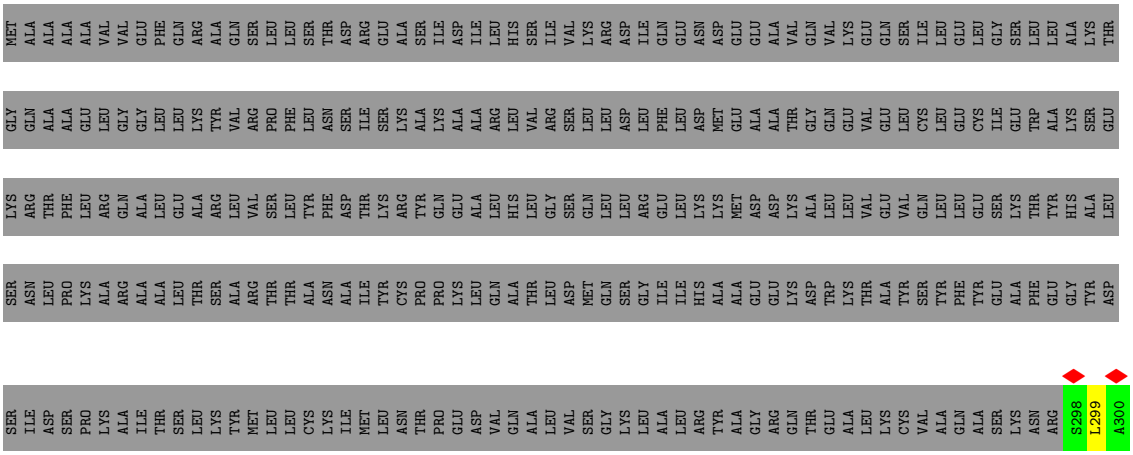
• Molecule 16: 26S proteasome non-ATPase regulatory subunit 12

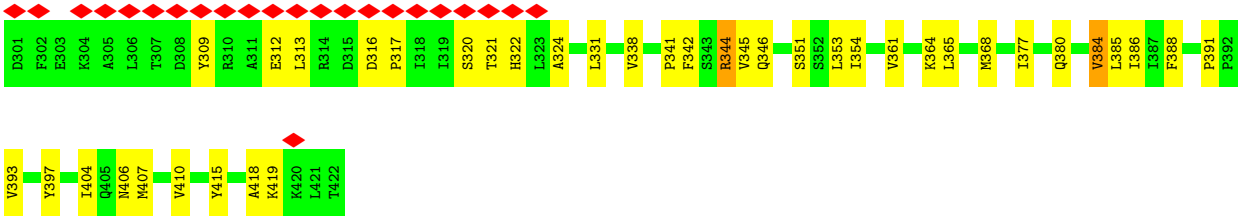
Chain W:



• Molecule 17: 26S proteasome non-ATPase regulatory subunit 11

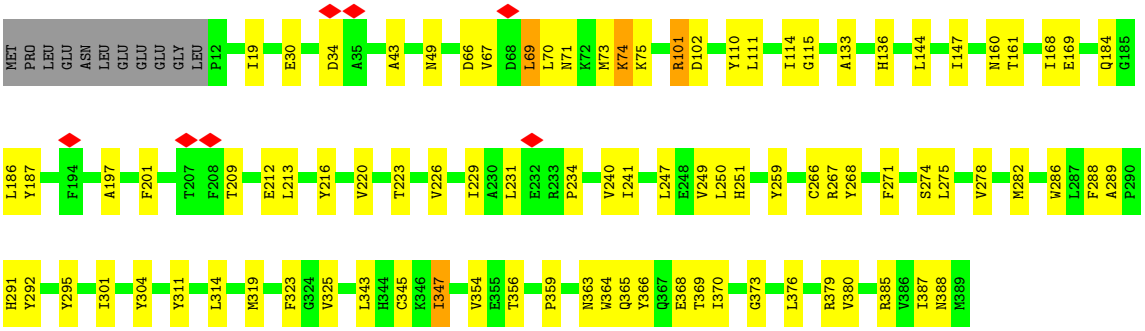
Chain X:





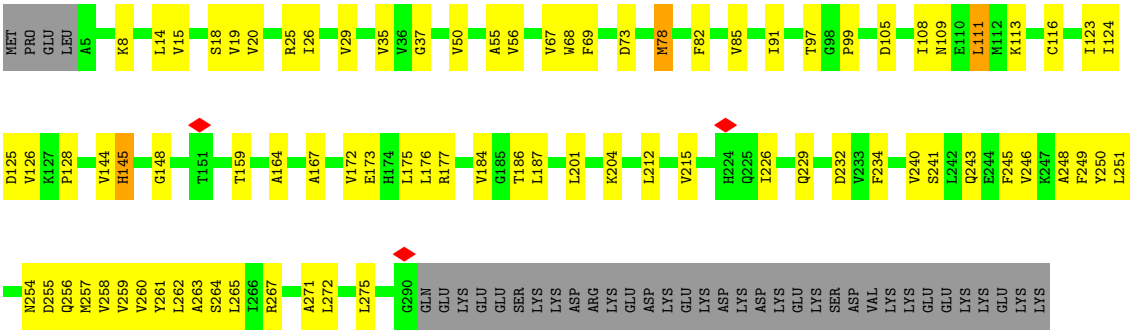
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:



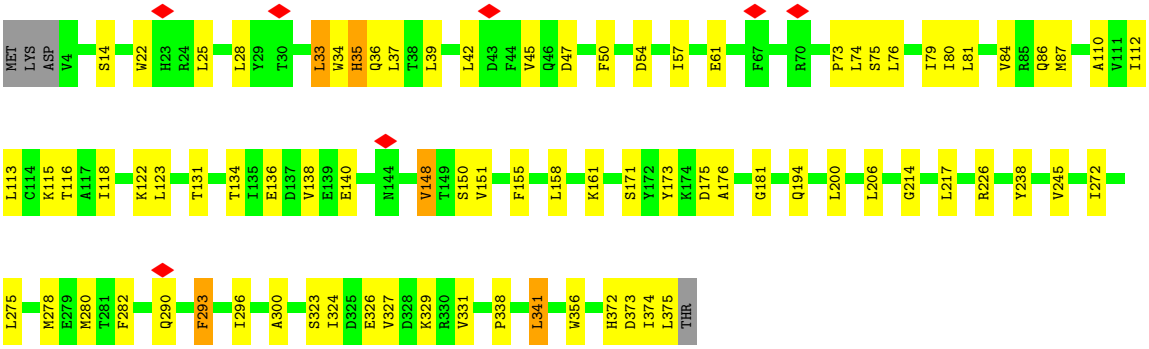
• Molecule 19: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:



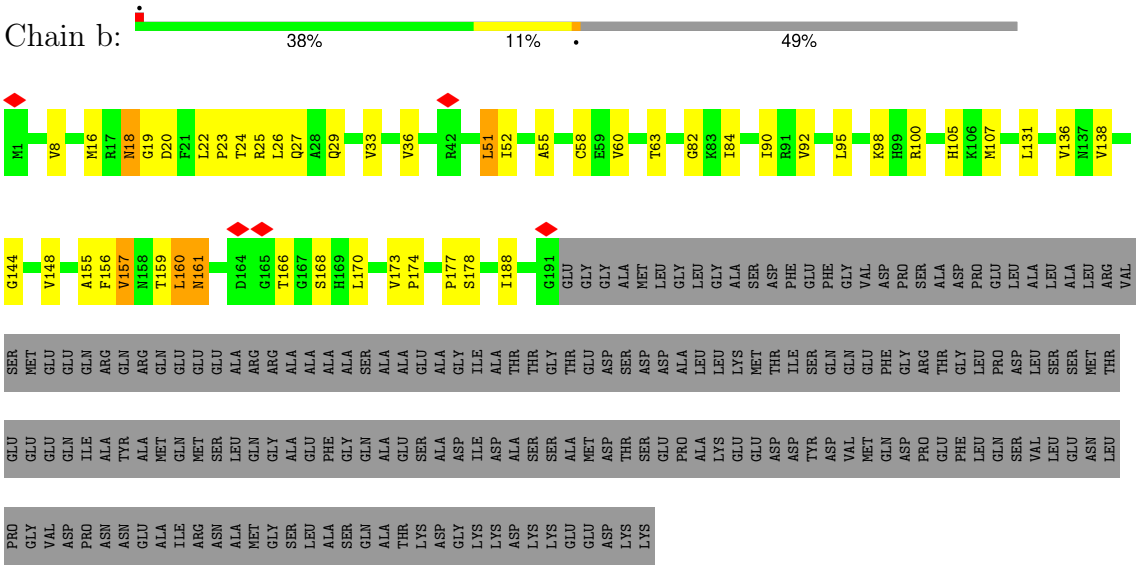
• Molecule 20: 26S proteasome non-ATPase regulatory subunit 13

Chain a:



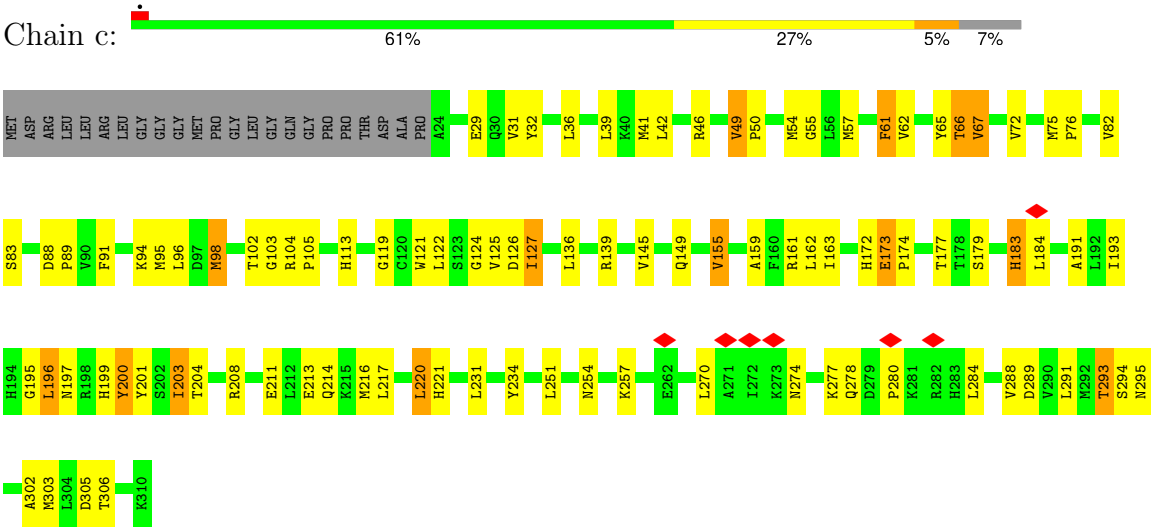
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



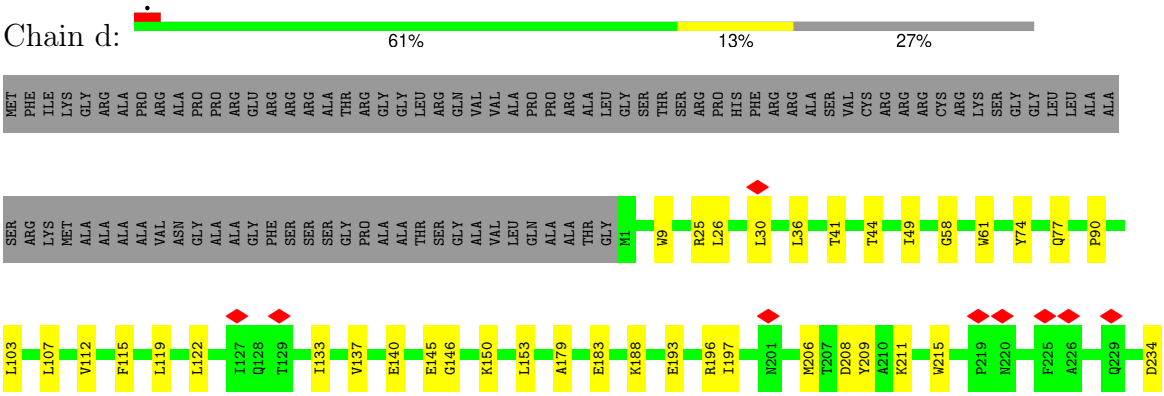
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 14

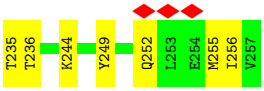
Chain c:



• Molecule 23: 26S proteasome non-ATPase regulatory subunit 8

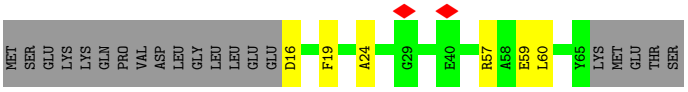
Chain d:





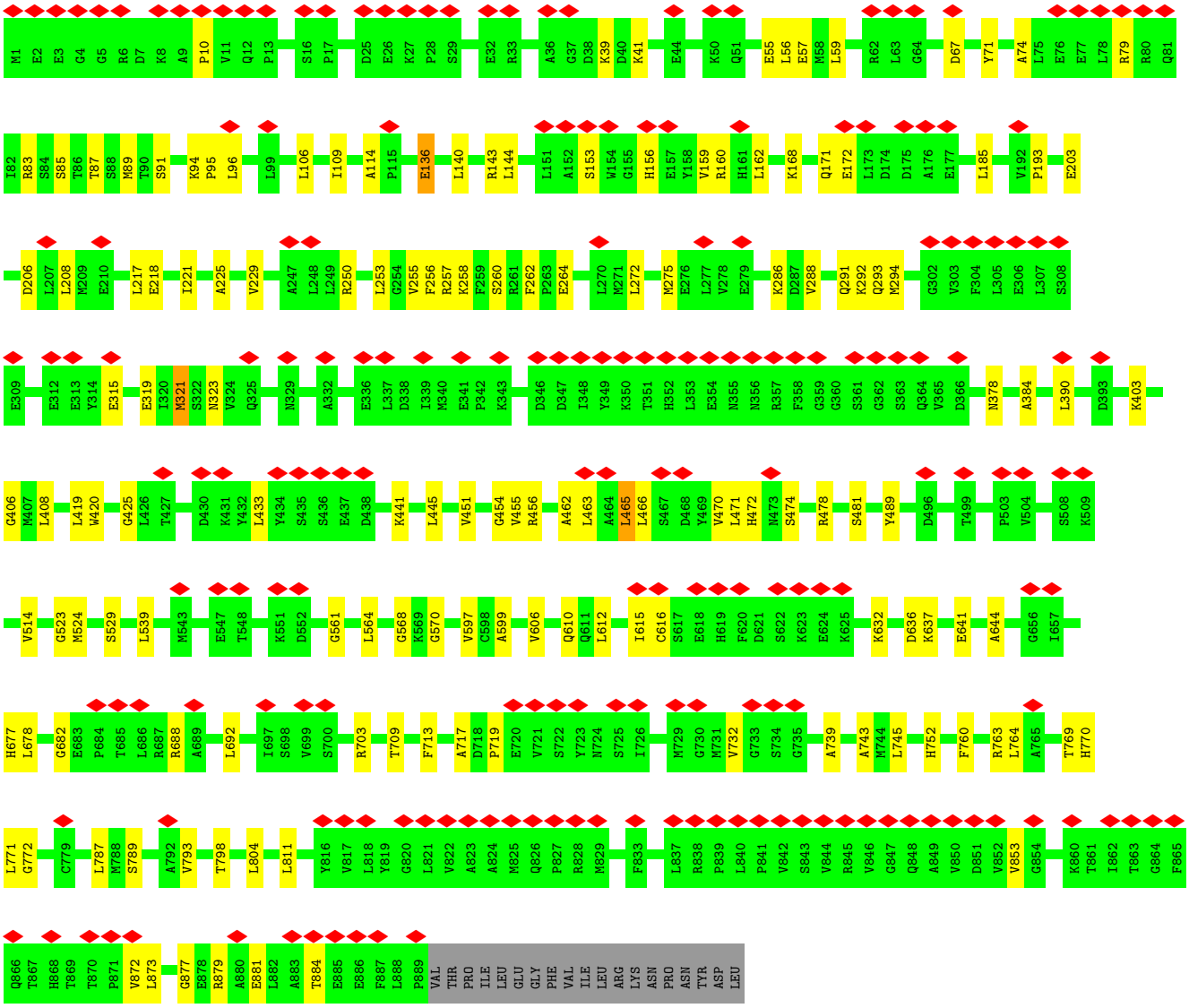
• Molecule 24: 26S proteasome complex subunit SEM1

Chain e:



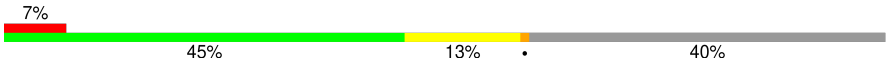
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 2

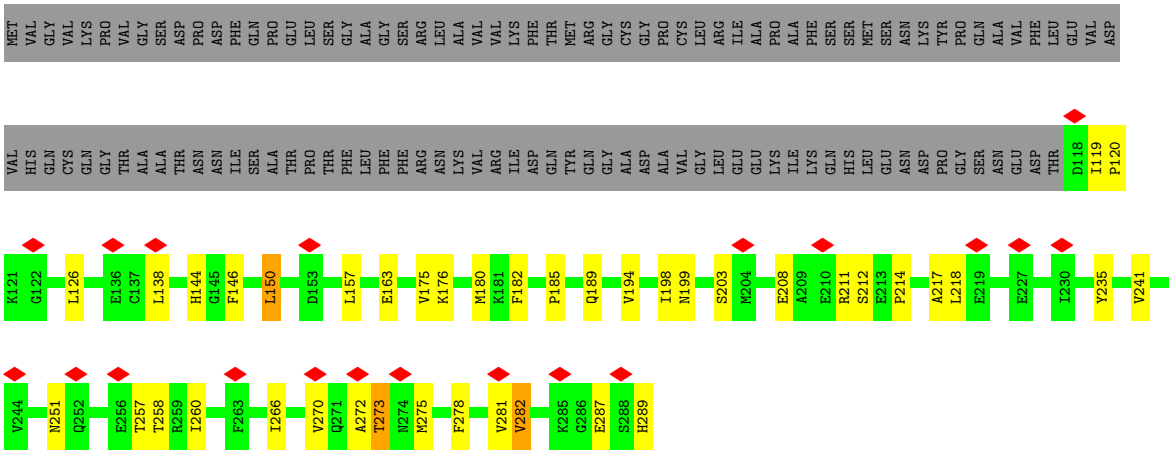
Chain f:



• Molecule 26: Thioredoxin-like protein 1

Chain g:


7%
45%
13%
40%


MET VAL GLY VAL LYS PRO VAL GLY SER ASP PRO ASP PHE GLN PRO GLU LEU SER GLY ALA GLY SER ARG LEU ALA VAL VAL LYS PHE THR MET ARG GLY CYS GLY PRO CYS LEU ARG ILE ALA PRO ALA PHE SER SER MET SER ASN LYS TYR PRO GLN ALA VAL PHE LEU GLU VAL ASP
VAL HIS GLN CYS GLN GLY THR ALA ALA THR ASN ASN ILE SER ALA THR PRO THR PHE LEU PHE PHE ARG ASN LYS VAL ARG ILE ASP GLN TYR GLN GLY ALA ASP ALA VAL GLY LEU GLU GLU LYS ILE LYS GLN HIS LEU GLU ASN ASP PRO GLY SER ASN GLU ASP THR D118 I119 P120

K121 G122 L126 E136 C137 L138 H144 G145 F146 L150 D153 L157 E163 V175 K176 M180 K181 F182 P185 Q189 V194 I198 N199 S203 M204 E208 A209 E210 R211 S212 E213 P214 A217 L218 E219 E227 I230 Y235 V241
V244 N251 Q252 E256 T257 T258 R259 I260 F263 I266 V270 Q271 A272 T273 N274 M275 F278 V281 V282 K285 G286 E287 S288 H289

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100351	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 ($e^-/Å^2$)	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	0.259	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	388.8, 388.8, 388.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.46	0/3290	0.79	0/4441
2	B	0.55	0/3002	0.89	0/4047
3	C	0.65	0/3027	0.92	0/4070
4	D	0.61	0/3089	0.89	0/4168
5	E	0.44	0/3145	0.75	0/4233
6	F	0.51	0/3152	0.80	0/4246
7	G	0.38	0/1937	0.67	0/2617
8	H	0.30	0/1852	0.56	0/2507
9	I	0.37	0/2001	0.69	0/2694
10	J	0.33	0/1913	0.64	0/2581
11	K	0.44	0/1805	0.71	0/2437
12	L	0.28	0/1908	0.53	0/2579
13	M	0.23	0/1909	0.58	0/2570
14	U	0.48	0/6786	0.79	0/9167
15	V	0.39	0/3661	0.66	0/4941
16	W	0.44	0/3683	0.79	0/4952
17	X	0.57	0/1021	0.94	0/1375
18	Y	0.47	0/3173	0.80	0/4273
19	Z	0.53	0/2324	0.84	0/3150
20	a	0.46	0/3045	0.84	0/4123
21	b	0.53	0/1478	0.89	0/2001
22	c	0.84	0/2302	1.08	0/3110
23	d	0.31	0/2162	0.75	0/2919
24	e	0.30	0/437	0.74	0/595
25	f	0.34	0/6980	0.70	0/9433
26	g	0.59	0/1403	0.93	0/1892
All	All	0.47	0/70485	0.78	0/95121

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 (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	3237	0	3291	52	0
2	B	2960	0	3010	67	0
3	C	2988	0	3089	65	0
4	D	3039	0	3076	61	0
5	E	3097	0	3174	49	0
6	F	3112	0	3198	57	0
7	G	1903	0	1911	17	0
8	H	1813	0	1806	17	0
9	I	1971	0	1992	23	0
10	J	1887	0	1905	25	0
11	K	1778	0	1764	27	0
12	L	1873	0	1860	21	0
13	M	1874	0	1861	15	0
14	U	6671	0	6738	106	0
15	V	3594	0	3666	53	0
16	W	3635	0	3762	59	0
17	X	1007	0	1038	41	0
18	Y	3115	0	3120	64	0
19	Z	2281	0	2312	83	0
20	a	2987	0	3005	55	0
21	b	1458	0	1505	32	0
22	c	2260	0	2276	87	0
23	d	2116	0	2146	31	0
24	e	425	0	328	6	0
25	f	6866	0	6866	88	0
26	g	1376	0	1324	27	0
27	A	31	0	12	4	0
27	D	31	0	12	1	0
27	E	31	0	12	2	0
27	F	31	0	12	2	0
28	A	1	0	0	0	0
28	D	1	0	0	0	0
28	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	F	1	0	0	0	0
29	B	27	0	12	1	0
29	C	27	0	12	4	0
30	c	1	0	0	0	0
All	All	69506	0	70095	1053	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 8.

All (1053) 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)
4:D:73:LEU:HB3	19:Z:184:VAL:HG12	1.61	0.83
23:d:41:THR:HG22	23:d:44:THR:HB	1.61	0.81
1:A:125:LEU:HG	1:A:134:ILE:HD11	1.63	0.80
2:B:197:ILE:HD13	2:B:235:LEU:HD13	1.65	0.79
22:c:122:LEU:H	22:c:196:LEU:HD11	1.47	0.79
16:W:373:ILE:HG23	20:a:326:GLU:HB2	1.67	0.77
3:C:193:GLY:HA2	29:C:501:ADP:H5'2	1.66	0.76
3:C:219:LEU:HB2	4:D:290:LEU:HD11	1.68	0.74
20:a:374:ILE:O	20:a:374:ILE:HG22	1.86	0.74
20:a:39:LEU:HB3	20:a:45:VAL:HG22	1.70	0.74
12:L:88:MET:HG2	12:L:112:ILE:HD11	1.68	0.73
10:J:10:PHE:HB2	11:K:26:TYR:HB3	1.69	0.73
15:V:416:ARG:HA	15:V:458:VAL:HB	1.70	0.72
1:A:260:LEU:HD21	1:A:272:ILE:HD13	1.71	0.72
2:B:224:LEU:HD21	2:B:235:LEU:HD12	1.70	0.72
20:a:293:PHE:HB2	20:a:329:LYS:HB3	1.71	0.71
2:B:342:ILE:HA	2:B:347:ILE:HD12	1.72	0.71
19:Z:263:ALA:HB1	22:c:288:VAL:HG13	1.71	0.71
2:B:219:PRO:HB3	2:B:348:ASP:HB3	1.73	0.71
4:D:232:GLY:HA3	4:D:266:GLU:HB2	1.72	0.70
15:V:479:ARG:HG2	19:Z:265:LEU:HA	1.73	0.70
17:X:377:ILE:HG22	17:X:386:ILE:HB	1.72	0.69
21:b:131:LEU:HD22	21:b:136:VAL:HG21	1.73	0.69
22:c:61:PHE:HA	22:c:67:VAL:HA	1.73	0.69
22:c:89:PRO:HG3	26:g:278:PHE:HB2	1.75	0.69
25:f:709:THR:HG21	25:f:745:LEU:HB3	1.75	0.69
22:c:32:TYR:HB3	22:c:208:ARG:HB2	1.74	0.68
13:M:175:GLU:HB3	13:M:196:ILE:HG12	1.74	0.68
19:Z:229:GLN:HB2	20:a:338:PRO:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:191:LYS:HA	14:U:194:ARG:HB3	1.75	0.68
2:B:230:THR:HG21	2:B:353:PHE:HB3	1.76	0.68
16:W:429:SER:HB2	22:c:231:LEU:HB2	1.74	0.68
15:V:251:LEU:HA	15:V:254:LEU:HD12	1.76	0.68
19:Z:125:ASP:HB3	19:Z:128:PRO:HG2	1.77	0.67
21:b:161:ASN:HA	21:b:166:THR:HB	1.76	0.67
25:f:384:ALA:H	25:f:419:LEU:HB3	1.60	0.67
12:L:72:ILE:HG12	12:L:134:ILE:HG23	1.77	0.67
18:Y:376:LEU:HD13	19:Z:265:LEU:HD11	1.76	0.66
25:f:106:LEU:HD22	25:f:109:ILE:HD12	1.75	0.66
6:F:283:ILE:HG22	6:F:326:VAL:HG22	1.78	0.66
20:a:113:LEU:HB3	20:a:151:VAL:HG23	1.78	0.65
21:b:22:LEU:HB2	21:b:23:PRO:HD3	1.77	0.65
5:E:116:ASP:HB3	5:E:119:VAL:HB	1.77	0.65
1:A:373:LEU:HD22	1:A:413:VAL:HG21	1.79	0.65
6:F:314:LEU:HB3	6:F:347:ARG:HH21	1.61	0.65
16:W:115:ILE:HB	16:W:120:ILE:HG21	1.79	0.65
21:b:157:VAL:HG13	21:b:168:SER:HB2	1.79	0.65
16:W:451:MET:O	16:W:455:LEU:HB2	1.97	0.65
16:W:47:LEU:HD11	16:W:70:VAL:HG11	1.79	0.65
14:U:383:ASP:HB3	14:U:386:LEU:HB3	1.78	0.64
15:V:480:ILE:O	23:d:252:GLN:NE2	2.26	0.64
16:W:378:MET:HE3	16:W:413:ILE:HD11	1.80	0.64
16:W:432:LEU:HD12	22:c:231:LEU:HD11	1.80	0.64
8:H:70:LYS:HB2	8:H:71:HIS:CE1	2.33	0.63
2:B:168:ASP:HB3	2:B:171:VAL:HG22	1.80	0.63
5:E:83:CYS:HB2	5:E:107:ILE:HG13	1.80	0.63
13:M:179:LEU:HB3	13:M:181:MET:HB3	1.81	0.63
4:D:278:GLN:NE2	4:D:286:GLN:HB2	2.14	0.63
15:V:465:ASP:OD1	19:Z:251:LEU:HD23	1.99	0.62
20:a:272:ILE:HA	20:a:275:LEU:HD12	1.81	0.62
18:Y:197:ALA:O	18:Y:201:PHE:HB2	2.00	0.62
25:f:171:GLN:HB3	25:f:208:LEU:HD11	1.80	0.62
3:C:219:LEU:HA	4:D:286:GLN:NE2	2.15	0.62
1:A:372:LEU:HD13	11:K:207:GLU:HA	1.80	0.62
11:K:49:ALA:HB1	11:K:202:LEU:HD11	1.81	0.62
25:f:466:LEU:HD12	25:f:481:SER:HA	1.82	0.62
1:A:134:ILE:HD12	1:A:134:ILE:H	1.64	0.61
25:f:140:LEU:HA	25:f:143:ARG:HB2	1.80	0.61
2:B:226:GLY:HA3	2:B:353:PHE:HB2	1.81	0.61
4:D:209:GLY:HA3	5:E:291:ARG:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:310:THR:HG22	16:W:311:THR:HG23	1.82	0.61
22:c:54:MET:HB2	22:c:82:VAL:HG22	1.81	0.61
6:F:185:TYR:HA	6:F:188:ILE:HG12	1.81	0.61
16:W:136:ILE:HD11	16:W:144:ARG:HD3	1.82	0.61
21:b:19:GLY:HA2	21:b:25:ARG:H	1.66	0.61
1:A:224:LEU:HD11	27:A:501:AGS:H2'	1.81	0.61
14:U:802:TYR:HB3	14:U:895:PRO:HD3	1.83	0.61
22:c:42:LEU:HD21	22:c:155:VAL:HG21	1.83	0.61
22:c:136:LEU:HD11	26:g:275:MET:HB3	1.82	0.61
25:f:472:HIS:HD2	25:f:474:SER:HB3	1.64	0.61
2:B:307:ARG:HH11	2:B:307:ARG:CG	2.14	0.61
14:U:603:LEU:HD13	14:U:622:LEU:HD21	1.83	0.61
8:H:153:GLY:HA3	9:I:81:SER:HB3	1.83	0.61
1:A:97:ARG:HA	2:B:131:HIS:HA	1.83	0.60
4:D:259:PRO:HB3	4:D:304:ASN:HB2	1.82	0.60
23:d:206:MET:HA	23:d:209:TYR:HB3	1.83	0.60
6:F:94:ILE:HD12	6:F:123:VAL:HG12	1.82	0.60
1:A:212:VAL:HG22	1:A:339:ARG:HB3	1.83	0.60
4:D:252:ARG:O	4:D:256:GLU:HB2	2.01	0.60
16:W:445:LEU:HD11	19:Z:226:ILE:HD12	1.84	0.60
3:C:103:ILE:HD12	3:C:123:LEU:HB3	1.84	0.60
14:U:510:GLU:HA	14:U:547:GLY:HA3	1.83	0.60
17:X:309:TYR:HB2	17:X:313:LEU:HD12	1.82	0.60
16:W:421:PRO:HG3	19:Z:251:LEU:CD1	2.32	0.60
25:f:425:GLY:HA3	25:f:451:VAL:HG21	1.83	0.60
14:U:559:ARG:HB3	14:U:562:GLU:HB2	1.84	0.59
11:K:77:ALA:HB3	11:K:142:LEU:HB2	1.83	0.59
26:g:281:VAL:HG23	26:g:282:VAL:HG12	1.83	0.59
14:U:11:LEU:HD12	14:U:19:LEU:HD11	1.83	0.59
1:A:220:THR:HA	27:A:501:AGS:HN61	1.67	0.59
10:J:229:VAL:HA	10:J:232:ILE:HG12	1.84	0.59
14:U:462:LEU:HG	14:U:463:ASN:N	2.15	0.59
15:V:480:ILE:HG23	19:Z:267:ARG:HH12	1.67	0.59
2:B:190:LEU:HD22	2:B:193:GLN:HE22	1.68	0.59
19:Z:259:VAL:CG2	22:c:295:ASN:HB2	2.32	0.59
19:Z:186:THR:HB	22:c:293:THR:HG21	1.85	0.59
1:A:130:ALA:HB3	1:A:133:ASP:HB3	1.85	0.59
10:J:13:ASP:HB2	10:J:15:HIS:CE1	2.38	0.59
19:Z:37:GLY:HA2	19:Z:56:VAL:HG12	1.84	0.59
22:c:161:ARG:HB3	22:c:201:TYR:HD1	1.67	0.59
25:f:478:ARG:HG2	25:f:514:VAL:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:16:SER:HB3	11:K:20:ARG:HG2	1.83	0.58
12:L:71:GLY:HA3	12:L:221:PHE:CE1	2.38	0.58
22:c:161:ARG:HB3	22:c:201:TYR:CD1	2.37	0.58
2:B:225:TYR:HB2	2:B:331:THR:H	1.69	0.58
14:U:216:VAL:HG23	14:U:220:LEU:HD12	1.85	0.58
20:a:37:LEU:HD11	20:a:79:ILE:HD13	1.84	0.58
25:f:292:LYS:HB3	25:f:771:LEU:HD12	1.84	0.58
25:f:445:LEU:HD12	25:f:465:LEU:HD12	1.84	0.58
22:c:57:MET:HB2	22:c:72:VAL:HG22	1.84	0.58
16:W:75:TYR:CE1	16:W:111:TYR:HB3	2.38	0.58
20:a:73:PRO:O	20:a:75:SER:N	2.35	0.58
22:c:172:HIS:NE2	22:c:174:PRO:HB3	2.18	0.58
3:C:53:ASN:HD21	14:U:643:SER:HA	1.67	0.58
22:c:65:TYR:CE2	22:c:66:THR:HG23	2.39	0.58
9:I:149:GLN:HG2	9:I:164:ILE:HD11	1.86	0.58
5:E:284:THR:HG22	6:F:297:ASP:HB2	1.86	0.58
6:F:191:LEU:HG	6:F:194:GLN:HB2	1.86	0.58
21:b:24:THR:O	21:b:27:GLN:N	2.36	0.58
25:f:144:LEU:HD11	25:f:159:VAL:HG21	1.85	0.58
25:f:403:LYS:HB2	25:f:406:GLY:H	1.69	0.58
1:A:336:ARG:NH1	27:F:501:AGS:S1G	2.73	0.57
16:W:231:ILE:HD12	16:W:243:ILE:HA	1.86	0.57
25:f:454:GLY:HA2	25:f:456:ARG:HH21	1.68	0.57
4:D:370:ILE:HG13	4:D:374:ASP:HB2	1.86	0.57
5:E:64:LEU:HD13	5:E:68:LYS:HB3	1.86	0.57
9:I:133:SER:HB3	9:I:164:ILE:HD13	1.86	0.57
15:V:283:ASN:HD21	24:e:16:ASP:HB2	1.68	0.57
17:X:365:LEU:HD21	17:X:385:LEU:HD21	1.85	0.57
21:b:157:VAL:HG21	21:b:170:LEU:HB2	1.86	0.57
6:F:219:PRO:HB2	6:F:324:THR:HG21	1.86	0.57
14:U:623:GLY:HA3	14:U:658:ILE:HG13	1.86	0.57
19:Z:14:LEU:HD12	22:c:39:LEU:HB3	1.85	0.57
3:C:42:LEU:HA	3:C:45:LEU:HD12	1.86	0.57
22:c:75:MET:HE1	22:c:88:ASP:HB2	1.86	0.57
1:A:122:VAL:HB	6:F:88:TYR:HB2	1.86	0.57
1:A:372:LEU:HD22	11:K:207:GLU:HG3	1.87	0.57
4:D:91:GLN:HA	4:D:129:SER:HA	1.87	0.57
18:Y:240:VAL:HG13	18:Y:241:ILE:HG13	1.85	0.57
21:b:16:MET:SD	21:b:29:GLN:NE2	2.77	0.57
6:F:282:ILE:HD11	6:F:327:LYS:HB2	1.85	0.57
20:a:34:TRP:HB2	21:b:18:ASN:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:349:THR:HB	4:D:354:LEU:HD21	1.87	0.57
16:W:428:TRP:HD1	19:Z:240:VAL:HB	1.70	0.57
18:Y:231:LEU:HB2	18:Y:234:PRO:HD2	1.85	0.57
19:Z:246:VAL:HA	19:Z:250:TYR:CD2	2.40	0.57
20:a:374:ILE:O	20:a:374:ILE:CG2	2.53	0.57
3:C:73:VAL:HG11	4:D:102:ILE:HD12	1.87	0.57
10:J:8:THR:HG23	10:J:18:GLN:HB2	1.87	0.57
2:B:257:GLN:HB2	2:B:262:ASP:HB2	1.86	0.57
10:J:17:PHE:O	10:J:21:TYR:HB2	2.05	0.57
18:Y:345:CYS:HA	18:Y:356:THR:HA	1.86	0.57
19:Z:73:ASP:HB2	21:b:63:THR:HG21	1.86	0.57
23:d:41:THR:CG2	23:d:44:THR:HB	2.33	0.57
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.87	0.56
6:F:249:LEU:HD23	6:F:283:ILE:HD13	1.87	0.56
6:F:268:VAL:HG22	6:F:316:GLN:HE22	1.70	0.56
14:U:790:GLY:H	14:U:880:ASN:HD22	1.54	0.56
5:E:56:ILE:HB	5:E:100:LEU:HB2	1.87	0.56
7:G:32:ILE:HD12	7:G:137:CYS:HB2	1.88	0.56
14:U:142:LEU:HD21	14:U:166:THR:HG22	1.87	0.56
16:W:370:TYR:CD1	20:a:324:ILE:HB	2.39	0.56
6:F:222:GLY:HA3	6:F:348:LEU:HA	1.88	0.56
11:K:195:ILE:HD11	11:K:217:LEU:HD11	1.86	0.56
15:V:479:ARG:HB3	19:Z:264:SER:HB2	1.86	0.56
20:a:373:ASP:O	20:a:374:ILE:HD13	2.05	0.56
2:B:219:PRO:CB	2:B:348:ASP:HB3	2.36	0.56
3:C:141:GLU:HA	4:D:326:ARG:NH2	2.20	0.56
9:I:3:ARG:HH12	12:L:124:GLY:HA2	1.69	0.56
15:V:315:LYS:HE2	18:Y:385:ARG:HB3	1.86	0.56
2:B:222:VAL:HB	2:B:349:ARG:HB2	1.88	0.56
14:U:600:ARG:O	14:U:604:HIS:HB3	2.06	0.56
25:f:470:VAL:HG22	25:f:471:LEU:HD12	1.88	0.56
14:U:619:VAL:HG13	14:U:651:GLY:HA3	1.88	0.56
15:V:337:LEU:HD21	15:V:364:THR:HG23	1.86	0.56
9:I:68:LEU:HD12	9:I:72:MET:HG3	1.86	0.56
6:F:324:THR:HB	6:F:327:LYS:HZ2	1.69	0.56
16:W:370:TYR:HD1	20:a:324:ILE:HB	1.71	0.56
20:a:74:LEU:HD22	20:a:110:ALA:HB2	1.88	0.56
2:B:103:ARG:HD3	2:B:138:PHE:HZ	1.72	0.55
2:B:190:LEU:HD22	2:B:193:GLN:NE2	2.21	0.55
3:C:246:ILE:HB	3:C:291:VAL:HG12	1.88	0.55
14:U:900:TYR:HB3	14:U:914:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:285:LEU:HD12	5:E:290:LEU:HD21	1.88	0.55
8:H:8:PHE:CZ	9:I:6:ASP:HA	2.41	0.55
15:V:480:ILE:HD13	23:d:249:TYR:HB2	1.88	0.55
16:W:409:LEU:HD23	17:X:384:VAL:HG11	1.87	0.55
3:C:100:ASP:HB2	3:C:123:LEU:O	2.06	0.55
3:C:346:LYS:O	3:C:350:LEU:HB2	2.06	0.55
4:D:278:GLN:HE21	4:D:286:GLN:HB2	1.72	0.55
15:V:470:ARG:HH11	23:d:235:THR:HA	1.70	0.55
24:e:57:ARG:HA	24:e:60:LEU:HD12	1.89	0.55
25:f:433:LEU:HA	25:f:441:LYS:HA	1.89	0.55
6:F:324:THR:HB	6:F:327:LYS:NZ	2.21	0.55
14:U:545:LEU:HD13	14:U:577:ILE:HG21	1.89	0.55
6:F:224:LEU:HD23	6:F:351:LYS:HG2	1.89	0.55
23:d:208:ASP:HA	23:d:211:LYS:HB2	1.88	0.55
15:V:287:ARG:HH21	24:e:19:PHE:HA	1.71	0.55
14:U:108:TYR:HD1	14:U:130:LEU:HD12	1.72	0.55
16:W:127:THR:HA	16:W:130:MET:HG2	1.89	0.55
17:X:365:LEU:CD2	17:X:385:LEU:HD21	2.36	0.55
18:Y:161:THR:HG21	18:Y:186:LEU:HD22	1.89	0.55
25:f:739:ALA:O	25:f:743:ALA:HB2	2.07	0.55
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.88	0.55
19:Z:91:ILE:HG13	19:Z:116:CYS:HB2	1.89	0.55
3:C:144:PRO:HD2	3:C:201:ARG:HD3	1.88	0.55
6:F:139:LEU:HD23	6:F:139:LEU:H	1.72	0.55
20:a:194:GLN:HB2	20:a:226:ARG:HD2	1.88	0.55
23:d:122:LEU:HD11	23:d:133:ILE:HG21	1.87	0.55
7:G:10:ASP:HA	7:G:15:ILE:HG13	1.89	0.54
10:J:196:LEU:HD13	10:J:199:VAL:HG13	1.89	0.54
4:D:62:LYS:HG2	23:d:255:MET:HB2	1.89	0.54
5:E:15:LYS:HE2	6:F:48:LEU:HD22	1.89	0.54
14:U:740:GLY:HA3	14:U:744:VAL:HG22	1.89	0.54
17:X:316:ASP:HB3	17:X:317:PRO:HD2	1.88	0.54
25:f:39:LYS:HG3	25:f:85:SER:HA	1.89	0.54
1:A:213:LEU:HA	1:A:319:MET:HB2	1.88	0.54
5:E:270:LEU:HD12	5:E:273:VAL:HB	1.88	0.54
7:G:84:THR:HB	13:M:156:VAL:HG22	1.90	0.54
14:U:503:GLN:HE22	14:U:505:ASP:HB2	1.72	0.54
18:Y:291:HIS:HB2	18:Y:295:TYR:H	1.73	0.54
20:a:372:HIS:HA	20:a:375:LEU:HD12	1.89	0.54
16:W:412:ILE:HD13	20:a:327:VAL:HG11	1.89	0.54
22:c:55:GLY:HA2	22:c:75:MET:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:11:SER:H	10:J:15:HIS:H	1.56	0.54
11:K:85:ALA:HA	11:K:88:LEU:HD13	1.89	0.54
15:V:486:ILE:HG23	19:Z:275:LEU:HD12	1.89	0.54
20:a:110:ALA:HA	20:a:113:LEU:HG	1.89	0.54
14:U:611:ASN:HB3	14:U:614:VAL:HG12	1.88	0.54
20:a:136:GLU:O	20:a:140:GLU:HB3	2.08	0.54
22:c:163:ILE:HD13	22:c:172:HIS:CD2	2.43	0.54
2:B:168:ASP:C	2:B:170:LEU:H	2.16	0.54
4:D:189:GLU:O	4:D:193:GLN:HG2	2.08	0.54
7:G:57:PRO:HD2	7:G:61:LEU:HD12	1.89	0.54
19:Z:19:VAL:HG21	19:Z:124:ILE:HG13	1.89	0.54
22:c:251:LEU:HD21	22:c:284:LEU:HB2	1.90	0.54
5:E:168:LYS:HA	5:E:274:LYS:HD2	1.90	0.54
11:K:51:GLU:HG2	11:K:53:ARG:H	1.72	0.54
20:a:131:THR:HA	20:a:134:THR:HG22	1.89	0.54
9:I:190:LEU:HB3	9:I:236:LEU:HD11	1.90	0.54
25:f:153:SER:H	25:f:156:HIS:HB3	1.72	0.54
2:B:234:LEU:HD21	29:B:501:ADP:H2'	1.89	0.53
3:C:197:THR:HG22	3:C:247:PHE:HE2	1.73	0.53
14:U:82:LEU:HD22	14:U:129:ARG:HB3	1.90	0.53
14:U:418:GLU:O	14:U:422:LEU:HB2	2.08	0.53
3:C:45:LEU:HD13	4:D:58:GLU:HA	1.90	0.53
14:U:713:TYR:O	14:U:717:ILE:HB	2.08	0.53
1:A:187:LEU:HD11	1:A:318:LEU:HD11	1.89	0.53
3:C:85:VAL:HG22	3:C:99:VAL:HG12	1.90	0.53
5:E:247:THR:HG22	5:E:249:ALA:H	1.74	0.53
6:F:365:ILE:HD13	6:F:393:GLY:HA2	1.90	0.53
6:F:387:CYS:HB3	12:L:166:GLN:HG2	1.90	0.53
11:K:31:ILE:HG21	11:K:140:ALA:HB2	1.90	0.53
19:Z:246:VAL:HA	19:Z:250:TYR:CE2	2.43	0.53
25:f:612:LEU:HD21	25:f:636:ASP:HA	1.91	0.53
5:E:313:LEU:HG	5:E:343:LEU:HD13	1.91	0.53
25:f:606:VAL:O	25:f:610:GLN:HB2	2.08	0.53
17:X:342:PHE:HB2	17:X:344:ARG:H	1.74	0.53
17:X:377:ILE:HB	17:X:388:PHE:HE2	1.73	0.53
19:Z:82:PHE:HA	19:Z:85:VAL:HG12	1.91	0.53
2:B:235:LEU:HD12	2:B:353:PHE:HZ	1.74	0.53
6:F:177:VAL:HB	6:F:248:PHE:HB3	1.90	0.53
18:Y:184:GLN:HA	18:Y:187:TYR:HD1	1.74	0.53
1:A:206:ILE:HG23	6:F:373:MET:HG2	1.90	0.53
3:C:44:ARG:HH11	3:C:48:GLN:HG2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:ILE:HD11	14:U:639:LEU:HD23	1.91	0.53
7:G:125:TYR:HB3	7:G:133:PRO:HA	1.91	0.53
8:H:70:LYS:HB2	8:H:71:HIS:NE2	2.24	0.53
18:Y:268:TYR:HB2	18:Y:323:PHE:HA	1.90	0.53
19:Z:260:VAL:HG23	19:Z:261:TYR:HD1	1.74	0.53
22:c:96:LEU:HD12	22:c:105:PRO:HB2	1.90	0.53
16:W:392:PHE:HA	16:W:395:ASN:HD21	1.73	0.53
17:X:345:VAL:HG12	17:X:385:LEU:HB2	1.90	0.53
22:c:211:GLU:C	22:c:213:GLU:H	2.16	0.53
3:C:191:PRO:HD2	3:C:317:PHE:O	2.09	0.53
18:Y:247:LEU:HA	18:Y:250:LEU:HG	1.89	0.53
3:C:197:THR:HG22	3:C:247:PHE:CE2	2.45	0.52
14:U:257:SER:HA	14:U:261:LEU:HD22	1.91	0.52
4:D:406:VAL:HG12	4:D:407:ILE:HG23	1.90	0.52
9:I:136:TYR:HD2	9:I:148:TYR:HB2	1.75	0.52
17:X:407:MET:HB2	18:Y:376:LEU:HD11	1.91	0.52
25:f:688:ARG:O	25:f:692:LEU:HB2	2.09	0.52
16:W:287:VAL:HA	16:W:290:ILE:HG12	1.91	0.52
18:Y:220:VAL:HA	18:Y:223:THR:HG22	1.91	0.52
21:b:23:PRO:O	21:b:24:THR:C	2.53	0.52
18:Y:319:MET:O	18:Y:323:PHE:HB3	2.10	0.52
19:Z:187:LEU:HB3	22:c:293:THR:HG22	1.89	0.52
2:B:54:PRO:HG3	2:B:60:LEU:HB2	1.90	0.52
14:U:701:ILE:HG21	14:U:810:THR:HG23	1.92	0.52
15:V:452:ASN:HD21	23:d:188:LYS:HB2	1.73	0.52
16:W:421:PRO:HG3	19:Z:251:LEU:HD12	1.92	0.52
25:f:419:LEU:HD11	25:f:804:LEU:HD21	1.91	0.52
1:A:373:LEU:HD22	1:A:413:VAL:CG2	2.39	0.52
9:I:119:GLN:O	9:I:123:GLN:HB2	2.09	0.52
17:X:322:HIS:C	17:X:324:ALA:H	2.17	0.52
22:c:32:TYR:HE2	22:c:66:THR:HB	1.75	0.52
22:c:49:VAL:HG13	22:c:50:PRO:HD3	1.90	0.52
3:C:20:LEU:HB3	14:U:153:ILE:HD13	1.92	0.52
14:U:229:VAL:HA	14:U:232:ILE:HG22	1.92	0.52
2:B:281:ILE:HD11	2:B:328:ILE:HD11	1.92	0.52
14:U:188:MET:HE3	14:U:193:PHE:CZ	2.45	0.52
20:a:171:SER:O	20:a:175:ASP:HB2	2.09	0.51
6:F:54:ILE:O	6:F:58:GLU:HB2	2.11	0.51
14:U:265:ILE:HD11	14:U:326:ILE:HG23	1.91	0.51
14:U:437:TYR:HA	14:U:472:ILE:HG21	1.92	0.51
6:F:217:ILE:HG22	6:F:218:GLN:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:71:HIS:HA	8:H:218:PHE:H	1.75	0.51
15:V:484:LEU:HD13	23:d:256:ILE:HD12	1.93	0.51
19:Z:35:VAL:H	19:Z:97:THR:HG22	1.75	0.51
22:c:162:LEU:HD22	22:c:200:TYR:HE2	1.74	0.51
3:C:307:ARG:HH21	3:C:310:ARG:HH22	1.58	0.51
9:I:2:SER:HA	9:I:5:TYR:HB2	1.92	0.51
19:Z:109:ASN:O	19:Z:113:LYS:HB2	2.10	0.51
26:g:208:GLU:O	26:g:212:SER:CB	2.59	0.51
1:A:75:PRO:HA	1:A:79:ASP:HB2	1.91	0.51
1:A:160:THR:HG21	1:A:256:MET:SD	2.51	0.51
2:B:307:ARG:CG	2:B:307:ARG:NH1	2.73	0.51
4:D:312:ASN:HB2	5:E:242:ARG:HH22	1.76	0.51
15:V:395:ILE:HA	15:V:398:LEU:HB2	1.93	0.51
19:Z:232:ASP:HB2	20:a:341:LEU:HD23	1.92	0.51
4:D:293:LEU:HD21	4:D:321:LEU:HD22	1.93	0.51
6:F:283:ILE:HG22	6:F:326:VAL:CG2	2.40	0.51
10:J:13:ASP:HB2	10:J:15:HIS:HE1	1.75	0.51
22:c:231:LEU:HD21	22:c:305:ASP:HB2	1.92	0.51
3:C:366:ALA:HB1	3:C:378:VAL:HG11	1.92	0.51
19:Z:26:ILE:HG23	22:c:103:GLY:HA2	1.93	0.51
20:a:245:VAL:HG21	20:a:300:ALA:HA	1.91	0.51
22:c:195:GLY:C	22:c:197:ASN:H	2.17	0.51
22:c:278:GLN:HG3	22:c:280:PRO:HD2	1.92	0.51
3:C:329:LEU:O	3:C:333:SER:HB3	2.11	0.51
6:F:344:ARG:HD3	6:F:347:ARG:HH11	1.76	0.51
16:W:441:LYS:HA	16:W:444:HIS:CE1	2.46	0.51
19:Z:259:VAL:HG23	22:c:295:ASN:HB2	1.92	0.51
25:f:221:ILE:HG21	25:f:255:VAL:HG11	1.92	0.51
15:V:321:ALA:HB1	15:V:324:PHE:HB3	1.92	0.51
18:Y:379:ARG:HG3	18:Y:379:ARG:HH11	1.76	0.51
15:V:345:ARG:HA	15:V:348:PHE:HD2	1.76	0.51
2:B:286:GLU:HG2	2:B:289:ALA:HB2	1.93	0.50
5:E:61:LEU:HD23	5:E:70:ILE:HG22	1.93	0.50
21:b:138:VAL:O	21:b:168:SER:HA	2.12	0.50
25:f:67:ASP:O	25:f:71:TYR:HB2	2.11	0.50
25:f:323:ASN:HD22	25:f:455:VAL:HA	1.76	0.50
10:J:192:ILE:HD11	10:J:232:ILE:HD11	1.94	0.50
14:U:886:PRO:HA	14:U:889:LEU:HB2	1.94	0.50
22:c:172:HIS:O	22:c:173:GLU:C	2.53	0.50
2:B:264:PRO:HA	2:B:311:GLU:HG2	1.92	0.50
4:D:90:GLY:HA2	4:D:106:THR:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:509:GLY:HA3	14:U:544:ILE:HG13	1.94	0.50
16:W:422:ASN:HA	22:c:234:TYR:HB2	1.93	0.50
18:Y:101:ARG:HG2	18:Y:102:ASP:N	2.20	0.50
1:A:86:THR:HB	2:B:102:LEU:HD13	1.92	0.50
1:A:97:ARG:HH22	1:A:115:VAL:HG13	1.77	0.50
2:B:222:VAL:HB	2:B:349:ARG:CB	2.41	0.50
6:F:439:ALA:HB1	12:L:74:ILE:HG13	1.93	0.50
13:M:116:ALA:HB2	13:M:151:ILE:HD12	1.94	0.50
14:U:736:ILE:HD12	14:U:779:LEU:HD21	1.94	0.50
18:Y:220:VAL:HG11	18:Y:249:VAL:HG21	1.94	0.50
22:c:124:GLY:O	22:c:127:ILE:HG12	2.11	0.50
25:f:253:LEU:HD12	25:f:256:PHE:HB2	1.92	0.50
16:W:397:VAL:HG11	17:X:341:PRO:HA	1.94	0.50
17:X:418:ALA:HB1	18:Y:387:ILE:HG13	1.94	0.50
3:C:25:LEU:HD23	4:D:40:LEU:HD11	1.93	0.50
3:C:232:ARG:O	3:C:232:ARG:HG3	2.11	0.50
4:D:60:TYR:OH	14:U:640:LEU:HD11	2.11	0.50
10:J:108:THR:HG21	10:J:145:TYR:CD1	2.46	0.50
12:L:81:ALA:HB2	12:L:130:VAL:HG21	1.94	0.50
14:U:221:ILE:HD13	14:U:255:SER:HB3	1.94	0.50
15:V:476:PHE:CZ	18:Y:370:ILE:HD12	2.47	0.50
19:Z:15:VAL:HG21	19:Z:50:VAL:HG12	1.93	0.50
14:U:586:VAL:O	14:U:590:TYR:HB2	2.10	0.50
14:U:633:CYS:SG	14:U:659:CYS:HB3	2.52	0.50
15:V:401:ASN:HA	23:d:145:GLU:HG2	1.92	0.50
15:V:479:ARG:HA	15:V:482:PHE:CD1	2.46	0.50
25:f:94:LYS:HG3	25:f:95:PRO:HD3	1.94	0.50
5:E:384:LEU:HG	6:F:340:PRO:HG2	1.94	0.50
26:g:163:GLU:HA	26:g:257:THR:HA	1.93	0.50
1:A:373:LEU:HD11	1:A:409:PHE:HB3	1.94	0.49
11:K:181:LEU:HA	11:K:184:VAL:HG22	1.94	0.49
18:Y:325:VAL:HG23	24:e:59:GLU:HB3	1.94	0.49
20:a:28:LEU:HD22	20:a:33:LEU:HD11	1.92	0.49
22:c:254:ASN:O	22:c:257:LYS:HB3	2.12	0.49
25:f:286:LYS:HG2	25:f:873:LEU:HD12	1.93	0.49
4:D:266:GLU:HG3	5:E:262:ASN:HB2	1.94	0.49
14:U:505:ASP:HB3	14:U:508:THR:HG22	1.92	0.49
14:U:529:ILE:HG21	14:U:556:MET:HE3	1.93	0.49
5:E:364:GLN:HA	5:E:367:PHE:HD2	1.76	0.49
15:V:451:ILE:HG23	15:V:458:VAL:HG22	1.94	0.49
19:Z:257:MET:HB2	19:Z:261:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:263:ALA:HB2	22:c:291:LEU:HD11	1.94	0.49
3:C:31:LEU:HB3	4:D:47:LEU:HD22	1.94	0.49
3:C:233:GLU:HA	3:C:236:VAL:HG22	1.95	0.49
5:E:4:PRO:HB2	5:E:7:LYS:HB2	1.94	0.49
23:d:150:LYS:HA	23:d:153:LEU:HG	1.94	0.49
13:M:134:SER:HB2	13:M:153:PRO:HD3	1.93	0.49
19:Z:263:ALA:HA	22:c:288:VAL:HG22	1.94	0.49
21:b:131:LEU:HB2	21:b:160:LEU:HD21	1.95	0.49
1:A:97:ARG:NH2	1:A:115:VAL:HG13	2.27	0.49
27:A:501:AGS:C4'	2:B:343:ARG:HH22	2.25	0.49
3:C:44:ARG:HG3	15:V:491:VAL:HG22	1.95	0.49
3:C:138:MET:O	3:C:141:GLU:HG2	2.12	0.49
6:F:47:LEU:O	6:F:51:GLU:HB2	2.12	0.49
22:c:61:PHE:CD1	22:c:139:ARG:HD2	2.47	0.49
1:A:312:ARG:HB3	1:A:315:ILE:HB	1.95	0.49
9:I:174:MET:SD	9:I:196:VAL:HG22	2.52	0.49
15:V:323:GLY:HA3	24:e:24:ALA:HA	1.94	0.49
3:C:337:ASN:HD22	3:C:377:HIS:HA	1.77	0.49
4:D:126:PRO:C	4:D:128:ALA:H	2.21	0.49
5:E:136:GLY:O	27:E:501:AGS:N6	2.46	0.49
17:X:397:TYR:HE2	19:Z:254:ASN:HB2	1.78	0.49
21:b:155:ALA:O	21:b:159:THR:HG22	2.13	0.49
14:U:520:MET:HB3	14:U:555:VAL:HG23	1.95	0.49
17:X:407:MET:HA	17:X:410:VAL:HG22	1.95	0.49
25:f:258:LYS:HB2	25:f:769:THR:HG23	1.93	0.49
25:f:688:ARG:HB3	25:f:692:LEU:HD23	1.94	0.49
9:I:122:THR:HG22	9:I:129:PRO:HB3	1.95	0.49
16:W:443:THR:HG21	19:Z:204:LYS:HB3	1.95	0.49
26:g:208:GLU:O	26:g:212:SER:HB2	2.13	0.49
25:f:71:TYR:HA	25:f:74:ALA:HB3	1.95	0.48
3:C:134:LEU:HA	3:C:137:LEU:HD12	1.94	0.48
13:M:77:VAL:HG11	13:M:84:ALA:HB1	1.95	0.48
15:V:486:ILE:HD13	19:Z:271:ALA:HB3	1.94	0.48
2:B:271:PHE:CD1	2:B:315:GLN:HB3	2.48	0.48
3:C:137:LEU:HB3	3:C:223:PHE:CE1	2.48	0.48
4:D:78:GLU:HA	4:D:81:ARG:HG2	1.95	0.48
14:U:819:VAL:HG12	14:U:821:LYS:H	1.77	0.48
16:W:421:PRO:HB3	19:Z:248:ALA:HA	1.95	0.48
17:X:406:ASN:HB3	17:X:407:MET:HE2	1.95	0.48
21:b:58:CYS:HB3	21:b:92:VAL:HG11	1.96	0.48
3:C:49:ARG:HB2	4:D:61:ILE:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:123:GLN:HG2	8:H:81:PRO:HB3	1.94	0.48
8:H:39:LYS:HE2	9:I:57:ASP:CG	2.39	0.48
16:W:359:VAL:HG23	16:W:382:LEU:HD12	1.95	0.48
18:Y:67:VAL:O	18:Y:71:ASN:HB2	2.14	0.48
19:Z:105:ASP:HA	19:Z:108:ILE:HG12	1.94	0.48
22:c:149:GLN:HE22	22:c:155:VAL:HA	1.78	0.48
25:f:294:MET:HE2	25:f:321:MET:HB2	1.95	0.48
14:U:262:SER:O	14:U:265:ILE:HG22	2.12	0.48
14:U:773:PHE:HB2	22:c:177:THR:HB	1.96	0.48
16:W:99:GLN:O	16:W:103:LYS:HG2	2.13	0.48
19:Z:172:VAL:HG13	22:c:217:LEU:HD22	1.94	0.48
21:b:24:THR:O	21:b:25:ARG:C	2.56	0.48
21:b:98:LYS:HE3	26:g:203:SER:O	2.14	0.48
1:A:365:GLU:HG2	1:A:367:ASP:H	1.79	0.48
2:B:293:LYS:HD2	2:B:293:LYS:HA	1.71	0.48
14:U:751:ARG:HG2	14:U:752:THR:HG23	1.96	0.48
14:U:792:ASN:HB3	14:U:914:LEU:HB3	1.95	0.48
17:X:364:LYS:O	17:X:368:MET:HB2	2.13	0.48
25:f:286:LYS:HG3	25:f:881:GLU:HB3	1.96	0.48
25:f:597:VAL:HG21	25:f:612:LEU:HD13	1.95	0.48
4:D:69:LYS:HB2	4:D:69:LYS:HE2	1.57	0.48
16:W:118:LEU:N	16:W:119:PRO:HD2	2.28	0.48
21:b:55:ALA:HA	21:b:82:GLY:HA3	1.94	0.48
22:c:88:ASP:HB3	22:c:91:PHE:HB3	1.96	0.48
25:f:789:SER:HA	25:f:793:VAL:HG13	1.96	0.48
6:F:70:LYS:HA	6:F:73:ILE:HG22	1.96	0.48
7:G:183:VAL:HG12	7:G:184:LYS:HD2	1.96	0.48
10:J:71:MET:HE1	10:J:133:ILE:HG12	1.96	0.48
12:L:72:ILE:HD13	12:L:134:ILE:HG12	1.95	0.48
14:U:616:ARG:HB2	14:U:647:HIS:HB3	1.95	0.48
14:U:633:CYS:HB2	14:U:634:PRO:HD3	1.96	0.48
16:W:427:ASP:O	16:W:431:LYS:HG3	2.13	0.48
25:f:288:VAL:HA	25:f:291:GLN:HB2	1.96	0.48
4:D:64:GLU:OE1	14:U:607:VAL:HG21	2.14	0.48
6:F:433:ALA:C	6:F:435:LEU:H	2.22	0.48
15:V:410:ILE:HG21	15:V:422:ILE:HG13	1.96	0.48
16:W:296:LEU:HD23	16:W:299:ILE:HD13	1.96	0.48
20:a:176:ALA:HB3	20:a:200:LEU:HD21	1.96	0.48
1:A:40:THR:HG21	25:f:136:GLU:HG3	1.95	0.48
1:A:109:PRO:HB2	1:A:125:LEU:H	1.79	0.48
4:D:104:GLY:HA2	4:D:110:ASN:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:26:LEU:HD12	8:H:151:PRO:CD	2.44	0.48
20:a:54:ASP:HB3	20:a:86:GLN:HG3	1.96	0.48
25:f:160:ARG:HH21	25:f:193:PRO:HB2	1.79	0.48
2:B:199:GLU:HA	2:B:203:LEU:HD23	1.96	0.47
4:D:159:LYS:HD2	4:D:221:HIS:HA	1.95	0.47
5:E:322:LYS:HD2	5:E:326:ILE:HG13	1.96	0.47
7:G:9:PHE:HB3	7:G:15:ILE:HD11	1.95	0.47
10:J:4:ASP:HA	10:J:122:ASN:HB3	1.95	0.47
13:M:37:ILE:HD12	13:M:176:ILE:HD11	1.96	0.47
16:W:148:THR:HA	16:W:151:THR:HG22	1.96	0.47
20:a:116:THR:HA	20:a:158:LEU:HD22	1.95	0.47
26:g:144:HIS:HB3	26:g:157:LEU:HA	1.94	0.47
8:H:11:THR:HG22	8:H:19:LEU:HD22	1.96	0.47
11:K:68:VAL:HG21	11:K:89:ILE:HG13	1.96	0.47
16:W:103:LYS:O	16:W:107:GLN:HG2	2.14	0.47
25:f:616:CYS:HB2	25:f:632:LYS:HG3	1.96	0.47
3:C:56:VAL:HG11	4:D:68:LEU:HD22	1.95	0.47
16:W:226:TYR:HD1	16:W:229:LEU:HD13	1.79	0.47
18:Y:144:LEU:HG	18:Y:160:ASN:HB3	1.96	0.47
22:c:125:VAL:HB	26:g:287:GLU:CG	2.43	0.47
15:V:333:ILE:HG21	15:V:360:TYR:HB3	1.95	0.47
19:Z:126:VAL:HA	22:c:216:MET:HE1	1.96	0.47
20:a:22:TRP:HA	20:a:25:LEU:HB3	1.96	0.47
2:B:122:ILE:HD11	2:B:130:GLU:HB3	1.96	0.47
3:C:186:VAL:HB	3:C:292:ILE:HG22	1.97	0.47
4:D:107:THR:HG22	5:E:77:PRO:HG3	1.96	0.47
6:F:241:ALA:HB2	6:F:248:PHE:CE1	2.49	0.47
7:G:183:VAL:HA	7:G:189:TRP:HZ2	1.80	0.47
20:a:173:TYR:HD2	20:a:200:LEU:HD22	1.80	0.47
21:b:100:ARG:HH11	21:b:105:HIS:HB2	1.79	0.47
25:f:739:ALA:O	25:f:743:ALA:CB	2.63	0.47
3:C:44:ARG:CZ	23:d:256:ILE:O	2.63	0.47
3:C:198:LEU:HD11	29:C:501:ADP:H2'	1.96	0.47
11:K:16:SER:CB	11:K:20:ARG:HG2	2.43	0.47
12:L:36:VAL:HG13	12:L:172:LEU:HD11	1.96	0.47
13:M:123:THR:HG22	13:M:130:PRO:HB3	1.96	0.47
14:U:524:LYS:HA	14:U:556:MET:HE1	1.96	0.47
16:W:271:VAL:HG11	16:W:299:ILE:HG21	1.96	0.47
20:a:148:VAL:HG22	20:a:150:SER:H	1.79	0.47
25:f:408:LEU:HD13	25:f:798:THR:HB	1.97	0.47
4:D:123:LEU:O	4:D:126:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:43:ASP:HB2	13:M:218:GLU:HG2	1.97	0.47
16:W:299:ILE:HG22	16:W:301:LYS:H	1.80	0.47
20:a:214:GLY:HA2	20:a:217:LEU:HD13	1.97	0.47
25:f:463:LEU:HB3	25:f:489:TYR:OH	2.14	0.47
3:C:368:MET:HA	3:C:371:LEU:HB3	1.95	0.47
4:D:352:MET:HE1	5:E:163:GLY:O	2.14	0.47
6:F:204:LEU:HG	6:F:212:PHE:HE1	1.79	0.47
12:L:104:PRO:HB2	12:L:107:ARG:HG3	1.97	0.47
20:a:28:LEU:HD13	20:a:36:GLN:HB3	1.95	0.47
26:g:146:PHE:CD2	26:g:150:LEU:HD23	2.50	0.47
6:F:95:GLU:HA	6:F:147:PRO:HG3	1.96	0.47
16:W:172:GLU:HG2	16:W:182:ARG:HE	1.80	0.47
18:Y:275:LEU:HA	18:Y:278:VAL:HG12	1.97	0.47
21:b:107:MET:HB3	21:b:136:VAL:HG13	1.97	0.47
22:c:196:LEU:HD22	22:c:200:TYR:HB2	1.97	0.47
4:D:160:PRO:HG2	4:D:217:LYS:O	2.16	0.46
4:D:282:ASP:HA	4:D:285:VAL:HG23	1.96	0.46
16:W:356:ASN:HA	16:W:359:VAL:HG12	1.97	0.46
17:X:380:GLN:HG2	18:Y:311:TYR:HE1	1.81	0.46
22:c:191:ALA:O	22:c:196:LEU:HB2	2.16	0.46
25:f:384:ALA:HA	25:f:420:TRP:HB2	1.97	0.46
3:C:44:ARG:HD2	3:C:48:GLN:HB2	1.98	0.46
6:F:154:ASN:HB2	6:F:161:LEU:HD11	1.96	0.46
14:U:97:VAL:HA	14:U:100:ILE:HG12	1.97	0.46
14:U:792:ASN:HA	14:U:913:ILE:HB	1.97	0.46
16:W:166:LEU:HD22	16:W:201:ARG:HB3	1.96	0.46
17:X:344:ARG:HA	17:X:385:LEU:O	2.15	0.46
12:L:72:ILE:HD12	12:L:88:MET:HE1	1.96	0.46
15:V:476:PHE:C	15:V:478:GLN:N	2.73	0.46
25:f:218:GLU:HA	25:f:221:ILE:HG12	1.97	0.46
25:f:811:LEU:H	25:f:853:VAL:HG13	1.81	0.46
1:A:35:THR:HG21	25:f:96:LEU:HA	1.96	0.46
3:C:133:PRO:O	3:C:134:LEU:C	2.59	0.46
4:D:373:ALA:HA	27:D:501:AGS:H1'	1.97	0.46
5:E:29:LEU:HB3	6:F:62:VAL:HG11	1.98	0.46
5:E:89:LYS:HA	5:E:92:LEU:HD23	1.97	0.46
16:W:421:PRO:HG3	19:Z:251:LEU:HD13	1.97	0.46
21:b:20:ASP:H	21:b:25:ARG:HB2	1.81	0.46
21:b:22:LEU:HD12	21:b:22:LEU:H	1.81	0.46
1:A:227:ARG:HH11	2:B:320:ASP:H	1.63	0.46
1:A:394:MET:HE1	2:B:219:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:ALA:HB2	2:B:413:LYS:HB3	1.96	0.46
3:C:115:ALA:HB2	3:C:127:LEU:HD21	1.97	0.46
11:K:12:VAL:HB	11:K:23:GLN:HG3	1.97	0.46
25:f:462:ALA:HB1	25:f:466:LEU:HD23	1.96	0.46
3:C:279:GLN:O	3:C:284:GLU:HB2	2.15	0.46
5:E:33:LEU:HD22	6:F:66:LEU:HD13	1.98	0.46
14:U:811:PHE:HZ	14:U:876:GLN:H	1.62	0.46
18:Y:289:ALA:HA	18:Y:292:TYR:CZ	2.50	0.46
22:c:183:HIS:HB2	22:c:184:LEU:HD12	1.98	0.46
25:f:764:LEU:HD21	25:f:771:LEU:HB2	1.98	0.46
2:B:379:THR:HG23	2:B:416:ASN:HD21	1.81	0.46
3:C:147:THR:H	3:C:150:MET:HG2	1.81	0.46
14:U:770:TRP:HA	22:c:179:SER:HB3	1.98	0.46
18:Y:301:ILE:HA	18:Y:304:TYR:HB2	1.98	0.46
22:c:251:LEU:CD2	22:c:284:LEU:HB2	2.45	0.46
7:G:50:ILE:HD13	7:G:79:VAL:HB	1.98	0.46
8:H:8:PHE:CE1	9:I:6:ASP:HA	2.51	0.46
14:U:669:ILE:HA	14:U:672:LEU:HB2	1.98	0.46
15:V:440:LYS:HB3	23:d:146:GLY:HA2	1.96	0.46
16:W:392:PHE:HA	16:W:395:ASN:ND2	2.31	0.46
19:Z:25:ARG:HH11	22:c:103:GLY:HA3	1.81	0.46
23:d:25:ARG:HH12	23:d:61:TRP:HH2	1.64	0.46
25:f:203:GLU:HA	25:f:206:ASP:HB2	1.98	0.46
1:A:306:LEU:HD23	1:A:336:ARG:HB3	1.98	0.46
11:K:217:LEU:HB3	11:K:229:PHE:HB2	1.96	0.46
12:L:72:ILE:CD1	12:L:88:MET:HE1	2.46	0.46
16:W:438:LEU:HD22	19:Z:234:PHE:HB2	1.98	0.46
3:C:206:HIS:C	3:C:208:ASP:H	2.24	0.45
10:J:64:ALA:HA	10:J:70:CYS:HA	1.97	0.45
15:V:486:ILE:HG21	19:Z:271:ALA:HB1	1.97	0.45
17:X:321:THR:OG1	17:X:322:HIS:N	2.49	0.45
20:a:217:LEU:HB3	20:a:238:TYR:HE2	1.80	0.45
21:b:33:VAL:HA	21:b:36:VAL:HG22	1.97	0.45
25:f:641:GLU:HB3	25:f:763:ARG:HH12	1.82	0.45
14:U:45:ILE:HD11	14:U:63:VAL:HG23	1.98	0.45
18:Y:110:TYR:O	18:Y:114:ILE:HB	2.16	0.45
18:Y:347:ILE:HG23	18:Y:354:VAL:HG22	1.98	0.45
20:a:138:VAL:HG11	20:a:155:PHE:HB2	1.98	0.45
22:c:277:LYS:HD2	22:c:277:LYS:HA	1.69	0.45
25:f:217:LEU:HD22	25:f:250:ARG:HE	1.82	0.45
25:f:524:MET:HB3	25:f:564:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:176:LYS:HG3	26:g:270:VAL:HG12	1.99	0.45
1:A:219:GLY:HA2	2:B:343:ARG:HH11	1.82	0.45
1:A:303:ILE:HD13	1:A:331:LEU:CD2	2.45	0.45
14:U:265:ILE:HB	14:U:329:LEU:HD22	1.98	0.45
15:V:476:PHE:CE2	18:Y:373:GLY:HA3	2.51	0.45
18:Y:43:ALA:O	18:Y:49:ASN:ND2	2.49	0.45
25:f:637:LYS:HB2	25:f:677:HIS:ND1	2.31	0.45
5:E:193:CYS:SG	5:E:194:ASN:N	2.90	0.45
6:F:134:LEU:HD12	6:F:134:LEU:HA	1.85	0.45
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.98	0.45
14:U:757:MET:HA	14:U:760:VAL:HG12	1.98	0.45
19:Z:173:GLU:O	19:Z:177:ARG:N	2.50	0.45
20:a:76:LEU:O	20:a:80:ILE:HG12	2.16	0.45
25:f:570:GLY:HA2	25:f:599:ALA:HB1	1.99	0.45
26:g:272:ALA:O	26:g:273:THR:C	2.58	0.45
2:B:149:SER:OG	2:B:163:LEU:HB2	2.17	0.45
2:B:350:LYS:H	2:B:350:LYS:HG2	1.50	0.45
5:E:234:GLU:HB2	6:F:311:LEU:HD13	1.98	0.45
6:F:319:GLY:O	6:F:320:PHE:C	2.59	0.45
8:H:22:ILE:HD12	8:H:22:ILE:HA	1.79	0.45
14:U:489:ALA:HA	14:U:520:MET:HE2	1.98	0.45
15:V:451:ILE:HG13	15:V:458:VAL:HG13	1.97	0.45
17:X:312:GLU:O	17:X:320:SER:HB3	2.17	0.45
5:E:280:ASN:HB3	6:F:295:ARG:HH22	1.82	0.45
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.98	0.45
14:U:61:ALA:HB3	14:U:84:ALA:HB2	1.99	0.45
15:V:487:HIS:O	15:V:491:VAL:HG23	2.16	0.45
19:Z:148:GLY:HA2	20:a:181:GLY:HA2	1.98	0.45
6:F:365:ILE:HG21	6:F:393:GLY:HA2	1.99	0.45
9:I:8:ARG:HD2	9:I:11:ILE:HG21	1.99	0.45
18:Y:247:LEU:O	18:Y:251:HIS:HB3	2.17	0.45
19:Z:69:PHE:HD1	21:b:60:VAL:HG11	1.82	0.45
26:g:138:LEU:HD23	26:g:138:LEU:HA	1.80	0.45
2:B:189:GLY:HA3	2:B:360:THR:HG22	1.98	0.45
2:B:256:ILE:HD12	2:B:305:ILE:HD12	1.99	0.45
4:D:167:ILE:HB	4:D:174:LYS:NZ	2.32	0.45
11:K:200:ILE:HD12	11:K:200:ILE:HA	1.86	0.45
22:c:122:LEU:HD12	22:c:126:ASP:HB3	1.97	0.45
25:f:253:LEU:HB3	25:f:256:PHE:HB2	1.98	0.45
2:B:380:LEU:HD13	2:B:383:LEU:HD12	1.97	0.45
3:C:380:GLN:HA	3:C:383:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:LEU:CB	19:Z:184:VAL:HG12	2.40	0.45
4:D:85:ILE:HB	4:D:86:PRO:HD3	1.99	0.45
6:F:176:GLU:HA	6:F:249:LEU:HD12	1.98	0.45
12:L:69:HIS:CE1	12:L:102:PRO:HB3	2.52	0.45
16:W:406:VAL:HG22	17:X:342:PHE:HB3	1.99	0.45
17:X:351:SER:HA	17:X:354:ILE:HG22	1.99	0.45
20:a:84:VAL:HA	20:a:87:MET:HG3	1.98	0.45
20:a:324:ILE:HG13	20:a:331:VAL:HG13	1.98	0.45
22:c:94:LYS:O	22:c:98:MET:HB3	2.17	0.45
25:f:763:ARG:HE	25:f:770:HIS:HB3	1.81	0.45
2:B:228:PRO:HB3	3:C:307:ARG:HH11	1.82	0.44
2:B:346:ARG:HE	2:B:346:ARG:HA	1.82	0.44
10:J:217:LEU:HD12	10:J:218:LYS:N	2.33	0.44
19:Z:78:MET:HE1	22:c:94:LYS:HG2	1.98	0.44
19:Z:212:LEU:HA	19:Z:215:VAL:HG12	1.99	0.44
19:Z:257:MET:O	19:Z:261:TYR:N	2.49	0.44
23:d:9:TRP:HE1	23:d:25:ARG:HD3	1.82	0.44
3:C:32:GLN:O	3:C:33:LEU:C	2.60	0.44
3:C:287:LYS:H	3:C:289:ILE:HD12	1.83	0.44
8:H:65:VAL:HG22	8:H:75:VAL:HG22	1.99	0.44
10:J:212:ARG:HD2	10:J:215:GLN:CD	2.43	0.44
12:L:44:ALA:HB2	12:L:142:PRO:HB3	1.99	0.44
13:M:176:ILE:HD13	13:M:196:ILE:HD13	1.99	0.44
15:V:283:ASN:HB3	24:e:19:PHE:HE1	1.80	0.44
15:V:489:MET:HE2	18:Y:388:ASN:HB3	2.00	0.44
19:Z:263:ALA:CB	22:c:288:VAL:HG13	2.42	0.44
25:f:10:PRO:HB2	25:f:59:LEU:HG	1.99	0.44
3:C:138:MET:HE3	3:C:138:MET:HB3	1.63	0.44
4:D:404:LYS:HA	4:D:408:LYS:HB2	1.98	0.44
14:U:656:LEU:HD13	14:U:656:LEU:HA	1.80	0.44
19:Z:176:LEU:HD23	22:c:214:GLN:NE2	2.32	0.44
19:Z:254:ASN:O	19:Z:257:MET:HG2	2.17	0.44
22:c:270:LEU:HG	22:c:274:ASN:HB3	1.98	0.44
4:D:169:GLY:O	4:D:170:MET:C	2.59	0.44
7:G:60:LEU:HD21	13:M:177:GLU:HA	1.97	0.44
8:H:26:LEU:HD12	8:H:151:PRO:HG2	1.99	0.44
13:M:49:VAL:HB	13:M:212:GLU:HB3	1.99	0.44
14:U:765:VAL:HG11	14:U:778:PHE:CD1	2.53	0.44
17:X:338:VAL:HG11	17:X:353:LEU:HD21	1.99	0.44
19:Z:241:SER:C	19:Z:243:GLN:N	2.73	0.44
19:Z:248:ALA:HA	19:Z:251:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:31:VAL:HG22	22:c:67:VAL:HG13	2.00	0.44
22:c:61:PHE:CE1	22:c:139:ARG:HD2	2.52	0.44
22:c:163:ILE:HD13	22:c:172:HIS:NE2	2.33	0.44
1:A:143:ASP:HB3	1:A:147:TYR:H	1.82	0.44
1:A:324:PRO:HA	1:A:327:LEU:HD23	1.98	0.44
5:E:287:PRO:HA	5:E:290:LEU:HB2	1.99	0.44
15:V:490:SER:HA	15:V:493:ALA:HB3	1.99	0.44
19:Z:164:ALA:HB2	22:c:220:LEU:HD13	2.00	0.44
25:f:637:LYS:HB3	25:f:678:LEU:HD13	1.99	0.44
14:U:780:SER:HA	14:U:783:TYR:CE2	2.52	0.44
19:Z:55:ALA:HB3	22:c:102:THR:HG23	2.00	0.44
19:Z:259:VAL:HG12	19:Z:260:VAL:HG13	1.99	0.44
22:c:303:MET:HB3	23:d:236:THR:HG22	1.99	0.44
25:f:323:ASN:HD21	25:f:420:TRP:CG	2.35	0.44
25:f:606:VAL:O	25:f:610:GLN:CB	2.66	0.44
1:A:109:PRO:HB3	1:A:125:LEU:HB3	1.99	0.44
2:B:56:THR:HG23	2:B:58:CYS:HB2	1.99	0.44
3:C:235:PHE:HB3	3:C:239:ARG:HB2	2.00	0.44
15:V:452:ASN:HB3	15:V:457:TYR:HB2	2.00	0.44
18:Y:363:ASN:HA	18:Y:366:TYR:HB3	1.99	0.44
20:a:293:PHE:HA	20:a:296:ILE:HD13	2.00	0.44
2:B:386:ALA:O	2:B:423:LYS:HE3	2.18	0.44
5:E:4:PRO:O	5:E:8:ALA:HB2	2.18	0.44
17:X:361:VAL:O	17:X:365:LEU:HB2	2.18	0.44
22:c:119:GLY:HA3	22:c:121:TRP:CD1	2.53	0.44
26:g:214:PRO:HG3	26:g:217:ALA:HB2	1.99	0.44
1:A:303:ILE:HD13	1:A:331:LEU:HD23	2.00	0.44
3:C:63:LEU:HD22	3:C:66:LEU:HD12	2.00	0.44
14:U:623:GLY:O	14:U:627:PHE:HB3	2.18	0.44
14:U:693:LEU:HB3	14:U:736:ILE:HD13	2.00	0.44
16:W:196:VAL:HG13	16:W:198:ASP:H	1.83	0.44
18:Y:212:GLU:HG2	18:Y:213:LEU:HG	2.00	0.44
1:A:390:THR:HG22	2:B:216:ILE:HG23	1.99	0.43
4:D:202:VAL:HG23	4:D:329:ARG:HB2	1.99	0.43
12:L:157:ARG:HG2	13:M:59:GLU:OE2	2.18	0.43
17:X:299:LEU:HD22	17:X:331:LEU:HD12	2.00	0.43
18:Y:74:LYS:HG3	18:Y:75:LYS:N	2.31	0.43
25:f:55:GLU:O	25:f:59:LEU:N	2.50	0.43
25:f:315:GLU:O	25:f:319:GLU:HB2	2.18	0.43
1:A:277:ILE:HD11	1:A:319:MET:HE3	1.99	0.43
3:C:100:ASP:H	3:C:123:LEU:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:234:GLU:HG3	6:F:311:LEU:HB3	2.00	0.43
8:H:134:LEU:HB2	8:H:149:SER:HB3	2.00	0.43
15:V:212:TYR:HA	15:V:253:LEU:HD11	2.00	0.43
17:X:391:PRO:HB2	17:X:393:VAL:HG22	1.99	0.43
19:Z:99:PRO:HA	19:Z:123:ILE:HG21	2.00	0.43
20:a:206:LEU:HD23	20:a:206:LEU:HA	1.87	0.43
25:f:262:PHE:HD1	25:f:568:GLY:HA2	1.84	0.43
25:f:272:LEU:HA	25:f:275:MET:HE3	2.00	0.43
3:C:32:GLN:HE21	3:C:32:GLN:HA	1.84	0.43
4:D:167:ILE:HB	4:D:174:LYS:HZ2	1.82	0.43
5:E:8:ALA:HA	6:F:44:ARG:HH12	1.82	0.43
16:W:144:ARG:NH2	16:W:145:LEU:HB2	2.33	0.43
16:W:200:ILE:HD12	16:W:200:ILE:H	1.82	0.43
19:Z:255:ASP:HA	19:Z:258:VAL:HG22	2.00	0.43
25:f:713:PHE:HB2	25:f:752:HIS:CE1	2.54	0.43
2:B:307:ARG:HH11	2:B:307:ARG:HG2	1.84	0.43
5:E:194:ASN:HB2	5:E:228:CYS:SG	2.59	0.43
7:G:80:MET:HE3	7:G:82:GLY:H	1.83	0.43
15:V:472:PRO:HB2	19:Z:256:GLN:HE22	1.81	0.43
15:V:483:CYS:O	15:V:487:HIS:ND1	2.50	0.43
18:Y:369:THR:HG22	19:Z:261:TYR:HD2	1.82	0.43
20:a:123:LEU:HD11	20:a:161:LYS:HB3	2.00	0.43
22:c:196:LEU:HA	22:c:200:TYR:HB2	2.00	0.43
1:A:249:TYR:HB3	6:F:259:MET:HB2	1.99	0.43
1:A:403:ILE:H	1:A:403:ILE:HG13	1.69	0.43
5:E:309:ARG:HG2	5:E:343:LEU:HD11	2.00	0.43
9:I:187:LYS:HD2	9:I:187:LYS:HA	1.75	0.43
14:U:177:LEU:H	14:U:177:LEU:HG	1.65	0.43
18:Y:133:ALA:HB3	18:Y:136:HIS:HB2	2.00	0.43
18:Y:169:GLU:CD	18:Y:169:GLU:H	2.27	0.43
18:Y:216:TYR:O	18:Y:220:VAL:HG13	2.19	0.43
19:Z:250:TYR:OH	23:d:234:ASP:HA	2.19	0.43
20:a:115:LYS:HA	20:a:118:ILE:HG22	2.00	0.43
2:B:313:LEU:HD22	2:B:316:LEU:HD11	1.99	0.43
5:E:12:TYR:O	5:E:16:LEU:HB2	2.17	0.43
9:I:136:TYR:HB2	9:I:148:TYR:HD2	1.83	0.43
14:U:789:ILE:HG12	14:U:881:PRO:HA	2.01	0.43
17:X:415:TYR:HD1	18:Y:379:ARG:NH1	2.16	0.43
21:b:156:PHE:O	21:b:160:LEU:HB2	2.18	0.43
21:b:174:PRO:HB2	21:b:178:SER:HB3	1.99	0.43
2:B:208:PRO:O	2:B:209:GLU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:LEU:HD13	4:D:73:LEU:HA	1.64	0.43
6:F:311:LEU:HD23	6:F:314:LEU:HD12	2.01	0.43
17:X:385:LEU:HD23	17:X:385:LEU:HA	1.80	0.43
17:X:397:TYR:HA	19:Z:257:MET:HE1	2.01	0.43
20:a:293:PHE:HB2	20:a:329:LYS:CB	2.46	0.43
25:f:717:ALA:HB2	25:f:760:PHE:HB2	2.01	0.43
3:C:338:LEU:HD22	3:C:342:ILE:HG21	2.01	0.43
5:E:341:ALA:HB2	27:E:501:AGS:H5'2	2.01	0.43
11:K:22:PHE:HB3	11:K:26:TYR:CE2	2.54	0.43
11:K:197:SER:O	11:K:200:ILE:HG22	2.19	0.43
12:L:19:ILE:HG22	12:L:22:ILE:H	1.82	0.43
14:U:9:ILE:HD12	14:U:9:ILE:H	1.83	0.43
15:V:131:LEU:HD22	15:V:171:VAL:HG11	2.00	0.43
16:W:412:ILE:HD13	20:a:327:VAL:CG1	2.49	0.43
17:X:309:TYR:O	17:X:313:LEU:HB2	2.18	0.43
22:c:32:TYR:CE2	22:c:66:THR:HB	2.54	0.43
22:c:122:LEU:N	22:c:196:LEU:HD11	2.25	0.43
23:d:26:LEU:O	23:d:30:LEU:HB2	2.19	0.43
25:f:79:ARG:O	25:f:83:ARG:HB2	2.17	0.43
25:f:264:GLU:HG3	25:f:529:SER:H	1.84	0.43
3:C:90:HIS:N	3:C:91:PRO:HD2	2.33	0.43
3:C:100:ASP:HB3	3:C:103:ILE:HG13	2.01	0.43
5:E:50:LEU:HD22	6:F:80:ILE:HD13	2.00	0.43
5:E:177:GLY:N	6:F:344:ARG:HD2	2.34	0.43
6:F:266:LYS:HA	6:F:269:ARG:HB2	1.99	0.43
8:H:29:VAL:HG21	8:H:151:PRO:HG3	2.01	0.43
8:H:118:MET:HG2	8:H:130:PHE:HD2	1.84	0.43
14:U:558:GLY:H	14:U:589:ALA:HA	1.84	0.43
16:W:30:GLU:O	16:W:34:LEU:HB2	2.19	0.43
16:W:120:ILE:HG13	16:W:121:LYS:N	2.31	0.43
16:W:452:ILE:HD12	16:W:455:LEU:HD13	2.00	0.43
18:Y:259:TYR:HB2	18:Y:274:SER:HB2	2.01	0.43
20:a:118:ILE:O	20:a:122:LYS:HB2	2.19	0.43
2:B:316:LEU:HB2	2:B:346:ARG:HD2	2.00	0.43
4:D:93:LEU:HD12	4:D:102:ILE:HG12	2.00	0.43
14:U:685:GLN:HG3	14:U:729:GLY:HA3	2.01	0.43
15:V:169:LEU:HD12	15:V:169:LEU:HA	1.91	0.43
17:X:322:HIS:C	17:X:324:ALA:N	2.76	0.43
17:X:346:GLN:HG2	17:X:384:VAL:HG22	2.01	0.43
17:X:377:ILE:CG2	17:X:386:ILE:HB	2.45	0.43
26:g:194:VAL:HB	26:g:218:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:LEU:CD1	2:B:353:PHE:HZ	2.32	0.42
5:E:210:GLU:H	5:E:210:GLU:HG3	1.62	0.42
6:F:344:ARG:HH21	6:F:346:GLY:HA3	1.84	0.42
10:J:40:ILE:HD13	10:J:184:ASP:HB2	2.00	0.42
10:J:50:VAL:HB	10:J:54:GLN:HB2	2.00	0.42
18:Y:144:LEU:HA	18:Y:147:ILE:HG22	2.01	0.42
27:A:501:AGS:H4'	2:B:343:ARG:HH22	1.84	0.42
9:I:8:ARG:HG3	9:I:11:ILE:HD13	2.01	0.42
11:K:206:MET:HG3	11:K:210:LEU:HB2	2.01	0.42
12:L:71:GLY:HA3	12:L:221:PHE:CZ	2.54	0.42
14:U:620:GLU:O	14:U:658:ILE:HD11	2.19	0.42
18:Y:282:MET:O	18:Y:288:PHE:HB2	2.19	0.42
19:Z:68:TRP:HZ3	19:Z:111:LEU:HD13	1.85	0.42
22:c:54:MET:HA	22:c:113:HIS:HA	2.00	0.42
25:f:288:VAL:HG11	25:f:879:ARG:HB2	2.01	0.42
21:b:26:LEU:HD13	21:b:26:LEU:HA	1.92	0.42
1:A:33:LEU:HD13	1:A:36:TYR:HD1	1.85	0.42
10:J:22:ALA:HB1	10:J:128:GLY:HA2	2.02	0.42
14:U:220:LEU:HD23	14:U:220:LEU:HA	1.85	0.42
1:A:26:ASP:HB2	1:A:29:ASP:HB2	2.02	0.42
1:A:227:ARG:HD3	2:B:320:ASP:H	1.85	0.42
2:B:237:LYS:HE2	3:C:282:GLY:HA2	2.01	0.42
2:B:283:PHE:HD1	2:B:328:ILE:HB	1.84	0.42
2:B:347:ILE:HG22	2:B:350:LYS:HD3	2.01	0.42
14:U:191:LYS:H	14:U:191:LYS:HG2	1.63	0.42
16:W:429:SER:HA	22:c:231:LEU:HD12	2.02	0.42
20:a:14:SER:HA	20:a:50:PHE:HE2	1.84	0.42
25:f:637:LYS:HD2	25:f:678:LEU:HD22	2.00	0.42
2:B:364:ILE:HD13	2:B:364:ILE:HA	1.84	0.42
5:E:180:LYS:H	5:E:180:LYS:HG3	1.65	0.42
6:F:217:ILE:HD13	6:F:217:ILE:HA	1.85	0.42
11:K:32:LYS:C	11:K:34:GLY:H	2.27	0.42
14:U:384:GLN:HG2	14:U:385:PHE:HD1	1.84	0.42
18:Y:66:ASP:HB3	18:Y:70:LEU:HD12	2.01	0.42
18:Y:209:THR:HA	18:Y:213:LEU:HD12	2.01	0.42
18:Y:266:CYS:HB3	18:Y:268:TYR:CZ	2.55	0.42
18:Y:359:PRO:HG2	18:Y:364:TRP:HB2	2.02	0.42
21:b:8:VAL:H	21:b:51:LEU:HA	1.84	0.42
2:B:171:VAL:HG12	2:B:273:VAL:HG13	2.02	0.42
7:G:113:MET:O	7:G:117:ARG:HG2	2.20	0.42
10:J:208:LEU:HD22	10:J:220:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:101:ILE:O	14:U:105:ILE:HG12	2.19	0.42
16:W:144:ARG:HH22	16:W:145:LEU:HD13	1.84	0.42
17:X:397:TYR:CE2	19:Z:254:ASN:HB2	2.55	0.42
18:Y:223:THR:HA	18:Y:226:VAL:HG12	2.01	0.42
20:a:57:ILE:HG13	20:a:61:GLU:HG2	2.02	0.42
22:c:231:LEU:CD2	22:c:302:ALA:HA	2.49	0.42
26:g:146:PHE:O	26:g:150:LEU:HG	2.19	0.42
4:D:214:MET:HB2	4:D:217:LYS:HE2	2.02	0.42
5:E:81:VAL:HG12	5:E:105:LEU:HB3	2.02	0.42
6:F:140:VAL:HG11	6:F:160:ILE:HG22	2.01	0.42
14:U:201:LEU:O	14:U:204:ILE:HG22	2.20	0.42
18:Y:268:TYR:HA	18:Y:271:PHE:HB3	2.01	0.42
21:b:84:ILE:HD12	21:b:84:ILE:H	1.85	0.42
26:g:185:PRO:HG2	26:g:189:GLN:HB2	2.02	0.42
5:E:173:TYR:CD2	5:E:282:PRO:HG3	2.55	0.42
7:G:9:PHE:CB	7:G:15:ILE:HD11	2.50	0.42
14:U:624:PHE:CD1	14:U:658:ILE:HD12	2.54	0.42
15:V:81:GLN:HB3	15:V:93:PHE:HB3	2.02	0.42
15:V:337:LEU:HD22	15:V:367:VAL:HG11	2.02	0.42
20:a:42:LEU:HD12	20:a:47:ASP:H	1.85	0.42
25:f:56:LEU:HD12	25:f:56:LEU:H	1.85	0.42
25:f:168:LYS:O	25:f:172:GLU:HB2	2.19	0.42
4:D:41:TYR:CD2	14:U:152:GLY:HA2	2.55	0.42
5:E:145:LEU:HA	5:E:148:VAL:HG12	2.02	0.42
5:E:172:LEU:HD23	5:E:299:ILE:HB	2.01	0.42
12:L:84:LEU:HD23	12:L:132:LEU:HD11	2.02	0.42
14:U:411:ILE:HD12	14:U:411:ILE:HA	1.86	0.42
14:U:554:LEU:HD12	14:U:554:LEU:HA	1.83	0.42
16:W:428:TRP:CZ3	22:c:231:LEU:HD13	2.55	0.42
18:Y:19:ILE:HD12	18:Y:19:ILE:HA	1.88	0.42
18:Y:69:LEU:O	18:Y:73:MET:HG2	2.20	0.42
18:Y:111:LEU:HD23	18:Y:115:GLY:HA3	2.00	0.42
2:B:172:THR:HA	2:B:175:LYS:HB3	2.02	0.41
3:C:328:ILE:HD11	29:C:501:ADP:N6	2.34	0.41
4:D:272:THR:HG21	5:E:251:ARG:HD3	2.02	0.41
6:F:225:MET:HB3	6:F:352:ILE:HB	2.02	0.41
11:K:197:SER:O	11:K:201:ILE:HG13	2.20	0.41
14:U:130:LEU:O	14:U:133:ILE:HG12	2.20	0.41
14:U:173:VAL:HB	14:U:176:MET:HG2	2.00	0.41
14:U:766:PHE:CE1	14:U:779:LEU:HD22	2.55	0.41
19:Z:259:VAL:HG12	19:Z:260:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:107:LEU:HD11	23:d:140:GLU:HB2	2.02	0.41
23:d:179:ALA:HA	23:d:215:TRP:HE1	1.85	0.41
25:f:225:ALA:HB1	25:f:644:ALA:HA	2.01	0.41
25:f:257:ARG:HA	25:f:260:SER:HB3	2.02	0.41
25:f:286:LYS:HE3	25:f:872:VAL:HG23	2.02	0.41
1:A:241:ILE:HB	1:A:244:GLU:HB2	2.02	0.41
4:D:60:TYR:HE2	14:U:640:LEU:HD21	1.85	0.41
18:Y:69:LEU:HD12	18:Y:70:LEU:HG	2.01	0.41
18:Y:365:GLN:HA	18:Y:368:GLU:HB2	2.01	0.41
19:Z:67:VAL:HG12	21:b:95:LEU:HD13	2.02	0.41
20:a:57:ILE:HD12	20:a:57:ILE:HA	1.86	0.41
22:c:211:GLU:C	22:c:213:GLU:N	2.78	0.41
23:d:74:TYR:HA	23:d:77:GLN:OE1	2.20	0.41
25:f:217:LEU:HD13	25:f:250:ARG:HD2	2.03	0.41
3:C:20:LEU:HB3	14:U:153:ILE:CD1	2.50	0.41
3:C:224:ILE:HG12	3:C:233:GLU:HG3	2.02	0.41
10:J:155:ALA:HB3	11:K:60:GLU:HB2	2.02	0.41
14:U:17:PRO:O	14:U:21:GLU:HG2	2.20	0.41
14:U:142:LEU:HD23	14:U:142:LEU:HA	1.85	0.41
14:U:177:LEU:HD12	14:U:178:ALA:N	2.36	0.41
15:V:109:ASN:HB2	15:V:112:VAL:HG23	2.02	0.41
22:c:83:SER:CB	26:g:287:GLU:HB2	2.49	0.41
25:f:87:THR:O	25:f:91:SER:HB2	2.20	0.41
26:g:198:ILE:HG21	26:g:241:VAL:HG22	2.02	0.41
1:A:327:LEU:HD12	1:A:331:LEU:HD12	2.01	0.41
4:D:130:VAL:HG12	4:D:142:VAL:HG22	2.02	0.41
6:F:310:MET:HE3	6:F:310:MET:HB3	1.90	0.41
10:J:134:VAL:HA	10:J:144:LEU:HA	2.02	0.41
14:U:554:LEU:HD11	14:U:761:VAL:HG13	2.02	0.41
21:b:107:MET:HB2	21:b:136:VAL:HA	2.02	0.41
22:c:159:ALA:HB3	22:c:203:ILE:HG23	2.02	0.41
22:c:302:ALA:O	22:c:306:THR:HG23	2.20	0.41
23:d:179:ALA:O	23:d:183:GLU:HB2	2.20	0.41
3:C:39:SER:O	3:C:43:ARG:HB2	2.20	0.41
3:C:197:THR:N	29:C:501:ADP:O1A	2.52	0.41
4:D:87:LEU:HB3	5:E:80:VAL:HB	2.02	0.41
5:E:295:LEU:HA	5:E:295:LEU:HD23	1.82	0.41
13:M:39:ILE:HG21	13:M:189:ILE:HD12	2.02	0.41
14:U:153:ILE:O	14:U:157:THR:HB	2.21	0.41
14:U:543:LYS:HE3	14:U:546:ARG:HH21	1.86	0.41
14:U:639:LEU:HD12	14:U:639:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:71:THR:HG22	15:V:107:ARG:HH21	1.86	0.41
18:Y:30:GLU:O	18:Y:34:ASP:HB3	2.20	0.41
18:Y:311:TYR:CG	18:Y:314:LEU:HD12	2.54	0.41
19:Z:144:VAL:HG23	19:Z:145:HIS:H	1.85	0.41
19:Z:245:PHE:HB3	19:Z:249:PHE:HB3	2.02	0.41
22:c:125:VAL:HB	26:g:287:GLU:HG3	2.01	0.41
23:d:256:ILE:HD13	23:d:256:ILE:HA	1.80	0.41
26:g:163:GLU:HB2	26:g:258:THR:HG23	2.02	0.41
3:C:136:SER:HA	3:C:139:MET:HB2	2.01	0.41
6:F:362:ARG:NH1	6:F:389:ASP:HA	2.35	0.41
9:I:76:VAL:HG11	9:I:83:ALA:HB1	2.01	0.41
14:U:801:GLN:HB3	14:U:877:LEU:HD12	2.01	0.41
15:V:489:MET:HE2	18:Y:388:ASN:HD22	1.85	0.41
17:X:346:GLN:HA	17:X:384:VAL:HA	2.02	0.41
19:Z:55:ALA:HB3	22:c:102:THR:CG2	2.50	0.41
23:d:103:LEU:HA	23:d:103:LEU:HD12	1.71	0.41
23:d:193:GLU:HA	23:d:197:ILE:HG23	2.02	0.41
25:f:293:GLN:HG2	25:f:772:GLY:H	1.86	0.41
2:B:317:ASP:OD2	2:B:343:ARG:NH2	2.53	0.41
14:U:838:LYS:O	14:U:842:LYS:HG3	2.21	0.41
15:V:251:LEU:O	15:V:255:LEU:HG	2.20	0.41
16:W:209:ILE:HA	16:W:209:ILE:HD13	1.83	0.41
17:X:317:PRO:O	17:X:321:THR:HB	2.20	0.41
18:Y:376:LEU:HD23	18:Y:376:LEU:HA	1.84	0.41
19:Z:15:VAL:O	19:Z:19:VAL:HG23	2.21	0.41
1:A:362:MET:HG2	2:B:215:GLY:O	2.20	0.41
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.36	0.41
4:D:275:PHE:HB2	5:E:251:ARG:NH2	2.36	0.41
9:I:105:ILE:HD13	9:I:110:LEU:HD13	2.03	0.41
14:U:191:LYS:O	14:U:192:GLN:C	2.63	0.41
14:U:619:VAL:HG11	14:U:648:VAL:HA	2.02	0.41
15:V:486:ILE:HG12	19:Z:272:LEU:HD23	2.01	0.41
16:W:231:ILE:HB	16:W:243:ILE:HG22	2.02	0.41
16:W:373:ILE:HG22	16:W:374:THR:N	2.36	0.41
22:c:46:ARG:O	22:c:46:ARG:HG2	2.20	0.41
23:d:196:ARG:HH21	23:d:206:MET:HG2	1.86	0.41
25:f:682:GLY:HA3	25:f:719:PRO:HA	2.03	0.41
1:A:243:SER:O	1:A:246:VAL:HG12	2.20	0.41
6:F:288:LEU:HD22	6:F:330:ALA:HB1	2.02	0.41
10:J:12:PRO:HA	11:K:26:TYR:CE1	2.55	0.41
10:J:41:VAL:HG23	10:J:211:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:41:VAL:O	10:J:211:MET:HE2	2.21	0.41
10:J:45:VAL:HG11	10:J:61:LYS:HB2	2.02	0.41
11:K:32:LYS:C	11:K:34:GLY:N	2.79	0.41
14:U:87:LEU:HA	14:U:90:VAL:HB	2.03	0.41
14:U:744:VAL:HG21	14:U:783:TYR:HB3	2.03	0.41
14:U:764:LEU:HD12	14:U:764:LEU:HA	1.91	0.41
17:X:419:LYS:NZ	18:Y:387:ILE:HD11	2.36	0.41
19:Z:18:SER:HB2	22:c:36:LEU:HD11	2.02	0.41
20:a:33:LEU:HD12	20:a:35:HIS:H	1.85	0.41
20:a:280:MET:SD	20:a:296:ILE:HG13	2.61	0.41
23:d:119:LEU:HD21	23:d:137:VAL:HG11	2.02	0.41
25:f:114:ALA:HB3	25:f:162:LEU:HD11	2.03	0.41
25:f:378:ASN:HD21	25:f:390:LEU:HD21	1.86	0.41
25:f:523:GLY:HA3	25:f:561:GLY:HA2	2.03	0.41
1:A:32:LEU:HD21	25:f:57:GLU:HB3	2.03	0.41
1:A:35:THR:HA	1:A:38:GLN:HG2	2.01	0.41
2:B:225:TYR:CB	2:B:331:THR:H	2.32	0.41
2:B:287:ILE:HD12	2:B:287:ILE:H	1.86	0.41
7:G:153:LYS:HB3	7:G:163:PHE:CE2	2.56	0.41
12:L:45:VAL:HG12	12:L:214:ILE:HG12	2.02	0.41
14:U:641:SER:HB2	14:U:675:MET:HE2	2.02	0.41
16:W:251:TYR:HE2	16:W:267:LEU:HD22	1.86	0.41
18:Y:229:ILE:HD13	18:Y:229:ILE:HA	1.91	0.41
20:a:81:LEU:HA	20:a:84:VAL:HG12	2.02	0.41
26:g:211:ARG:O	26:g:211:ARG:HG2	2.17	0.41
1:A:111:TYR:OH	1:A:134:ILE:HD13	2.21	0.40
4:D:42:SER:HA	14:U:187:LEU:HD21	2.03	0.40
5:E:302:ASP:OD1	5:E:302:ASP:N	2.54	0.40
6:F:189:GLY:HA3	27:F:501:AGS:N1	2.35	0.40
14:U:197:VAL:O	14:U:201:LEU:N	2.54	0.40
19:Z:20:VAL:HG11	22:c:213:GLU:HB3	2.03	0.40
19:Z:260:VAL:C	19:Z:262:LEU:H	2.29	0.40
11:K:31:ILE:HG21	11:K:140:ALA:CB	2.52	0.40
17:X:322:HIS:O	17:X:324:ALA:N	2.41	0.40
18:Y:343:LEU:O	18:Y:343:LEU:HG	2.21	0.40
18:Y:376:LEU:O	18:Y:380:VAL:HG12	2.21	0.40
22:c:41:MET:HB3	22:c:145:VAL:HG21	2.03	0.40
25:f:292:LYS:HZ1	25:f:877:GLY:HA2	1.85	0.40
26:g:251:ASN:HB3	26:g:258:THR:HG22	2.03	0.40
1:A:245:LEU:HD12	1:A:280:ILE:HG21	2.02	0.40
2:B:86:LYS:HA	2:B:87:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:VAL:C	2:B:164:MET:H	2.29	0.40
4:D:47:LEU:O	4:D:48:GLN:C	2.65	0.40
4:D:247:VAL:HG21	4:D:288:ILE:HG13	2.04	0.40
4:D:323:ARG:HB2	4:D:326:ARG:HD2	2.03	0.40
9:I:194:ILE:HD12	9:I:194:ILE:HA	1.91	0.40
12:L:133:LEU:HD23	12:L:133:LEU:HA	1.94	0.40
14:U:130:LEU:HD23	14:U:130:LEU:H	1.85	0.40
15:V:208:ALA:HA	15:V:211:TYR:CD2	2.56	0.40
16:W:371:THR:OG1	20:a:323:SER:HB2	2.20	0.40
17:X:406:ASN:O	17:X:410:VAL:HG13	2.20	0.40
19:Z:243:GLN:H	19:Z:243:GLN:CD	2.29	0.40
22:c:104:ARG:HG3	26:g:199:ASN:HB3	2.03	0.40
23:d:58:GLY:HA2	23:d:61:TRP:CE3	2.57	0.40
26:g:119:ILE:HG22	26:g:266:ILE:HG12	2.04	0.40
26:g:180:MET:HG2	26:g:182:PHE:H	1.86	0.40
3:C:105:ILE:HD12	3:C:105:ILE:HA	1.92	0.40
4:D:212:LYS:HD2	4:D:312:ASN:HA	2.04	0.40
9:I:192:LEU:O	9:I:196:VAL:HG23	2.21	0.40
14:U:65:SER:O	14:U:69:TYR:HB3	2.21	0.40
18:Y:267:ARG:O	18:Y:271:PHE:CB	2.70	0.40
19:Z:8:LYS:HB2	19:Z:159:THR:HG23	2.04	0.40
19:Z:85:VAL:HA	22:c:76:PRO:HB3	2.03	0.40
19:Z:167:ALA:HB3	22:c:46:ARG:HD2	2.04	0.40
20:a:278:MET:O	20:a:282:PHE:HB2	2.20	0.40
22:c:119:GLY:HA3	22:c:121:TRP:NE1	2.37	0.40
25:f:185:LEU:HD13	25:f:185:LEU:HA	1.95	0.40
25:f:615:ILE:HD13	25:f:615:ILE:HA	1.98	0.40
25:f:703:ARG:HB2	25:f:787:LEU:HD11	2.02	0.40
26:g:119:ILE:HA	26:g:120:PRO:HD3	1.97	0.40
2:B:203:LEU:O	2:B:204:PRO:C	2.64	0.40
3:C:88:LYS:HB2	3:C:94:LYS:HA	2.03	0.40
3:C:229:ARG:HD2	3:C:231:VAL:HG23	2.03	0.40
8:H:39:LYS:HE2	9:I:57:ASP:OD1	2.21	0.40
11:K:19:GLY:O	11:K:20:ARG:HB3	2.22	0.40
14:U:95:GLU:O	14:U:99:THR:HG23	2.22	0.40
15:V:278:GLU:HA	15:V:285:TRP:HZ2	1.85	0.40
15:V:428:LEU:HD12	15:V:428:LEU:HA	1.96	0.40
17:X:404:ILE:HG23	18:Y:376:LEU:HD12	2.04	0.40
21:b:144:GLY:HA2	21:b:177:PRO:HA	2.04	0.40
23:d:49:ILE:HD11	23:d:90:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/433 (95%)	365 (89%)	45 (11%)	0	100	100
2	B	373/440 (85%)	330 (88%)	43 (12%)	0	100	100
3	C	379/398 (95%)	341 (90%)	38 (10%)	0	100	100
4	D	378/418 (90%)	344 (91%)	34 (9%)	0	100	100
5	E	387/403 (96%)	357 (92%)	30 (8%)	0	100	100
6	F	393/439 (90%)	348 (88%)	45 (12%)	0	100	100
7	G	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
8	H	230/234 (98%)	221 (96%)	9 (4%)	0	100	100
9	I	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
11	K	231/241 (96%)	214 (93%)	17 (7%)	0	100	100
12	L	236/269 (88%)	231 (98%)	5 (2%)	0	100	100
13	M	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
14	U	845/953 (89%)	791 (94%)	54 (6%)	0	100	100
15	V	440/534 (82%)	423 (96%)	17 (4%)	0	100	100
16	W	444/456 (97%)	419 (94%)	25 (6%)	0	100	100
17	X	123/422 (29%)	116 (94%)	7 (6%)	0	100	100
18	Y	376/389 (97%)	346 (92%)	30 (8%)	0	100	100
19	Z	284/324 (88%)	248 (87%)	36 (13%)	0	100	100
20	a	370/376 (98%)	342 (92%)	28 (8%)	0	100	100
21	b	189/377 (50%)	172 (91%)	17 (9%)	0	100	100
22	c	285/310 (92%)	245 (86%)	40 (14%)	0	100	100
23	d	255/350 (73%)	220 (86%)	35 (14%)	0	100	100
24	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
25	f	887/908 (98%)	796 (90%)	91 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	g	170/289 (59%)	157 (92%)	13 (8%)	0	100	100
All	All	8697/10043 (87%)	7991 (92%)	706 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/372 (95%)	344 (98%)	9 (2%)	42	62
2	B	333/385 (86%)	314 (94%)	19 (6%)	18	43
3	C	329/346 (95%)	299 (91%)	30 (9%)	9	30
4	D	333/366 (91%)	310 (93%)	23 (7%)	14	39
5	E	341/353 (97%)	334 (98%)	7 (2%)	47	65
6	F	342/379 (90%)	332 (97%)	10 (3%)	37	58
7	G	208/210 (99%)	205 (99%)	3 (1%)	59	71
8	H	190/191 (100%)	186 (98%)	4 (2%)	47	65
9	I	210/221 (95%)	207 (99%)	3 (1%)	59	71
10	J	203/211 (96%)	197 (97%)	6 (3%)	36	57
11	K	195/203 (96%)	192 (98%)	3 (2%)	57	70
12	L	204/230 (89%)	204 (100%)	0	100	100
13	M	197/212 (93%)	194 (98%)	3 (2%)	57	70
14	U	730/816 (90%)	713 (98%)	17 (2%)	44	64
15	V	388/460 (84%)	381 (98%)	7 (2%)	51	68
16	W	410/416 (99%)	403 (98%)	7 (2%)	53	68
17	X	114/362 (32%)	112 (98%)	2 (2%)	51	68
18	Y	334/344 (97%)	328 (98%)	6 (2%)	51	68
19	Z	257/295 (87%)	251 (98%)	6 (2%)	44	64
20	a	332/336 (99%)	324 (98%)	8 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	b	167/312 (54%)	157 (94%)	10 (6%)	17	42
22	c	252/268 (94%)	229 (91%)	23 (9%)	9	30
23	d	231/294 (79%)	227 (98%)	4 (2%)	53	68
24	e	44/63 (70%)	44 (100%)	0	100	100
25	f	745/763 (98%)	736 (99%)	9 (1%)	63	73
26	g	156/253 (62%)	148 (95%)	8 (5%)	21	45
All	All	7598/8661 (88%)	7371 (97%)	227 (3%)	37	57

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	LEU
1	A	129	VAL
1	A	133	ASP
1	A	134	ILE
1	A	138	MET
1	A	270	CYS
1	A	388	VAL
1	A	403	ILE
1	A	430	MET
2	B	150	VAL
2	B	152	LEU
2	B	203	LEU
2	B	210	TYR
2	B	222	VAL
2	B	225	TYR
2	B	255	LEU
2	B	262	ASP
2	B	268	ARG
2	B	307	ARG
2	B	313	LEU
2	B	316	LEU
2	B	320	ASP
2	B	334	ILE
2	B	342	ILE
2	B	346	ARG
2	B	350	LYS
2	B	351	ILE
2	B	364	ILE
3	C	21	ARG

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Mol	Chain	Res	Type
3	C	22	GLN
3	C	28	ILE
3	C	31	LEU
3	C	32	GLN
3	C	39	SER
3	C	40	GLN
3	C	42	LEU
3	C	52	LEU
3	C	63	LEU
3	C	85	VAL
3	C	89	VAL
3	C	108	VAL
3	C	119	ASP
3	C	130	LYS
3	C	138	MET
3	C	147	THR
3	C	210	THR
3	C	214	VAL
3	C	218	GLU
3	C	219	LEU
3	C	224	ILE
3	C	231	VAL
3	C	237	MET
3	C	274	LEU
3	C	286	THR
3	C	298	ILE
3	C	300	ILE
3	C	369	TYR
3	C	378	VAL
4	D	40	LEU
4	D	46	LYS
4	D	47	LEU
4	D	48	GLN
4	D	69	LYS
4	D	73	LEU
4	D	76	GLN
4	D	82	ILE
4	D	102	ILE
4	D	116	LEU
4	D	143	LEU
4	D	193	GLN
4	D	219	VAL

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Mol	Chain	Res	Type
4	D	235	PHE
4	D	240	LEU
4	D	253	LEU
4	D	278	GLN
4	D	282	ASP
4	D	284	GLU
4	D	330	LYS
4	D	335	LEU
4	D	385	LEU
4	D	393	ILE
5	E	98	VAL
5	E	191	LEU
5	E	195	PHE
5	E	253	ILE
5	E	271	HIS
5	E	302	ASP
5	E	303	LEU
6	F	90	VAL
6	F	93	VAL
6	F	136	VAL
6	F	191	LEU
6	F	192	ASP
6	F	257	VAL
6	F	282	ILE
6	F	323	ASN
6	F	347	ARG
6	F	406	ILE
7	G	10	ASP
7	G	56	VAL
7	G	73	THR
8	H	7	SER
8	H	26	LEU
8	H	74	LEU
8	H	203	MET
9	I	10	THR
9	I	30	HIS
9	I	59	VAL
10	J	10	PHE
10	J	50	VAL
10	J	118	TYR
10	J	145	TYR
10	J	211	MET

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Mol	Chain	Res	Type
10	J	217	LEU
11	K	28	ILE
11	K	152	GLN
11	K	199	LEU
13	M	8	ASP
13	M	136	MET
13	M	184	MET
14	U	35	TRP
14	U	130	LEU
14	U	177	LEU
14	U	189	GLN
14	U	200	VAL
14	U	250	PHE
14	U	410	VAL
14	U	462	LEU
14	U	501	LEU
14	U	541	HIS
14	U	544	ILE
14	U	574	LYS
14	U	588	MET
14	U	603	LEU
14	U	656	LEU
14	U	788	VAL
14	U	828	VAL
15	V	210	CYS
15	V	300	LEU
15	V	314	ARG
15	V	346	LEU
15	V	438	VAL
15	V	443	ARG
15	V	470	ARG
16	W	115	ILE
16	W	120	ILE
16	W	382	LEU
16	W	384	LEU
16	W	393	LEU
16	W	406	VAL
16	W	438	LEU
17	X	344	ARG
17	X	384	VAL
18	Y	69	LEU
18	Y	74	LYS

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Mol	Chain	Res	Type
18	Y	101	ARG
18	Y	168	ILE
18	Y	286	TRP
18	Y	347	ILE
19	Z	29	VAL
19	Z	78	MET
19	Z	111	LEU
19	Z	145	HIS
19	Z	175	LEU
19	Z	201	LEU
20	a	33	LEU
20	a	35	HIS
20	a	112	ILE
20	a	148	VAL
20	a	290	GLN
20	a	293	PHE
20	a	341	LEU
20	a	356	TRP
21	b	18	ASN
21	b	51	LEU
21	b	52	ILE
21	b	90	ILE
21	b	148	VAL
21	b	157	VAL
21	b	160	LEU
21	b	161	ASN
21	b	173	VAL
21	b	188	ILE
22	c	29	GLU
22	c	49	VAL
22	c	61	PHE
22	c	62	VAL
22	c	66	THR
22	c	67	VAL
22	c	95	MET
22	c	98	MET
22	c	127	ILE
22	c	155	VAL
22	c	173	GLU
22	c	183	HIS
22	c	193	ILE
22	c	196	LEU

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Mol	Chain	Res	Type
22	c	199	HIS
22	c	200	TYR
22	c	203	ILE
22	c	204	THR
22	c	220	LEU
22	c	221	HIS
22	c	289	ASP
22	c	293	THR
22	c	294	SER
23	d	36	LEU
23	d	112	VAL
23	d	115	PHE
23	d	244	LYS
25	f	41	LYS
25	f	89	MET
25	f	136	GLU
25	f	229	VAL
25	f	321	MET
25	f	465	LEU
25	f	539	LEU
25	f	732	VAL
25	f	884	THR
26	g	126	LEU
26	g	150	LEU
26	g	175	VAL
26	g	235	TYR
26	g	260	ILE
26	g	273	THR
26	g	282	VAL
26	g	289	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	322	ASN
1	A	433	ASN
2	B	81	ASN
2	B	416	ASN
3	C	32	GLN
3	C	41	ASN
3	C	46	GLN

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Mol	Chain	Res	Type
4	D	49	GLN
4	D	57	GLN
4	D	76	GLN
4	D	110	ASN
4	D	173	GLN
4	D	312	ASN
4	D	353	ASN
5	E	280	ASN
5	E	345	ASN
6	F	208	HIS
6	F	243	GLN
6	F	316	GLN
6	F	321	GLN
7	G	24	GLN
7	G	128	ASN
7	G	150	GLN
8	H	109	GLN
8	H	112	GLN
8	H	189	HIS
11	K	41	GLN
11	K	152	GLN
11	K	155	HIS
11	K	182	GLN
12	L	21	GLN
12	L	69	HIS
14	U	18	GLN
14	U	192	GLN
14	U	258	GLN
14	U	346	ASN
14	U	389	ASN
14	U	503	GLN
14	U	596	ASN
14	U	632	GLN
14	U	647	HIS
14	U	665	ASN
14	U	801	GLN
14	U	880	ASN
15	V	283	ASN
16	W	96	GLN
16	W	107	GLN
16	W	167	GLN
16	W	395	ASN

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Mol	Chain	Res	Type
16	W	440	ASN
17	X	333	GLN
17	X	405	GLN
18	Y	196	GLN
18	Y	280	GLN
18	Y	363	ASN
18	Y	367	GLN
18	Y	388	ASN
19	Z	32	GLN
19	Z	72	HIS
19	Z	174	HIS
19	Z	189	GLN
19	Z	256	GLN
19	Z	273	HIS
20	a	9	GLN
20	a	12	GLN
20	a	23	HIS
20	a	264	ASN
20	a	337	GLN
21	b	56	ASN
21	b	76	HIS
21	b	142	ASN
22	c	30	GLN
22	c	128	ASN
22	c	199	HIS
22	c	219	ASN
22	c	241	ASN
22	c	287	HIS
23	d	60	GLN
23	d	88	GLN
23	d	102	ASN
23	d	149	ASN
25	f	81	GLN
25	f	118	ASN
25	f	199	ASN
25	f	245	ASN
25	f	325	GLN
25	f	472	HIS
25	f	758	ASN
25	f	782	HIS
25	f	848	GLN
26	g	148	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 11 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
27	AGS	F	501	28	32,33,33	0.66	1 (3%)	45,52,52	0.55	0
29	ADP	B	501	-	28,29,29	0.46	0	43,45,45	0.51	0
27	AGS	D	501	28	32,33,33	0.66	1 (3%)	45,52,52	0.52	0
27	AGS	E	501	28	32,33,33	0.67	1 (3%)	45,52,52	0.48	0
27	AGS	A	501	28	32,33,33	0.66	1 (3%)	45,52,52	0.53	0
29	ADP	C	501	-	28,29,29	0.45	0	43,45,45	0.55	0

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
27	AGS	F	501	28	-	5/21/38/38	0/3/3/3
29	ADP	B	501	-	-	3/16/32/32	0/3/3/3
27	AGS	D	501	28	-	3/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	AGS	E	501	28	-	0/21/38/38	0/3/3/3
27	AGS	A	501	28	-	2/21/38/38	0/3/3/3
29	ADP	C	501	-	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	501	AGS	PG-S1G	2.12	1.95	1.90
27	A	501	AGS	PG-S1G	2.12	1.95	1.90
27	D	501	AGS	PG-S1G	2.11	1.95	1.90
27	F	501	AGS	PG-S1G	2.09	1.95	1.90

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	D	501	AGS	C5'-O5'-PA-O3A
27	F	501	AGS	C5'-O5'-PA-O3A
29	C	501	ADP	C5'-O5'-PA-O3A
27	D	501	AGS	C4'-C5'-O5'-PA
29	B	501	ADP	PB-O3A-PA-O5'
29	B	501	ADP	C3'-C4'-C5'-O5'
27	D	501	AGS	C5'-O5'-PA-O1A
27	F	501	AGS	C5'-O5'-PA-O1A
29	C	501	ADP	C5'-O5'-PA-O1A
27	F	501	AGS	C4'-C5'-O5'-PA
27	A	501	AGS	C2'-C1'-N9-C8
27	A	501	AGS	C2'-C1'-N9-C4
27	F	501	AGS	C3'-C4'-C5'-O5'
27	F	501	AGS	O4'-C4'-C5'-O5'
29	B	501	ADP	O4'-C4'-C5'-O5'
29	C	501	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	F	501	AGS	2	0
29	B	501	ADP	1	0

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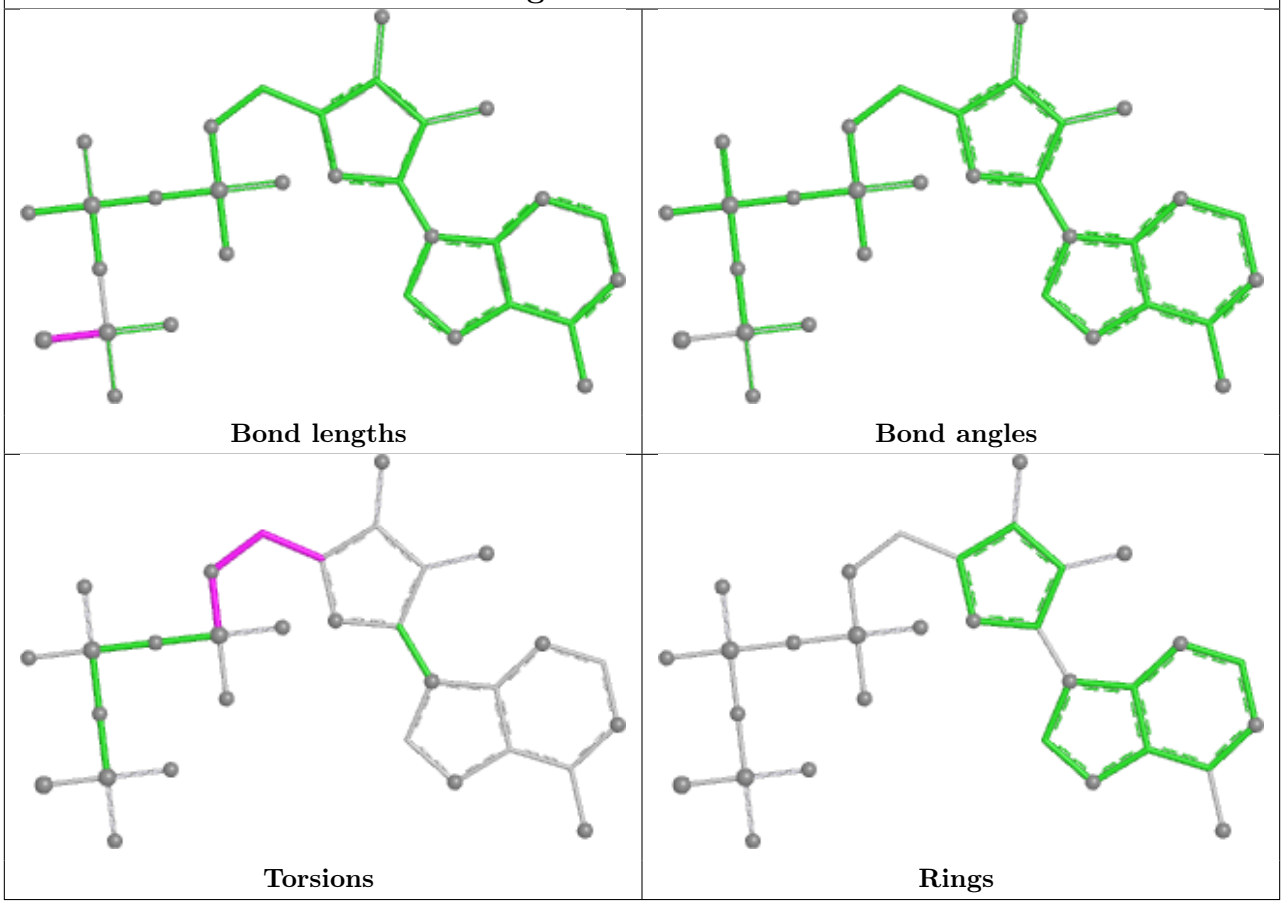
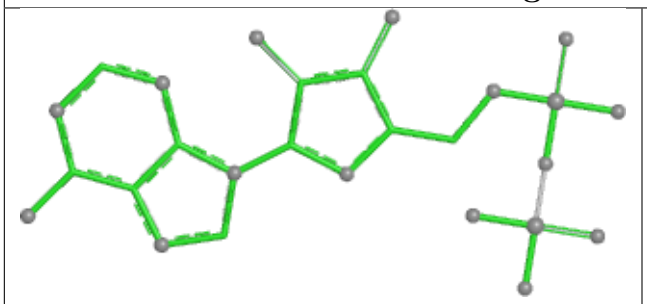
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	501	AGS	1	0
27	E	501	AGS	2	0
27	A	501	AGS	4	0
29	C	501	ADP	4	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

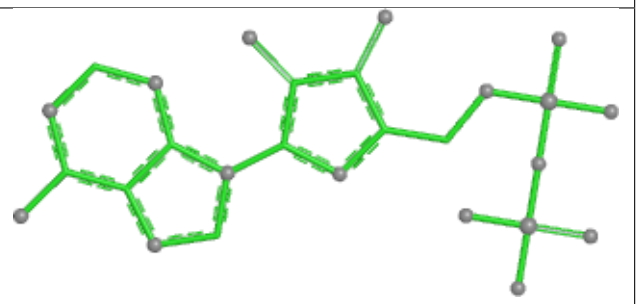
Ligand AGS F 501



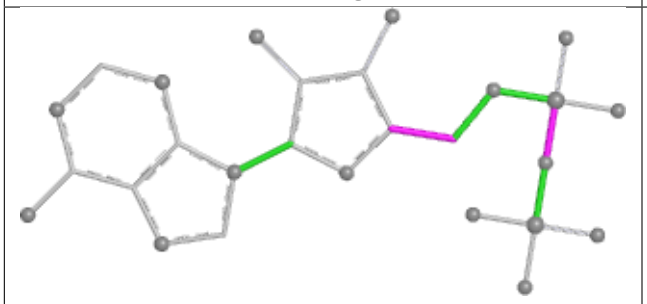
Ligand ADP B 501



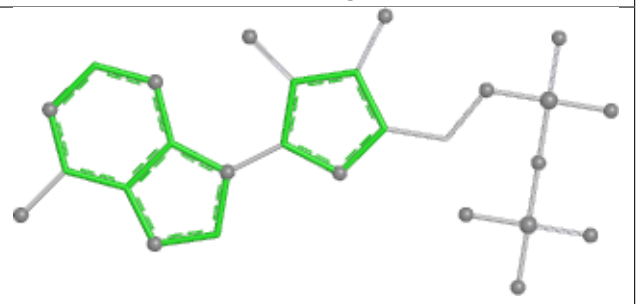
Bond lengths



Bond angles

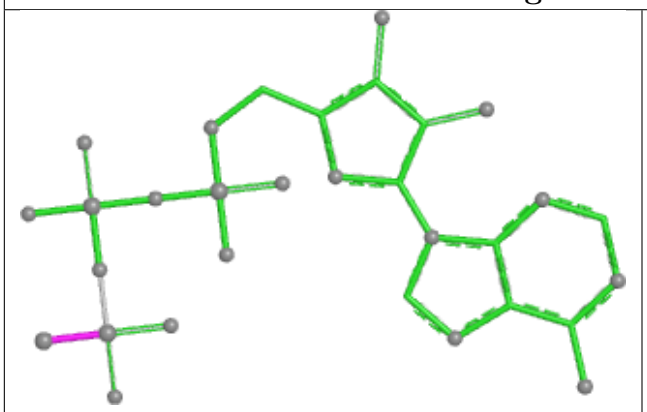


Torsions

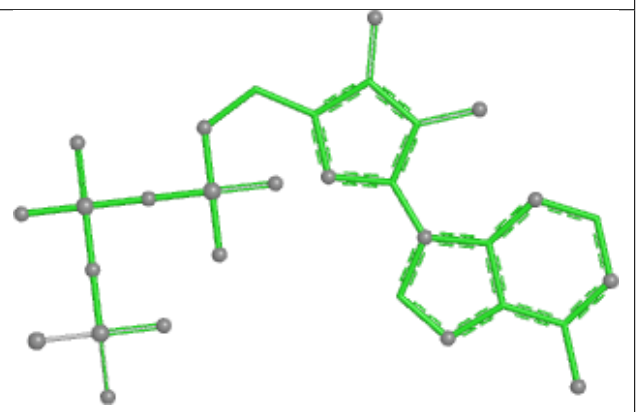


Rings

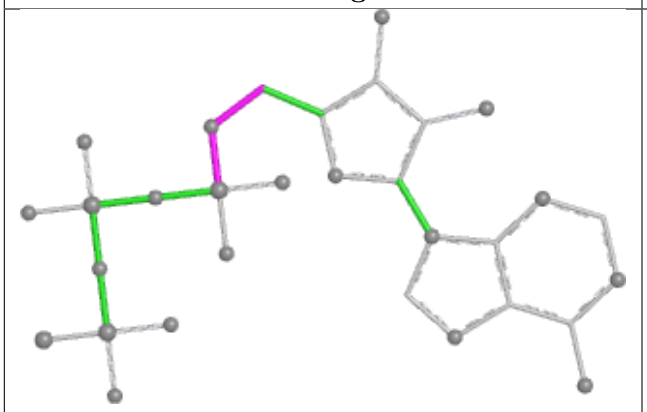
Ligand AGS D 501



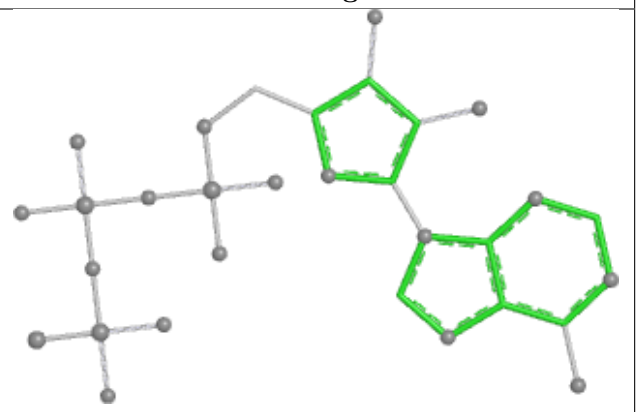
Bond lengths



Bond angles

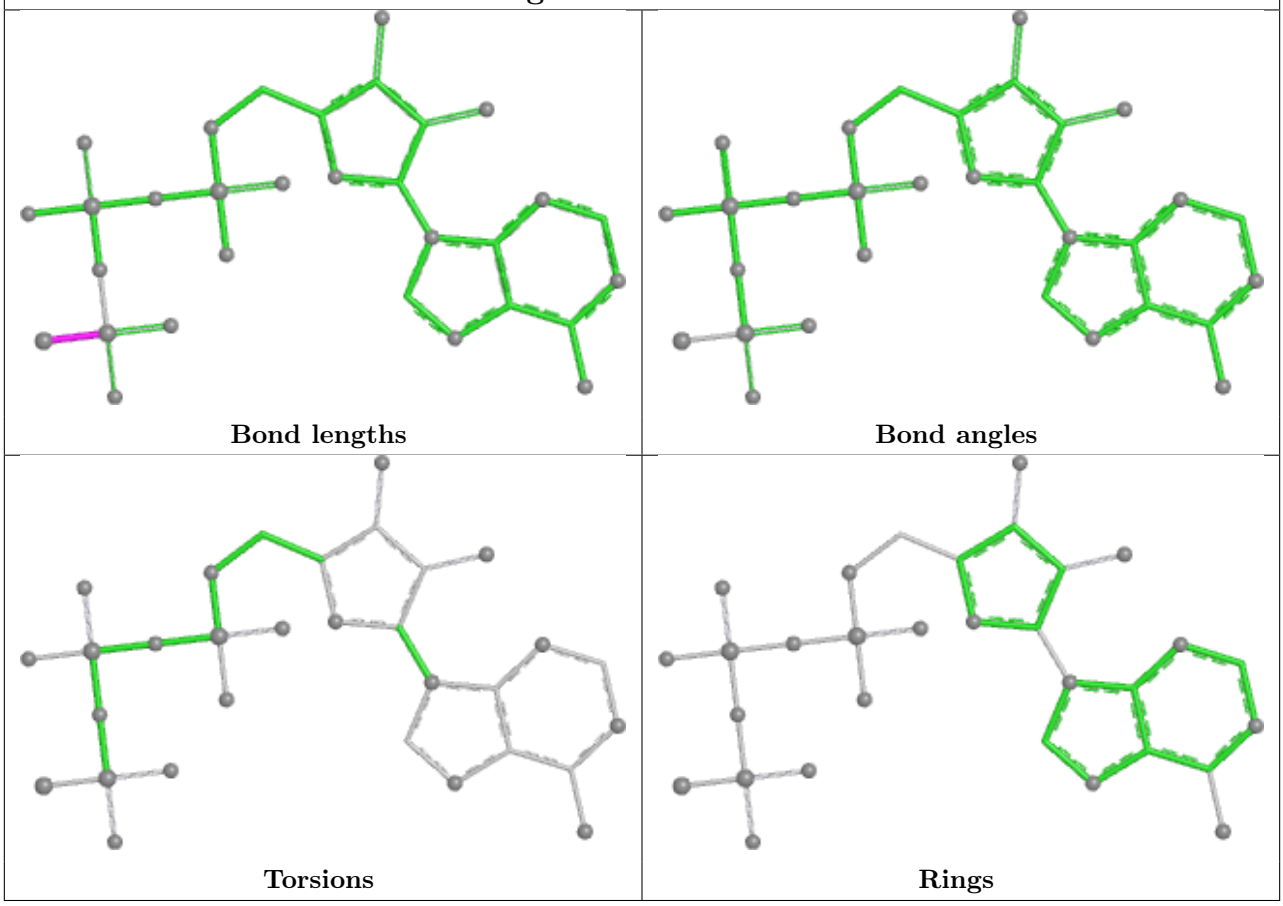


Torsions

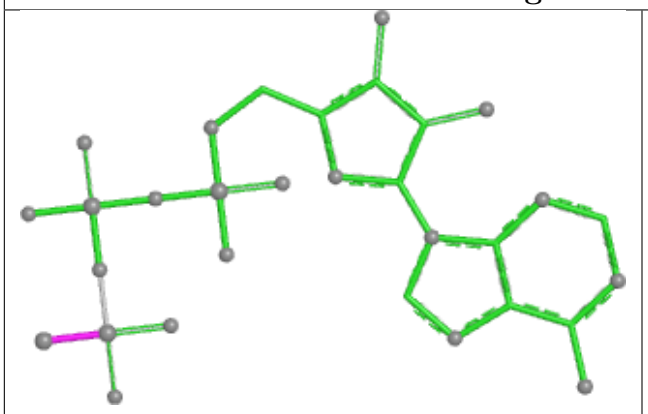


Rings

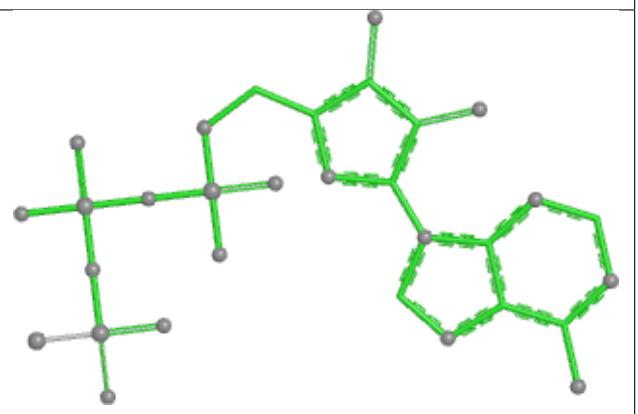
Ligand AGS E 501



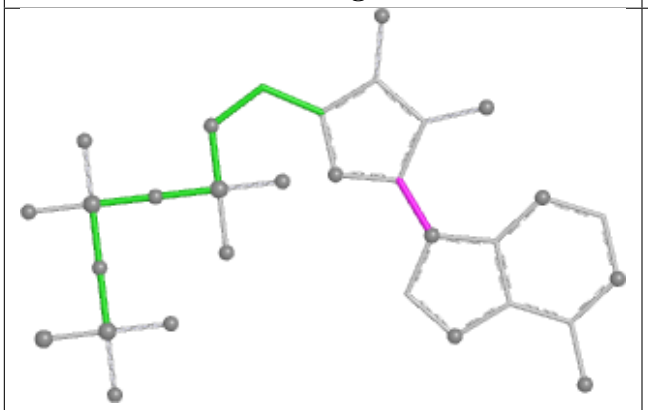
Ligand AGS A 501



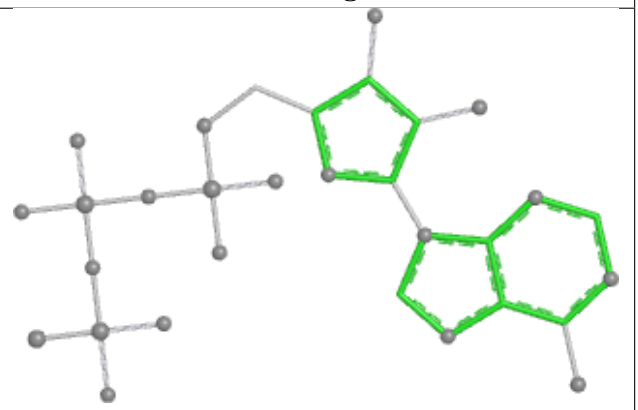
Bond lengths



Bond angles

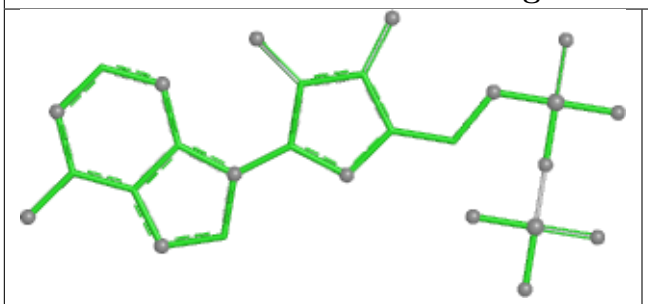


Torsions

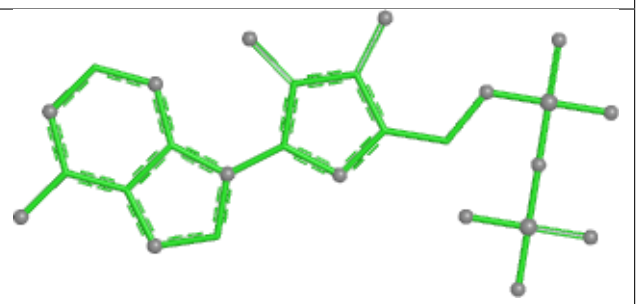


Rings

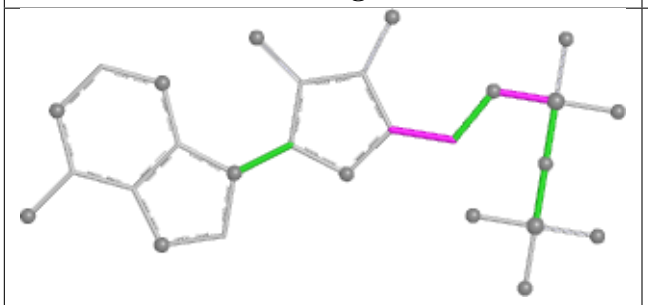
Ligand ADP C 501



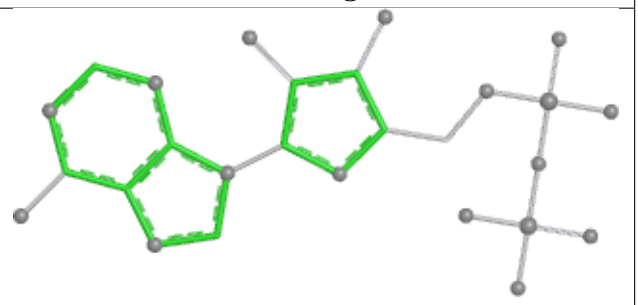
Bond lengths



Bond angles



Torsions



Rings

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.

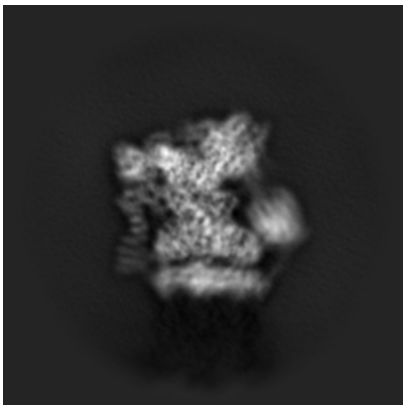
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-71741. These allow visual inspection of the internal detail of the map and identification of artifacts.

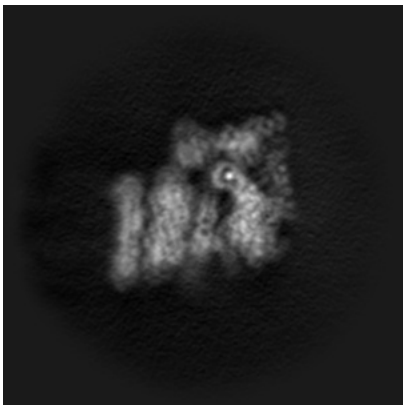
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

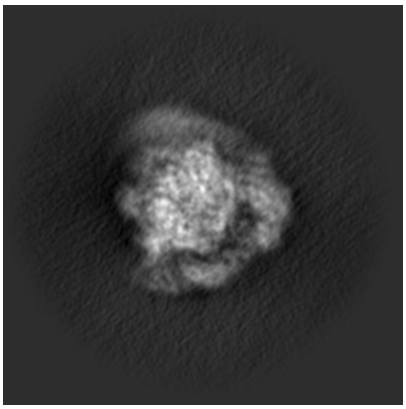
6.1.1 Primary map



X

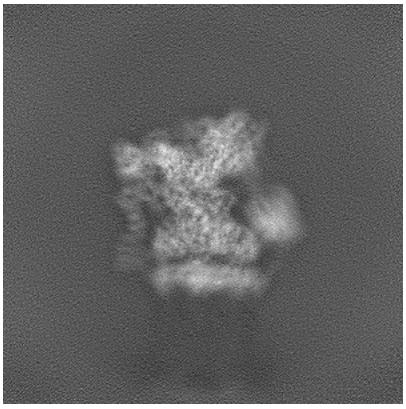


Y

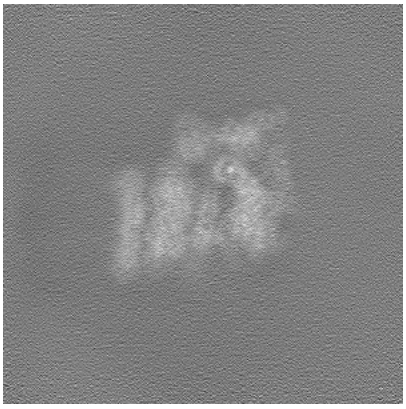


Z

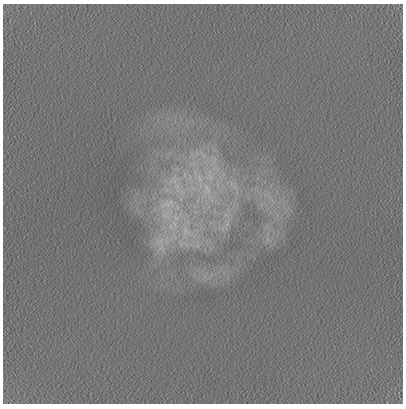
6.1.2 Raw map



X



Y

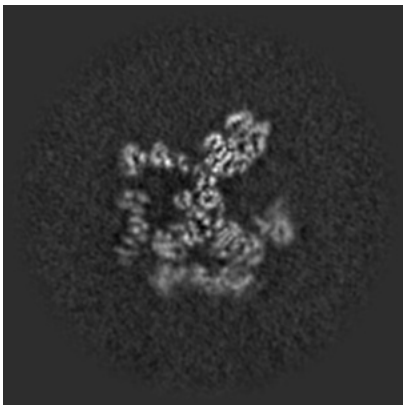


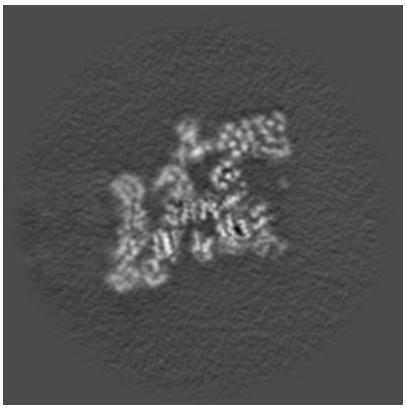
Z

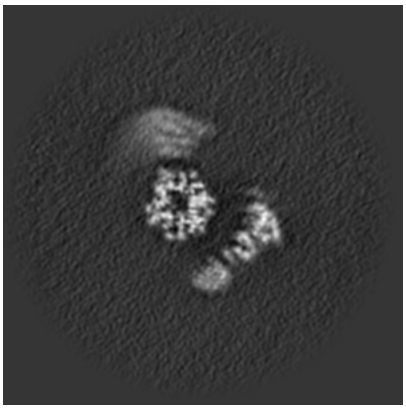
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

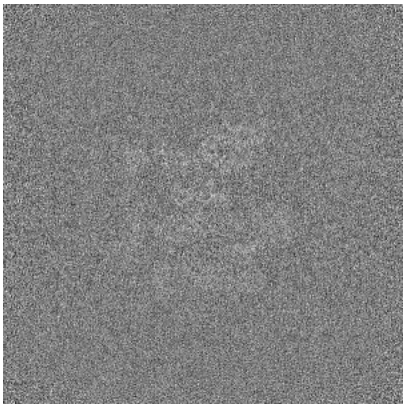
6.2.1 Primary map

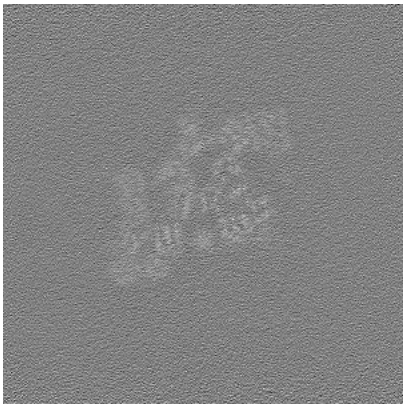

X Index: 240

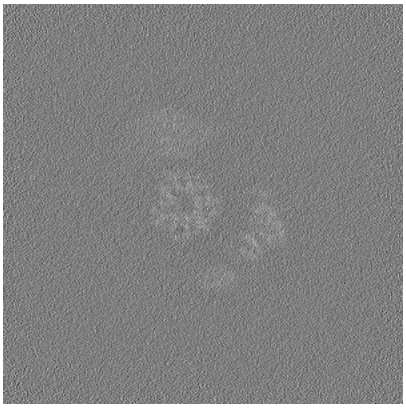

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

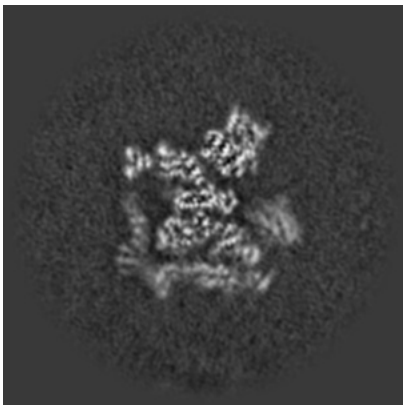

Y Index: 240


Z Index: 240

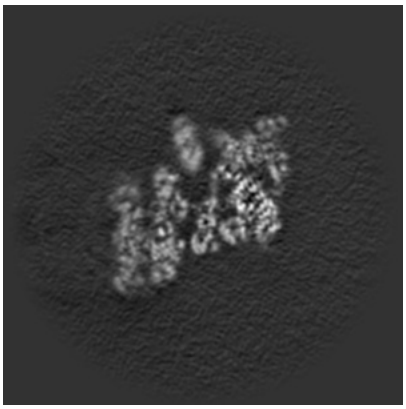
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

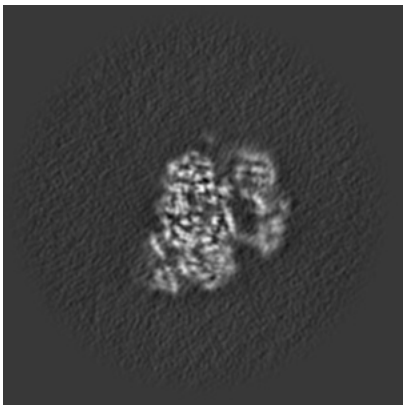
6.3.1 Primary map



X Index: 228

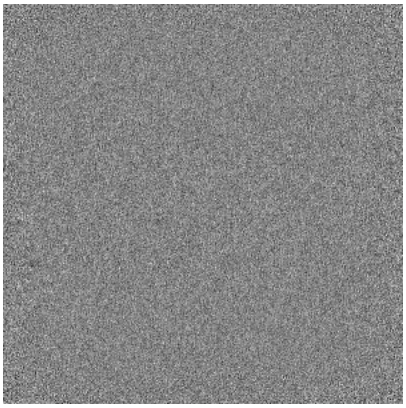


Y Index: 257

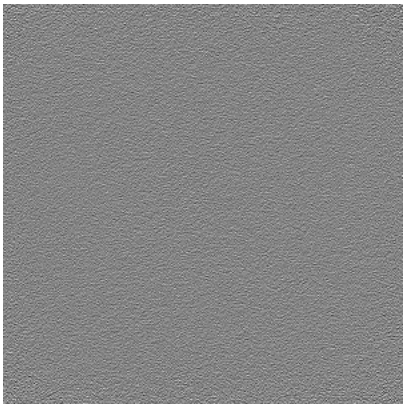


Z Index: 288

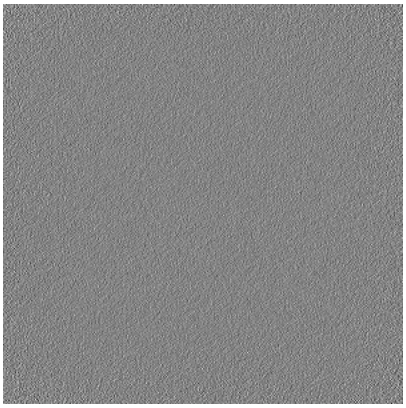
6.3.2 Raw map



X Index: 0



Y Index: 0

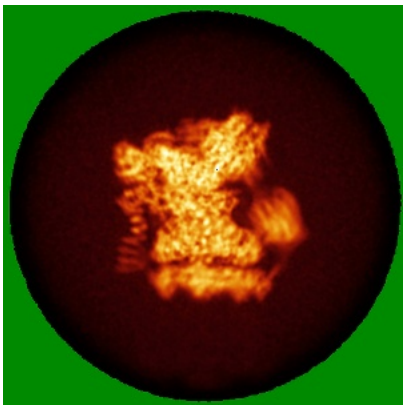


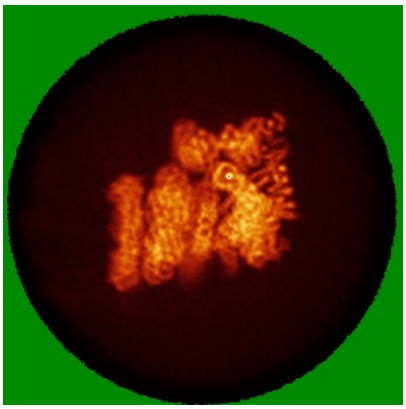
Z Index: 0

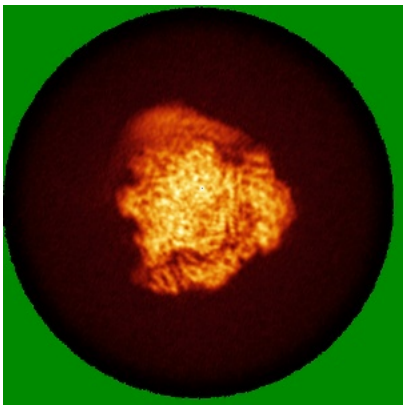
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

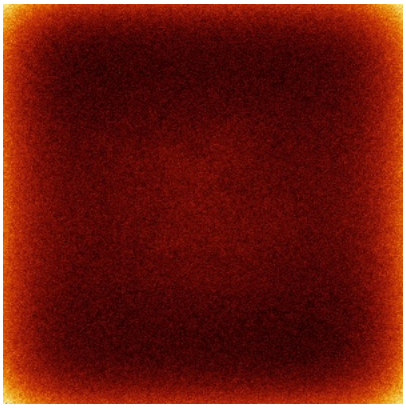
6.4.1 Primary map

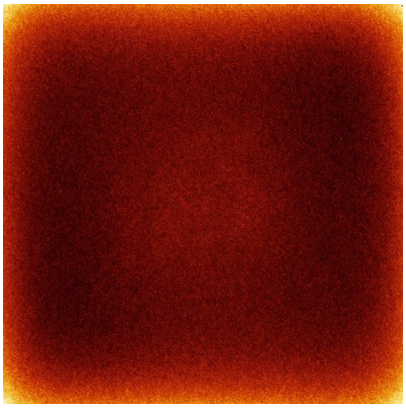

X

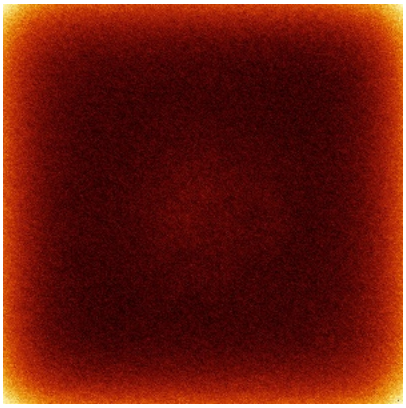

Y


Z

6.4.2 Raw map


X

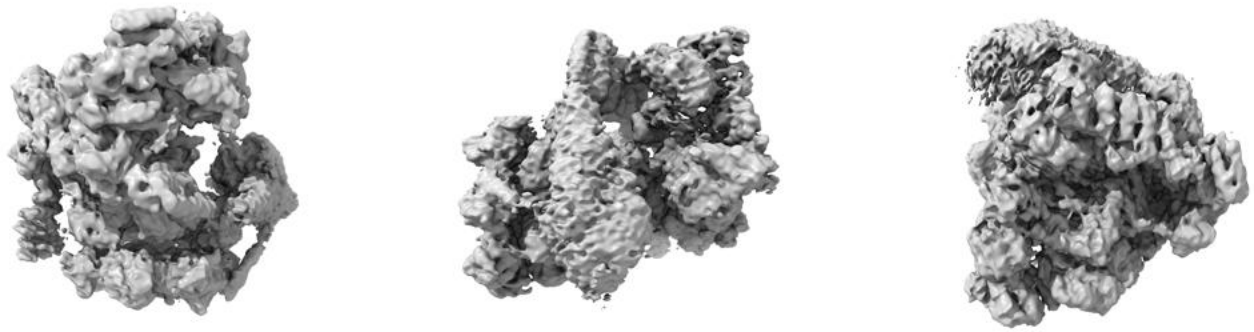

Y


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)

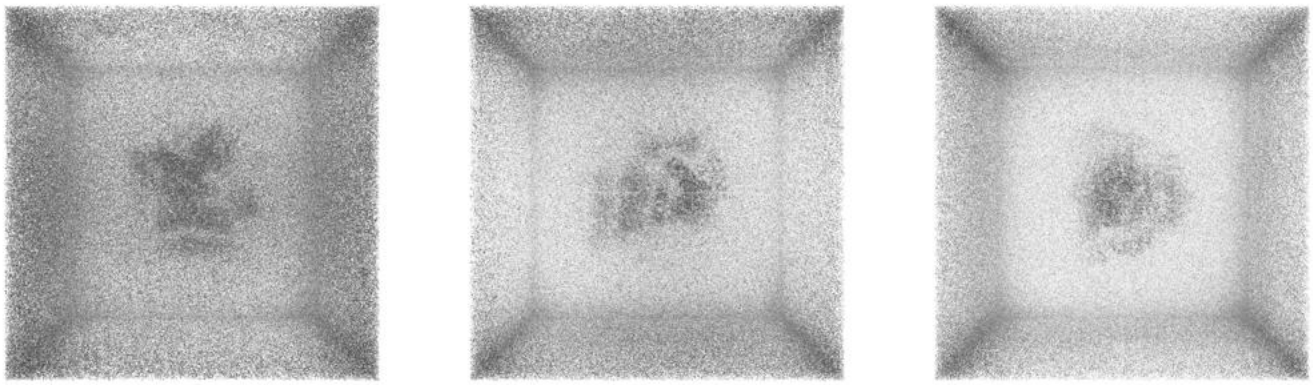
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



X Y Z

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.

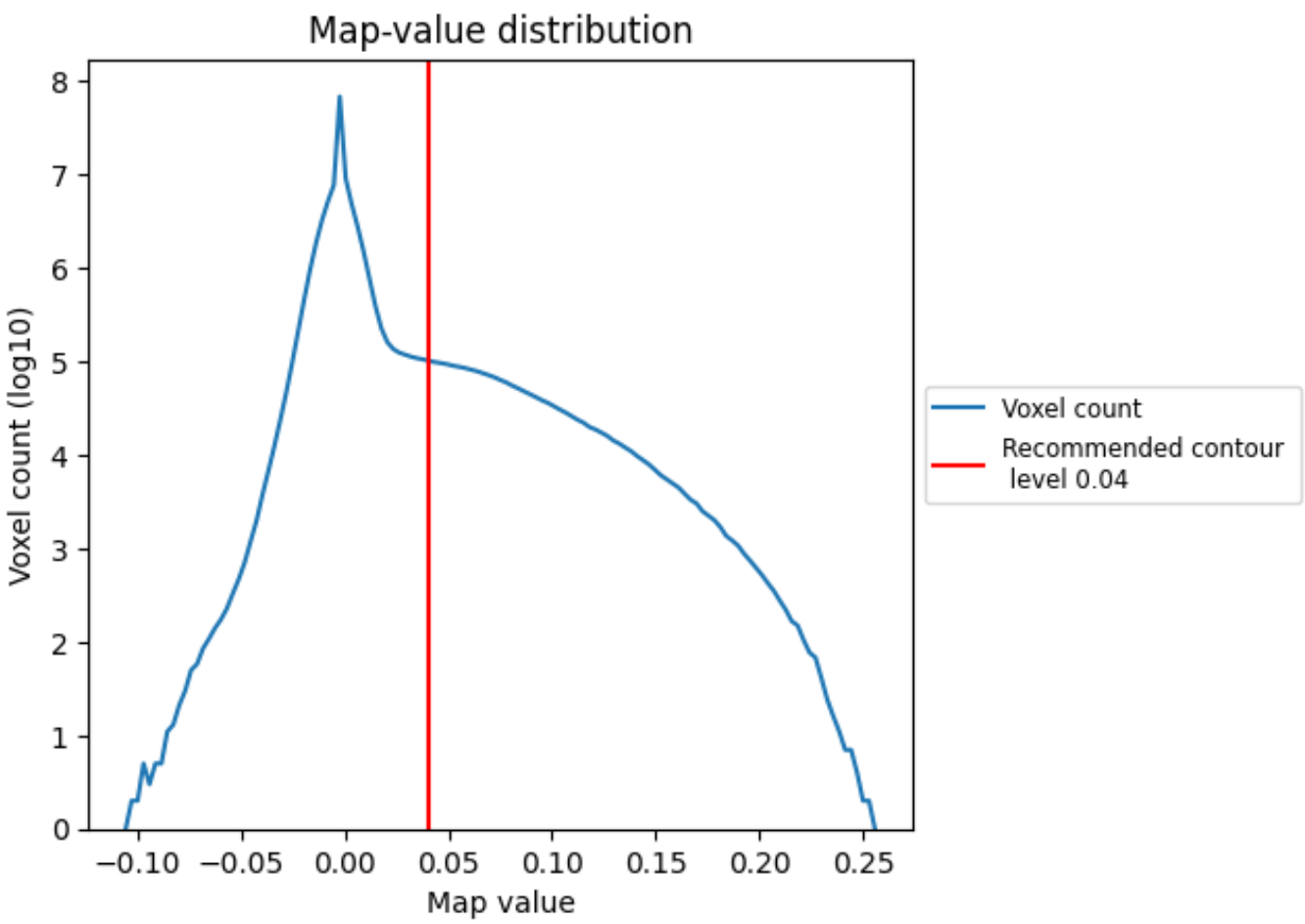
6.6 Mask visualisation (i)

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

7 Map analysis (i)

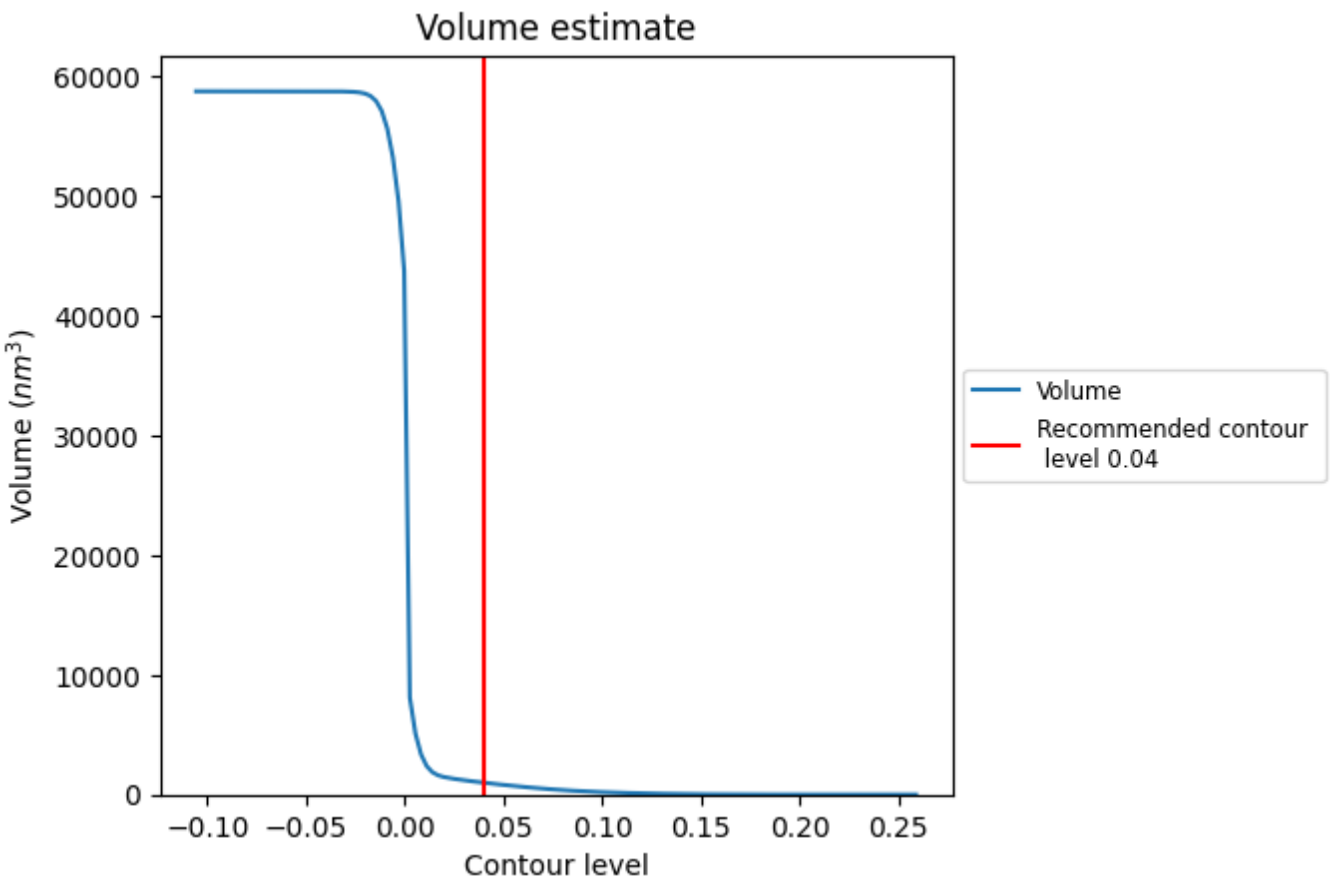
This section contains the results of statistical analysis of the map.

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.

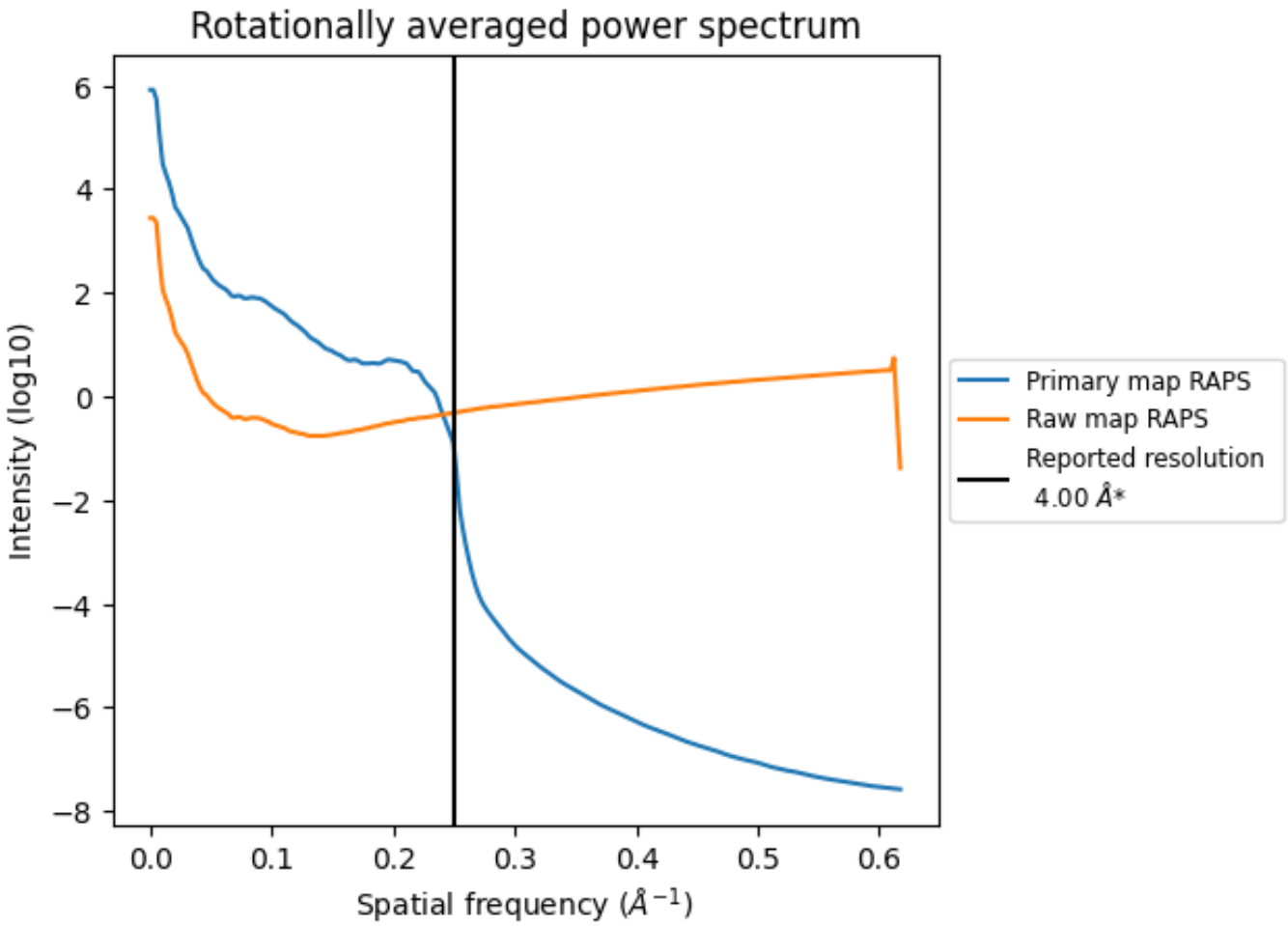
7.2 Volume estimate (i)



The volume at the recommended contour level is 989 nm^3; this corresponds to an approximate mass of 893 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)

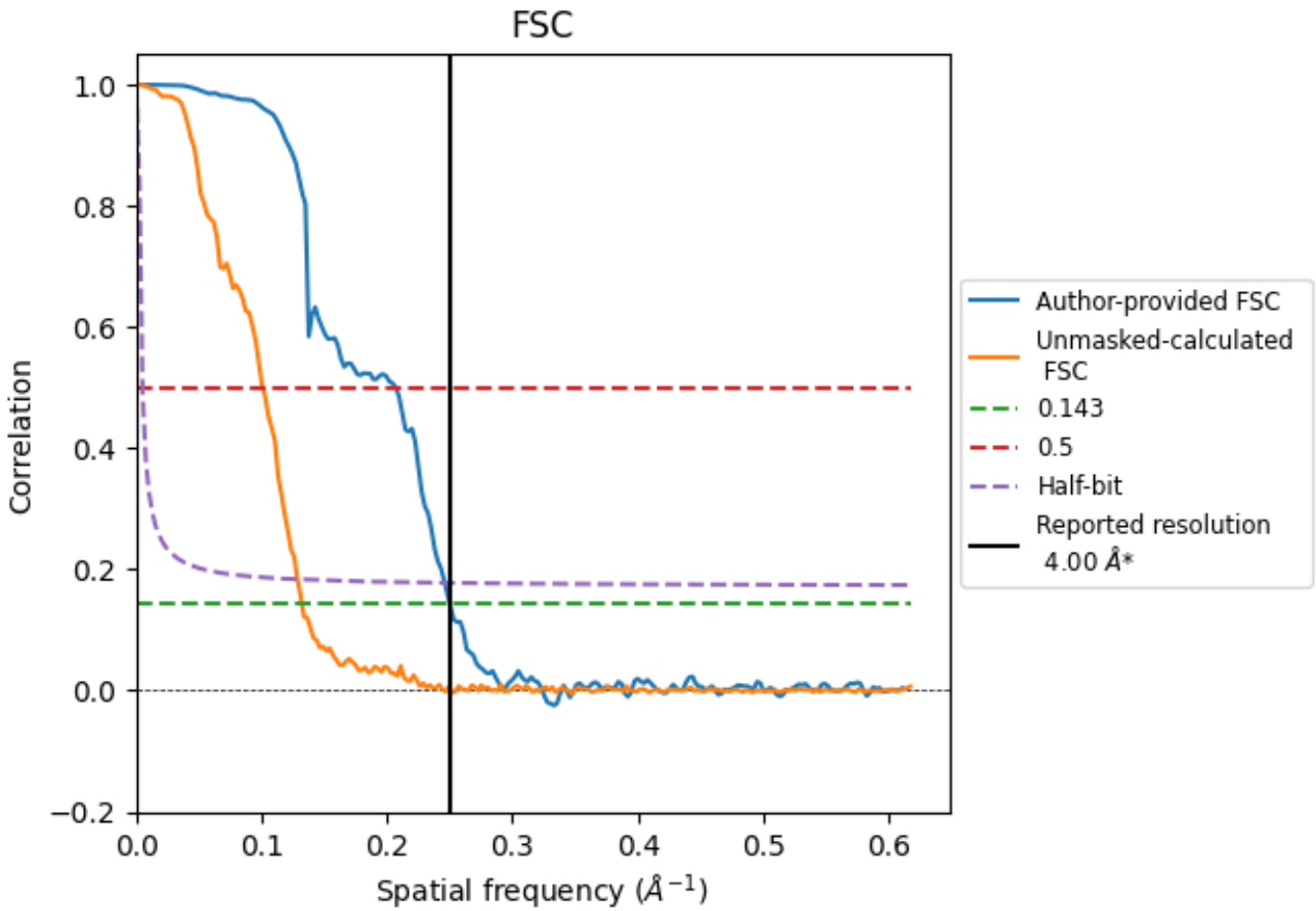


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

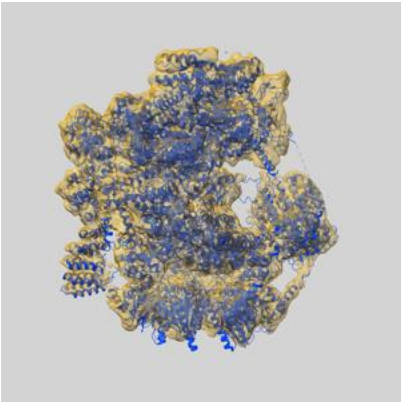
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	4.83	4.07
Unmasked-calculated*	7.57	9.92	7.78

*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 7.57 differs from the reported value 4.0 by more than 10 %

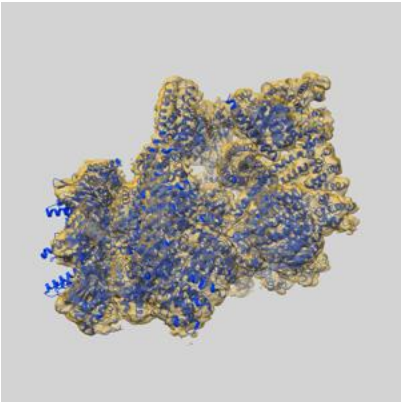
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-71741 and PDB model 9PMQ. Per-residue inclusion information can be found in section 3 on page 10.

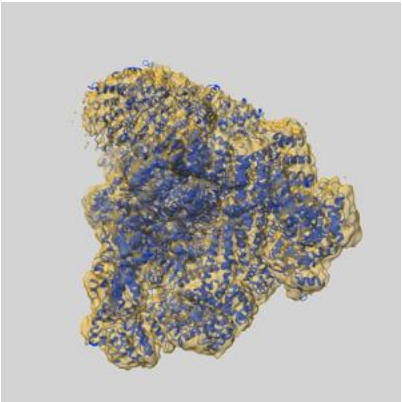
9.1 Map-model overlay (i)



X



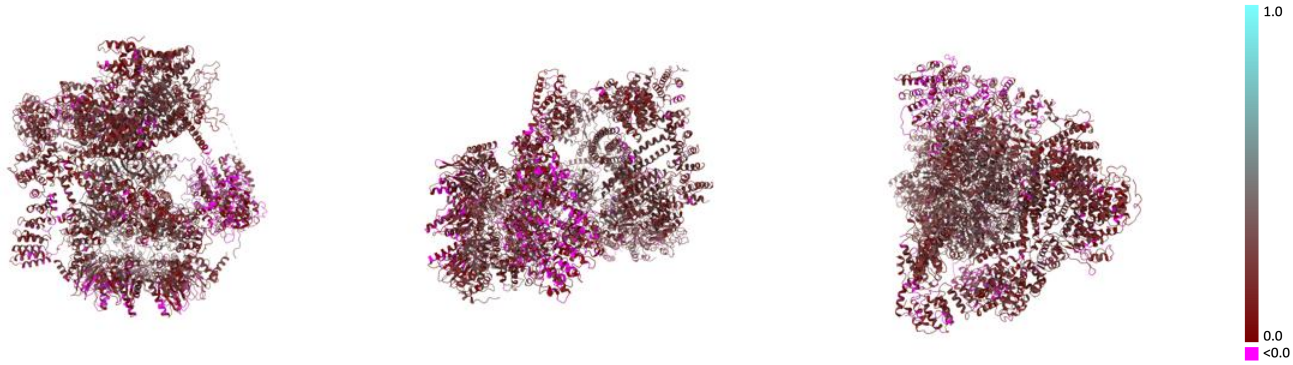
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

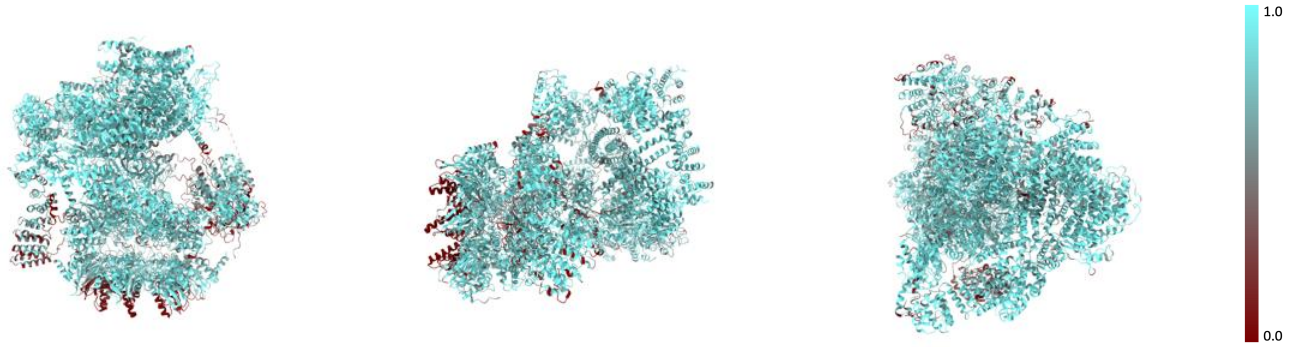
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

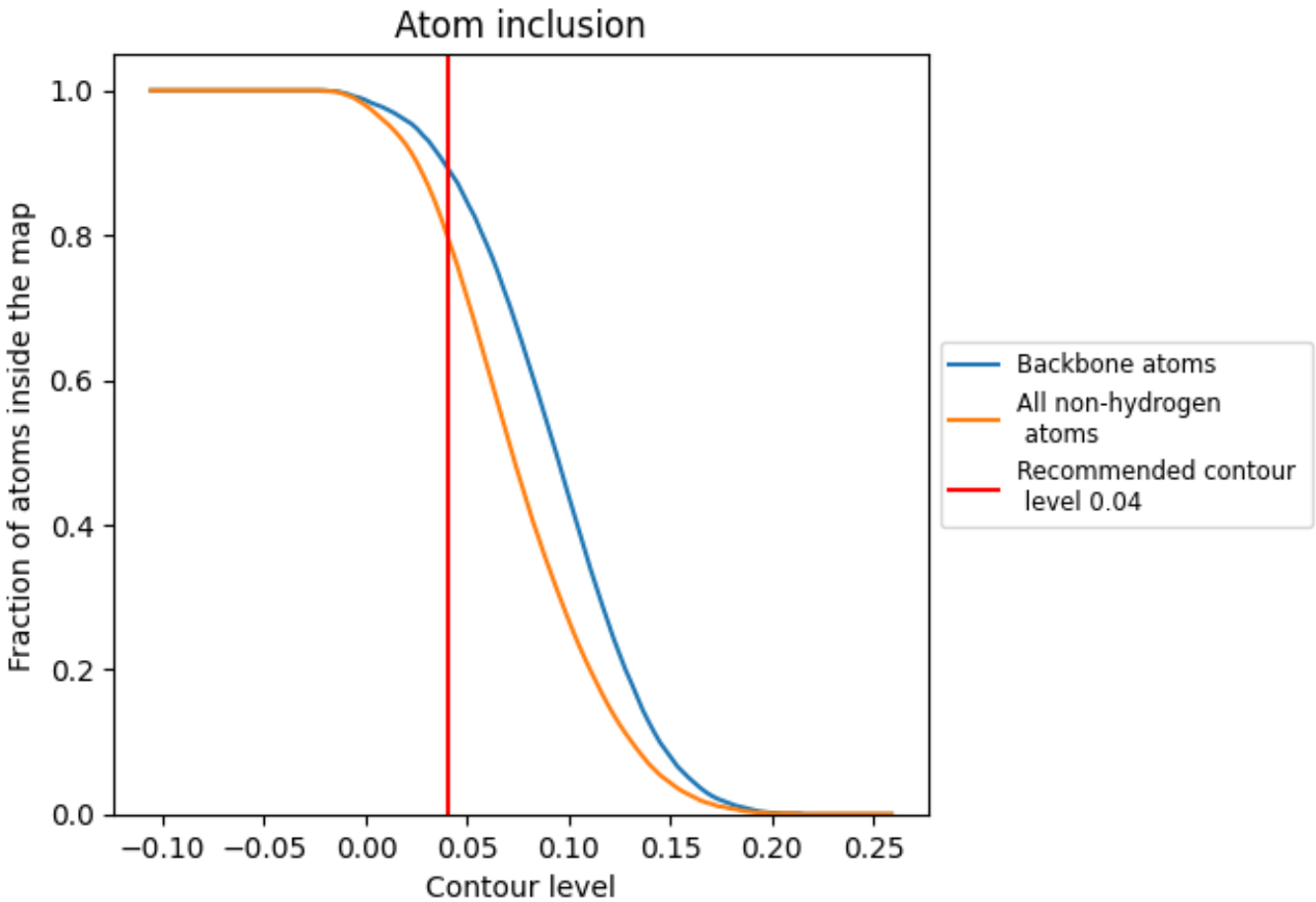
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.1900
A	0.8160	0.2190
B	0.7970	0.2040
C	0.8340	0.2240
D	0.8650	0.2430
E	0.8740	0.2340
F	0.8580	0.2380
G	0.6280	0.1520
H	0.7700	0.1740
I	0.7410	0.1810
J	0.6490	0.1500
K	0.6710	0.1710
L	0.7890	0.2120
M	0.6860	0.1750
U	0.8580	0.2250
V	0.8870	0.1990
W	0.6490	0.1560
X	0.7350	0.1730
Y	0.8900	0.1720
Z	0.8980	0.2510
a	0.8920	0.1790
b	0.8950	0.2200
c	0.8610	0.2610
d	0.8440	0.1460
e	0.9070	0.2020
f	0.7150	0.0620
g	0.6660	0.2490