Full wwPDB EM Validation Report ⓘ

Nov 8, 2021 – 05:13 pm GMT

PDB ID	:	7PG9
EMDB ID	:	EMD-13389
Title	:	human 20S proteasome
Authors	:	Xu, C.; Cong, Y.
Deposited on	:	2021-08-13
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

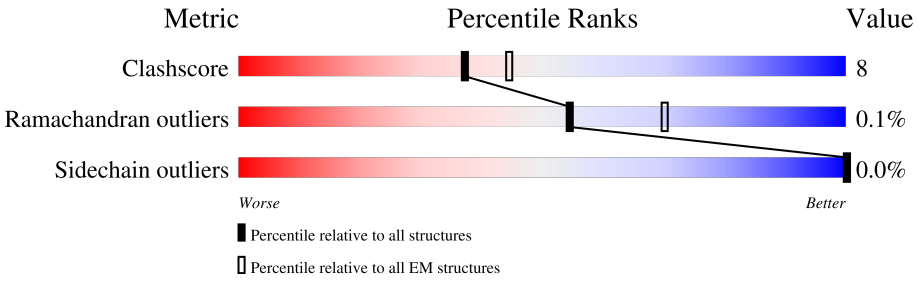
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	246	5% 79% 18% ·
1	O	246	· 76% 21% ·
2	B	234	· 81% 17% ·
2	P	234	· 83% 15% ·
3	C	261	8% 79% 16% 5%
3	Q	261	7% 79% 15% 5%
4	D	248	· 78% 15% 6%
4	R	248	· 79% 15% 6%

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Mol	Chain	Length	Quality of chain
5	E	241	6% 80% 17%
5	S	241	6% 78% 18%
6	F	263	70% 18% 11%
6	T	263	71% 17% 11%
7	G	255	77% 16% 6%
7	U	255	79% 15% 6%
8	H	205	82% 17%
8	V	205	81% 17%
9	I	234	79% 15% 6%
9	W	234	77% 17% 6%
10	J	205	75% 25%
10	X	205	74% 25%
11	K	201	74% 23%
11	Y	201	73% 24%
12	L	204	77% 21%
12	Z	204	77% 21%
13	M	213	82% 18%
13	a	213	100%
14	N	219	79% 18%
14	b	219	97%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 45326 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1729	1101	303	313	12		
1	O	238	Total	C	N	O	S	0	0
			1725	1099	302	312	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		
2	P	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		
3	Q	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		
4	R	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		
5	S	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		
6	T	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		
7	U	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		
8	V	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		
9	W	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		
11	Y	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		
12	Z	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		
13	a	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

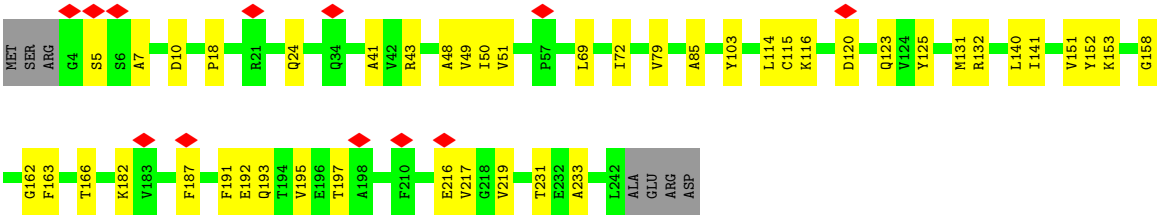
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		
14	b	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		

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.

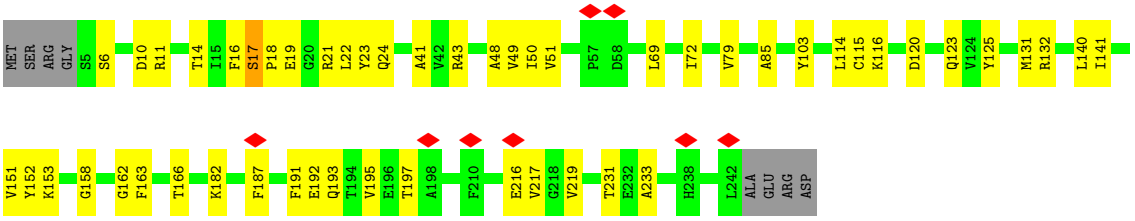
• Molecule 1: Proteasome subunit alpha type-6

Chain A:



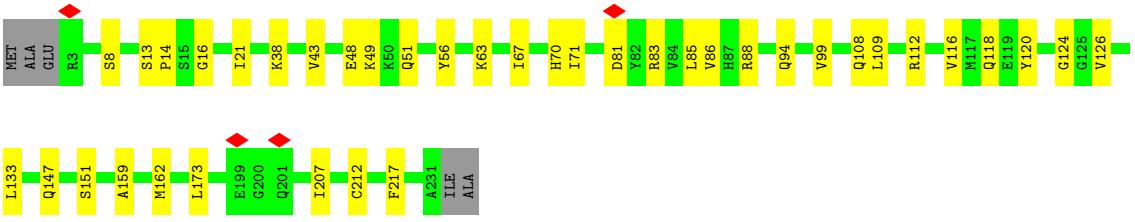
• Molecule 1: Proteasome subunit alpha type-6

Chain O:



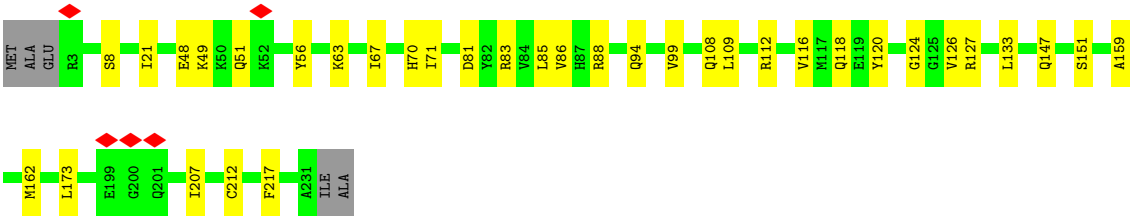
• Molecule 2: Proteasome subunit alpha type-2

Chain B:

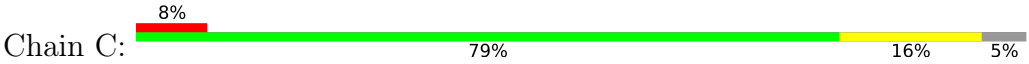


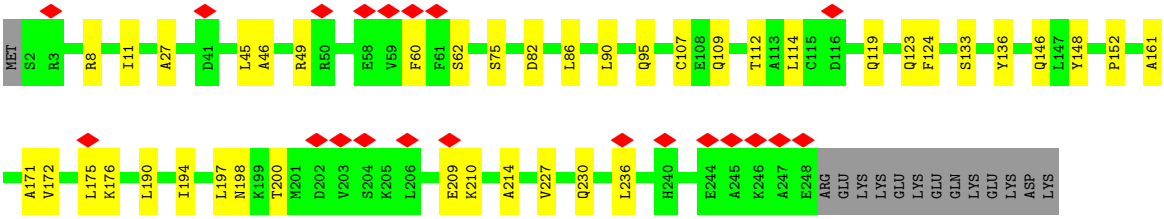
• Molecule 2: Proteasome subunit alpha type-2

Chain P:

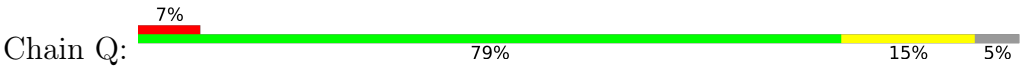


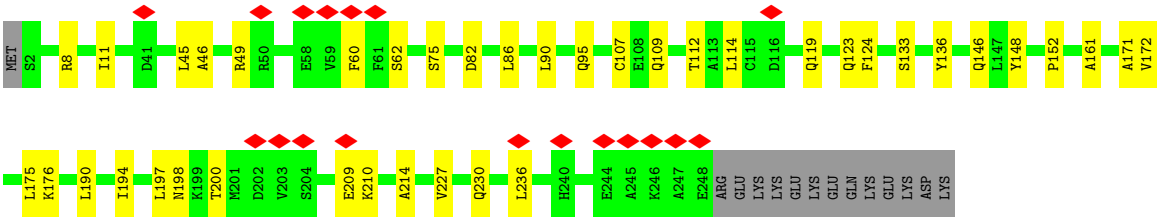
• Molecule 3: Proteasome subunit alpha type-4



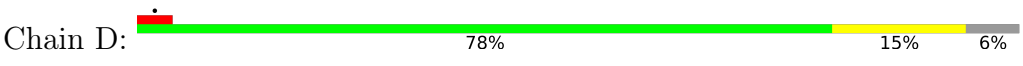


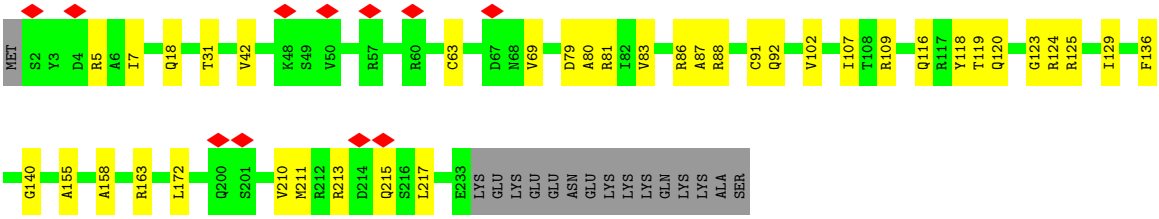
• Molecule 3: Proteasome subunit alpha type-4



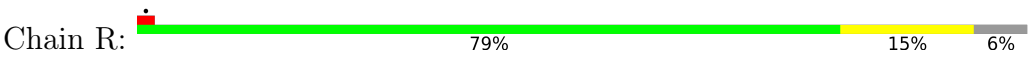


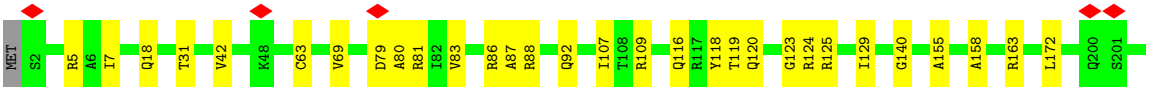
• Molecule 4: Proteasome subunit alpha type-7

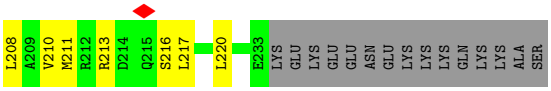




• Molecule 4: Proteasome subunit alpha type-7

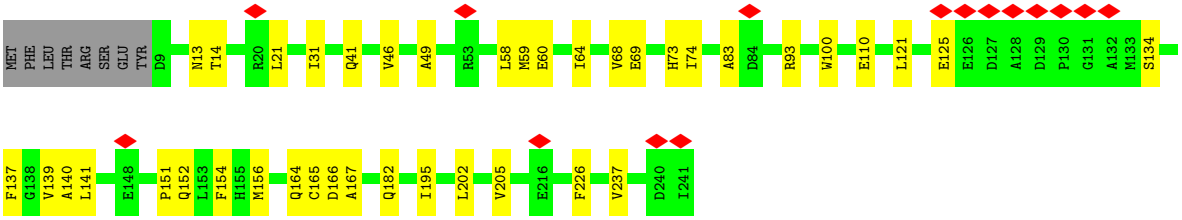






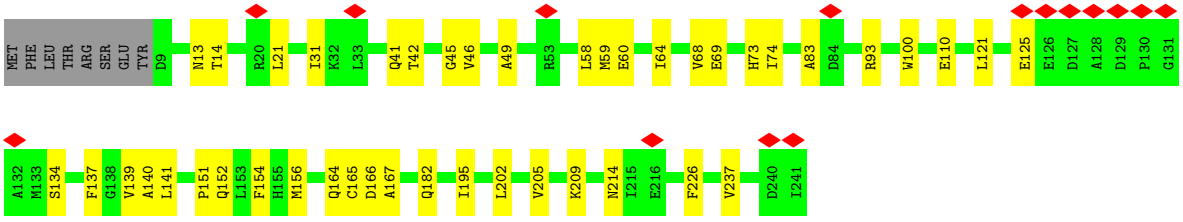
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



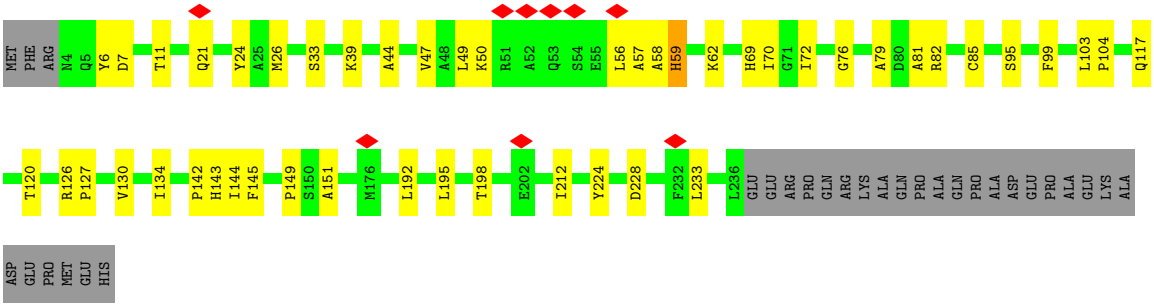
• Molecule 5: Proteasome subunit alpha type-5

Chain S:



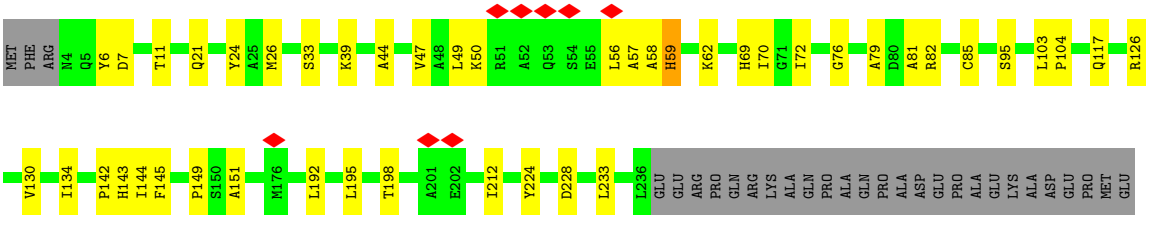
• Molecule 6: Proteasome subunit alpha type-1

Chain F:



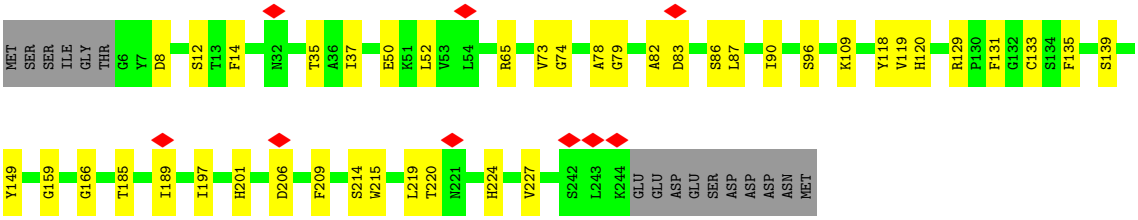
• Molecule 6: Proteasome subunit alpha type-1

Chain T:



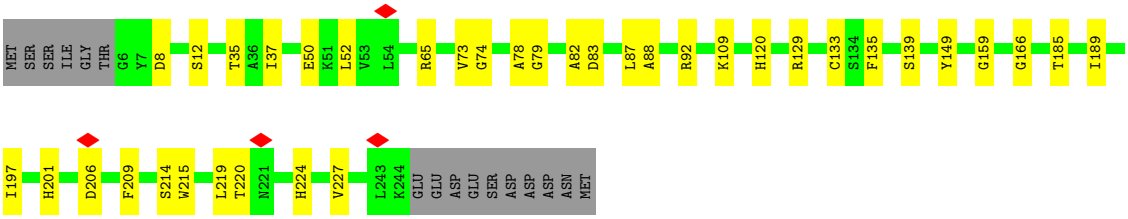
• Molecule 7: Proteasome subunit alpha type-3

Chain G:



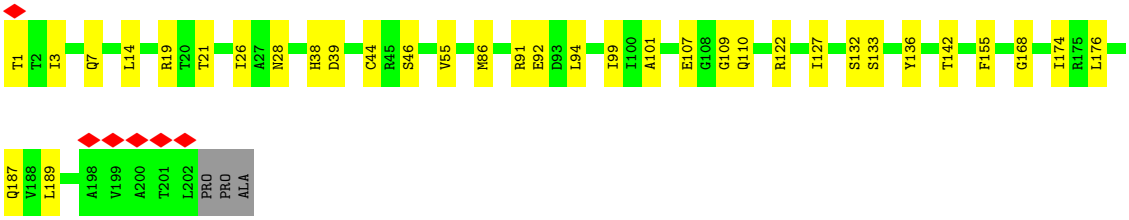
• Molecule 7: Proteasome subunit alpha type-3

Chain U:



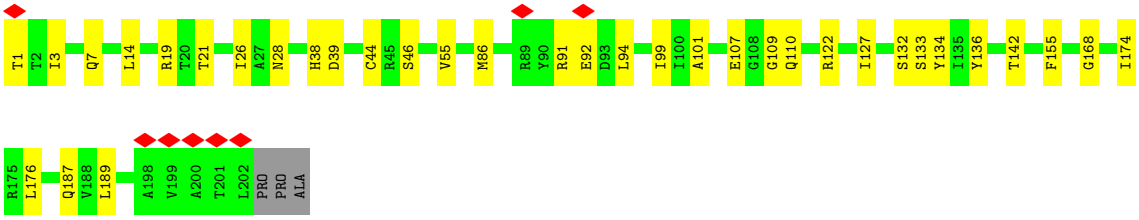
• Molecule 8: Proteasome subunit beta type-6

Chain H:



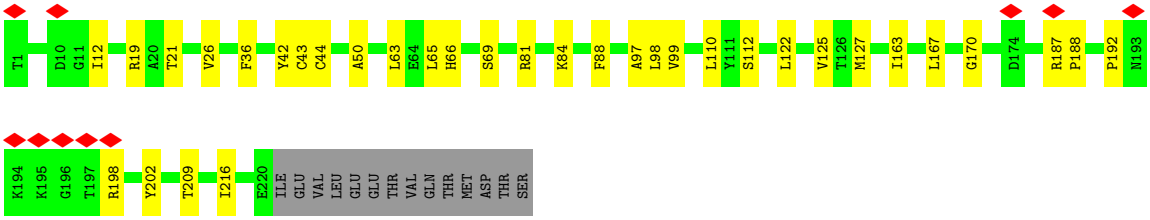
• Molecule 8: Proteasome subunit beta type-6

Chain V:



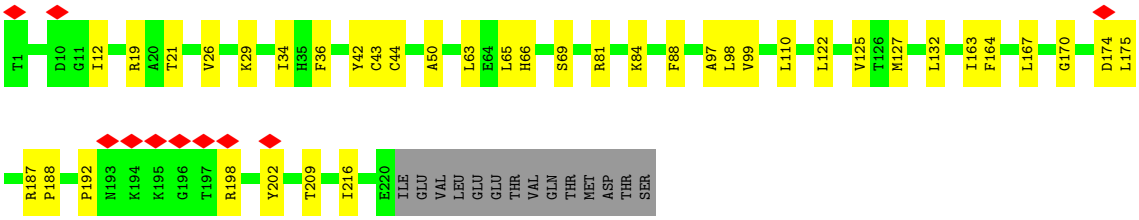
• Molecule 9: Proteasome subunit beta type-7

Chain I:



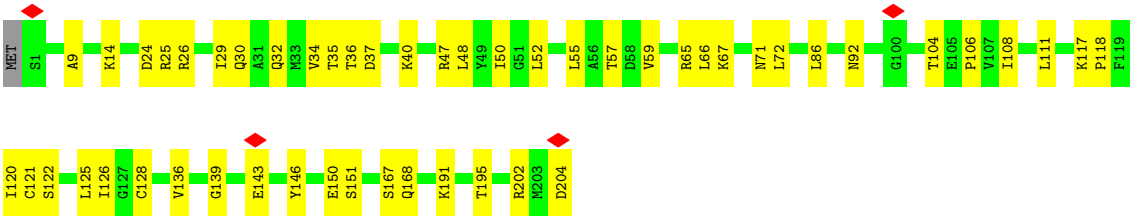
• Molecule 9: Proteasome subunit beta type-7

Chain W:



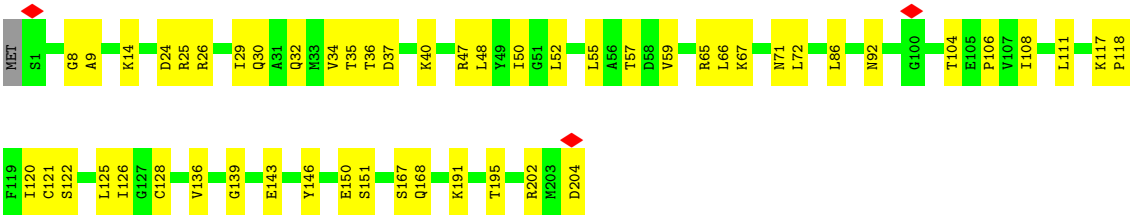
• Molecule 10: Proteasome subunit beta type-3

Chain J:



• Molecule 10: Proteasome subunit beta type-3

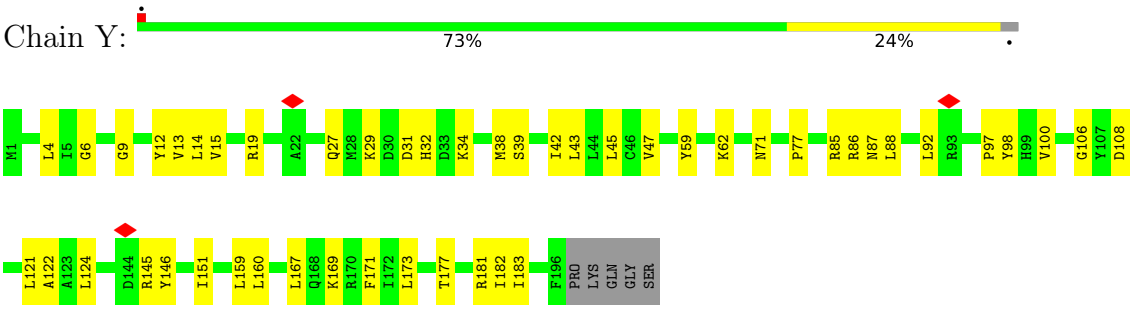
Chain X:



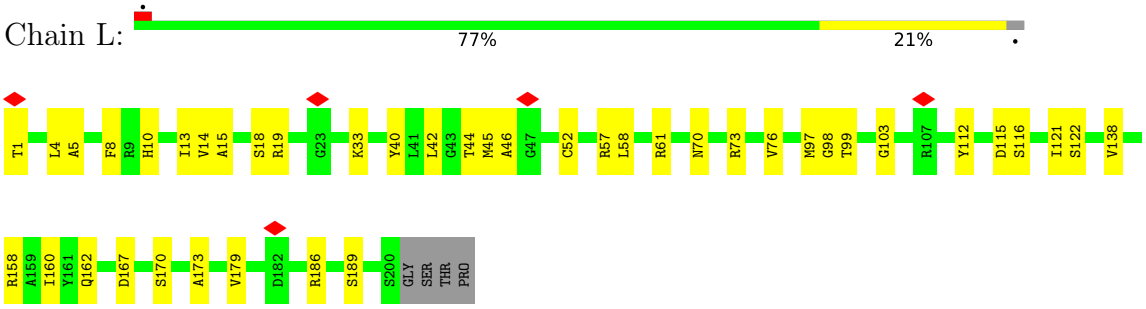
• Molecule 11: Proteasome subunit beta type-2

Chain K:

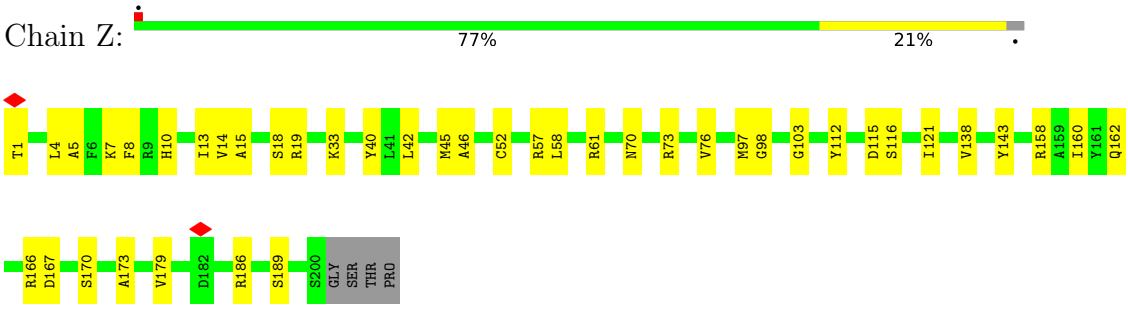
• Molecule 11: Proteasome subunit beta type-2



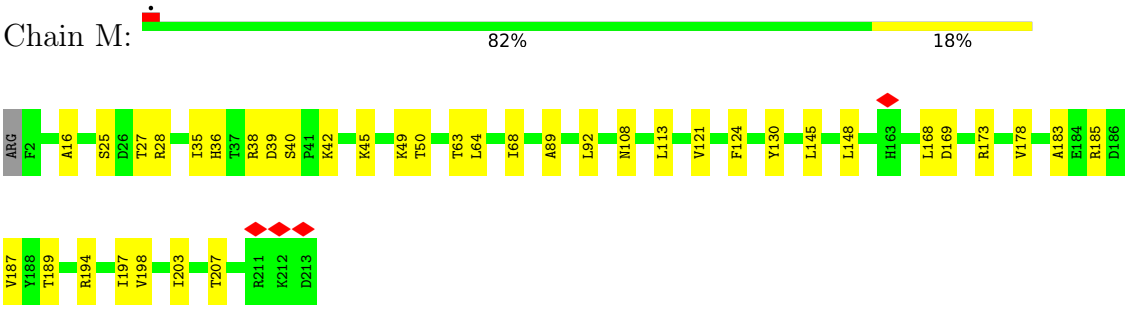
• Molecule 12: Proteasome subunit beta type-5



• Molecule 12: Proteasome subunit beta type-5

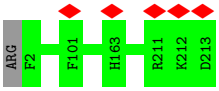


• Molecule 13: Proteasome subunit beta type-1



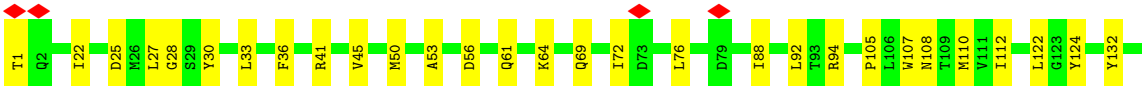
• Molecule 13: Proteasome subunit beta type-1

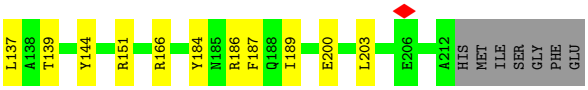
Chain a:



• Molecule 14: Proteasome subunit beta type-4

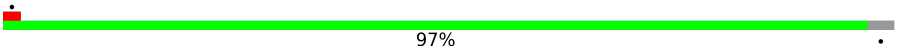
Chain N:

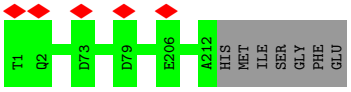




• Molecule 14: Proteasome subunit beta type-4

Chain b:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.022	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0153	Depositor
Map size (Å)	289.96, 289.96, 289.96	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality

5.1 Standard geometry

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	0.26	0/1758	0.44	0/2386
1	O	0.27	0/1754	0.44	0/2381
2	B	0.26	0/1701	0.42	0/2318
2	P	0.25	0/1701	0.42	0/2318
3	C	0.24	0/1815	0.43	0/2466
3	Q	0.24	0/1815	0.43	0/2466
4	D	0.24	0/1657	0.44	0/2261
4	R	0.24	0/1657	0.43	0/2261
5	E	0.25	0/1685	0.43	0/2290
5	S	0.24	0/1685	0.43	0/2290
6	F	0.24	0/1738	0.43	0/2364
6	T	0.24	0/1738	0.43	0/2364
7	G	0.26	0/1795	0.42	0/2434
7	U	0.26	0/1795	0.42	0/2434
8	H	0.25	0/1491	0.43	0/2021
8	V	0.25	0/1491	0.43	0/2021
9	I	0.25	0/1603	0.45	0/2180
9	W	0.25	0/1603	0.45	0/2180
10	J	0.25	0/1563	0.45	0/2113
10	X	0.25	0/1563	0.45	0/2113
11	K	0.25	0/1538	0.46	0/2088
11	Y	0.25	0/1538	0.45	0/2088
12	L	0.25	0/1531	0.44	0/2076
12	Z	0.25	0/1531	0.44	0/2076
13	M	0.25	0/1613	0.45	0/2178
13	a	0.25	0/1613	0.45	0/2178
14	N	0.25	0/1598	0.45	0/2170
14	b	0.25	0/1598	0.45	0/2170
All	All	0.25	0/46168	0.44	0/62685

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	1729	0	1650	28	0
1	O	1725	0	1647	40	0
2	B	1662	0	1590	28	0
2	P	1662	0	1590	25	0
3	C	1786	0	1717	28	0
3	Q	1786	0	1717	27	0
4	D	1633	0	1518	31	0
4	R	1633	0	1518	29	0
5	E	1659	0	1589	30	0
5	S	1659	0	1589	32	0
6	F	1704	0	1638	39	0
6	T	1704	0	1638	35	0
7	G	1760	0	1680	31	0
7	U	1760	0	1680	27	0
8	H	1465	0	1419	20	0
8	V	1465	0	1419	22	0
9	I	1576	0	1558	29	0
9	W	1576	0	1558	35	0
10	J	1534	0	1539	34	0
10	X	1534	0	1539	36	0
11	K	1506	0	1475	41	0
11	Y	1506	0	1475	40	0
12	L	1500	0	1441	30	0
12	Z	1500	0	1441	32	0
13	M	1583	0	1579	29	0
13	a	1583	0	1579	0	0
14	N	1568	0	1513	28	0
14	b	1568	0	1513	0	0
All	All	45326	0	43809	679	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 (679) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.24	1.19
9:I:187:ARG:HB2	9:I:188:PRO:HD3	1.26	1.16
5:S:121:LEU:HD12	6:T:79:ALA:HB3	1.59	0.84
5:E:121:LEU:HD12	6:F:79:ALA:HB3	1.59	0.83
9:I:187:ARG:CB	9:I:188:PRO:HD3	2.09	0.83
1:O:17:SER:OG	1:O:18:PRO:HD2	1.78	0.82
9:W:187:ARG:HB3	9:W:188:PRO:CD	2.06	0.82
9:I:187:ARG:HB2	9:I:188:PRO:CD	2.08	0.80
9:W:187:ARG:CB	9:W:188:PRO:HD3	2.10	0.78
1:O:14:THR:HG22	1:O:24:GLN:HG2	1.66	0.75
7:G:35:THR:HA	7:G:166:GLY:HA3	1.69	0.74
1:O:19:GLU:CB	1:O:21:ARG:HG3	2.17	0.73
12:L:97:MET:HG2	12:L:98:GLY:H	1.54	0.73
7:U:35:THR:HA	7:U:166:GLY:HA3	1.70	0.73
12:L:97:MET:HB3	12:L:116:SER:HB3	1.71	0.72
1:O:14:THR:CG2	1:O:24:GLN:HG2	2.21	0.71
12:Z:97:MET:HG2	12:Z:98:GLY:H	1.54	0.71
12:Z:97:MET:HB3	12:Z:116:SER:HB3	1.71	0.71
10:X:34:VAL:HG12	10:X:35:THR:HG23	1.74	0.70
10:J:34:VAL:HG12	10:J:35:THR:HG23	1.74	0.69
1:O:14:THR:HG22	1:O:24:GLN:CG	2.22	0.69
9:I:110:LEU:HD21	9:I:125:VAL:HG22	1.74	0.69
11:K:12:TYR:HB2	11:K:182:ILE:HD11	1.75	0.69
11:Y:12:TYR:HB2	11:Y:182:ILE:HD11	1.75	0.69
1:O:19:GLU:HB3	1:O:21:ARG:HG3	1.75	0.69
2:P:159:ALA:HB1	2:P:173:LEU:HD23	1.76	0.68
2:B:159:ALA:HB1	2:B:173:LEU:HD23	1.76	0.68
9:W:110:LEU:HD21	9:W:125:VAL:HG22	1.74	0.68
11:K:169:LYS:O	11:Y:27:GLN:NE2	2.27	0.67
12:Z:14:VAL:HG21	12:Z:42:LEU:HD11	1.76	0.67
2:B:85:LEU:HD21	2:B:133:LEU:HD11	1.77	0.67
10:J:24:ASP:OD1	10:J:40:LYS:NZ	2.27	0.67
6:F:95:SER:HB3	6:F:103:LEU:HD12	1.76	0.66
6:T:95:SER:HB3	6:T:103:LEU:HD12	1.76	0.66
11:K:19:ARG:HB3	11:K:31:ASP:HA	1.77	0.66
7:G:50:GLU:OE2	7:G:201:HIS:ND1	2.29	0.66
10:J:29:ILE:HG22	10:J:30:GLN:H	1.61	0.66
12:L:14:VAL:HG21	12:L:42:LEU:HD11	1.76	0.66
11:K:27:GLN:NE2	11:Y:169:LYS:O	2.29	0.65
2:P:85:LEU:HD21	2:P:133:LEU:HD11	1.77	0.65
10:X:29:ILE:HG22	10:X:30:GLN:H	1.61	0.65
6:F:44:ALA:HB2	6:F:142:PRO:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:163:ILE:HG12	9:W:170:GLY:HA2	1.78	0.65
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.79	0.65
11:Y:19:ARG:HB3	11:Y:31:ASP:HA	1.77	0.65
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.79	0.65
2:P:51:GLN:HB3	2:P:56:TYR:HD2	1.61	0.65
6:T:39:LYS:HB3	6:T:144:ILE:HD11	1.78	0.65
14:N:33:LEU:HD13	8:V:134:TYR:CZ	2.32	0.64
2:B:51:GLN:HB3	2:B:56:TYR:HD2	1.61	0.64
6:T:44:ALA:HB2	6:T:142:PRO:HB3	1.78	0.64
4:D:211:MET:HB2	4:D:217:LEU:HD12	1.80	0.64
1:O:19:GLU:HB2	1:O:21:ARG:HG3	1.79	0.64
4:R:5:ARG:O	4:R:123:GLY:N	2.30	0.64
4:R:211:MET:HB2	4:R:217:LEU:HD12	1.80	0.64
9:I:163:ILE:HG12	9:I:170:GLY:HA2	1.78	0.64
13:M:148:LEU:HD23	13:M:178:VAL:HG23	1.78	0.64
13:M:38:ARG:NH2	9:W:164:PHE:O	2.30	0.63
4:D:5:ARG:O	4:D:123:GLY:N	2.30	0.63
5:E:164:GLN:HB3	6:F:58:ALA:HB3	1.81	0.63
13:M:49:LYS:O	13:M:50:THR:OG1	2.14	0.63
13:M:198:VAL:HG22	13:M:203:ILE:HG12	1.81	0.63
14:N:56:ASP:O	14:N:108:ASN:ND2	2.24	0.63
6:F:39:LYS:HB3	6:F:144:ILE:HD11	1.78	0.62
5:S:164:GLN:HB3	6:T:58:ALA:HB3	1.81	0.62
7:U:50:GLU:OE2	7:U:201:HIS:ND1	2.29	0.62
8:V:107:GLU:OE1	8:V:110:GLN:NE2	2.33	0.61
3:C:46:ALA:HB1	3:C:197:LEU:HD11	1.81	0.61
3:Q:46:ALA:HB1	3:Q:197:LEU:HD11	1.81	0.61
12:Z:19:ARG:O	12:Z:33:LYS:NZ	2.31	0.61
8:H:107:GLU:OE1	8:H:110:GLN:NE2	2.33	0.61
2:B:83:ARG:HA	2:B:86:VAL:HG12	1.83	0.61
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.83	0.61
2:P:83:ARG:HA	2:P:86:VAL:HG12	1.83	0.61
3:Q:194:ILE:O	3:Q:198:ASN:ND2	2.35	0.60
13:M:45:LYS:HE3	13:M:203:ILE:HD12	1.84	0.60
2:P:48:GLU:O	2:P:63:LYS:NZ	2.35	0.60
5:S:31:ILE:HD13	5:S:140:ALA:HB2	1.83	0.60
3:C:194:ILE:O	3:C:198:ASN:ND2	2.35	0.59
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.83	0.59
5:E:41:GLN:NE2	5:E:151:PRO:O	2.36	0.59
9:W:36:PHE:HD1	9:W:42:TYR:HE1	1.50	0.59
5:E:31:ILE:HD13	5:E:140:ALA:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:GLU:O	2:B:63:LYS:NZ	2.35	0.59
13:M:27:THR:HB	13:M:39:ASP:HA	1.84	0.59
5:S:14:THR:HG23	6:T:21:GLN:HE22	1.68	0.59
5:S:41:GLN:NE2	5:S:151:PRO:O	2.36	0.59
8:V:28:ASN:ND2	9:W:122:LEU:HD11	2.18	0.59
14:N:61:GLN:HA	14:N:64:LYS:HD3	1.85	0.59
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.84	0.59
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.84	0.59
10:J:26:ARG:NH2	10:J:32:GLN:O	2.36	0.58
10:X:24:ASP:OD1	10:X:40:LYS:NZ	2.27	0.58
8:H:7:GLN:NE2	8:H:109:GLY:O	2.36	0.58
9:I:36:PHE:HD1	9:I:42:TYR:HE1	1.50	0.58
10:X:26:ARG:NH2	10:X:32:GLN:O	2.36	0.58
13:M:169:ASP:HB3	13:M:173:ARG:HH22	1.68	0.58
6:T:39:LYS:HD3	6:T:144:ILE:HG12	1.85	0.58
1:A:41:ALA:HB3	1:A:166:THR:HB	1.86	0.57
9:I:44:CYS:HB2	9:I:99:VAL:HB	1.86	0.57
1:O:41:ALA:HB3	1:O:166:THR:HB	1.86	0.57
5:E:14:THR:HG23	6:F:21:GLN:HE22	1.68	0.57
6:F:39:LYS:HD3	6:F:144:ILE:HG12	1.84	0.57
13:M:64:LEU:HD21	13:M:108:ASN:HD21	1.69	0.57
8:V:7:GLN:NE2	8:V:109:GLY:O	2.37	0.57
2:B:108:GLN:HB3	2:B:112:ARG:HH12	1.69	0.57
1:O:120:ASP:OD1	2:P:83:ARG:NH1	2.38	0.57
8:H:28:ASN:ND2	9:I:122:LEU:HD11	2.18	0.57
13:M:35:ILE:O	14:N:151:ARG:NH2	2.30	0.57
9:W:34:ILE:HD12	9:W:174:ASP:CG	2.25	0.57
9:W:44:CYS:HB2	9:W:99:VAL:HB	1.86	0.57
1:A:120:ASP:OD1	2:B:83:ARG:NH1	2.38	0.56
4:D:86:ARG:NH1	4:D:118:TYR:OH	2.29	0.56
12:L:19:ARG:O	12:L:33:LYS:NZ	2.31	0.56
10:X:125:LEU:HD12	10:X:126:ILE:HG23	1.86	0.56
10:J:48:LEU:HD21	10:J:86:LEU:HD22	1.88	0.56
2:P:67:ILE:HG21	2:P:109:LEU:HD11	1.88	0.56
10:J:125:LEU:HD12	10:J:126:ILE:HG23	1.86	0.56
13:M:68:ILE:HD11	13:M:92:LEU:HD13	1.87	0.56
4:R:86:ARG:NH1	4:R:118:TYR:OH	2.29	0.56
2:P:108:GLN:HB3	2:P:112:ARG:HH12	1.69	0.56
12:Z:98:GLY:HA2	12:Z:115:ASP:HA	1.88	0.56
14:N:28:GLY:N	14:N:36:PHE:O	2.39	0.56
10:X:48:LEU:HD21	10:X:86:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:LYS:HB3	6:F:59:HIS:HB2	1.88	0.55
1:O:19:GLU:OE1	1:O:19:GLU:HA	2.06	0.55
8:V:176:LEU:HD12	8:V:187:GLN:HE21	1.71	0.55
3:C:190:LEU:HD23	3:C:236:LEU:HD11	1.88	0.55
9:I:209:THR:OG1	10:J:168:GLN:NE2	2.38	0.55
11:K:4:LEU:HD22	11:K:45:LEU:HD23	1.89	0.55
6:F:7:ASP:HB2	6:F:24:TYR:HE2	1.72	0.55
13:M:145:LEU:HD22	13:M:178:VAL:HG22	1.88	0.55
9:W:209:THR:OG1	10:X:168:GLN:NE2	2.38	0.55
12:L:98:GLY:HA2	12:L:115:ASP:HA	1.88	0.55
13:M:36:HIS:HB3	14:N:132:TYR:CZ	2.41	0.55
14:N:25:ASP:OD1	14:N:41:ARG:NH2	2.40	0.55
14:N:27:LEU:HD13	14:N:184:TYR:HB2	1.88	0.55
6:T:50:LYS:HB3	6:T:59:HIS:HB2	1.88	0.55
5:E:41:GLN:HA	5:E:46:VAL:HG12	1.89	0.55
3:Q:190:LEU:HD23	3:Q:236:LEU:HD11	1.87	0.55
2:B:147:GLN:NE2	2:B:162:MET:SD	2.80	0.54
5:S:41:GLN:HA	5:S:46:VAL:HG12	1.89	0.54
12:Z:45:MET:HG3	12:Z:52:CYS:HB2	1.89	0.54
8:H:176:LEU:HD12	8:H:187:GLN:HE21	1.71	0.54
2:P:147:GLN:NE2	2:P:162:MET:SD	2.80	0.54
9:W:198:ARG:NH2	10:X:150:GLU:O	2.40	0.54
11:Y:4:LEU:HD22	11:Y:45:LEU:HD23	1.89	0.54
11:Y:19:ARG:HE	11:Y:177:THR:HB	1.72	0.54
2:B:67:ILE:HG21	2:B:109:LEU:HD11	1.88	0.54
13:M:28:ARG:NH1	13:M:187:VAL:O	2.40	0.54
11:Y:171:PHE:CE2	11:Y:173:LEU:HB2	2.42	0.54
7:G:215:TRP:CZ3	7:G:227:VAL:HG13	2.43	0.54
7:U:79:GLY:HA3	7:U:133:CYS:HA	1.89	0.54
11:K:171:PHE:CE2	11:K:173:LEU:HB2	2.42	0.54
9:I:198:ARG:NH2	10:J:150:GLU:O	2.40	0.54
3:C:109:GLN:HE21	11:K:71:ASN:HD21	1.56	0.54
3:Q:109:GLN:HE21	11:Y:71:ASN:HD21	1.56	0.54
7:G:79:GLY:HA3	7:G:133:CYS:HA	1.89	0.53
14:N:25:ASP:HA	14:N:187:PHE:HA	1.90	0.53
1:O:49:VAL:HG22	1:O:219:VAL:HG12	1.90	0.53
9:I:97:ALA:HB1	9:I:127:MET:HE2	1.90	0.53
10:J:47:ARG:HD3	10:J:111:LEU:HD12	1.91	0.53
12:L:45:MET:HG3	12:L:52:CYS:HB2	1.89	0.53
4:R:69:VAL:HG11	4:R:107:ILE:HG21	1.91	0.53
4:R:80:ALA:HA	4:R:129:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:ALA:HA	4:D:129:ILE:HD13	1.90	0.53
10:J:25:ARG:HH11	10:J:37:ASP:HA	1.74	0.53
11:K:19:ARG:HE	11:K:177:THR:HB	1.73	0.53
5:E:13:ASN:HB3	6:F:126:ARG:HB3	1.91	0.53
11:K:19:ARG:HH21	11:K:177:THR:HB	1.73	0.53
10:X:47:ARG:HD3	10:X:111:LEU:HD12	1.91	0.53
2:B:13:SER:HB2	2:B:14:PRO:HD2	1.90	0.53
7:U:215:TRP:CZ3	7:U:227:VAL:HG13	2.43	0.53
10:X:25:ARG:HH11	10:X:37:ASP:HA	1.74	0.53
12:Z:18:SER:HB2	12:Z:173:ALA:H	1.73	0.53
11:Y:29:LYS:HB2	12:Z:121:ILE:HD12	1.91	0.53
6:F:47:VAL:HG12	6:F:195:LEU:HD22	1.90	0.53
9:I:19:ARG:NH1	9:I:167:LEU:O	2.42	0.52
10:J:104:THR:HG23	10:J:106:PRO:HD3	1.91	0.52
6:T:7:ASP:HB2	6:T:24:TYR:HE2	1.72	0.52
4:D:69:VAL:HG11	4:D:107:ILE:HG21	1.91	0.52
9:I:12:ILE:HD11	9:I:110:LEU:HD12	1.92	0.52
6:T:49:LEU:HG	6:T:195:LEU:HD11	1.91	0.52
7:G:96:SER:OG	14:N:69:GLN:NE2	2.42	0.52
3:Q:209:GLU:OE2	3:Q:230:GLN:NE2	2.42	0.52
9:I:50:ALA:HB2	10:J:128:CYS:HB2	1.91	0.52
10:J:143:GLU:HA	10:J:146:TYR:HD2	1.75	0.52
12:L:4:LEU:HB2	12:L:160:ILE:HD11	1.92	0.52
12:L:138:VAL:HG21	12:L:162:GLN:HG3	1.91	0.52
1:O:10:ASP:OD2	1:O:17:SER:HA	2.10	0.52
8:V:133:SER:HA	8:V:136:TYR:HE2	1.75	0.52
11:Y:19:ARG:HH21	11:Y:177:THR:HB	1.73	0.52
12:Z:138:VAL:HG21	12:Z:162:GLN:HG3	1.91	0.52
1:A:49:VAL:HG22	1:A:219:VAL:HG12	1.90	0.52
3:C:209:GLU:OE2	3:C:230:GLN:NE2	2.42	0.52
6:T:47:VAL:HG12	6:T:195:LEU:HD22	1.90	0.52
9:W:12:ILE:HD11	9:W:110:LEU:HD12	1.92	0.52
9:W:19:ARG:NH1	9:W:167:LEU:O	2.42	0.52
6:F:72:ILE:HG22	6:F:134:ILE:HG12	1.92	0.52
11:K:29:LYS:HD2	12:L:121:ILE:HB	1.92	0.52
12:L:18:SER:HB2	12:L:173:ALA:H	1.73	0.52
4:R:31:THR:OG1	4:R:163:ARG:O	2.23	0.52
6:T:76:GLY:HA3	6:T:130:VAL:HA	1.92	0.52
3:C:112:THR:HG23	4:D:81:ARG:HD2	1.92	0.52
8:H:133:SER:HA	8:H:136:TYR:HE2	1.75	0.52
9:I:187:ARG:CB	9:I:188:PRO:CD	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:29:LYS:HB2	12:L:121:ILE:HD12	1.91	0.52
3:Q:112:THR:HG23	4:R:81:ARG:HD2	1.92	0.52
3:C:124:PHE:HB3	4:D:124:ARG:HG2	1.92	0.52
1:O:17:SER:OG	1:O:18:PRO:CD	2.53	0.52
5:S:13:ASN:HB3	6:T:126:ARG:HB3	1.91	0.52
10:X:25:ARG:HB3	10:X:36:THR:O	2.10	0.52
11:Y:14:LEU:HD12	11:Y:182:ILE:HD13	1.91	0.51
6:F:49:LEU:HG	6:F:195:LEU:HD11	1.91	0.51
10:X:143:GLU:HA	10:X:146:TYR:HD2	1.75	0.51
12:Z:4:LEU:HB2	12:Z:160:ILE:HD11	1.92	0.51
14:N:92:LEU:HD23	14:N:112:ILE:HD11	1.91	0.51
14:N:189:ILE:HD12	14:N:203:LEU:HD22	1.91	0.51
9:W:50:ALA:HB2	10:X:128:CYS:HB2	1.91	0.51
10:J:25:ARG:HB3	10:J:36:THR:O	2.10	0.51
2:P:88:ARG:HD2	2:P:116:VAL:HG11	1.91	0.51
2:B:88:ARG:HD2	2:B:116:VAL:HG11	1.91	0.51
9:W:34:ILE:HD12	9:W:174:ASP:OD2	2.10	0.51
3:Q:124:PHE:HB3	4:R:124:ARG:HG2	1.92	0.51
2:P:51:GLN:HB3	2:P:56:TYR:CD2	2.45	0.51
6:T:72:ILE:HG22	6:T:134:ILE:HG12	1.92	0.51
8:V:21:THR:HG22	8:V:26:ILE:HG12	1.92	0.51
7:G:215:TRP:HZ3	7:G:227:VAL:HG13	1.76	0.51
3:Q:119:GLN:HE22	4:R:79:ASP:HA	1.76	0.51
3:C:45:LEU:HD13	3:C:75:SER:HB2	1.92	0.51
8:H:3:ILE:HD12	8:H:99:ILE:HG22	1.92	0.51
13:M:168:LEU:HD11	13:M:197:ILE:HD11	1.93	0.51
7:U:215:TRP:CE3	7:U:227:VAL:HG22	2.46	0.51
10:X:67:LYS:HE3	10:X:71:ASN:HD21	1.76	0.51
10:X:104:THR:HG23	10:X:106:PRO:HD3	1.91	0.51
11:Y:29:LYS:HD2	12:Z:121:ILE:HB	1.92	0.51
7:G:215:TRP:CE3	7:G:227:VAL:HG22	2.46	0.51
14:N:53:ALA:HB2	14:N:110:MET:HG2	1.93	0.51
9:W:36:PHE:CD1	9:W:42:TYR:HE1	2.29	0.51
10:J:9:ALA:HA	10:J:139:GLY:HA3	1.93	0.50
11:K:14:LEU:HD12	11:K:182:ILE:HD13	1.91	0.50
3:Q:45:LEU:HD13	3:Q:75:SER:HB2	1.92	0.50
9:W:97:ALA:HB1	9:W:127:MET:HE2	1.92	0.50
10:X:47:ARG:NH2	10:X:191:LYS:O	2.45	0.50
2:B:51:GLN:HB3	2:B:56:TYR:CD2	2.45	0.50
13:M:49:LYS:HD2	13:M:113:LEU:HB2	1.92	0.50
6:T:11:THR:HA	7:U:129:ARG:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:215:TRP:HZ3	7:U:227:VAL:HG13	1.76	0.50
8:V:3:ILE:HD12	8:V:99:ILE:HG22	1.92	0.50
9:W:81:ARG:HA	9:W:84:LYS:HG2	1.93	0.50
6:F:76:GLY:HA3	6:F:130:VAL:HA	1.92	0.50
6:F:82:ARG:HA	6:F:85:CYS:HB3	1.93	0.50
9:I:81:ARG:HA	9:I:84:LYS:HG2	1.92	0.50
10:J:67:LYS:HE3	10:J:71:ASN:HD21	1.76	0.50
2:P:99:VAL:HG13	10:X:92:ASN:HD22	1.76	0.50
3:Q:161:ALA:HB1	3:Q:175:LEU:HD13	1.94	0.50
6:T:143:HIS:HB3	6:T:145:PHE:CD2	2.46	0.50
3:C:161:ALA:HB1	3:C:175:LEU:HD13	1.93	0.50
3:Q:171:ALA:HB2	3:Q:200:THR:HG21	1.94	0.50
10:X:9:ALA:HA	10:X:139:GLY:HA3	1.93	0.50
3:C:119:GLN:HE22	4:D:79:ASP:HA	1.76	0.50
4:D:31:THR:OG1	4:D:163:ARG:O	2.23	0.50
10:J:47:ARG:NH2	10:J:191:LYS:O	2.45	0.50
13:M:108:ASN:HB2	13:M:124:PHE:HB2	1.92	0.50
12:Z:8:PHE:CE1	12:Z:10:HIS:HB2	2.47	0.50
12:L:8:PHE:CE1	12:L:10:HIS:HB2	2.47	0.50
1:O:158:GLY:O	2:P:83:ARG:NH2	2.45	0.50
6:F:143:HIS:HB3	6:F:145:PHE:CD2	2.47	0.50
7:U:109:LYS:HA	7:U:149:TYR:HE2	1.77	0.50
2:B:99:VAL:HG13	10:J:92:ASN:HD22	1.76	0.49
3:C:171:ALA:HB2	3:C:200:THR:HG21	1.94	0.49
7:G:109:LYS:HA	7:G:149:TYR:HE2	1.77	0.49
11:K:13:VAL:HB	11:K:183:ILE:HB	1.94	0.49
11:Y:13:VAL:HB	11:Y:183:ILE:HB	1.94	0.49
6:F:11:THR:HA	7:G:129:ARG:HD3	1.93	0.49
6:F:117:GLN:HE22	7:G:83:ASP:HA	1.77	0.49
6:T:117:GLN:HE22	7:U:83:ASP:HA	1.77	0.49
8:H:21:THR:HG22	8:H:26:ILE:HG12	1.92	0.49
12:Z:103:GLY:HA2	12:Z:179:VAL:HG11	1.94	0.49
9:I:36:PHE:CD1	9:I:42:TYR:HE1	2.29	0.49
11:K:59:TYR:HE2	11:K:87:ASN:HD22	1.61	0.49
1:A:153:LYS:HB3	1:A:163:PHE:CE2	2.48	0.49
3:C:86:LEU:HD22	3:C:114:LEU:HD11	1.95	0.49
8:H:133:SER:HA	8:H:136:TYR:CE2	2.47	0.49
12:L:103:GLY:HA2	12:L:179:VAL:HG11	1.94	0.49
6:T:82:ARG:HA	6:T:85:CYS:HB3	1.93	0.49
8:V:133:SER:HA	8:V:136:TYR:CE2	2.47	0.49
1:A:158:GLY:O	2:B:83:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:216:ILE:HG12	10:J:195:THR:HG22	1.95	0.49
1:O:43:ARG:HA	1:O:48:ALA:HA	1.95	0.49
3:Q:136:TYR:HB2	3:Q:148:TYR:HB2	1.95	0.49
14:N:45:VAL:HG11	14:N:88:ILE:HD13	1.93	0.49
1:A:43:ARG:HA	1:A:48:ALA:HA	1.95	0.49
4:D:5:ARG:HA	5:E:125:GLU:HB2	1.95	0.49
3:Q:86:LEU:HD22	3:Q:114:LEU:HD11	1.95	0.49
10:J:202:ARG:NH2	10:J:204:ASP:OD2	2.46	0.48
4:R:140:GLY:O	4:R:213:ARG:NH1	2.46	0.48
3:C:136:TYR:HB2	3:C:148:TYR:HB2	1.95	0.48
13:M:25:SER:HB2	13:M:42:LYS:HB2	1.95	0.48
1:O:153:LYS:HB3	1:O:163:PHE:CE2	2.48	0.48
2:B:120:TYR:HD1	2:B:126:VAL:HG21	1.79	0.48
7:G:73:VAL:HG22	7:G:139:SER:HB3	1.94	0.48
7:U:149:TYR:HD1	7:U:159:GLY:HA2	1.78	0.48
11:K:43:LEU:HD12	11:K:183:ILE:HD11	1.95	0.48
9:I:21:THR:HG22	9:I:26:VAL:HA	1.96	0.48
1:A:51:VAL:HG22	1:A:217:VAL:HG22	1.96	0.48
2:P:120:TYR:HD1	2:P:126:VAL:HG21	1.79	0.48
6:T:26:MET:HA	6:T:149:PRO:HG2	1.96	0.48
11:Y:38:MET:HB2	11:Y:42:ILE:HG13	1.96	0.48
11:K:38:MET:HB2	11:K:42:ILE:HG13	1.96	0.48
5:E:165:CYS:HA	6:F:57:ALA:HA	1.96	0.48
7:U:219:LEU:HD12	7:U:220:THR:HG23	1.96	0.48
11:Y:59:TYR:HE2	11:Y:87:ASN:HD22	1.60	0.48
6:F:26:MET:HA	6:F:149:PRO:HG2	1.96	0.48
6:T:69:HIS:CD2	6:T:70:ILE:HG13	2.49	0.48
7:U:73:VAL:HG22	7:U:139:SER:HB3	1.94	0.48
10:X:202:ARG:NH2	10:X:204:ASP:OD2	2.46	0.48
2:B:8:SER:HA	2:B:124:GLY:HA2	1.96	0.47
1:A:191:PHE:CE1	1:A:193:GLN:HB2	2.49	0.47
2:B:16:GLY:O	3:C:27:ALA:HB2	2.14	0.47
6:F:69:HIS:CD2	6:F:70:ILE:HG13	2.49	0.47
2:P:118:GLN:HE22	3:Q:82:ASP:HA	1.78	0.47
4:R:5:ARG:HA	5:S:125:GLU:HB2	1.96	0.47
9:W:216:ILE:HG12	10:X:195:THR:HG22	1.95	0.47
11:K:43:LEU:HD11	11:K:181:ARG:HD2	1.97	0.47
1:O:103:TYR:O	9:W:81:ARG:HD3	2.15	0.47
2:P:8:SER:HA	2:P:124:GLY:HA2	1.96	0.47
5:S:100:TRP:O	12:Z:57:ARG:NH2	2.47	0.47
10:X:8:GLY:HA3	10:X:40:LYS:HZ3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:GLN:HE22	3:C:82:ASP:HA	1.78	0.47
5:E:182:GLN:HA	6:F:56:LEU:HD11	1.96	0.47
11:K:6:GLY:HA2	11:K:15:VAL:HA	1.97	0.47
13:M:36:HIS:O	14:N:151:ARG:NH2	2.48	0.47
2:P:212:CYS:HB2	2:P:217:PHE:HD1	1.80	0.47
9:W:21:THR:HG22	9:W:26:VAL:HA	1.96	0.47
3:C:172:VAL:O	3:C:176:LYS:HG3	2.15	0.47
5:E:100:TRP:O	12:L:57:ARG:NH2	2.47	0.47
14:N:56:ASP:H	14:N:107:TRP:HD1	1.61	0.47
1:O:191:PHE:CE1	1:O:193:GLN:HB2	2.49	0.47
4:R:120:GLN:O	5:S:134:SER:N	2.33	0.47
5:S:165:CYS:HA	6:T:57:ALA:HA	1.96	0.47
12:Z:8:PHE:HE1	12:Z:10:HIS:HB2	1.80	0.47
1:A:103:TYR:O	9:I:81:ARG:HD3	2.15	0.47
2:B:212:CYS:HB2	2:B:217:PHE:HD1	1.80	0.47
5:E:41:GLN:N	5:E:166:ASP:O	2.39	0.47
7:G:149:TYR:HD1	7:G:159:GLY:HA2	1.78	0.47
7:G:219:LEU:HD12	7:G:220:THR:HG23	1.95	0.47
1:O:49:VAL:HG11	1:O:195:VAL:HA	1.97	0.47
3:Q:172:VAL:O	3:Q:176:LYS:HG3	2.15	0.47
11:Y:43:LEU:HD12	11:Y:183:ILE:HD11	1.96	0.47
4:D:7:ILE:HG22	4:D:18:GLN:HG3	1.97	0.47
13:M:16:ALA:HB2	13:M:121:VAL:HG23	1.96	0.47
1:O:115:CYS:SG	1:O:140:LEU:HD12	2.55	0.47
6:T:192:LEU:HD21	6:T:212:ILE:HD11	1.95	0.47
10:X:52:LEU:HB2	10:X:59:VAL:HG13	1.97	0.47
12:L:4:LEU:N	12:L:15:ALA:O	2.46	0.47
13:M:27:THR:O	13:M:40:SER:N	2.47	0.47
1:O:51:VAL:HG22	1:O:217:VAL:HG22	1.96	0.46
6:F:192:LEU:HD21	6:F:212:ILE:HD11	1.95	0.46
8:H:91:ARG:NH1	8:H:92:GLU:OE2	2.49	0.46
8:H:174:ILE:HB	8:H:189:LEU:HB2	1.98	0.46
11:K:145:ARG:HD3	12:Z:158:ARG:HD3	1.97	0.46
11:K:173:LEU:HD23	11:Y:173:LEU:HD23	1.97	0.46
12:L:158:ARG:HD3	11:Y:145:ARG:HD3	1.97	0.46
13:M:113:LEU:HD13	13:M:198:VAL:HG12	1.95	0.46
8:V:91:ARG:NH1	8:V:92:GLU:OE2	2.49	0.46
11:Y:88:LEU:HG	11:Y:122:ALA:HB2	1.98	0.46
12:Z:97:MET:CG	12:Z:98:GLY:H	2.26	0.46
1:A:152:TYR:HD1	1:A:162:GLY:HA2	1.81	0.46
1:A:182:LYS:NZ	1:A:197:THR:HG23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:182:GLN:HA	6:T:56:LEU:HD11	1.96	0.46
8:V:142:THR:HG23	8:V:155:PHE:HE1	1.80	0.46
12:Z:4:LEU:N	12:Z:15:ALA:O	2.46	0.46
10:J:55:LEU:HD11	11:K:121:LEU:HD13	1.98	0.46
4:R:7:ILE:HG22	4:R:18:GLN:HG3	1.97	0.46
10:X:14:LYS:HE3	10:X:120:ILE:HG12	1.98	0.46
1:A:49:VAL:HG11	1:A:195:VAL:HA	1.97	0.46
4:D:136:PHE:CD1	4:D:213:ARG:HG3	2.51	0.46
8:H:94:LEU:HD21	9:I:88:PHE:HZ	1.80	0.46
12:L:97:MET:CG	12:L:98:GLY:H	2.26	0.46
11:Y:39:SER:HB2	11:Y:42:ILE:HG12	1.98	0.46
1:A:123:GLN:NE2	2:B:81:ASP:HA	2.31	0.46
8:H:38:HIS:CD2	8:H:39:ASP:H	2.34	0.46
8:H:142:THR:HG23	8:H:155:PHE:HE1	1.80	0.46
10:J:52:LEU:HB2	10:J:59:VAL:HG13	1.97	0.46
11:K:39:SER:HB2	11:K:42:ILE:HG12	1.98	0.46
12:L:8:PHE:HE1	12:L:10:HIS:HB2	1.80	0.46
6:T:6:TYR:OH	7:U:8:ASP:OD2	2.29	0.46
11:Y:43:LEU:HD11	11:Y:181:ARG:HD2	1.97	0.46
3:C:11:ILE:HG22	4:D:7:ILE:HG23	1.98	0.46
1:O:123:GLN:NE2	2:P:81:ASP:HA	2.31	0.46
1:O:182:LYS:NZ	1:O:197:THR:HG23	2.30	0.46
8:V:19:ARG:NH1	8:V:168:GLY:O	2.46	0.46
8:V:94:LEU:HD21	9:W:88:PHE:HZ	1.80	0.46
11:Y:6:GLY:HA2	11:Y:15:VAL:HA	1.97	0.46
12:Z:58:LEU:HD12	12:Z:61:ARG:HD3	1.97	0.46
1:A:115:CYS:SG	1:A:140:LEU:HD12	2.55	0.46
1:O:152:TYR:HD1	1:O:162:GLY:HA2	1.81	0.46
3:Q:49:ARG:N	3:Q:210:LYS:O	2.41	0.46
13:M:194:ARG:HH11	13:M:207:THR:HB	1.81	0.46
8:V:38:HIS:CD2	8:V:39:ASP:H	2.34	0.46
8:V:174:ILE:HB	8:V:189:LEU:HB2	1.98	0.46
4:D:42:VAL:HG22	4:D:210:VAL:HG22	1.98	0.45
2:P:70:HIS:CD2	2:P:71:ILE:HG13	2.51	0.45
5:S:202:LEU:HA	5:S:205:VAL:HG22	1.98	0.45
11:Y:98:TYR:HB3	11:Y:100:VAL:HG22	1.98	0.45
3:C:107:CYS:HB2	3:C:146:GLN:OE1	2.16	0.45
7:G:185:THR:O	7:G:189:ILE:HG12	2.17	0.45
10:J:14:LYS:HE3	10:J:120:ILE:HG12	1.98	0.45
14:N:124:TYR:HE1	14:N:139:THR:HG22	1.81	0.45
3:Q:11:ILE:HG22	4:R:7:ILE:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:107:CYS:HB2	3:Q:146:GLN:OE1	2.16	0.45
6:F:224:TYR:HD1	6:F:228:ASP:HB3	1.81	0.45
10:J:55:LEU:HG	10:J:57:THR:HG22	1.99	0.45
3:Q:8:ARG:HE	4:R:5:ARG:HH22	1.64	0.45
4:R:42:VAL:HG22	4:R:210:VAL:HG22	1.98	0.45
6:T:195:LEU:O	6:T:198:THR:OG1	2.29	0.45
6:T:224:TYR:HD1	6:T:228:ASP:HB3	1.81	0.45
10:X:55:LEU:HG	10:X:57:THR:HG22	1.99	0.45
3:C:60:PHE:O	3:C:62:SER:N	2.49	0.45
11:K:88:LEU:HG	11:K:122:ALA:HB2	1.98	0.45
4:R:158:ALA:HB3	5:S:58:LEU:HD13	1.99	0.45
4:D:158:ALA:HB3	5:E:58:LEU:HD13	1.99	0.45
2:B:70:HIS:CD2	2:B:71:ILE:HG13	2.51	0.45
4:D:116:GLN:O	4:D:119:THR:OG1	2.28	0.45
12:L:8:PHE:HE2	12:L:13:ILE:HG12	1.82	0.45
12:L:58:LEU:HD12	12:L:61:ARG:HD3	1.97	0.45
5:S:69:GLU:HG2	5:S:226:PHE:CD2	2.52	0.45
10:X:55:LEU:HD11	11:Y:121:LEU:HD13	1.98	0.45
10:X:121:CYS:SG	10:X:122:SER:N	2.90	0.45
5:E:137:PHE:HB3	5:E:139:VAL:HG22	1.99	0.45
10:J:50:ILE:HG13	10:J:108:ILE:HG22	1.99	0.45
8:V:55:VAL:HG13	8:V:86:MET:HG2	1.99	0.45
1:A:116:LYS:NZ	9:I:69:SER:OG	2.50	0.45
3:C:8:ARG:HE	4:D:5:ARG:HH22	1.64	0.45
5:E:202:LEU:HA	5:E:205:VAL:HG22	1.98	0.45
8:H:55:VAL:HG13	8:H:86:MET:HG2	1.99	0.45
11:K:98:TYR:HB3	11:K:100:VAL:HG22	1.98	0.45
14:N:72:ILE:O	14:N:76:LEU:HG	2.17	0.45
7:U:185:THR:O	7:U:189:ILE:HG12	2.17	0.45
7:U:214:SER:HA	7:U:227:VAL:HG23	1.99	0.45
1:A:192:GLU:OE1	1:A:193:GLN:NE2	2.50	0.44
5:E:69:GLU:HG2	5:E:226:PHE:CD2	2.52	0.44
5:E:69:GLU:O	5:E:93:ARG:NE	2.50	0.44
1:O:116:LYS:NZ	9:W:69:SER:OG	2.50	0.44
7:G:214:SER:HA	7:G:227:VAL:HG23	1.99	0.44
11:K:19:ARG:NH2	11:K:177:THR:HB	2.32	0.44
10:X:66:LEU:HD21	10:X:86:LEU:HD11	1.99	0.44
10:J:121:CYS:SG	10:J:122:SER:N	2.90	0.44
1:O:192:GLU:OE1	1:O:193:GLN:NE2	2.50	0.44
3:C:49:ARG:N	3:C:210:LYS:O	2.41	0.44
11:K:92:LEU:HA	11:K:97:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:5:ALA:HA	12:L:13:ILE:O	2.18	0.44
3:Q:60:PHE:O	3:Q:62:SER:N	2.49	0.44
9:W:43:CYS:SG	9:W:98:LEU:HB3	2.58	0.44
12:Z:8:PHE:HE2	12:Z:13:ILE:HG12	1.81	0.44
6:F:117:GLN:NE2	7:G:83:ASP:HA	2.33	0.44
13:M:63:THR:HG23	14:N:94:ARG:HH12	1.82	0.44
2:P:94:GLN:HG3	9:W:65:LEU:HD12	1.99	0.44
2:B:13:SER:HB2	2:B:14:PRO:CD	2.48	0.44
4:D:116:GLN:NE2	5:E:83:ALA:O	2.51	0.44
5:E:14:THR:O	5:E:21:LEU:HA	2.18	0.44
13:M:187:VAL:HB	9:W:167:LEU:HB3	1.99	0.44
14:N:166:ARG:NH2	14:N:200:GLU:OE1	2.43	0.44
1:O:22:LEU:HD23	1:O:22:LEU:HA	1.85	0.44
6:T:117:GLN:NE2	7:U:83:ASP:HA	2.33	0.44
10:X:50:ILE:HG13	10:X:108:ILE:HG22	1.99	0.44
2:B:94:GLN:HG3	9:I:65:LEU:HD12	1.99	0.44
6:F:192:LEU:HD13	6:F:233:LEU:HD23	1.99	0.44
9:I:43:CYS:SG	9:I:98:LEU:HB3	2.58	0.44
14:N:92:LEU:HD21	14:N:110:MET:SD	2.56	0.44
12:Z:5:ALA:HA	12:Z:13:ILE:O	2.17	0.44
12:Z:7:LYS:O	12:Z:143:TYR:OH	2.28	0.44
7:G:65:ARG:HH21	7:G:78:ALA:HA	1.83	0.44
4:R:87:ALA:HB1	4:R:107:ILE:HD11	2.00	0.44
14:N:22:ILE:HG12	14:N:50:MET:CE	2.48	0.43
13:M:185:ARG:HA	9:W:26:VAL:HB	1.99	0.43
5:S:14:THR:O	5:S:21:LEU:HA	2.18	0.43
10:X:57:THR:O	11:Y:85:ARG:NH2	2.52	0.43
11:Y:19:ARG:NH2	11:Y:177:THR:HB	2.32	0.43
11:Y:77:PRO:HD2	11:Y:108:ASP:HB2	2.00	0.43
2:B:21:ILE:HG21	2:B:151:SER:HB3	2.01	0.43
7:G:149:TYR:CD1	7:G:159:GLY:HA2	2.54	0.43
8:H:7:GLN:HE22	8:H:122:ARG:HH21	1.67	0.43
1:O:16:PHE:CE2	2:P:127:ARG:NH1	2.86	0.43
4:R:116:GLN:NE2	5:S:83:ALA:O	2.51	0.43
9:W:163:ILE:HD13	9:W:192:PRO:HG2	2.01	0.43
11:Y:29:LYS:HD3	11:Y:32:HIS:HD2	1.84	0.43
2:B:49:LYS:H	2:B:207:ILE:HA	1.84	0.43
10:J:66:LEU:HD21	10:J:86:LEU:HD11	1.99	0.43
11:K:19:ARG:NE	11:K:177:THR:HB	2.33	0.43
11:K:77:PRO:HD2	11:K:108:ASP:HB2	2.00	0.43
3:Q:95:GLN:HG3	10:X:72:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:192:LEU:HD13	6:T:233:LEU:HD23	1.99	0.43
5:E:73:HIS:CD2	5:E:74:ILE:HG13	2.54	0.43
5:S:73:HIS:CD2	5:S:74:ILE:HG13	2.54	0.43
3:C:123:GLN:HG3	4:D:125:ARG:HG2	1.99	0.43
5:E:110:GLU:HA	5:E:154:PHE:HE2	1.83	0.43
2:P:21:ILE:HG21	2:P:151:SER:HB3	2.01	0.43
7:U:149:TYR:CD1	7:U:159:GLY:HA2	2.53	0.43
11:Y:19:ARG:NE	11:Y:177:THR:HB	2.33	0.43
4:D:136:PHE:CG	4:D:213:ARG:HG3	2.53	0.43
11:K:29:LYS:HD3	11:K:32:HIS:HD2	1.84	0.43
2:P:118:GLN:NE2	3:Q:82:ASP:HA	2.34	0.43
4:R:63:CYS:HB3	4:R:88:ARG:HH21	1.83	0.43
7:U:52:LEU:HD23	7:U:209:PHE:HB3	2.01	0.43
11:Y:92:LEU:HA	11:Y:97:PRO:HB3	2.00	0.43
6:F:151:ALA:HB3	7:G:82:ALA:HB1	2.01	0.43
13:M:185:ARG:HG2	9:W:29:LYS:NZ	2.34	0.43
5:S:137:PHE:HB3	5:S:139:VAL:HG22	1.99	0.43
4:D:87:ALA:HB1	4:D:107:ILE:HD11	2.00	0.43
6:F:117:GLN:O	6:F:120:THR:OG1	2.28	0.43
5:S:69:GLU:O	5:S:93:ARG:NE	2.51	0.43
4:D:140:GLY:HA2	4:D:213:ARG:HD3	2.01	0.43
9:I:163:ILE:HD13	9:I:192:PRO:HG2	2.01	0.43
8:V:7:GLN:HE22	8:V:122:ARG:HH21	1.67	0.43
4:D:63:CYS:HB3	4:D:88:ARG:HH21	1.83	0.42
10:J:65:ARG:CZ	11:K:86:ARG:HH12	2.32	0.42
4:R:109:ARG:NH2	12:Z:70:ASN:OD1	2.52	0.42
5:S:110:GLU:HA	5:S:154:PHE:HE2	1.83	0.42
6:T:33:SER:HB2	6:T:62:LYS:HE2	2.00	0.42
8:V:1:THR:HG21	8:V:46:SER:HA	2.01	0.42
11:Y:85:ARG:HD2	11:Y:124:LEU:HB2	2.01	0.42
12:Z:1:THR:HG21	12:Z:46:ALA:HA	2.01	0.42
1:A:231:THR:HG22	1:A:233:ALA:H	1.84	0.42
5:E:195:ILE:HG22	5:E:237:VAL:HG11	2.02	0.42
12:Z:40:TYR:CD2	12:Z:73:ARG:HD3	2.54	0.42
8:H:1:THR:HG21	8:H:46:SER:HA	2.01	0.42
10:J:57:THR:O	11:K:85:ARG:NH2	2.51	0.42
1:O:231:THR:HG22	1:O:233:ALA:H	1.84	0.42
5:E:59:MET:SD	5:E:64:ILE:HD11	2.60	0.42
6:F:33:SER:HB2	6:F:62:LYS:HE2	2.00	0.42
11:K:12:TYR:HH	11:K:151:ILE:HG23	1.84	0.42
14:N:1:THR:N	14:N:105:PRO:O	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:30:TYR:O	14:N:33:LEU:HB3	2.19	0.42
1:O:11:ARG:H	1:O:11:ARG:HG2	1.63	0.42
1:O:85:ALA:HB1	7:U:120:HIS:HD2	1.85	0.42
2:P:49:LYS:H	2:P:207:ILE:HA	1.84	0.42
3:Q:123:GLN:HG3	4:R:125:ARG:HG2	1.99	0.42
4:D:109:ARG:NH2	12:L:70:ASN:OD1	2.53	0.42
11:K:85:ARG:HD2	11:K:124:LEU:HB2	2.01	0.42
11:K:167:LEU:O	11:K:171:PHE:HB3	2.19	0.42
13:M:169:ASP:HB3	13:M:173:ARG:NH2	2.32	0.42
1:O:6:SER:CB	1:O:11:ARG:HD3	2.50	0.42
10:X:65:ARG:CZ	11:Y:86:ARG:HH12	2.32	0.42
3:C:95:GLN:HG3	10:J:72:LEU:HD12	2.01	0.42
3:C:172:VAL:HG12	3:C:176:LYS:HE2	2.02	0.42
6:F:81:ALA:HA	6:F:130:VAL:HG11	2.02	0.42
6:F:95:SER:O	6:F:99:PHE:N	2.48	0.42
11:K:12:TYR:OH	11:K:151:ILE:HG23	2.20	0.42
1:O:123:GLN:HE22	2:P:81:ASP:HA	1.85	0.42
5:S:59:MET:SD	5:S:64:ILE:HD11	2.60	0.42
6:T:81:ALA:HA	6:T:130:VAL:HG11	2.02	0.42
10:X:122:SER:HB2	10:X:136:VAL:HB	2.02	0.42
11:Y:12:TYR:OH	11:Y:151:ILE:HG23	2.20	0.42
14:N:187:PHE:HE1	14:N:189:ILE:HD11	1.85	0.42
5:S:41:GLN:N	5:S:166:ASP:O	2.39	0.42
5:S:209:LYS:O	5:S:214:ASN:ND2	2.51	0.42
11:Y:14:LEU:HD21	11:Y:160:LEU:HD22	2.01	0.42
3:C:214:ALA:HB2	3:C:227:VAL:HG22	2.01	0.42
7:G:37:ILE:HG12	7:G:197:ILE:HD11	2.02	0.42
7:G:52:LEU:HD23	7:G:209:PHE:HB3	2.00	0.42
13:M:183:ALA:HA	13:M:189:THR:HG23	2.01	0.42
1:O:69:LEU:HD13	1:O:216:GLU:HG3	2.01	0.42
4:R:155:ALA:HB3	5:S:60:GLU:HB3	2.02	0.42
12:Z:1:THR:HA	12:Z:33:LYS:NZ	2.35	0.42
1:A:69:LEU:HD13	1:A:216:GLU:HG3	2.01	0.42
2:B:118:GLN:NE2	3:C:82:ASP:HA	2.34	0.42
5:E:68:VAL:HB	5:E:93:ARG:HH21	1.84	0.42
5:E:167:ALA:HB3	6:F:56:LEU:HD13	2.02	0.42
6:F:144:ILE:O	6:F:144:ILE:HG22	2.20	0.42
12:L:1:THR:HG21	12:L:46:ALA:HA	2.02	0.42
5:S:49:ALA:HB1	5:S:202:LEU:HD11	2.02	0.42
5:S:68:VAL:HB	5:S:93:ARG:HH21	1.84	0.42
6:T:103:LEU:HD23	6:T:104:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:202:TYR:HD2	10:X:151:SER:HB3	1.85	0.41
5:E:49:ALA:HB1	5:E:202:LEU:HD11	2.02	0.41
6:F:6:TYR:OH	7:G:8:ASP:OD2	2.29	0.41
10:J:122:SER:HB2	10:J:136:VAL:HB	2.02	0.41
11:K:42:ILE:HG22	11:K:106:GLY:HA3	2.01	0.41
12:L:1:THR:HA	12:L:33:LYS:NZ	2.35	0.41
13:M:89:ALA:HB1	13:M:130:TYR:HE1	1.86	0.41
5:S:41:GLN:NE2	5:S:152:GLN:HA	2.35	0.41
6:T:151:ALA:HB3	7:U:82:ALA:HB1	2.01	0.41
7:U:65:ARG:HH21	7:U:78:ALA:HA	1.83	0.41
4:D:63:CYS:HB3	4:D:88:ARG:NH2	2.35	0.41
6:F:103:LEU:HD23	6:F:104:PRO:O	2.20	0.41
4:R:63:CYS:HB3	4:R:88:ARG:NH2	2.35	0.41
6:T:144:ILE:HG22	6:T:144:ILE:O	2.20	0.41
11:Y:34:LYS:HD3	11:Y:47:VAL:HG12	2.03	0.41
11:Y:42:ILE:HG22	11:Y:106:GLY:HA3	2.01	0.41
1:A:24:GLN:NE2	7:G:14:PHE:HB2	2.36	0.41
4:D:158:ALA:HB1	4:D:172:LEU:HD13	2.03	0.41
9:I:202:TYR:HD2	10:J:151:SER:HB3	1.85	0.41
9:I:209:THR:HG21	10:J:167:SER:HB2	2.02	0.41
11:K:34:LYS:HD3	11:K:47:VAL:HG12	2.02	0.41
11:K:144:ASP:OD1	12:Z:166:ARG:NH2	2.40	0.41
12:L:40:TYR:CD2	12:L:73:ARG:HD3	2.54	0.41
1:O:14:THR:HG23	1:O:24:GLN:HG2	2.01	0.41
5:S:195:ILE:HG22	5:S:237:VAL:HG11	2.02	0.41
9:W:209:THR:HG21	10:X:167:SER:HB2	2.02	0.41
12:Z:33:LYS:O	12:Z:45:MET:N	2.50	0.41
1:A:72:ILE:HG21	1:A:114:LEU:HD21	2.02	0.41
1:A:85:ALA:HB1	7:G:120:HIS:HD2	1.85	0.41
7:G:87:LEU:HD13	7:G:135:PHE:CE2	2.56	0.41
4:R:92:GLN:HB3	11:Y:62:LYS:HG3	2.02	0.41
5:S:141:LEU:HB2	5:S:156:MET:HE2	2.01	0.41
4:D:83:VAL:HG21	4:D:129:ILE:HD11	2.01	0.41
7:G:74:GLY:HA3	7:G:224:HIS:CD2	2.56	0.41
3:Q:172:VAL:HG12	3:Q:176:LYS:HE2	2.02	0.41
1:A:50:ILE:HD12	1:A:79:VAL:HB	2.03	0.41
1:A:123:GLN:HE22	2:B:81:ASP:HA	1.85	0.41
10:J:117:LYS:HD2	10:J:118:PRO:HD2	2.03	0.41
4:R:83:VAL:HG21	4:R:129:ILE:HD11	2.01	0.41
3:C:90:LEU:HD21	3:C:114:LEU:HB2	2.03	0.41
1:O:72:ILE:HG21	1:O:114:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:214:ALA:HB2	3:Q:227:VAL:HG22	2.01	0.41
4:R:158:ALA:HB1	4:R:172:LEU:HD13	2.03	0.41
7:U:87:LEU:HD13	7:U:135:PHE:CE2	2.56	0.41
8:V:38:HIS:CG	8:V:39:ASP:H	2.39	0.41
8:V:44:CYS:HB2	8:V:99:ILE:CG2	2.51	0.41
11:Y:167:LEU:O	11:Y:171:PHE:HB3	2.19	0.41
12:Z:167:ASP:HB3	12:Z:170:SER:HB2	2.02	0.41
1:A:5:SER:O	1:A:18:PRO:HD2	2.20	0.41
2:B:38:LYS:HG3	2:B:43:VAL:HG22	2.03	0.41
5:E:41:GLN:NE2	5:E:152:GLN:HA	2.35	0.41
7:G:90:ILE:HG13	7:G:118:TYR:CE2	2.56	0.41
11:K:14:LEU:HD21	11:K:160:LEU:HD22	2.01	0.41
12:L:44:THR:O	12:L:99:THR:OG1	2.36	0.41
12:L:167:ASP:HB3	12:L:170:SER:HB2	2.02	0.41
1:O:50:ILE:HD12	1:O:79:VAL:HB	2.03	0.41
1:O:132:ARG:HB3	7:U:12:SER:O	2.21	0.41
7:U:74:GLY:HA3	7:U:224:HIS:CD2	2.56	0.41
1:A:7:ALA:O	1:A:10:ASP:OD1	2.39	0.41
7:G:206:ASP:N	7:G:206:ASP:OD1	2.49	0.41
8:H:19:ARG:NH1	8:H:168:GLY:O	2.46	0.41
12:L:76:VAL:HG12	12:L:112:TYR:CD2	2.56	0.41
3:Q:133:SER:HB2	3:Q:152:PRO:HD3	2.03	0.41
7:U:37:ILE:HG12	7:U:197:ILE:HD11	2.02	0.41
7:U:206:ASP:OD1	7:U:206:ASP:N	2.50	0.41
10:X:117:LYS:HD2	10:X:118:PRO:HD2	2.03	0.41
11:Y:9:GLY:HA3	11:Y:12:TYR:CZ	2.56	0.41
12:Z:76:VAL:HG12	12:Z:112:TYR:CD2	2.56	0.41
4:D:91:CYS:HA	4:D:102:VAL:HG11	2.03	0.40
4:D:92:GLN:HB3	11:K:62:LYS:HG3	2.02	0.40
4:D:120:GLN:O	5:E:134:SER:N	2.33	0.40
4:D:155:ALA:HB3	5:E:60:GLU:HB3	2.02	0.40
5:E:141:LEU:HB2	5:E:156:MET:HE2	2.02	0.40
9:I:112:SER:HB3	9:I:125:VAL:HG11	2.03	0.40
14:N:122:LEU:HG	14:N:137:LEU:HD12	2.03	0.40
1:A:132:ARG:HB3	7:G:12:SER:O	2.21	0.40
12:L:112:TYR:HE1	12:L:122:SER:HB2	1.86	0.40
14:N:184:TYR:HE2	14:N:186:ARG:HB2	1.85	0.40
4:R:116:GLN:O	4:R:119:THR:OG1	2.28	0.40
4:R:208:LEU:HD22	4:R:220:LEU:HD12	2.03	0.40
8:V:127:ILE:HD12	8:V:132:SER:HB2	2.03	0.40
11:Y:146:TYR:HB2	11:Y:159:LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:195:LEU:O	6:F:198:THR:OG1	2.29	0.40
7:G:119:VAL:HG13	7:G:131:PHE:HD2	1.87	0.40
8:H:127:ILE:HD12	8:H:132:SER:HB2	2.03	0.40
12:L:186:ARG:NH1	12:L:189:SER:HB2	2.36	0.40
5:S:167:ALA:HB3	6:T:56:LEU:HD13	2.02	0.40
9:W:63:LEU:HA	9:W:66:HIS:HB3	2.03	0.40
8:H:44:CYS:HB2	8:H:99:ILE:CG2	2.51	0.40
1:O:125:TYR:HA	1:O:131:MET:HG3	2.03	0.40
5:S:42:THR:OG1	5:S:45:GLY:O	2.31	0.40
10:X:146:TYR:O	10:X:150:GLU:HG2	2.21	0.40
12:Z:4:LEU:HB3	12:Z:15:ALA:HB3	2.03	0.40
12:Z:186:ARG:NH1	12:Z:189:SER:HB2	2.36	0.40
1:A:125:TYR:HA	1:A:131:MET:HG3	2.03	0.40
3:C:133:SER:HB2	3:C:152:PRO:HD3	2.03	0.40
6:F:117:GLN:OE1	7:G:86:SER:HB2	2.22	0.40
6:F:120:THR:HG22	6:F:127:PRO:HG3	2.03	0.40
9:I:63:LEU:HA	9:I:66:HIS:HB3	2.03	0.40
11:K:14:LEU:HB2	11:K:182:ILE:HD12	2.03	0.40
14:N:144:TYR:HB3	9:W:132:LEU:HB3	2.02	0.40
3:Q:90:LEU:HD21	3:Q:114:LEU:HB2	2.03	0.40
7:U:88:ALA:O	7:U:92:ARG:HG3	2.22	0.40
9:W:174:ASP:OD1	9:W:175:LEU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	237/246 (96%)	229 (97%)	7 (3%)	1 (0%)	34 69
1	O	236/246 (96%)	229 (97%)	6 (2%)	1 (0%)	34 69
2	B	227/234 (97%)	222 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	227/234 (97%)	222 (98%)	5 (2%)	0	100	100
3	C	245/261 (94%)	231 (94%)	14 (6%)	0	100	100
3	Q	245/261 (94%)	231 (94%)	14 (6%)	0	100	100
4	D	230/248 (93%)	221 (96%)	8 (4%)	1 (0%)	34	69
4	R	230/248 (93%)	223 (97%)	6 (3%)	1 (0%)	34	69
5	E	231/241 (96%)	226 (98%)	5 (2%)	0	100	100
5	S	231/241 (96%)	226 (98%)	5 (2%)	0	100	100
6	F	231/263 (88%)	227 (98%)	3 (1%)	1 (0%)	34	69
6	T	231/263 (88%)	227 (98%)	3 (1%)	1 (0%)	34	69
7	G	237/255 (93%)	232 (98%)	5 (2%)	0	100	100
7	U	237/255 (93%)	232 (98%)	5 (2%)	0	100	100
8	H	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
8	V	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
9	I	218/234 (93%)	204 (94%)	14 (6%)	0	100	100
9	W	218/234 (93%)	204 (94%)	14 (6%)	0	100	100
10	J	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	X	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
11	K	194/201 (96%)	189 (97%)	5 (3%)	0	100	100
11	Y	194/201 (96%)	189 (97%)	5 (3%)	0	100	100
12	L	198/204 (97%)	194 (98%)	4 (2%)	0	100	100
12	Z	198/204 (97%)	194 (98%)	4 (2%)	0	100	100
13	M	210/213 (99%)	204 (97%)	6 (3%)	0	100	100
13	a	210/213 (99%)	204 (97%)	6 (3%)	0	100	100
14	N	210/219 (96%)	205 (98%)	5 (2%)	0	100	100
14	b	210/219 (96%)	205 (98%)	5 (2%)	0	100	100
All	All	6139/6458 (95%)	5952 (97%)	181 (3%)	6 (0%)	54	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	R	216	SER
1	A	187	PHE
1	O	187	PHE

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Mol	Chain	Res	Type
4	D	215	GLN
6	F	59	HIS
6	T	59	HIS

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	163/210 (78%)	163 (100%)	0	100	100
1	O	163/210 (78%)	161 (99%)	2 (1%)	71	84
2	B	150/191 (78%)	150 (100%)	0	100	100
2	P	150/191 (78%)	150 (100%)	0	100	100
3	C	160/221 (72%)	160 (100%)	0	100	100
3	Q	160/221 (72%)	160 (100%)	0	100	100
4	D	136/211 (64%)	136 (100%)	0	100	100
4	R	136/211 (64%)	136 (100%)	0	100	100
5	E	158/203 (78%)	158 (100%)	0	100	100
5	S	158/203 (78%)	158 (100%)	0	100	100
6	F	160/224 (71%)	160 (100%)	0	100	100
6	T	160/224 (71%)	160 (100%)	0	100	100
7	G	162/212 (76%)	162 (100%)	0	100	100
7	U	162/212 (76%)	162 (100%)	0	100	100
8	H	140/159 (88%)	140 (100%)	0	100	100
8	V	140/159 (88%)	140 (100%)	0	100	100
9	I	157/195 (80%)	157 (100%)	0	100	100
9	W	157/195 (80%)	157 (100%)	0	100	100
10	J	155/174 (89%)	155 (100%)	0	100	100
10	X	155/174 (89%)	155 (100%)	0	100	100
11	K	148/171 (86%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	148/171 (86%)	148 (100%)	0	100	100
12	L	138/159 (87%)	138 (100%)	0	100	100
12	Z	138/159 (87%)	138 (100%)	0	100	100
13	M	158/178 (89%)	158 (100%)	0	100	100
13	a	158/178 (89%)	158 (100%)	0	100	100
14	N	149/181 (82%)	149 (100%)	0	100	100
14	b	149/181 (82%)	149 (100%)	0	100	100
All	All	4268/5378 (79%)	4266 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	17	SER
1	O	23	TYR

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

Mol	Chain	Res	Type
1	A	24	GLN
1	A	128	ASN
1	A	193	GLN
2	B	51	GLN
2	B	87	HIS
3	C	40	ASN
3	C	109	GLN
3	C	119	GLN
3	C	167	ASN
3	C	198	ASN
4	D	54	GLN
5	E	97	GLN
6	F	43	HIS
6	F	60	GLN
8	H	7	GLN
8	H	38	HIS
8	H	187	GLN
9	I	66	HIS
10	J	92	ASN
10	J	168	GLN

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Mol	Chain	Res	Type
11	K	32	HIS
11	K	63	ASN
11	K	101	ASN
13	M	79	ASN
13	M	108	ASN
13	M	157	ASN
14	N	69	GLN
14	N	81	HIS
1	O	128	ASN
1	O	193	GLN
2	P	51	GLN
2	P	87	HIS
3	Q	40	ASN
3	Q	109	GLN
3	Q	119	GLN
3	Q	167	ASN
3	Q	198	ASN
4	R	54	GLN
4	R	154	HIS
5	S	97	GLN
6	T	43	HIS
6	T	60	GLN
8	V	7	GLN
8	V	38	HIS
8	V	187	GLN
9	W	66	HIS
10	X	92	ASN
10	X	168	GLN
10	X	172	ASN
11	Y	32	HIS
11	Y	63	ASN
11	Y	71	ASN
11	Y	101	ASN
13	a	79	ASN
13	a	108	ASN
13	a	157	ASN
14	b	69	GLN
14	b	81	HIS

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

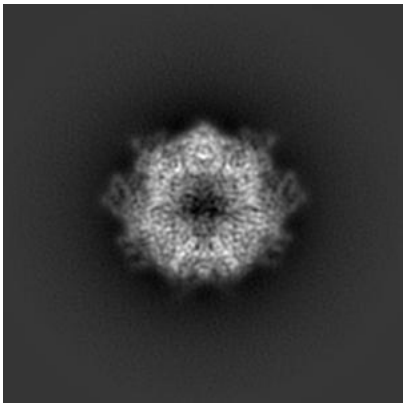
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13389. These allow visual inspection of the internal detail of the map and identification of artifacts.

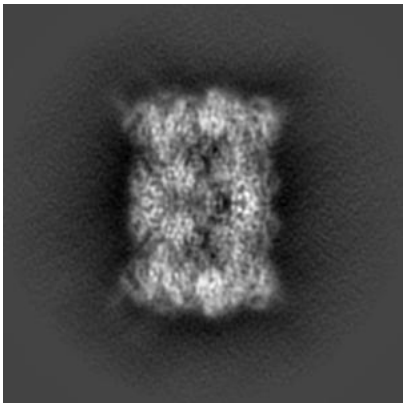
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

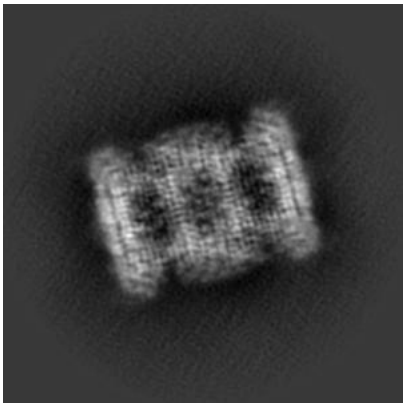
6.1.1 Primary map



X



Y

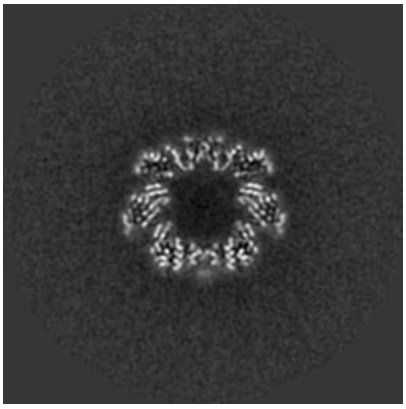


Z

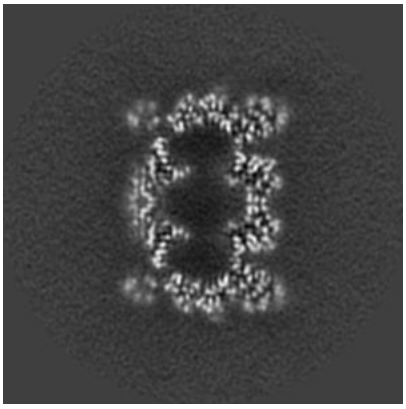
The images above show the map projected in three orthogonal directions.

6.2 Central slices

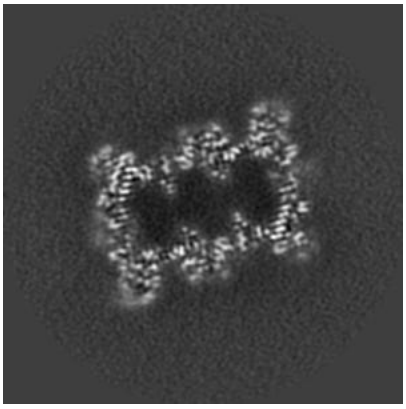
6.2.1 Primary map



X Index: 110



Y Index: 110

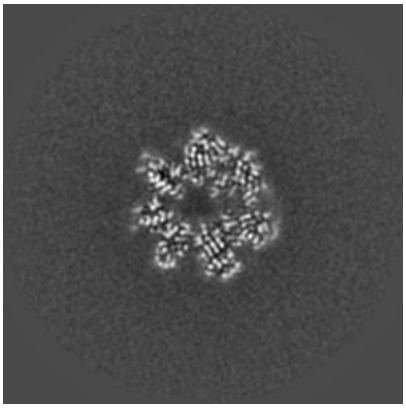


Z Index: 110

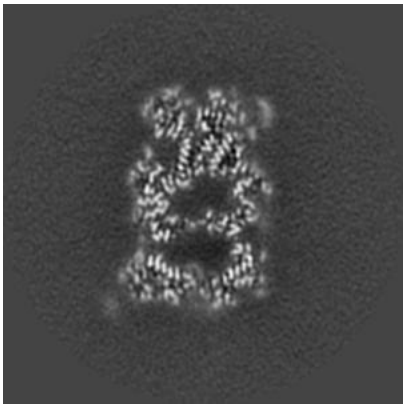
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

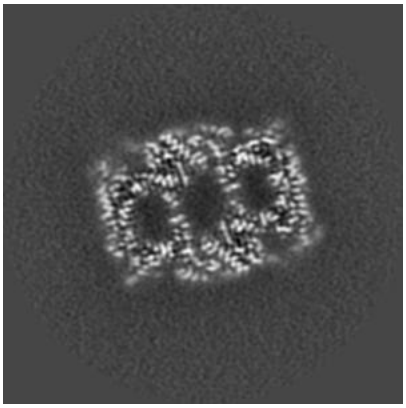
6.3.1 Primary map



X Index: 95



Y Index: 96



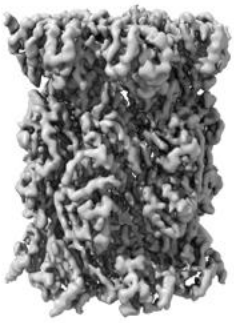
Z Index: 97

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

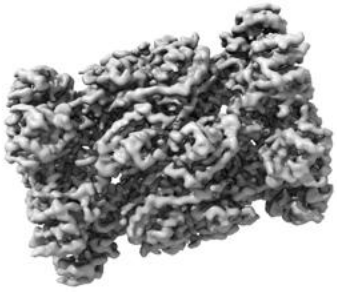
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0153. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

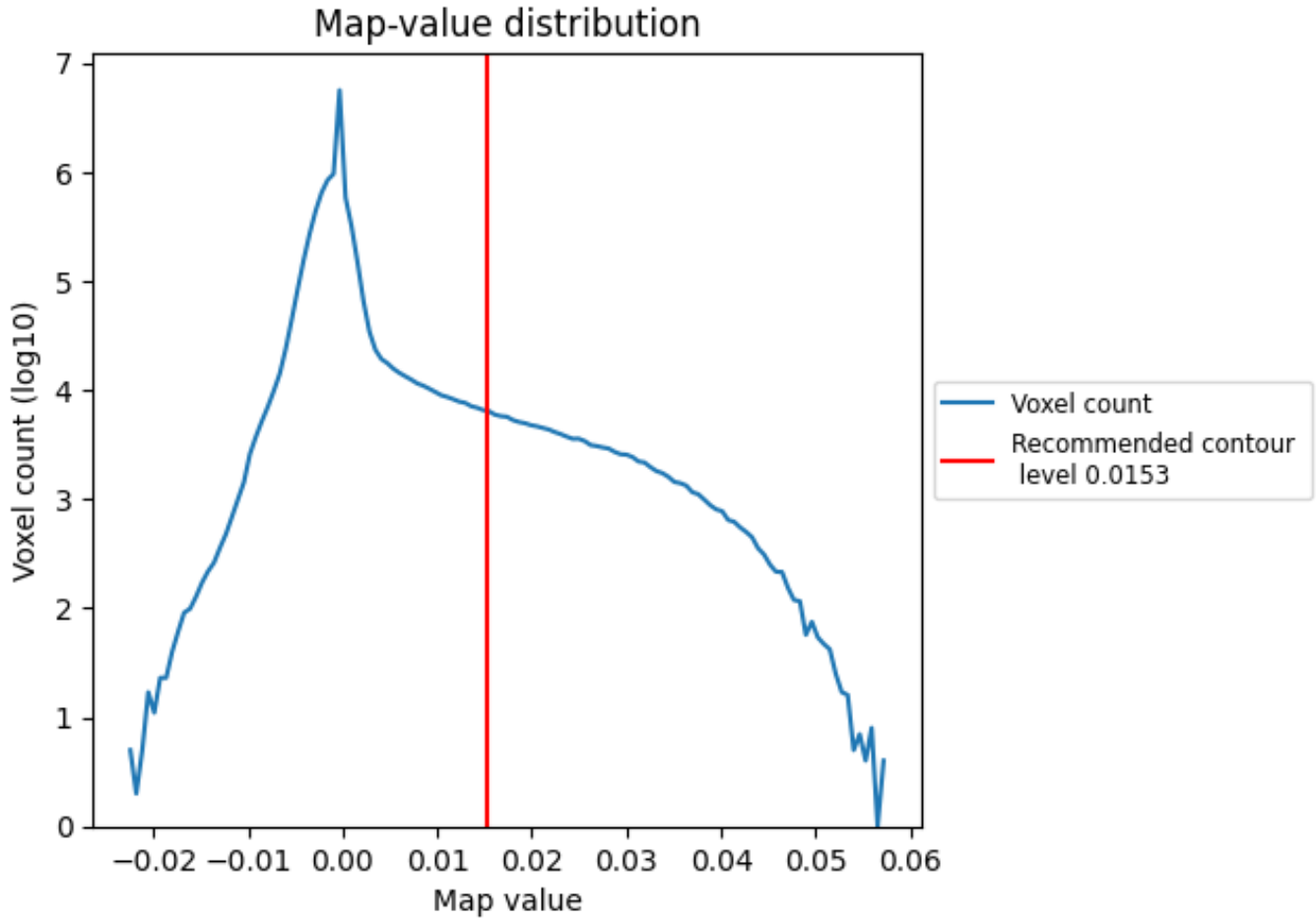
6.5 Mask visualisation (i)

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

7 Map analysis

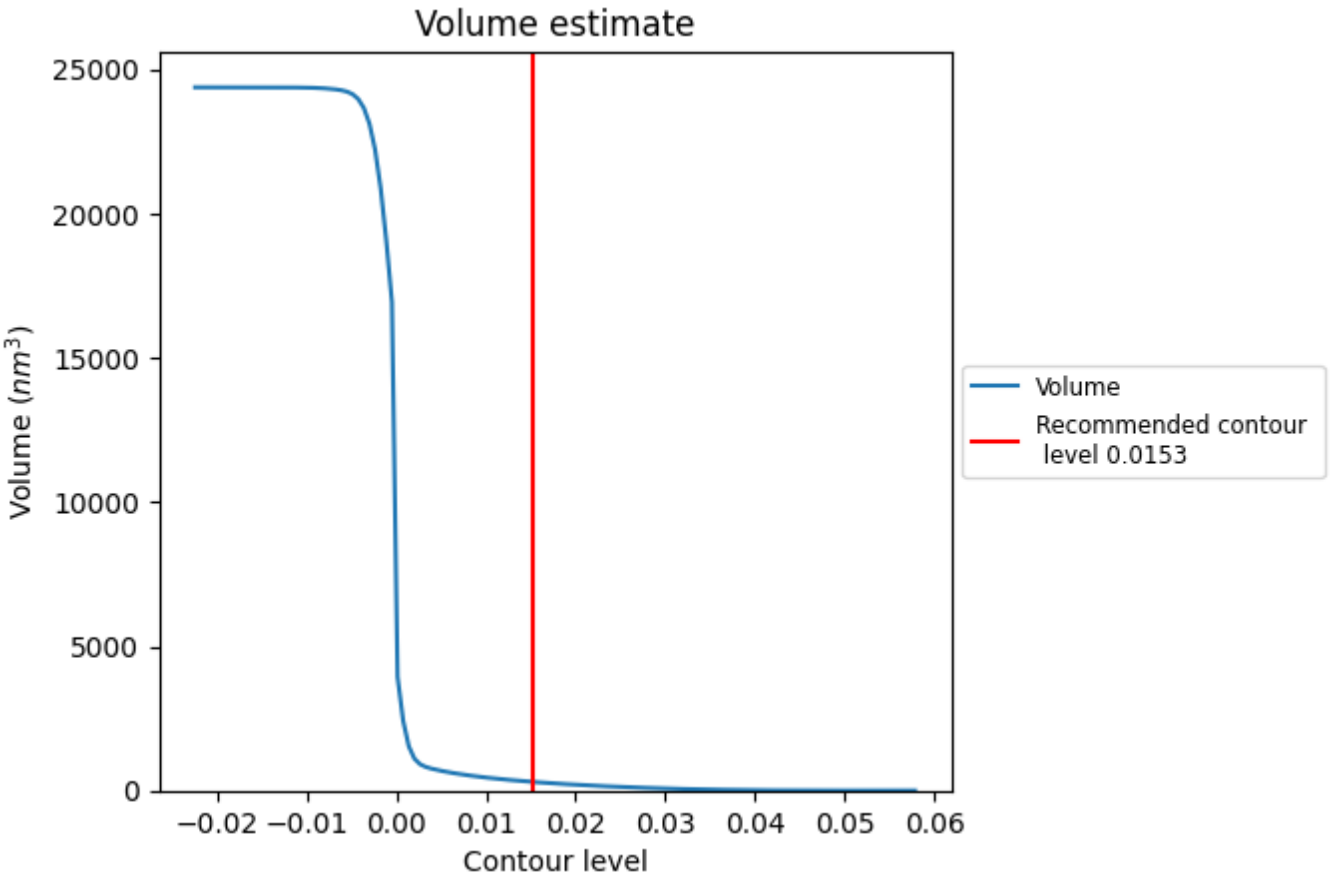
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

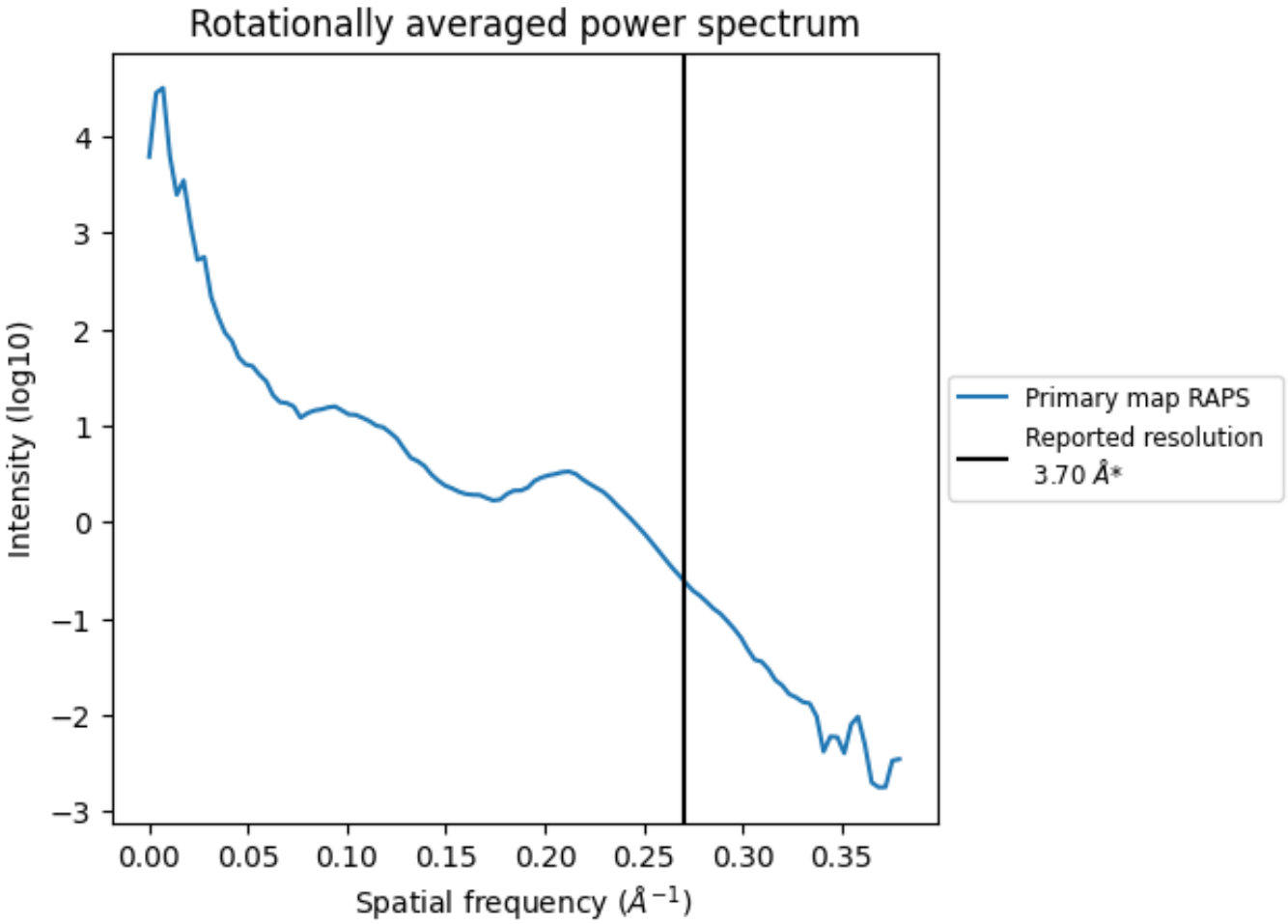
7.2 Volume estimate



The volume at the recommended contour level is 298 nm^3; this corresponds to an approximate mass of 270 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 0.270 Å^{-1}

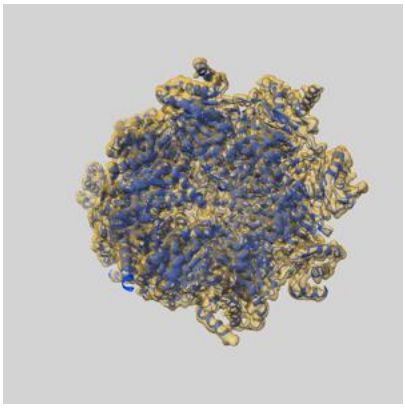
8 Fourier-Shell correlation (i)

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

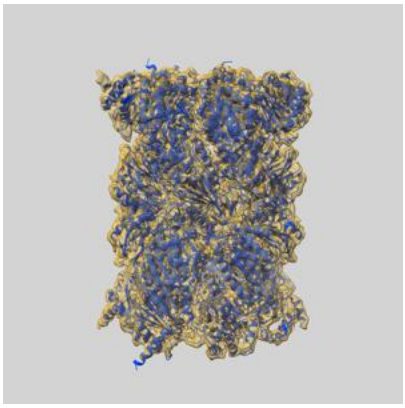
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13389 and PDB model 7PG9. Per-residue inclusion information can be found in section 3 on page 7.

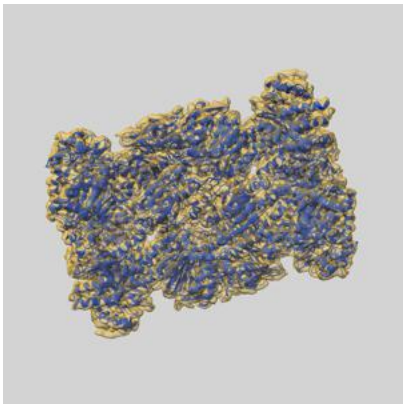
9.1 Map-model overlay



X



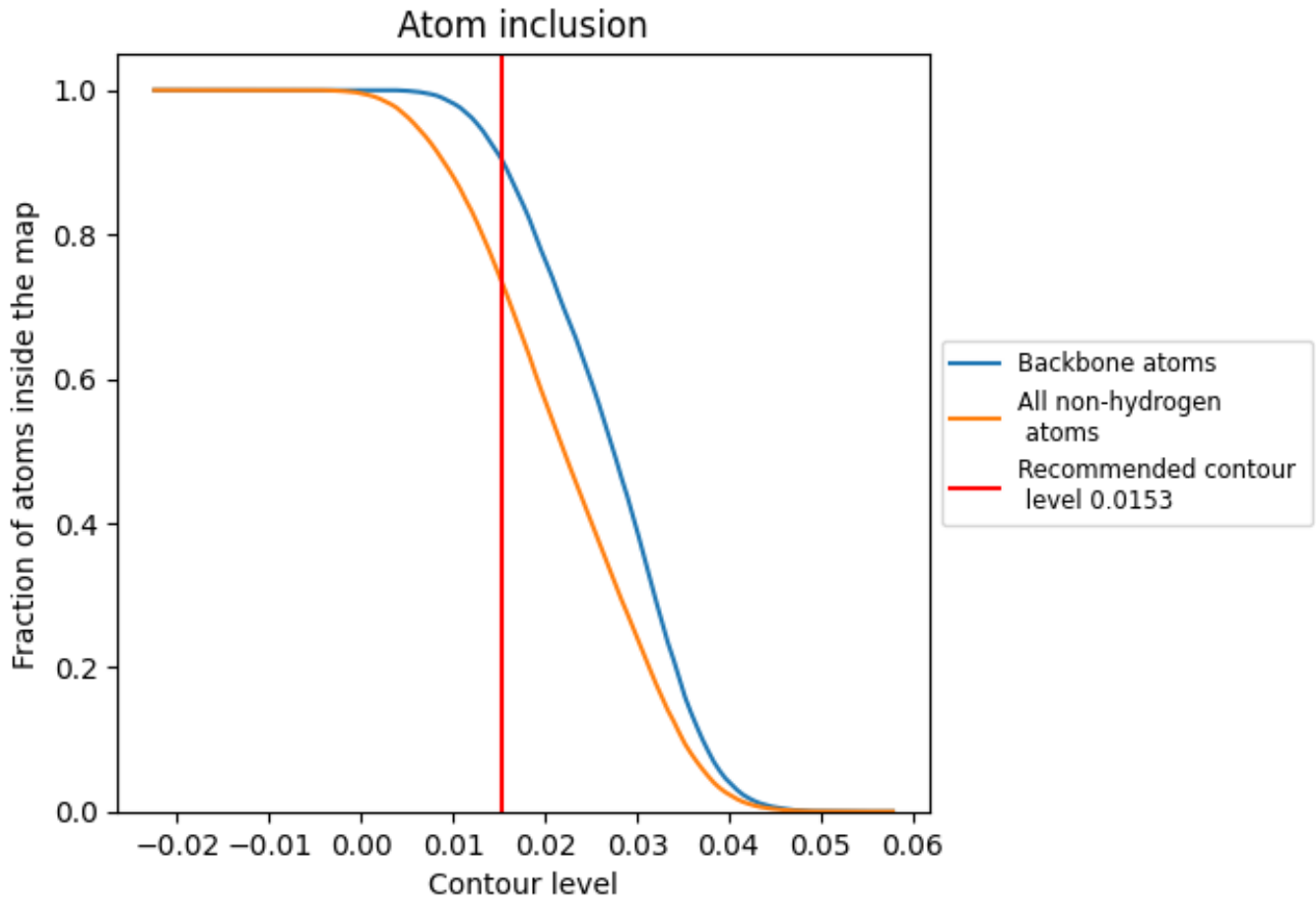
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0153 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 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.