Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 11:12 AM JST

PDB ID	:	7V5G
EMDB ID	:	EMD-31724
Title	:	20S+monoUb-CyclinB1-NT (S1)
Authors	:	Xu, C.; Cong, Y.
Deposited on	:	2021-08-17
Resolution	:	4.47 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

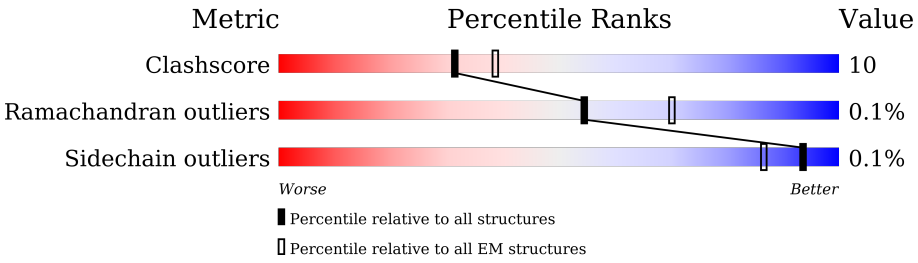
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.47 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	205	30% 84% 14% ·
1	H	205	32% 80% 18% ·
2	B	234	30% 76% 18% 6%
2	I	234	27% 74% 20% 6%
3	C	205	40% 70% 29%
3	J	205	24% 70% 29%
4	D	201	32% 78% 20% ·
4	K	201	27% 73% 24% ·

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Mol	Chain	Length	Quality of chain
5	E	204	25% 75% 23%
5	L	204	23% 72% 26%
6	F	213	26% 79% 20%
6	M	213	27% 82% 17%
7	G	219	27% 80% 16%
7	N	219	28% 77% 20%
8	O	246	48% 73% 23%
8	V	246	51% 83% 14%
9	P	234	41% 76% 21%
9	W	234	61% 73% 24%
10	Q	261	38% 76% 19% 5%
10	X	261	60% 78% 16% 5%
11	R	248	40% 72% 21% 6%
11	Y	248	59% 74% 19% 6%
12	S	241	44% 80% 17%
12	Z	241	57% 82% 14%
13	T	263	34% 65% 24% 11%
13	a	263	40% 89% 11%
14	U	255	40% 72% 22% 6%
14	b	255	35% 94% 6%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 48150 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 beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
1	H	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
2	I	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
3	J	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 4 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		
4	K	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		
5	L	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
6	M	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	212	Total	C	N	O	S	0	0
			1655	1044	285	315	11		
7	N	212	Total	C	N	O	S	0	0
			1655	1044	285	315	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	238	Total	C	N	O	S	0	0
			1857	1181	308	355	13		
8	O	238	Total	C	N	O	S	0	0
			1857	1181	308	355	13		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	228	Total	C	N	O	S	0	0
			1779	1138	300	335	6		
9	P	228	Total	C	N	O	S	0	0
			1779	1138	300	335	6		

- Molecule 10 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	247	Total	C	N	O	S	0	0
			1942	1228	332	372	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	248	Total	C	N	O	S	0	0
			1950	1233	333	373	11		

- Molecule 11 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	232	Total	C	N	O	S	0	0
			1825	1147	324	349	5		
11	R	232	Total	C	N	O	S	0	0
			1825	1147	324	349	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	233	Total	C	N	O	S	0	0
			1828	1146	328	343	11		
13	T	233	Total	C	N	O	S	0	0
			1828	1146	328	343	11		

- Molecule 14 is a protein called Proteasome subunit alpha type-3.

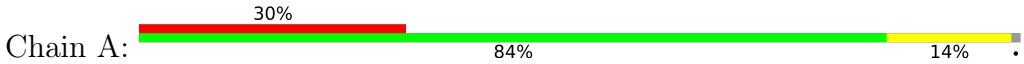
Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	239	Total	C	N	O	S	0	0
			1874	1189	320	354	11		
14	U	239	Total	C	N	O	S	0	0
			1874	1189	320	354	11		

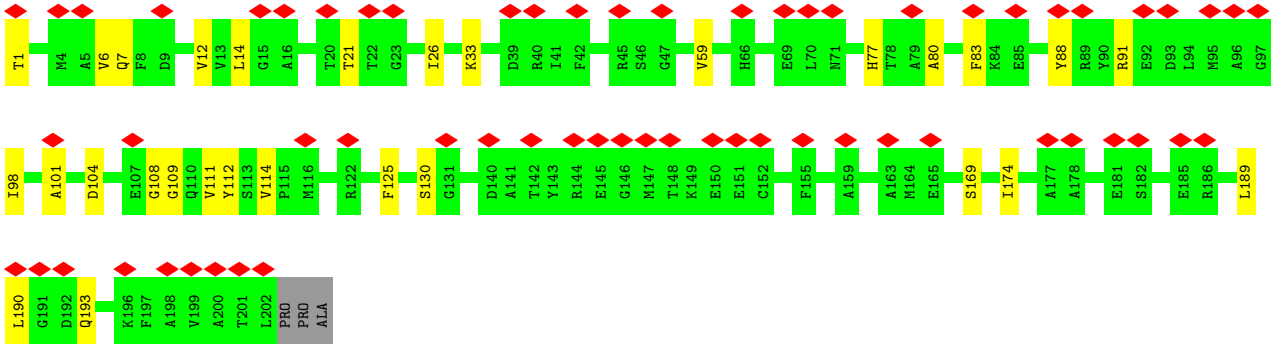
3 Residue-property plots (i)

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 beta type-6

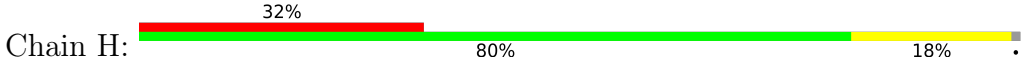
Chain A:

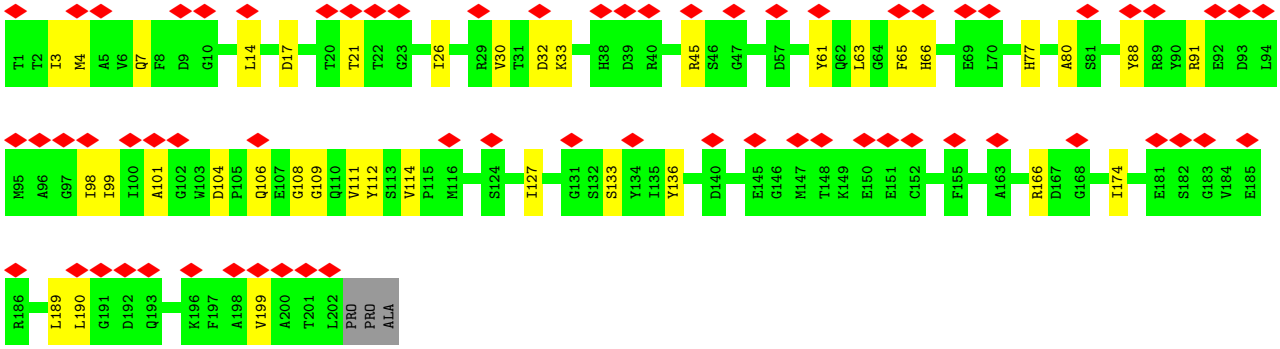




• Molecule 1: Proteasome subunit beta type-6

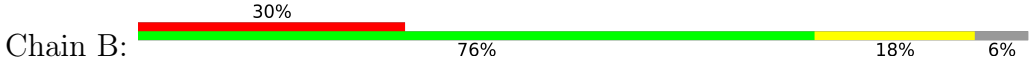
Chain H:

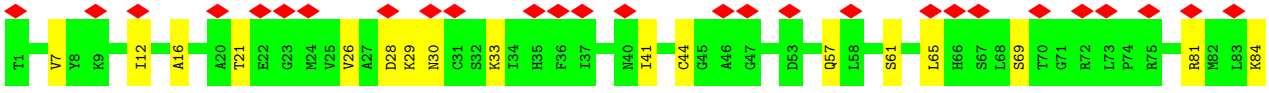


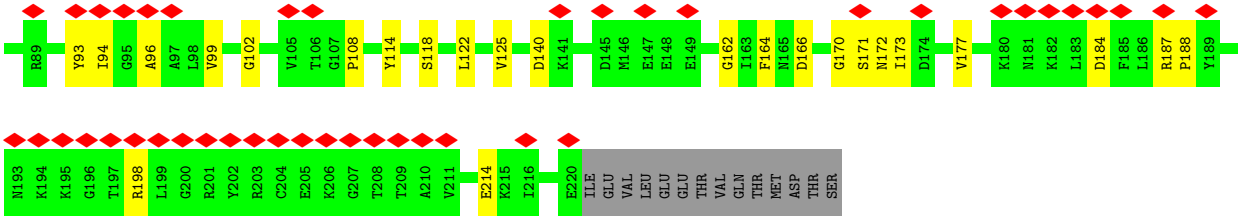


• Molecule 2: Proteasome subunit beta type-7

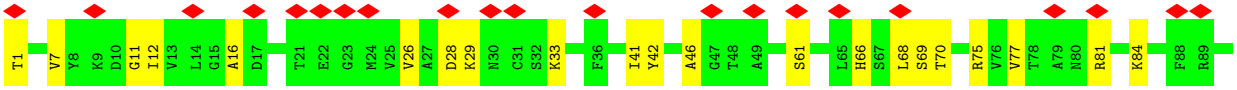
Chain B:

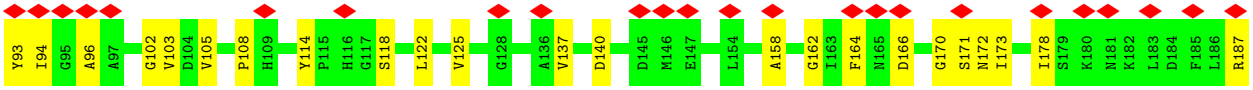


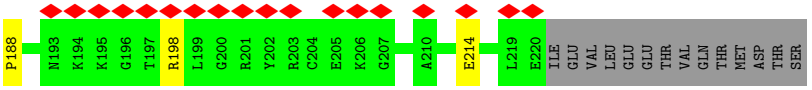




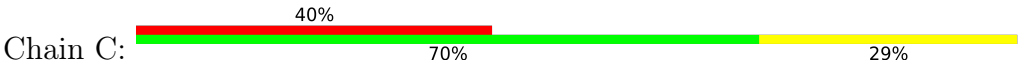
• Molecule 2: Proteasome subunit beta type-7

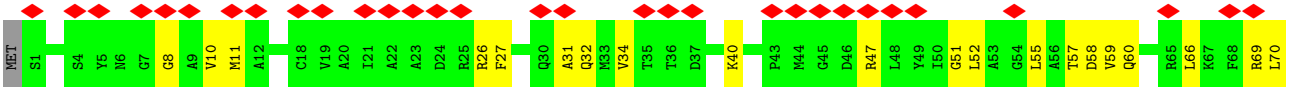


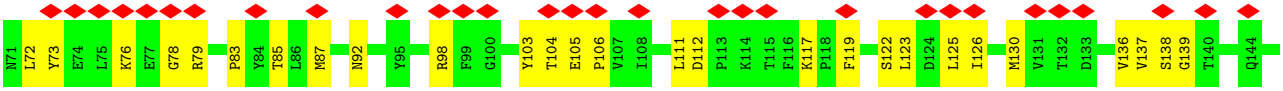


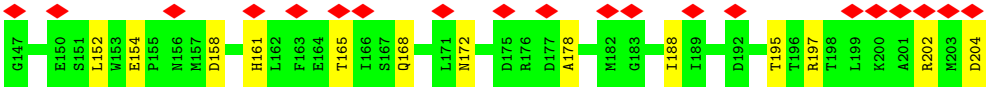


• Molecule 3: Proteasome subunit beta type-3

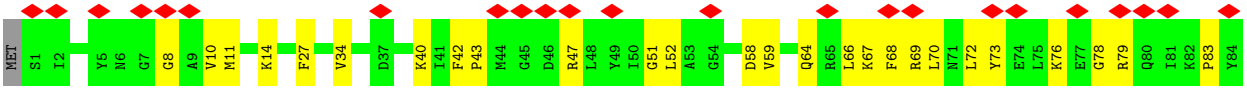


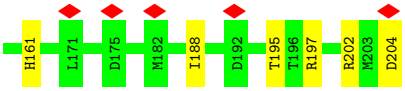






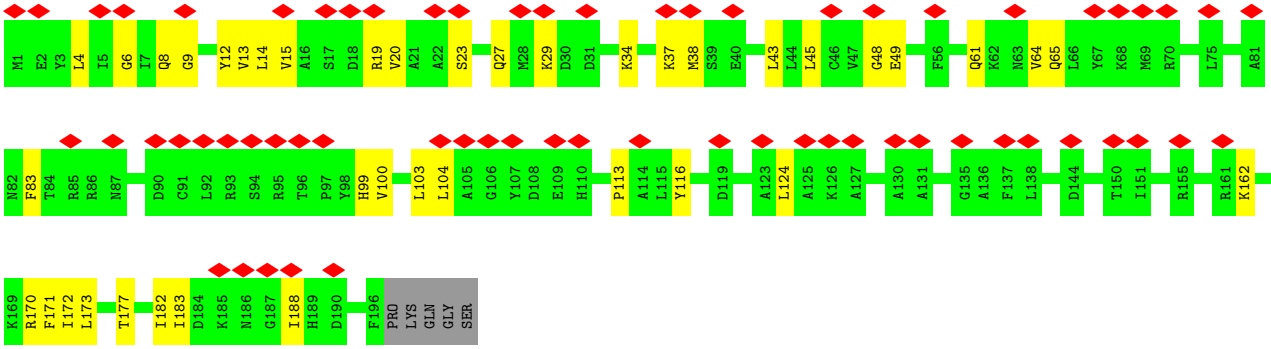
• Molecule 3: Proteasome subunit beta type-3





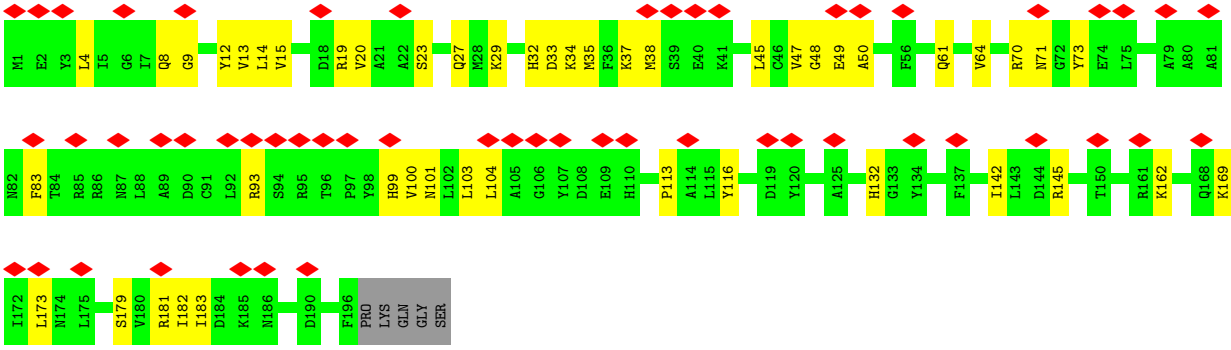
• Molecule 4: Proteasome subunit beta type-2

Chain D:



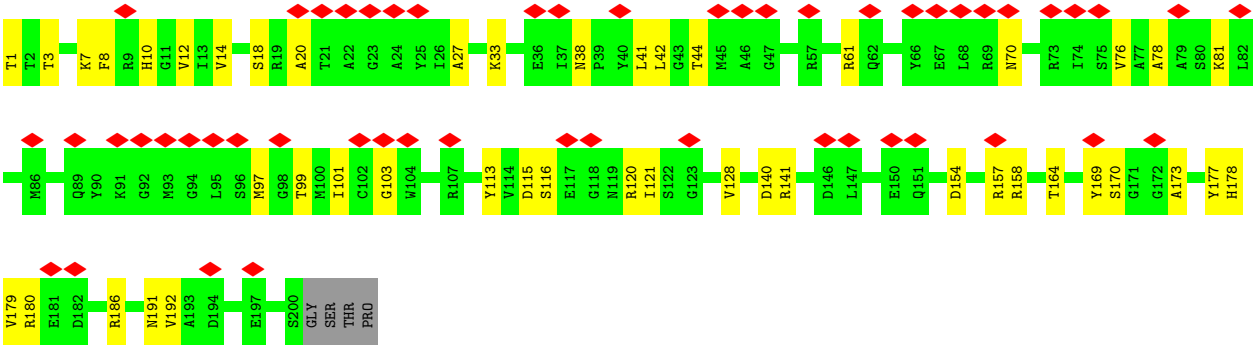
• Molecule 4: Proteasome subunit beta type-2

Chain K:



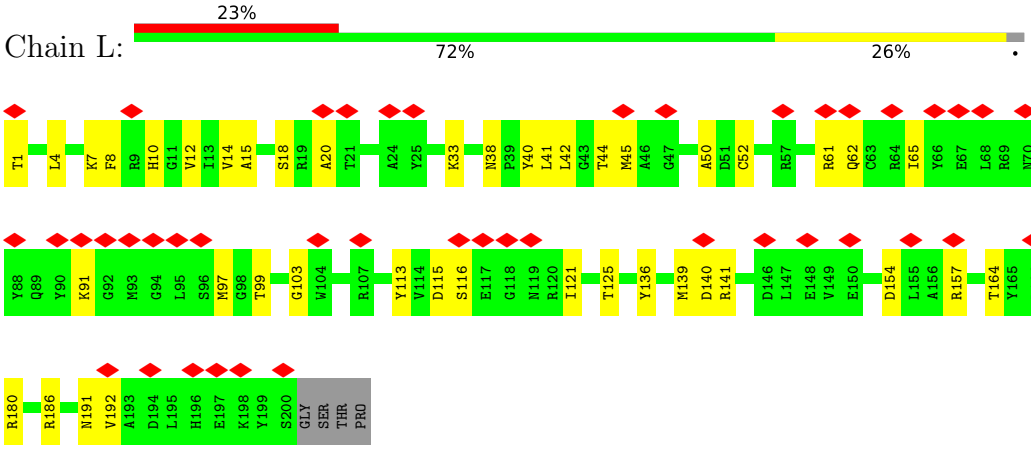
• Molecule 5: Proteasome subunit beta type-5

Chain E:



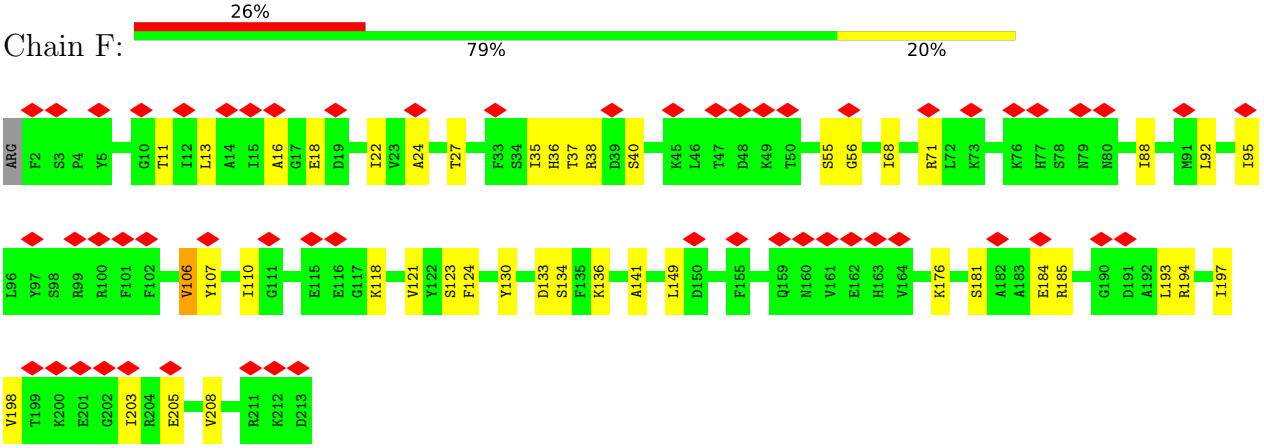
• Molecule 5: Proteasome subunit beta type-5

Chain L:



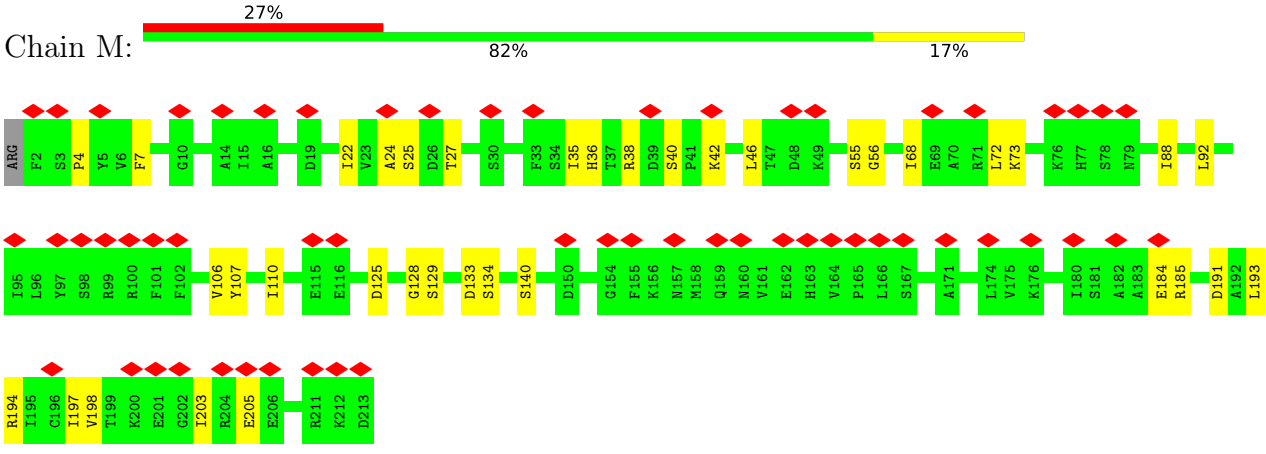
• Molecule 6: Proteasome subunit beta type-1

Chain F:



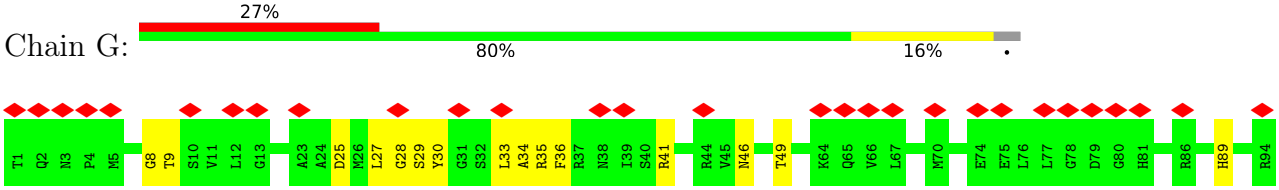
• Molecule 6: Proteasome subunit beta type-1

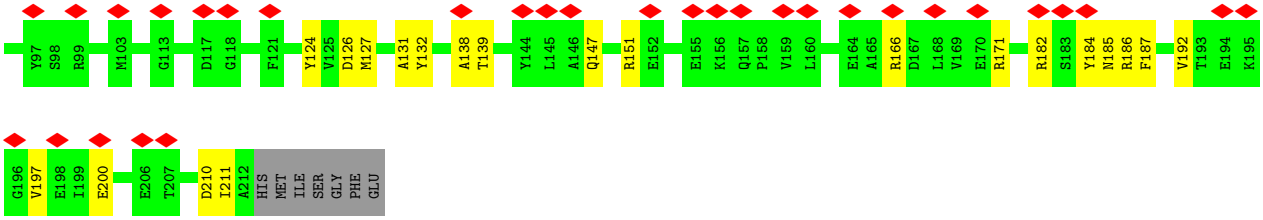
Chain M:



• Molecule 7: Proteasome subunit beta type-4

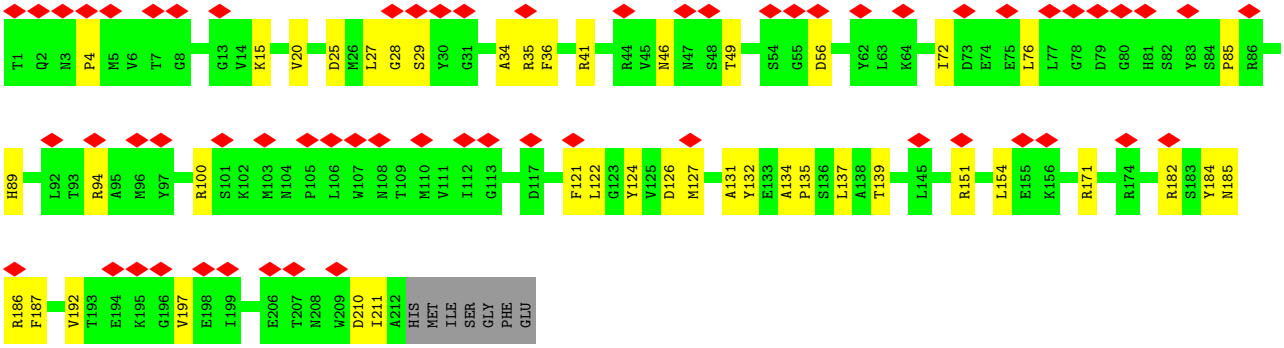
Chain G:





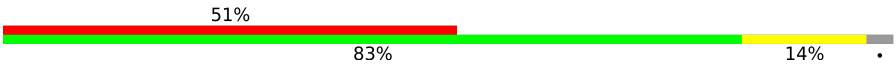
• Molecule 7: Proteasome subunit beta type-4

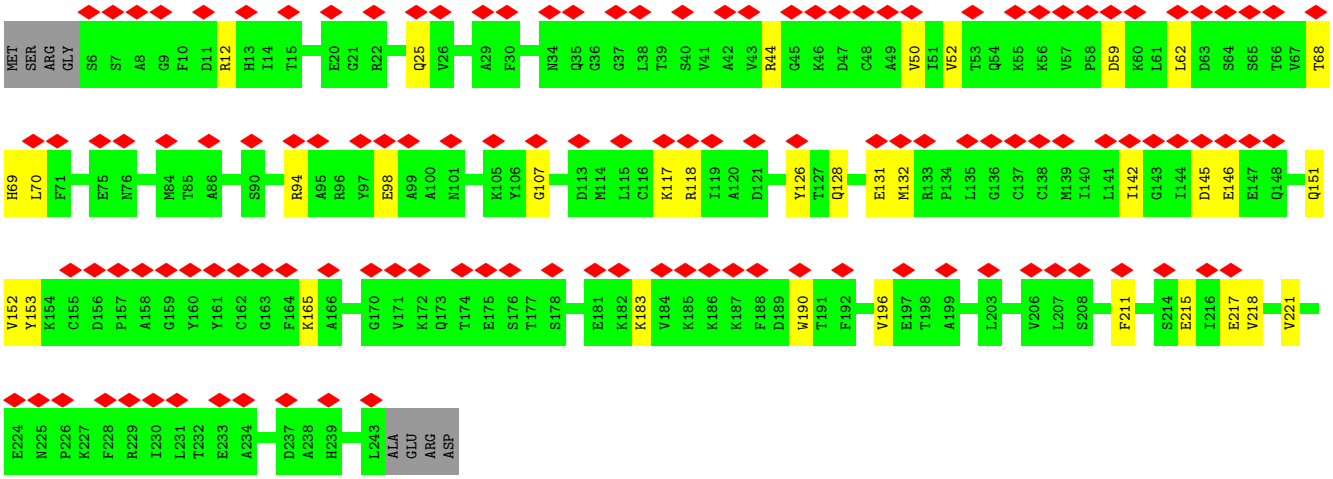
Chain N:



• Molecule 8: Proteasome subunit alpha type-6

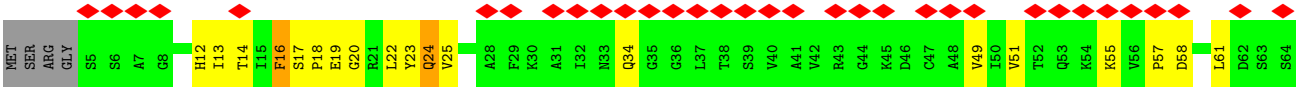
Chain V:

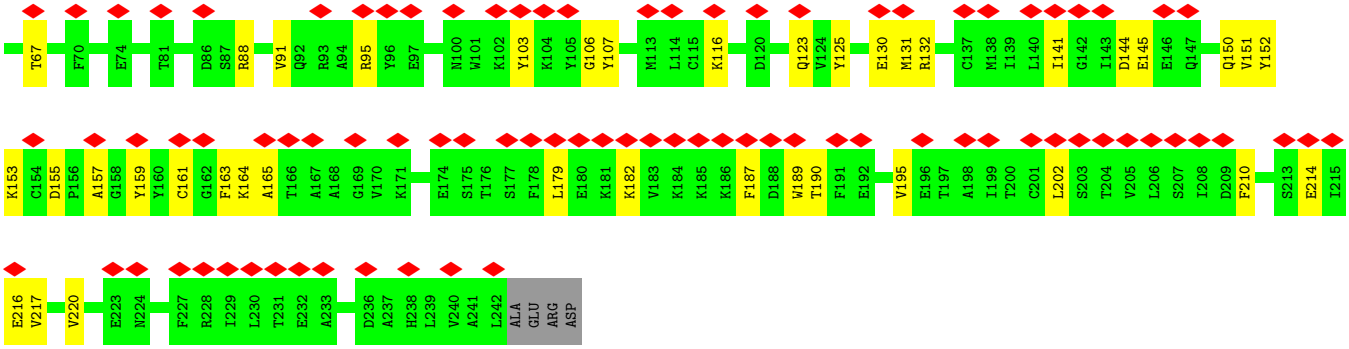




• Molecule 8: Proteasome subunit alpha type-6

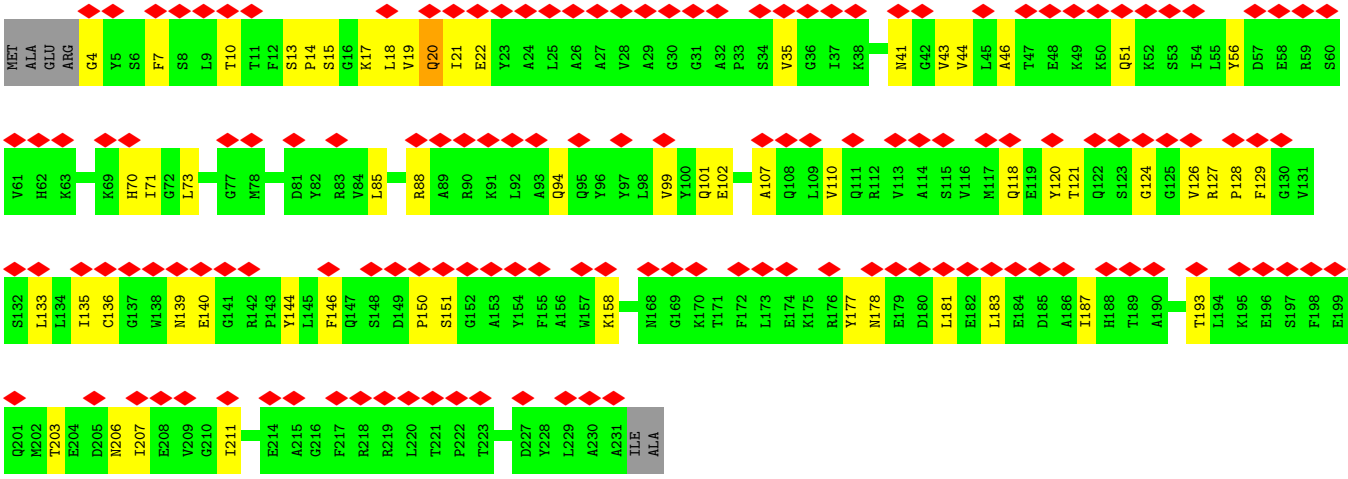
Chain O:





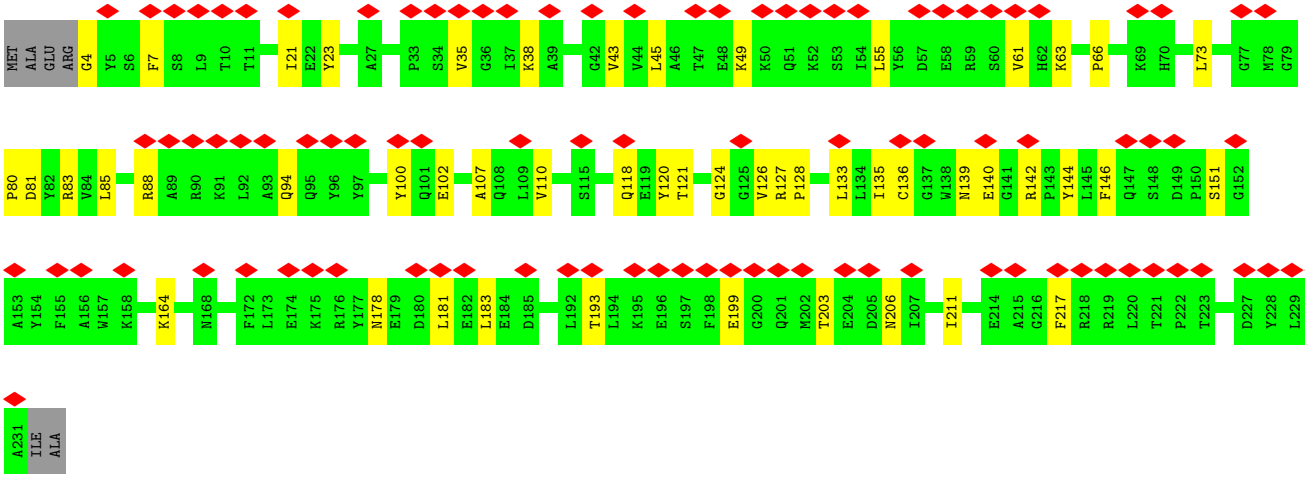
• Molecule 9: Proteasome subunit alpha type-2

Chain W:



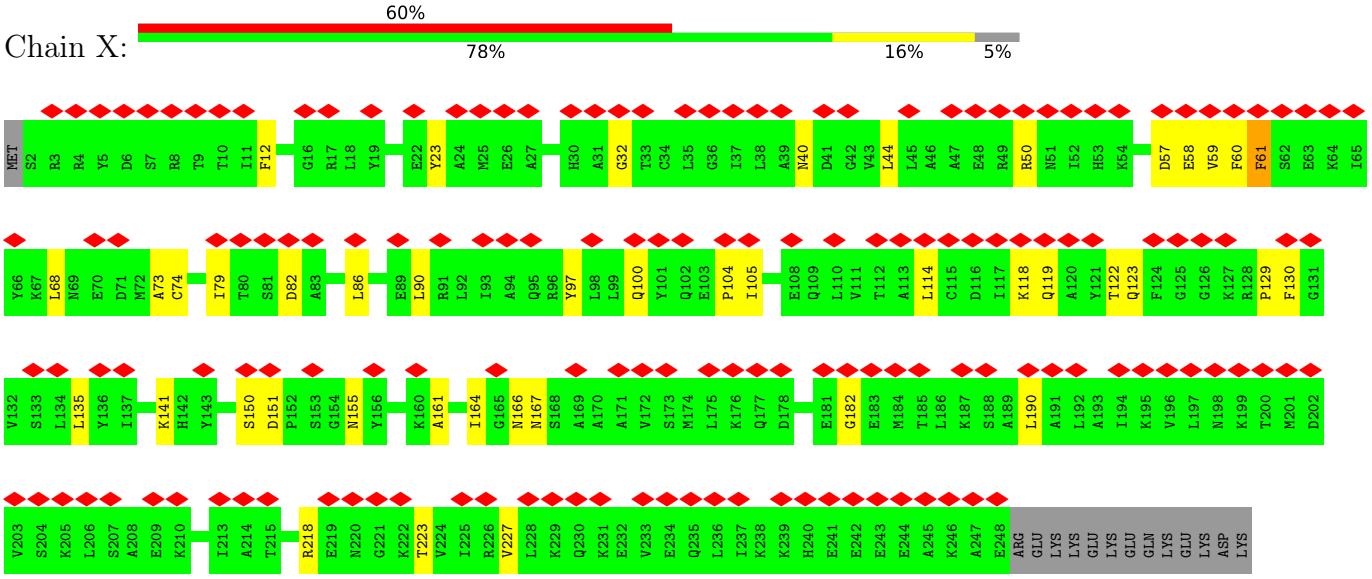
• Molecule 9: Proteasome subunit alpha type-2

Chain P:



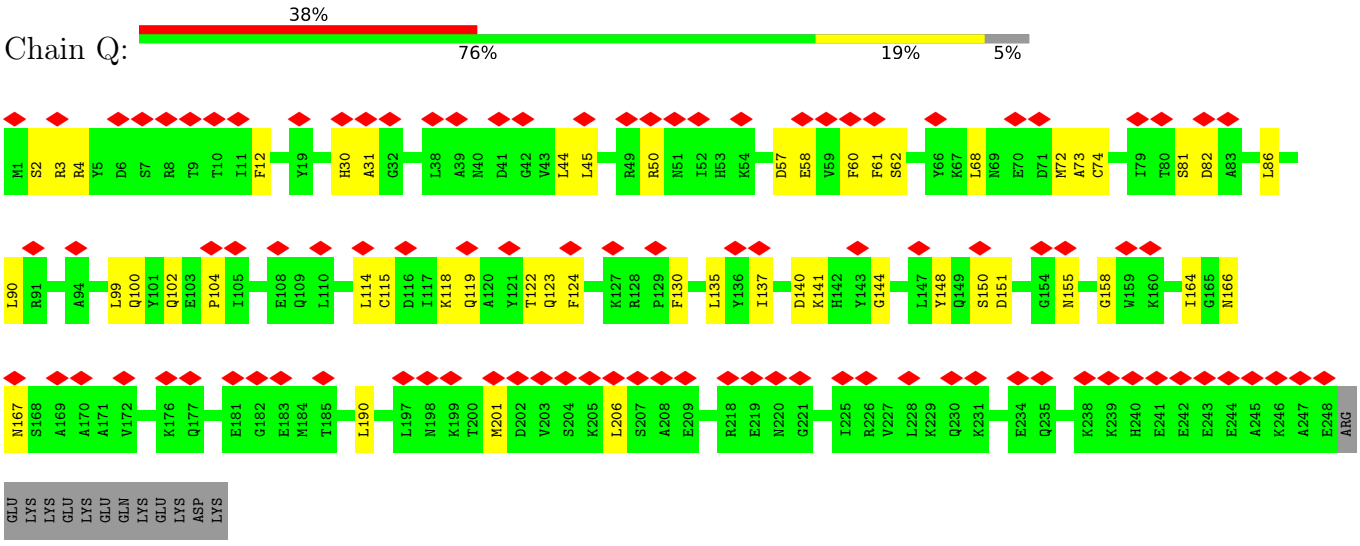
• Molecule 10: Proteasome subunit alpha type-4

Chain X:



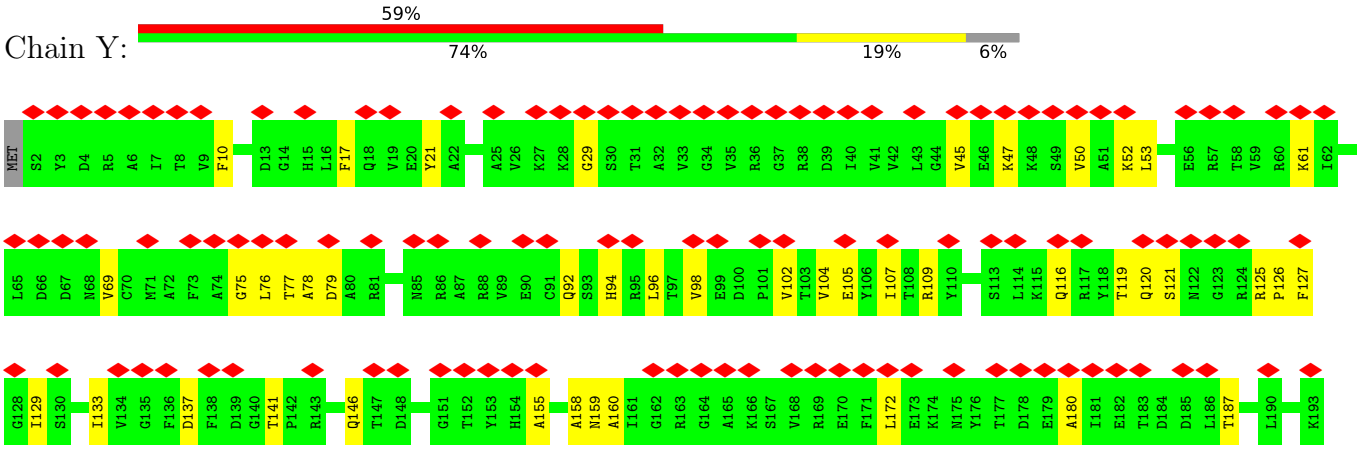
• Molecule 10: Proteasome subunit alpha type-4

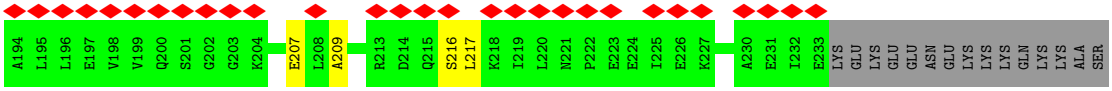
Chain Q:



• Molecule 11: Proteasome subunit alpha type-7

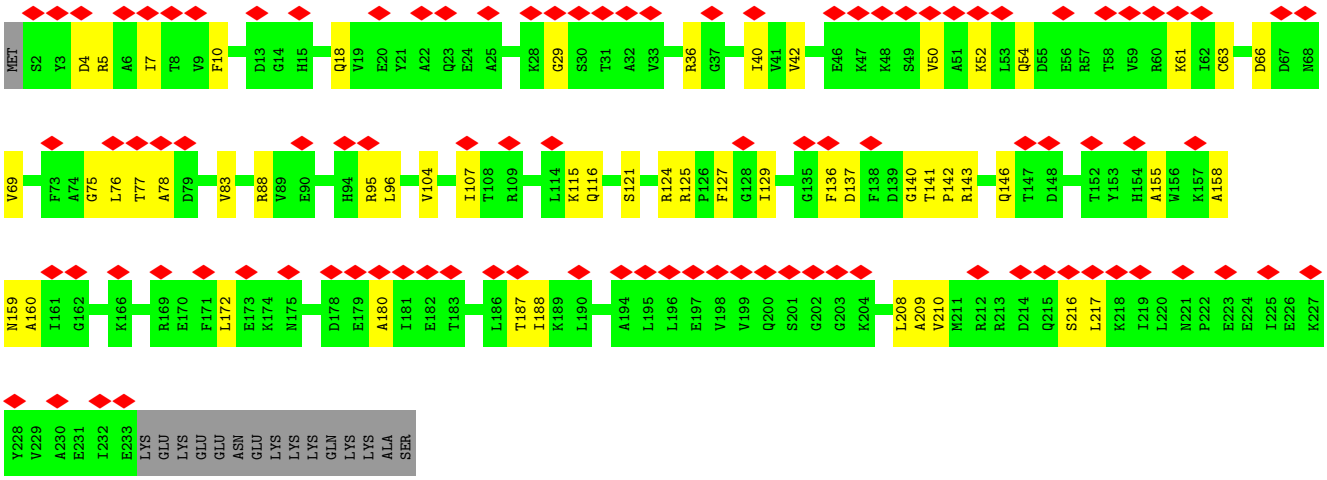
Chain Y:





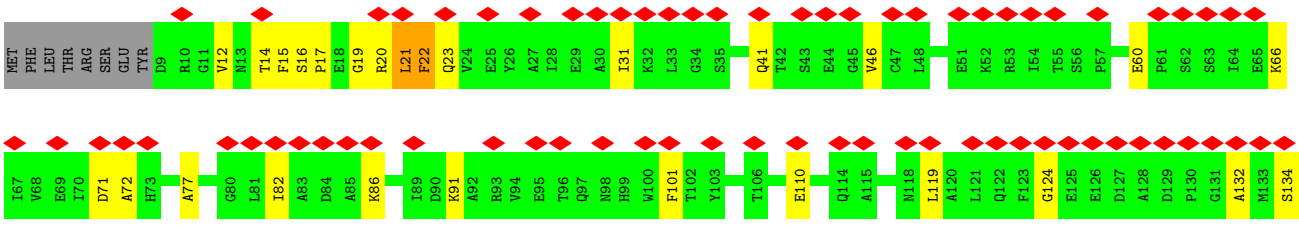
• Molecule 11: Proteasome subunit alpha type-7

Chain R:



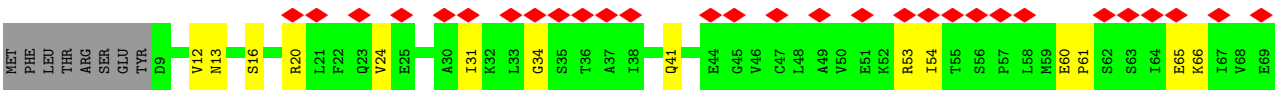
• Molecule 12: Proteasome subunit alpha type-5

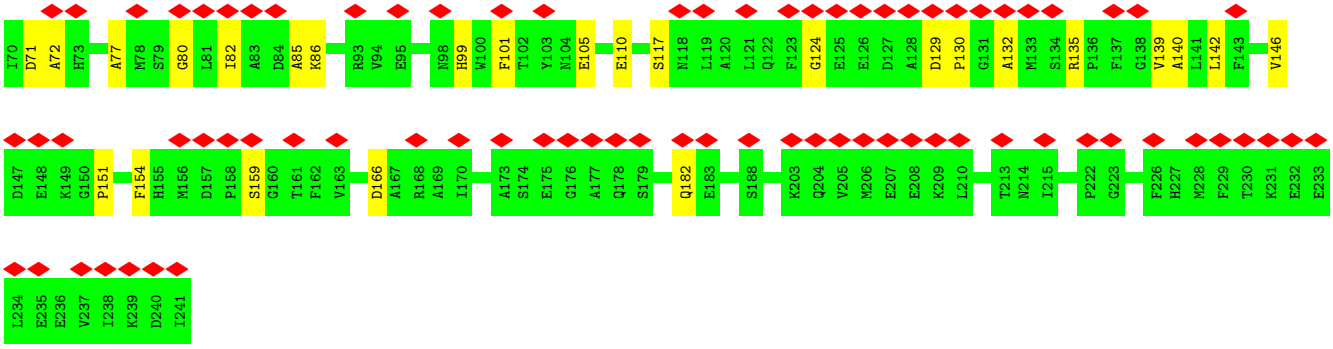
Chain Z:



• Molecule 12: Proteasome subunit alpha type-5

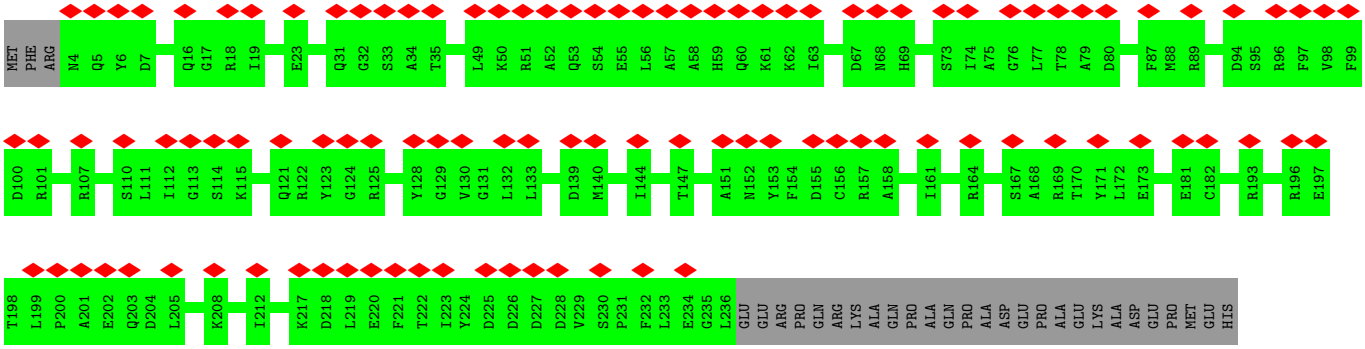
Chain S:





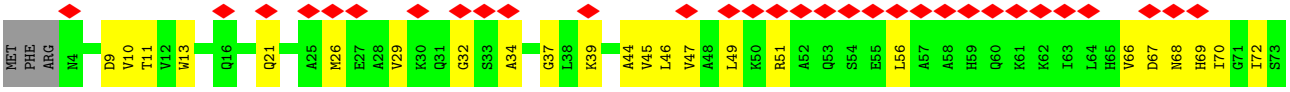
• Molecule 13: Proteasome subunit alpha type-1

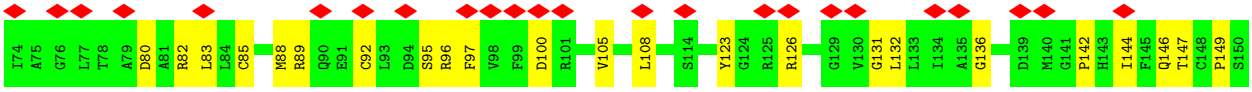
Chain a:

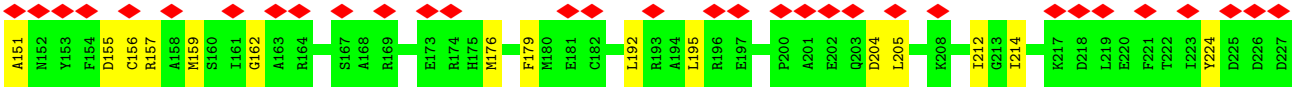


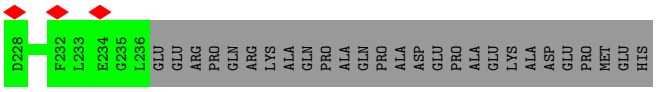
• Molecule 13: Proteasome subunit alpha type-1

Chain T:



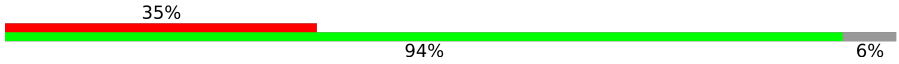


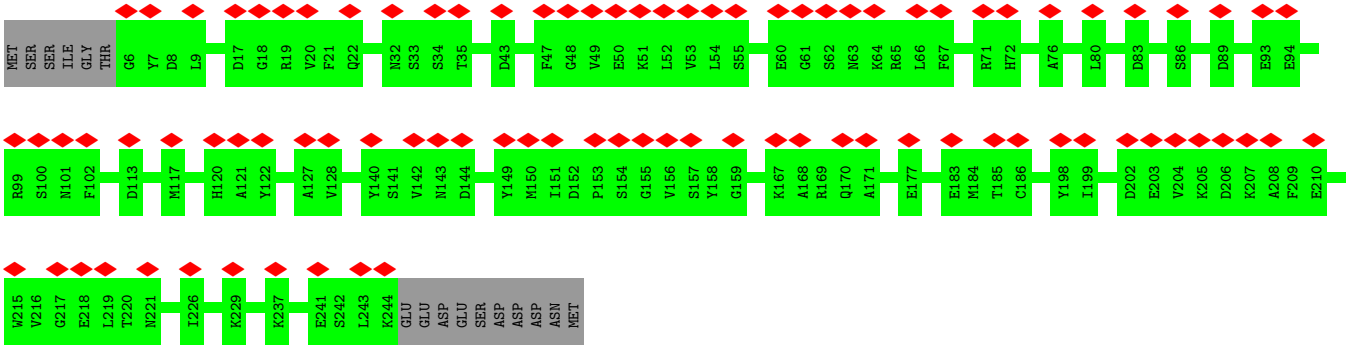




• Molecule 14: Proteasome subunit alpha type-3

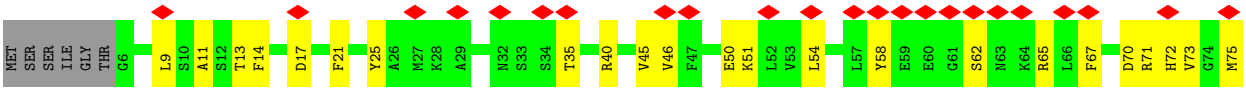
Chain b:

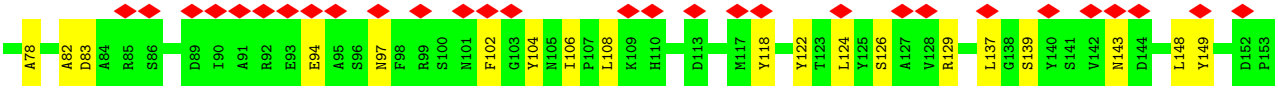


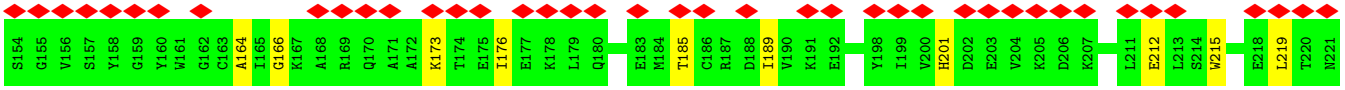


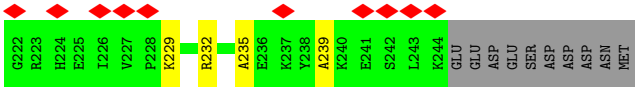
• Molecule 14: Proteasome subunit alpha type-3

Chain U:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72086	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	0.032	Depositor
Minimum map value	-0.013	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	263.6, 263.6, 263.6	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3180001, 1.3180001, 1.3180001	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	0.24	0/1540	0.42	0/2085
1	H	0.24	0/1540	0.42	0/2085
2	B	0.24	0/1686	0.43	0/2282
2	I	0.24	0/1686	0.43	0/2282
3	C	0.24	0/1620	0.44	0/2184
3	J	0.24	0/1620	0.44	0/2184
4	D	0.24	0/1603	0.41	0/2168
4	K	0.24	0/1603	0.41	0/2168
5	E	0.24	0/1586	0.41	0/2142
5	L	0.24	0/1586	0.41	0/2142
6	F	0.24	0/1673	0.42	0/2254
6	M	0.24	0/1673	0.42	0/2254
7	G	0.25	0/1687	0.42	0/2284
7	N	0.25	0/1687	0.42	0/2284
8	O	0.25	0/1891	0.43	0/2557
8	V	0.24	0/1891	0.41	0/2557
9	P	0.24	0/1818	0.40	0/2463
9	W	0.26	0/1818	0.42	0/2463
10	Q	0.24	0/1980	0.42	0/2667
10	X	0.24	0/1972	0.42	0/2657
11	R	0.23	0/1851	0.42	0/2500
11	Y	0.23	0/1851	0.42	0/2500
12	S	0.24	0/1805	0.41	0/2437
12	Z	0.26	0/1805	0.43	0/2437
13	T	0.24	0/1862	0.42	0/2517
13	a	0.23	0/1862	0.41	0/2517
14	U	0.25	0/1909	0.43	0/2570
14	b	0.25	0/1909	0.40	0/2570
All	All	0.24	0/49014	0.42	0/66210

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	1514	0	1487	17	0
1	H	1514	0	1487	27	0
2	B	1659	0	1681	34	0
2	I	1659	0	1681	37	0
3	C	1591	0	1612	50	0
3	J	1591	0	1612	42	0
4	D	1571	0	1573	27	0
4	K	1571	0	1573	34	0
5	E	1555	0	1520	33	0
5	L	1555	0	1520	37	0
6	F	1643	0	1640	27	0
6	M	1643	0	1640	27	0
7	G	1655	0	1634	30	0
7	N	1655	0	1634	30	0
8	O	1857	0	1866	92	0
8	V	1857	0	1866	23	0
9	P	1779	0	1771	59	0
9	W	1779	0	1771	60	0
10	Q	1950	0	1972	47	0
10	X	1942	0	1960	48	0
11	R	1825	0	1849	39	0
11	Y	1825	0	1849	36	0
12	S	1778	0	1764	26	0
12	Z	1778	0	1764	34	0
13	T	1828	0	1820	44	0
13	a	1828	0	1820	0	0
14	U	1874	0	1861	54	0
14	b	1874	0	1861	0	0
All	All	48150	0	48088	819	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 10.

All (819) 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)
10:X:61:PHE:CZ	10:X:227:VAL:HB	1.38	1.59
8:V:68:THR:HG23	8:V:217:GLU:OE1	1.36	1.25
10:X:61:PHE:HZ	10:X:227:VAL:CB	1.56	1.17
3:C:55:LEU:HG	3:C:57:THR:HG22	1.19	1.17
8:O:16:PHE:CZ	9:P:127:ARG:HD2	1.82	1.15
8:O:16:PHE:HE1	9:P:127:ARG:HB2	1.03	1.15
3:C:55:LEU:CG	3:C:57:THR:HG22	1.77	1.14
10:X:61:PHE:CZ	10:X:227:VAL:CB	2.27	1.12
10:Q:4:ARG:CZ	14:U:9:LEU:HD22	1.80	1.11
8:O:16:PHE:CE1	9:P:127:ARG:HD2	1.88	1.08
2:I:187:ARG:HB3	2:I:188:PRO:HD3	1.32	1.07
12:Z:16:SER:HB3	12:Z:22:PHE:CE1	1.91	1.06
9:W:21:ILE:HD11	9:W:121:THR:CG2	1.86	1.05
8:O:16:PHE:CZ	9:P:127:ARG:NH1	2.24	1.04
2:B:187:ARG:HB3	2:B:188:PRO:HD3	1.39	1.04
8:O:16:PHE:CE1	9:P:127:ARG:HB2	1.92	1.03
8:V:68:THR:HG22	8:V:70:LEU:H	1.20	1.01
3:C:55:LEU:CD2	3:C:57:THR:CG2	2.40	0.99
3:C:55:LEU:CD2	3:C:57:THR:HG22	1.94	0.96
9:W:21:ILE:HD11	9:W:121:THR:HG22	1.47	0.95
3:C:55:LEU:HD21	3:C:57:THR:HG21	1.49	0.94
8:O:132:ARG:HH11	14:U:14:PHE:HZ	1.01	0.94
10:X:61:PHE:CE2	10:X:227:VAL:CG2	2.52	0.93
3:C:55:LEU:HD21	3:C:57:THR:CG2	1.98	0.93
8:O:132:ARG:HG2	14:U:124:LEU:HD12	1.50	0.93
10:X:61:PHE:HE2	10:X:227:VAL:CG2	1.82	0.92
8:O:132:ARG:HB2	14:U:14:PHE:HE2	1.33	0.92
14:U:11:ALA:HB3	14:U:126:SER:HA	1.52	0.92
8:O:16:PHE:HE1	9:P:127:ARG:CB	1.83	0.91
8:O:14:THR:HG22	8:O:24:GLN:HB2	1.51	0.90
8:O:22:LEU:HD11	9:P:127:ARG:CZ	2.02	0.89
10:Q:4:ARG:NE	14:U:9:LEU:HD22	1.87	0.89
2:I:187:ARG:HB3	2:I:188:PRO:CD	2.06	0.85
10:X:61:PHE:CE2	10:X:227:VAL:HG21	2.08	0.85
9:W:14:PRO:HA	10:X:23:TYR:CE1	2.12	0.85
10:X:61:PHE:HE2	10:X:227:VAL:HG21	1.40	0.85
8:O:17:SER:CB	8:O:23:TYR:HE2	1.89	0.84
8:O:16:PHE:HZ	9:P:127:ARG:NH1	1.67	0.84
8:O:16:PHE:HZ	9:P:127:ARG:HH11	0.85	0.81
8:O:132:ARG:HD2	14:U:14:PHE:CZ	2.17	0.80
12:Z:16:SER:HB3	12:Z:22:PHE:HE1	1.43	0.80
9:W:14:PRO:HA	10:X:23:TYR:CD1	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:22:LEU:HD11	9:P:127:ARG:NH1	1.97	0.79
9:W:21:ILE:HD11	9:W:121:THR:HG21	1.63	0.79
8:O:16:PHE:CZ	9:P:127:ARG:CD	2.64	0.79
9:W:20:GLN:OE1	9:W:20:GLN:HA	1.83	0.78
5:E:97:MET:HB2	5:E:116:SER:HB3	1.66	0.77
8:V:68:THR:CG2	8:V:217:GLU:OE1	2.27	0.77
8:O:22:LEU:CD1	9:P:127:ARG:CZ	2.63	0.77
8:O:16:PHE:CE2	9:P:127:ARG:NH1	2.53	0.75
10:X:61:PHE:CE2	10:X:227:VAL:HB	2.17	0.74
12:Z:15:PHE:HB3	12:Z:19:GLY:HA2	1.68	0.74
8:O:14:THR:HG22	8:O:24:GLN:CB	2.17	0.74
8:O:16:PHE:CE1	9:P:127:ARG:CD	2.70	0.74
5:L:18:SER:HB2	5:L:173:ALA:H	1.52	0.73
3:C:10:VAL:HG11	3:C:51:GLY:HA3	1.70	0.73
4:D:27:GLN:NE2	4:K:169:LYS:O	2.21	0.73
2:B:187:ARG:HB3	2:B:188:PRO:CD	2.18	0.72
12:Z:20:ARG:O	12:Z:21:LEU:HB3	1.90	0.72
3:C:92:ASN:HD21	9:W:99:VAL:HA	1.54	0.71
10:X:61:PHE:CE2	10:X:227:VAL:CB	2.74	0.71
8:O:16:PHE:CZ	8:O:22:LEU:HD21	2.26	0.71
12:Z:21:LEU:O	12:Z:23:GLN:N	2.23	0.71
6:F:68:ILE:HD11	6:F:92:LEU:HD13	1.74	0.69
12:Z:16:SER:HB2	12:Z:17:PRO:HD2	1.75	0.69
10:X:119:GLN:NE2	11:Y:79:ASP:OD1	2.26	0.69
9:W:18:LEU:HD11	10:X:79:ILE:CD1	2.24	0.68
3:C:188:ILE:HB	3:C:195:THR:HB	1.76	0.68
8:O:13:ILE:CA	8:O:24:GLN:HE21	2.06	0.68
8:O:17:SER:O	8:O:20:GLY:N	2.27	0.68
8:O:132:ARG:NH1	14:U:14:PHE:HZ	1.83	0.68
6:M:68:ILE:HD11	6:M:92:LEU:HD13	1.73	0.68
8:O:17:SER:CB	8:O:23:TYR:CE2	2.74	0.67
5:L:97:MET:HB2	5:L:116:SER:HB3	1.76	0.67
4:K:83:PHE:HE1	10:Q:100:GLN:HG2	1.59	0.67
3:J:10:VAL:HG11	3:J:51:GLY:HA3	1.75	0.67
8:O:17:SER:HB3	8:O:23:TYR:CE2	2.28	0.67
10:Q:3:ARG:HH22	13:T:9:ASP:HB2	1.60	0.66
13:T:132:LEU:HB2	13:T:147:THR:HB	1.78	0.66
8:O:130:GLU:O	14:U:126:SER:HB3	1.95	0.66
2:B:61:SER:O	9:W:94:GLN:NE2	2.29	0.66
3:J:188:ILE:HB	3:J:195:THR:HB	1.77	0.66
8:O:17:SER:C	8:O:20:GLY:H	1.99	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:194:ARG:NH1	6:F:205:GLU:OE2	2.29	0.66
12:Z:20:ARG:O	12:Z:21:LEU:CB	2.44	0.66
13:T:72:ILE:HD11	13:T:132:LEU:HB3	1.78	0.66
8:O:132:ARG:HB2	14:U:14:PHE:CE2	2.24	0.65
10:Q:158:GLY:O	11:R:54:GLN:NE2	2.29	0.65
4:K:19:ARG:HD3	4:K:179:SER:HB2	1.79	0.65
5:E:18:SER:HB2	5:E:173:ALA:H	1.61	0.65
6:M:198:VAL:HG22	6:M:203:ILE:HG12	1.78	0.65
9:W:88:ARG:NH2	9:W:120:TYR:OH	2.30	0.65
8:O:141:ILE:HG22	8:O:151:VAL:HG22	1.79	0.64
5:E:154:ASP:OD1	5:E:157:ARG:NH2	2.30	0.64
9:W:118:GLN:NE2	10:X:82:ASP:OD1	2.30	0.64
6:F:22:ILE:HG12	6:F:197:ILE:HG12	1.79	0.64
8:V:12:ARG:O	8:V:25:GLN:NE2	2.30	0.64
5:E:14:VAL:HG21	5:E:42:LEU:HD11	1.79	0.64
9:P:203:THR:OG1	9:P:206:ASN:ND2	2.29	0.64
10:X:44:LEU:HD22	10:X:190:LEU:HD23	1.80	0.64
1:H:7:GLN:NE2	1:H:109:GLY:O	2.31	0.64
9:W:21:ILE:CD1	9:W:121:THR:CG2	2.72	0.64
9:P:88:ARG:NH2	9:P:120:TYR:OH	2.31	0.64
3:C:202:ARG:HH12	5:L:191:ASN:HD21	1.46	0.63
12:Z:31:ILE:HD13	12:Z:140:ALA:HB2	1.80	0.63
5:L:154:ASP:OD1	5:L:157:ARG:NH2	2.31	0.63
7:G:9:THR:HG21	7:G:25:ASP:HB2	1.78	0.63
6:M:194:ARG:NH1	6:M:205:GLU:OE2	2.32	0.63
8:V:142:ILE:HG22	8:V:152:VAL:HG22	1.81	0.63
8:O:12:HIS:O	8:O:24:GLN:NE2	2.32	0.63
13:T:66:VAL:O	13:T:89:ARG:NH1	2.31	0.62
6:F:198:VAL:HG22	6:F:203:ILE:HG12	1.79	0.62
9:W:21:ILE:CD1	9:W:121:THR:HG21	2.27	0.62
1:A:7:GLN:NE2	1:A:109:GLY:O	2.31	0.62
2:B:172:ASN:OD1	2:B:173:ILE:N	2.33	0.62
7:N:185:ASN:OD1	7:N:186:ARG:N	2.32	0.62
8:O:16:PHE:CE1	8:O:22:LEU:HD21	2.33	0.62
9:P:118:GLN:NE2	10:Q:82:ASP:OD1	2.33	0.62
4:D:45:LEU:HD12	4:D:103:LEU:HD22	1.81	0.62
3:C:79:ARG:NH1	9:W:140:GLU:OE2	2.33	0.61
6:F:24:ALA:HB1	6:F:193:LEU:HD11	1.82	0.61
5:E:103:GLY:HA2	5:E:179:VAL:HG11	1.83	0.61
9:W:14:PRO:HA	10:X:23:TYR:CZ	2.35	0.61
9:W:203:THR:OG1	9:W:206:ASN:ND2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:66:LYS:HE2	12:Z:82:ILE:HD11	1.82	0.61
3:J:79:ARG:NH1	9:P:140:GLU:OE2	2.34	0.61
9:W:158:LYS:HB3	9:W:177:TYR:OH	2.00	0.61
11:R:69:VAL:HG11	11:R:107:ILE:HG21	1.83	0.61
3:C:57:THR:HG23	3:C:58:ASP:N	2.15	0.61
5:L:14:VAL:HG21	5:L:42:LEU:HD11	1.81	0.61
14:U:215:TRP:HH2	14:U:219:LEU:HB2	1.66	0.61
2:I:172:ASN:OD1	2:I:173:ILE:N	2.34	0.60
4:D:14:LEU:HD13	4:D:182:ILE:HB	1.83	0.60
2:I:93:TYR:O	3:J:98:ARG:NH2	2.34	0.60
9:W:139:ASN:HB2	9:W:144:TYR:HE2	1.67	0.60
11:R:159:ASN:OD1	11:R:160:ALA:N	2.33	0.60
12:S:13:ASN:HB3	13:T:126:ARG:HB3	1.82	0.60
9:W:85:LEU:HD13	9:W:133:LEU:HD11	1.84	0.60
11:Y:209:ALA:HB1	11:Y:217:LEU:HD11	1.83	0.60
14:U:67:PHE:HB2	14:U:75:MET:HB3	1.83	0.60
2:B:29:LYS:NZ	6:M:184:GLU:OE1	2.35	0.60
8:V:94:ARG:NH1	8:V:126:TYR:OH	2.35	0.60
11:R:209:ALA:HB1	11:R:217:LEU:HD11	1.84	0.60
2:I:61:SER:O	9:P:94:GLN:NE2	2.35	0.60
11:Y:159:ASN:OD1	11:Y:160:ALA:N	2.35	0.60
11:R:116:GLN:HE22	12:S:86:LYS:HB2	1.67	0.59
1:A:130:SER:HG	1:A:169:SER:HG	1.50	0.59
4:K:20:VAL:O	4:K:34:LYS:NZ	2.32	0.59
9:W:18:LEU:CD1	10:X:79:ILE:HD11	2.32	0.59
4:D:83:PHE:HE1	10:X:100:GLN:HG2	1.66	0.59
5:E:191:ASN:OD1	5:E:192:VAL:N	2.36	0.59
4:D:8:GLN:HE21	4:D:113:PRO:HG2	1.66	0.59
10:X:40:ASN:ND2	10:X:182:GLY:O	2.36	0.59
10:Q:44:LEU:HD22	10:Q:190:LEU:HD23	1.84	0.59
6:F:184:GLU:OE1	2:I:29:LYS:NZ	2.35	0.59
10:Q:151:ASP:OD1	10:Q:155:ASN:N	2.35	0.59
13:T:44:ALA:HB2	13:T:142:PRO:HB2	1.85	0.59
3:C:158:ASP:HB2	3:C:161:HIS:HD2	1.67	0.59
3:C:122:SER:HB2	3:C:136:VAL:HB	1.84	0.59
3:J:122:SER:HB2	3:J:136:VAL:HB	1.84	0.59
10:X:151:ASP:OD1	10:X:155:ASN:N	2.35	0.59
8:O:132:ARG:HG2	14:U:124:LEU:CD1	2.28	0.59
13:T:10:VAL:HG23	13:T:11:THR:HG23	1.84	0.59
8:V:52:VAL:HG22	8:V:218:VAL:HG22	1.85	0.58
11:R:146:GLN:OE1	11:R:159:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:78:GLY:HA3	10:Q:60:PHE:HE1	1.68	0.58
8:O:14:THR:CG2	8:O:24:GLN:HG3	2.34	0.58
7:G:29:SER:OG	7:G:182:ARG:NH1	2.36	0.58
10:Q:4:ARG:NE	14:U:9:LEU:CD2	2.62	0.58
3:C:66:LEU:O	3:C:70:LEU:N	2.31	0.58
6:M:22:ILE:HG12	6:M:197:ILE:HG12	1.86	0.58
9:P:139:ASN:HB2	9:P:144:TYR:HE2	1.69	0.58
5:E:61:ARG:HH22	12:Z:101:PHE:HA	1.69	0.57
1:H:21:THR:HG22	1:H:26:ILE:HG12	1.86	0.57
11:Y:61:LYS:NZ	11:Y:77:THR:OG1	2.37	0.57
4:D:20:VAL:O	4:D:34:LYS:NZ	2.29	0.57
2:I:81:ARG:NH1	8:O:106:GLY:O	2.36	0.57
7:N:27:LEU:HD22	7:N:184:TYR:HB2	1.86	0.57
8:O:51:VAL:HG22	8:O:217:VAL:HG22	1.85	0.57
5:E:38:ASN:OD1	5:E:41:LEU:N	2.38	0.57
7:N:29:SER:OG	7:N:182:ARG:NH1	2.37	0.57
13:T:39:LYS:HB3	13:T:144:ILE:HG12	1.85	0.57
4:K:14:LEU:HD13	4:K:182:ILE:HB	1.87	0.57
5:L:191:ASN:OD1	5:L:192:VAL:N	2.38	0.57
6:M:73:LYS:O	13:T:89:ARG:NH2	2.37	0.57
10:Q:31:ALA:O	10:Q:50:ARG:NH2	2.37	0.57
14:U:73:VAL:HG22	14:U:139:SER:HB2	1.87	0.57
10:X:123:GLN:HA	11:Y:125:ARG:HE	1.70	0.57
10:Q:4:ARG:HD2	14:U:9:LEU:HD13	1.87	0.57
7:G:185:ASN:OD1	7:G:186:ARG:N	2.37	0.57
7:G:27:LEU:HD11	7:G:34:ALA:HB1	1.86	0.56
10:X:119:GLN:HE22	11:Y:79:ASP:HA	1.70	0.56
5:E:20:ALA:HB2	5:E:33:LYS:HZ1	1.70	0.56
8:O:58:ASP:HB3	8:O:61:LEU:HG	1.87	0.56
1:H:174:ILE:HB	1:H:189:LEU:HB2	1.86	0.56
7:N:25:ASP:O	7:N:41:ARG:NH2	2.38	0.56
8:O:16:PHE:CD1	8:O:16:PHE:N	2.73	0.56
8:O:22:LEU:HD21	9:P:127:ARG:HD2	1.87	0.56
5:L:38:ASN:OD1	5:L:41:LEU:N	2.38	0.56
3:J:11:MET:HG3	3:J:137:VAL:HG22	1.88	0.56
3:J:158:ASP:HB2	3:J:161:HIS:HD2	1.70	0.56
6:M:27:THR:O	6:M:40:SER:N	2.38	0.56
8:O:14:THR:HG23	8:O:24:GLN:HG3	1.87	0.56
8:O:130:GLU:HG2	9:P:4:GLY:HA2	1.86	0.56
9:P:73:LEU:HD11	9:P:133:LEU:HD22	1.87	0.56
4:D:29:LYS:HD2	5:E:121:ILE:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:LEU:O	3:C:76:LYS:N	2.39	0.56
9:W:18:LEU:HD11	10:X:79:ILE:HD11	1.85	0.56
10:Q:68:LEU:H	10:Q:73:ALA:HA	1.70	0.56
5:E:44:THR:O	5:E:99:THR:OG1	2.22	0.56
3:C:58:ASP:OD2	3:C:103:TYR:N	2.33	0.56
11:Y:29:GLY:HA3	11:Y:75:GLY:HA2	1.86	0.56
8:O:34:GLN:NE2	14:U:17:ASP:O	2.39	0.56
10:Q:30:HIS:O	10:Q:50:ARG:NH1	2.35	0.56
11:R:137:ASP:OD1	11:R:141:THR:N	2.36	0.56
5:L:44:THR:O	5:L:99:THR:OG1	2.22	0.56
10:Q:60:PHE:O	10:Q:62:SER:N	2.39	0.56
5:L:8:PHE:CE1	5:L:10:HIS:HB2	2.42	0.55
9:P:142:ARG:NH2	10:Q:57:ASP:OD2	2.39	0.55
3:J:87:MET:HG3	3:J:123:LEU:HD11	1.88	0.55
13:T:13:TRP:HE1	14:U:129:ARG:HB2	1.71	0.55
2:B:41:ILE:HG12	2:B:102:GLY:HA3	1.88	0.55
5:E:140:ASP:OD2	4:K:170:ARG:NH2	2.37	0.55
10:X:68:LEU:H	10:X:73:ALA:HA	1.71	0.55
12:S:66:LYS:HE2	12:S:82:ILE:HD11	1.89	0.55
13:T:151:ALA:HB3	14:U:82:ALA:HB1	1.87	0.55
14:U:83:ASP:OD1	14:U:129:ARG:NH2	2.31	0.55
3:C:26:ARG:NH1	3:C:178:ALA:O	2.39	0.55
7:N:210:ASP:OD1	7:N:211:ILE:N	2.39	0.55
13:T:32:GLY:O	13:T:51:ARG:NH2	2.40	0.55
4:D:49:GLU:OE2	4:D:99:HIS:ND1	2.40	0.55
2:I:7:VAL:HG22	2:I:12:ILE:HG22	1.89	0.55
11:R:115:LYS:HG2	11:R:127:PHE:HD2	1.71	0.55
11:R:136:PHE:HB3	11:R:140:GLY:HA2	1.87	0.55
12:S:12:VAL:HG21	12:S:124:GLY:HA2	1.88	0.55
5:E:78:ALA:HB2	11:Y:98:VAL:HA	1.89	0.55
6:M:24:ALA:HB1	6:M:193:LEU:HD11	1.88	0.55
2:B:30:ASN:O	2:B:187:ARG:NH2	2.37	0.55
2:B:81:ARG:HD2	8:V:107:GLY:HA3	1.89	0.55
2:I:69:SER:O	8:O:116:LYS:NZ	2.40	0.55
2:I:162:GLY:O	2:I:166:ASP:N	2.40	0.55
5:E:1:THR:N	5:E:169:TYR:O	2.40	0.55
6:F:185:ARG:HA	2:I:26:VAL:HB	1.89	0.55
10:Q:4:ARG:CD	14:U:9:LEU:HD13	2.37	0.55
2:B:162:GLY:O	2:B:166:ASP:N	2.38	0.55
1:H:106:GLN:NE2	14:U:143:ASN:OD1	2.40	0.54
3:J:58:ASP:OD2	3:J:103:TYR:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:171:PHE:CE2	4:K:173:LEU:HB2	2.42	0.54
3:C:87:MET:HG3	3:C:123:LEU:HD11	1.89	0.54
7:G:192:VAL:HG22	7:G:197:VAL:HG22	1.89	0.54
3:J:68:PHE:HB2	10:Q:99:LEU:HD21	1.89	0.54
12:Z:41:GLN:NE2	12:Z:151:PRO:O	2.41	0.54
10:Q:57:ASP:OD1	10:Q:58:GLU:N	2.38	0.54
13:T:39:LYS:HE2	13:T:157:ARG:HA	1.87	0.54
6:F:123:SER:HB2	6:F:136:LYS:HG2	1.89	0.54
4:K:8:GLN:HE21	4:K:113:PRO:HG2	1.72	0.54
2:I:214:GLU:HG3	3:J:197:ARG:HG2	1.88	0.54
1:A:174:ILE:HB	1:A:189:LEU:HB2	1.88	0.54
3:C:11:MET:HG3	3:C:137:VAL:HG22	1.88	0.54
1:H:77:HIS:HE1	14:U:104:TYR:HE1	1.55	0.54
5:L:103:GLY:HA2	5:L:179:VAL:HG11	1.90	0.54
10:X:32:GLY:HA2	10:X:50:ARG:HE	1.72	0.54
10:X:118:LYS:NZ	10:X:150:SER:OG	2.34	0.54
2:B:93:TYR:O	3:C:98:ARG:NH2	2.41	0.54
3:C:69:ARG:HH22	3:C:92:ASN:HD22	1.54	0.54
5:E:178:HIS:CE1	5:E:180:ARG:HE	2.26	0.54
8:O:13:ILE:HA	8:O:24:GLN:HE21	1.71	0.54
11:Y:155:ALA:HB3	12:Z:60:GLU:HB3	1.89	0.54
2:I:187:ARG:CB	2:I:188:PRO:HD3	2.21	0.54
6:M:35:ILE:HB	7:N:151:ARG:HH12	1.73	0.54
8:O:164:LYS:N	9:P:55:LEU:O	2.41	0.54
10:Q:123:GLN:HA	11:R:125:ARG:HE	1.73	0.54
4:K:49:GLU:OE2	4:K:99:HIS:ND1	2.41	0.54
8:O:132:ARG:HD2	14:U:14:PHE:CE2	2.43	0.54
13:T:214:ILE:HD12	13:T:224:TYR:HE2	1.73	0.54
3:C:55:LEU:HD23	3:C:57:THR:CG2	2.38	0.53
10:Q:4:ARG:CZ	14:U:9:LEU:CD2	2.71	0.53
11:R:158:ALA:HB1	11:R:172:LEU:HD13	1.90	0.53
10:X:57:ASP:OD1	10:X:58:GLU:N	2.38	0.53
11:Y:137:ASP:OD1	11:Y:141:THR:N	2.37	0.53
12:S:34:GLY:HA3	12:S:80:GLY:HA2	1.90	0.53
9:W:18:LEU:CD1	10:X:79:ILE:CD1	2.86	0.53
5:L:164:THR:HG22	5:L:170:SER:HB3	1.90	0.53
2:B:26:VAL:HB	6:M:185:ARG:HA	1.90	0.53
7:G:89:HIS:NE2	7:G:124:TYR:O	2.39	0.53
7:G:124:TYR:HE1	7:G:139:THR:HG22	1.74	0.53
3:J:202:ARG:NH2	3:J:204:ASP:OD2	2.38	0.53
2:B:7:VAL:HG22	2:B:12:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:HIS:HA	1:H:80:ALA:HB3	1.90	0.53
7:N:89:HIS:CE1	7:N:131:ALA:HB1	2.43	0.53
12:Z:91:LYS:HE2	12:Z:119:LEU:HD11	1.90	0.53
5:E:115:ASP:OD1	5:E:116:SER:N	2.42	0.53
6:M:55:SER:O	6:M:107:TYR:N	2.34	0.53
10:Q:123:GLN:HA	11:R:125:ARG:NE	2.23	0.53
11:R:61:LYS:NZ	11:R:77:THR:OG1	2.41	0.53
6:F:36:HIS:HB3	7:G:132:TYR:CE2	2.44	0.52
2:B:198:ARG:NH2	3:C:154:GLU:OE2	2.35	0.52
4:D:37:LYS:O	4:D:61:GLN:NE2	2.42	0.52
5:E:158:ARG:HD2	4:K:145:ARG:HH11	1.74	0.52
3:J:67:LYS:HA	3:J:70:LEU:HB3	1.92	0.52
6:M:56:GLY:HA3	6:M:106:VAL:HA	1.91	0.52
9:P:35:VAL:HG11	9:P:193:THR:HG21	1.90	0.52
3:J:66:LEU:HD11	3:J:90:VAL:HG22	1.90	0.52
9:W:21:ILE:HG21	9:W:151:SER:HB3	1.91	0.52
8:O:67:THR:OG1	8:O:216:GLU:OE1	2.24	0.52
3:C:47:ARG:HE	3:C:111:LEU:HB2	1.74	0.52
5:E:8:PHE:CE1	5:E:10:HIS:HB2	2.44	0.52
6:F:88:ILE:HG22	6:F:110:ILE:HD13	1.91	0.52
8:O:210:PHE:HB3	8:O:214:GLU:HB2	1.90	0.52
11:R:7:ILE:HG22	11:R:18:GLN:HG3	1.92	0.52
1:H:3:ILE:HG13	1:H:99:ILE:HD12	1.91	0.52
7:N:27:LEU:HD11	7:N:34:ALA:HB1	1.91	0.52
14:U:40:ARG:HG3	14:U:45:VAL:HG22	1.92	0.52
10:X:90:LEU:HD21	10:X:114:LEU:HD22	1.92	0.52
7:G:211:ILE:HB	1:H:30:VAL:HG11	1.92	0.52
3:J:73:TYR:HA	3:J:76:LYS:HB3	1.92	0.52
1:H:32:ASP:O	1:H:45:ARG:NH2	2.43	0.51
6:M:133:ASP:OD1	6:M:134:SER:N	2.43	0.51
13:T:47:VAL:HG22	13:T:212:ILE:HG12	1.93	0.51
1:A:21:THR:HG22	1:A:26:ILE:HG12	1.92	0.51
9:W:118:GLN:HE22	10:X:82:ASP:HA	1.75	0.51
8:O:16:PHE:CE1	9:P:127:ARG:CB	2.72	0.51
7:G:89:HIS:CE1	7:G:131:ALA:HB1	2.46	0.51
14:U:35:THR:HA	14:U:166:GLY:HA3	1.92	0.51
1:H:98:ILE:HB	1:H:114:VAL:HB	1.92	0.51
7:N:124:TYR:HB2	7:N:137:LEU:HD13	1.92	0.51
8:V:44:ARG:HH21	8:V:165:LYS:HG2	1.75	0.51
13:T:10:VAL:HG12	13:T:21:GLN:HG2	1.92	0.51
5:E:177:TYR:HD1	5:E:186:ARG:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:28:ASP:HB2	3:J:130:MET:HG3	1.92	0.51
3:J:78:GLY:HA3	10:Q:60:PHE:CE1	2.45	0.51
8:O:155:ASP:OD1	8:O:159:TYR:N	2.35	0.51
8:O:179:LEU:HB3	9:P:55:LEU:HD21	1.93	0.51
1:A:77:HIS:HA	1:A:80:ALA:HB3	1.91	0.51
4:D:43:LEU:HD12	4:D:183:ILE:HD11	1.92	0.51
5:E:141:ARG:HH21	4:K:142:ILE:HD13	1.74	0.51
5:L:33:LYS:O	5:L:45:MET:N	2.33	0.51
2:B:65:LEU:HG	9:W:94:GLN:HE22	1.76	0.51
10:Q:124:PHE:HB3	11:R:124:ARG:HG2	1.93	0.51
14:U:50:GLU:OE2	14:U:201:HIS:ND1	2.44	0.51
11:Y:69:VAL:HG11	11:Y:107:ILE:HG21	1.93	0.51
3:J:69:ARG:HA	3:J:72:LEU:HD12	1.93	0.50
6:M:36:HIS:HB3	7:N:132:TYR:CZ	2.46	0.50
7:N:28:GLY:N	7:N:36:PHE:O	2.44	0.50
10:X:135:LEU:HG	10:X:164:ILE:HD13	1.92	0.50
2:I:122:LEU:HD12	2:I:125:VAL:HG12	1.93	0.50
5:L:115:ASP:OD1	5:L:116:SER:N	2.43	0.50
1:H:88:TYR:O	1:H:91:ARG:NH1	2.45	0.50
8:O:17:SER:HB2	8:O:23:TYR:HE2	1.71	0.50
3:C:85:THR:OG1	9:W:102:GLU:OE2	2.27	0.50
5:E:61:ARG:HH12	12:Z:101:PHE:HD1	1.59	0.50
3:C:73:TYR:HA	3:C:76:LYS:HB3	1.93	0.50
4:K:35:MET:SD	4:K:181:ARG:NE	2.84	0.50
8:V:98:GLU:OE1	8:V:118:ARG:NE	2.40	0.50
12:Z:21:LEU:O	12:Z:21:LEU:HG	2.11	0.50
8:O:16:PHE:CE2	8:O:22:LEU:HD21	2.47	0.50
14:U:72:HIS:CD2	14:U:73:VAL:HG23	2.46	0.50
9:W:121:THR:HA	9:W:128:PRO:HG3	1.93	0.50
10:X:68:LEU:HD11	10:X:74:CYS:HB3	1.94	0.50
12:Z:12:VAL:HG21	12:Z:124:GLY:HA2	1.93	0.50
9:P:110:VAL:HG22	9:P:135:ILE:HD12	1.94	0.50
13:T:49:LEU:HB2	13:T:195:LEU:HD11	1.93	0.50
9:W:73:LEU:HD21	9:W:133:LEU:HD22	1.94	0.50
1:A:88:TYR:O	1:A:91:ARG:NH1	2.40	0.50
3:J:76:LYS:HZ3	9:P:100:TYR:HE2	1.59	0.50
9:W:14:PRO:HA	10:X:23:TYR:CG	2.46	0.50
11:Y:105:GLU:OE2	11:Y:109:ARG:NH2	2.41	0.50
13:T:204:ASP:OD1	13:T:205:LEU:N	2.44	0.50
1:A:104:ASP:OD1	1:A:108:GLY:N	2.45	0.49
12:Z:46:VAL:HG23	12:Z:151:PRO:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:THR:CG2	3:C:58:ASP:N	2.75	0.49
7:G:8:GLY:HA3	7:G:41:ARG:NH1	2.26	0.49
2:I:66:HIS:CE1	2:I:70:THR:HG21	2.46	0.49
8:O:55:LYS:HG2	8:O:57:PRO:HD3	1.94	0.49
4:K:29:LYS:HD2	5:L:121:ILE:HB	1.94	0.49
9:W:10:THR:HG23	9:W:20:GLN:HB2	1.94	0.49
10:X:12:PHE:CE1	11:Y:125:ARG:HD2	2.47	0.49
4:D:19:ARG:HB2	4:D:177:THR:HG22	1.94	0.49
5:L:125:THR:HB	5:L:139:MET:SD	2.52	0.49
10:Q:122:THR:O	11:R:125:ARG:NE	2.39	0.49
4:D:171:PHE:CE2	4:D:173:LEU:HB2	2.47	0.49
10:Q:68:LEU:HD11	10:Q:74:CYS:HB3	1.94	0.49
13:T:95:SER:O	13:T:100:ASP:N	2.45	0.49
14:U:45:VAL:HG11	14:U:148:LEU:HD13	1.95	0.49
6:F:56:GLY:HA3	6:F:106:VAL:HA	1.94	0.49
3:C:78:GLY:HA3	10:X:60:PHE:CZ	2.48	0.49
3:C:112:ASP:HB3	3:C:117:LYS:H	1.77	0.49
2:I:77:VAL:HG12	8:O:107:TYR:OH	2.12	0.49
9:P:118:GLN:HE22	10:Q:82:ASP:HA	1.78	0.49
11:R:29:GLY:HA3	11:R:75:GLY:HA2	1.94	0.49
2:B:65:LEU:HG	9:W:94:GLN:NE2	2.28	0.49
3:J:8:GLY:HA3	3:J:40:LYS:HE2	1.95	0.49
3:J:125:LEU:HD12	3:J:126:ILE:HG23	1.95	0.49
5:L:178:HIS:CE1	5:L:180:ARG:HE	2.30	0.49
9:W:73:LEU:HD11	9:W:133:LEU:HD22	1.95	0.49
10:X:12:PHE:HE1	11:Y:125:ARG:HD2	1.78	0.49
10:X:161:ALA:HB3	11:Y:53:LEU:HD22	1.94	0.49
11:Y:50:VAL:HG12	11:Y:52:LYS:H	1.77	0.49
6:F:133:ASP:OD1	6:F:134:SER:N	2.43	0.48
2:I:198:ARG:NH2	3:J:154:GLU:OE2	2.37	0.48
5:L:7:LYS:HB3	5:L:12:VAL:HG22	1.95	0.48
6:M:35:ILE:O	7:N:151:ARG:NH2	2.45	0.48
9:W:110:VAL:HG21	9:W:146:PHE:HD2	1.78	0.48
8:V:126:TYR:HD1	8:V:132:MET:HG3	1.79	0.48
8:O:22:LEU:HD13	9:P:127:ARG:CZ	2.44	0.48
5:E:164:THR:HG22	5:E:170:SER:HB3	1.94	0.48
7:N:15:LYS:HA	7:N:20:VAL:HG12	1.95	0.48
9:W:44:VAL:HG11	9:W:187:ILE:HA	1.95	0.48
8:O:17:SER:HB3	8:O:23:TYR:CD2	2.48	0.48
9:P:21:ILE:HG21	9:P:151:SER:HB3	1.95	0.48
10:Q:2:SER:OG	10:Q:3:ARG:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:ARG:NH2	2:I:164:PHE:HB3	2.28	0.48
8:O:12:HIS:C	8:O:24:GLN:NE2	2.66	0.48
2:I:75:ARG:HB2	8:O:107:TYR:HE2	1.79	0.48
4:K:19:ARG:O	4:K:32:HIS:N	2.46	0.48
6:M:46:LEU:HB3	6:M:72:LEU:HD11	1.95	0.48
6:M:88:ILE:HG22	6:M:110:ILE:HD13	1.95	0.48
13:T:88:MET:HG2	13:T:108:LEU:HD11	1.94	0.48
4:D:170:ARG:NH2	5:L:140:ASP:OD2	2.41	0.48
7:N:192:VAL:HG22	7:N:197:VAL:HG22	1.96	0.48
10:Q:201:MET:HG2	10:Q:206:LEU:HD21	1.94	0.48
1:A:98:ILE:HB	1:A:114:VAL:HB	1.96	0.48
2:I:68:LEU:HD22	9:P:66:PRO:HG2	1.96	0.48
3:J:72:LEU:O	3:J:76:LYS:N	2.45	0.48
11:Y:158:ALA:HB1	11:Y:172:LEU:HD13	1.96	0.48
9:P:73:LEU:HD13	9:P:135:ILE:HG12	1.94	0.48
4:D:13:VAL:HG22	4:D:183:ILE:HB	1.95	0.48
1:H:14:LEU:HD11	1:H:101:ALA:HB3	1.95	0.48
8:O:14:THR:HG22	8:O:24:GLN:CG	2.43	0.48
9:P:7:PHE:HD2	11:R:5:ARG:HH21	1.60	0.48
2:B:69:SER:O	8:V:117:LYS:NZ	2.47	0.48
5:L:136:TYR:HA	5:L:139:MET:HE2	1.96	0.48
5:E:27:ALA:O	6:F:136:LYS:NZ	2.37	0.47
6:F:27:THR:O	6:F:40:SER:N	2.46	0.47
4:K:104:LEU:HB3	4:K:116:TYR:HB2	1.96	0.47
1:A:7:GLN:HA	1:A:12:VAL:HG12	1.96	0.47
3:C:60:GLN:NE2	4:D:124:LEU:O	2.46	0.47
13:T:34:ALA:HA	13:T:162:GLY:HA3	1.94	0.47
2:I:41:ILE:HG12	2:I:102:GLY:HA3	1.95	0.47
3:C:168:GLN:O	3:C:172:ASN:ND2	2.47	0.47
2:I:16:ALA:HB1	2:I:33:LYS:HB2	1.97	0.47
4:K:38:MET:HB3	4:K:64:VAL:HG11	1.96	0.47
7:N:94:ARG:NH1	13:T:97:PHE:HA	2.29	0.47
6:F:181:SER:HB3	3:J:150:GLU:HB3	1.97	0.47
4:K:45:LEU:HD12	4:K:103:LEU:HD22	1.95	0.47
5:L:20:ALA:HB2	5:L:33:LYS:HZ1	1.80	0.47
7:N:124:TYR:HE1	7:N:139:THR:HG22	1.80	0.47
8:V:183:LYS:HD2	8:V:190:TRP:CD1	2.48	0.47
8:O:16:PHE:CE1	9:P:127:ARG:CG	2.98	0.47
9:P:61:VAL:HG13	9:P:83:ARG:NH2	2.29	0.47
2:B:28:ASP:HB2	3:C:130:MET:HG3	1.96	0.47
5:E:7:LYS:HB3	5:E:12:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:25:SER:HB2	6:M:42:LYS:HB2	1.96	0.47
9:P:49:LYS:HG3	9:P:63:LYS:HE2	1.97	0.47
3:C:8:GLY:HA3	3:C:40:LYS:HE2	1.97	0.47
6:F:185:ARG:HD2	3:J:146:TYR:HB3	1.97	0.47
2:I:187:ARG:CB	2:I:188:PRO:CD	2.80	0.47
8:V:50:VAL:HG21	8:V:196:VAL:HA	1.96	0.47
9:W:13:SER:O	10:X:23:TYR:HB3	2.14	0.47
12:Z:71:ASP:OD1	12:Z:72:ALA:N	2.43	0.47
13:T:26:MET:HG2	13:T:149:PRO:HG2	1.97	0.47
3:C:125:LEU:HD12	3:C:126:ILE:HG23	1.96	0.47
3:J:64:GLN:HE21	10:Q:102:GLN:NE2	2.13	0.47
5:L:61:ARG:HD3	12:S:101:PHE:CE1	2.50	0.47
11:R:10:PHE:CE2	12:S:135:ARG:HB2	2.50	0.47
11:R:63:CYS:HB3	11:R:88:ARG:HH21	1.80	0.47
11:R:180:ALA:O	11:R:187:THR:OG1	2.32	0.47
2:B:164:PHE:HB3	6:M:38:ARG:NH2	2.29	0.47
13:T:192:LEU:HD22	13:T:205:LEU:HD21	1.97	0.47
12:S:71:ASP:OD1	12:S:72:ALA:N	2.43	0.47
2:B:16:ALA:HB1	2:B:33:LYS:HB2	1.97	0.46
4:K:37:LYS:O	4:K:61:GLN:NE2	2.47	0.46
2:B:81:ARG:HG2	2:B:84:LYS:HE2	1.97	0.46
8:V:131:GLU:HG2	9:W:4:GLY:HA2	1.96	0.46
9:W:110:VAL:HG22	9:W:135:ILE:HD12	1.96	0.46
2:B:57:GLN:HE22	9:W:101:GLN:HG2	1.80	0.46
5:L:61:ARG:CZ	12:S:101:PHE:HA	2.45	0.46
8:V:211:PHE:HB3	8:V:215:GLU:HB2	1.96	0.46
8:O:182:LYS:HD2	8:O:189:TRP:CD1	2.49	0.46
13:T:29:VAL:HG11	13:T:131:GLY:H	1.81	0.46
9:W:21:ILE:HD13	9:W:151:SER:HA	1.97	0.46
10:Q:12:PHE:HZ	11:R:125:ARG:HH11	1.64	0.46
12:S:41:GLN:N	12:S:166:ASP:O	2.48	0.46
2:B:122:LEU:HD12	2:B:125:VAL:HG12	1.97	0.46
7:N:134:ALA:HB3	7:N:137:LEU:HD21	1.97	0.46
10:Q:140:ASP:OD1	10:Q:144:GLY:N	2.49	0.46
11:R:40:ILE:HD11	11:R:210:VAL:HB	1.96	0.46
13:T:155:ASP:HB3	14:U:62:SER:HB2	1.97	0.46
7:G:27:LEU:HD22	7:G:184:TYR:HB2	1.97	0.46
7:G:46:ASN:OD1	7:G:49:THR:N	2.48	0.46
2:I:170:GLY:O	2:I:171:SER:OG	2.30	0.46
3:C:83:PRO:HG2	3:C:119:PHE:HB2	1.97	0.46
4:K:47:VAL:O	4:K:101:ASN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:4:PRO:O	7:N:100:ARG:NH1	2.49	0.46
9:W:178:ASN:HB2	9:W:181:LEU:HG	1.97	0.46
12:S:16:SER:OG	12:S:20:ARG:N	2.42	0.46
13:T:105:VAL:HG11	13:T:136:GLY:HA3	1.98	0.46
14:U:185:THR:O	14:U:189:ILE:HG12	2.16	0.46
14:U:229:LYS:HA	14:U:232:ARG:HB3	1.96	0.46
4:D:43:LEU:HD11	4:D:188:ILE:HG12	1.97	0.46
5:E:61:ARG:NH2	12:Z:101:PHE:HA	2.30	0.46
6:F:13:LEU:HD11	6:F:149:LEU:HD11	1.97	0.46
4:K:71:ASN:HB3	4:K:73:TYR:CE2	2.50	0.46
13:T:96:ARG:HA	13:T:100:ASP:HA	1.98	0.46
4:D:9:GLY:HA3	4:D:12:TYR:CE2	2.51	0.46
2:I:75:ARG:HD2	8:O:107:TYR:CE2	2.51	0.46
2:I:81:ARG:HA	2:I:84:LYS:HE2	1.97	0.46
5:L:4:LEU:N	5:L:15:ALA:O	2.46	0.46
6:M:36:HIS:HB3	7:N:132:TYR:CE2	2.51	0.46
6:M:38:ARG:HB3	6:M:191:ASP:OD2	2.16	0.46
9:W:121:THR:HG22	9:W:128:PRO:HB3	1.97	0.46
11:Y:116:GLN:HE22	12:Z:86:LYS:HB2	1.81	0.46
11:Y:127:PHE:HB3	11:Y:129:ILE:HG12	1.97	0.46
8:O:23:TYR:C	8:O:25:VAL:H	2.19	0.46
12:S:31:ILE:HD13	12:S:140:ALA:HB2	1.97	0.46
11:R:4:ASP:O	11:R:5:ARG:NH1	2.43	0.45
14:U:235:ALA:O	14:U:239:ALA:N	2.49	0.45
3:C:104:THR:HG23	3:C:106:PRO:HD3	1.97	0.45
7:G:25:ASP:HB3	7:G:184:TYR:HB3	1.97	0.45
11:Y:119:THR:HG22	11:Y:126:PRO:HB3	1.98	0.45
8:O:49:VAL:HG21	8:O:195:VAL:HA	1.97	0.45
12:S:77:ALA:HB3	12:S:142:LEU:HB2	1.98	0.45
13:T:9:ASP:OD1	13:T:10:VAL:N	2.49	0.45
3:C:105:GLU:HB3	3:C:138:SER:HB3	1.97	0.45
5:L:177:TYR:HD1	5:L:186:ARG:HA	1.81	0.45
11:R:66:ASP:HB2	11:R:95:ARG:NH2	2.31	0.45
14:U:65:ARG:HH21	14:U:78:ALA:HA	1.81	0.45
7:N:135:PRO:HB2	7:N:154:LEU:HD13	1.99	0.45
9:W:15:SER:HB2	9:W:17:LYS:HE3	1.98	0.45
9:W:46:ALA:HB1	9:W:207:ILE:HD11	1.99	0.45
10:X:104:PRO:HD2	10:X:141:LYS:HE3	1.98	0.45
8:O:23:TYR:C	8:O:25:VAL:N	2.69	0.45
14:U:46:VAL:HA	14:U:215:TRP:HB3	1.98	0.45
2:B:81:ARG:NH1	8:V:107:GLY:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:28:GLY:N	7:G:36:PHE:O	2.50	0.45
12:S:146:VAL:HG22	12:S:151:PRO:HB3	1.98	0.45
14:U:72:HIS:NE2	14:U:106:ILE:O	2.39	0.45
6:F:176:LYS:HE3	6:F:208:VAL:HG21	1.99	0.45
3:J:104:THR:HG23	3:J:106:PRO:HD3	1.99	0.45
5:L:81:LYS:NZ	11:R:96:LEU:O	2.34	0.45
9:W:18:LEU:H	9:W:18:LEU:HD12	1.81	0.45
12:Z:15:PHE:HB3	12:Z:19:GLY:CA	2.44	0.45
2:B:164:PHE:HB3	6:M:38:ARG:HH22	1.82	0.45
11:Y:47:LYS:HE3	11:Y:207:GLU:HB2	1.99	0.45
8:O:19:GLU:OE1	8:O:19:GLU:HA	2.17	0.45
12:S:110:GLU:HA	12:S:154:PHE:HE2	1.82	0.45
1:A:14:LEU:HD11	1:A:101:ALA:HB3	1.99	0.45
1:H:17:ASP:OD1	1:H:33:LYS:NZ	2.48	0.45
4:D:23:SER:OG	4:D:27:GLN:HA	2.17	0.45
1:H:4:MET:HG3	1:H:127:ILE:HG22	1.98	0.45
12:Z:157:ASP:HB3	12:Z:161:THR:H	1.82	0.45
10:Q:166:ASN:OD1	10:Q:167:ASN:N	2.50	0.45
4:D:4:LEU:HD22	4:D:45:LEU:HD13	1.99	0.45
5:E:70:ASN:HA	11:Y:109:ARG:HH12	1.82	0.45
8:V:145:ASP:OD1	8:V:146:GLU:N	2.50	0.45
10:X:61:PHE:HE2	10:X:227:VAL:HG23	1.72	0.45
1:A:1:THR:HG23	1:A:33:LYS:HZ3	1.83	0.44
1:A:6:VAL:HG23	1:A:125:PHE:HB3	2.00	0.44
2:B:187:ARG:CB	2:B:188:PRO:HD3	2.27	0.44
3:J:42:PHE:HB3	3:J:43:PRO:HD2	1.98	0.44
3:J:105:GLU:OE1	3:J:139:GLY:N	2.42	0.44
5:L:50:ALA:HB2	6:M:129:SER:HB3	1.99	0.44
7:N:85:PRO:HG2	7:N:121:PHE:HD2	1.81	0.44
2:B:94:ILE:HG22	2:B:96:ALA:H	1.82	0.44
3:C:152:LEU:HG	3:C:165:THR:HG23	1.99	0.44
6:F:16:ALA:HB2	6:F:121:VAL:HG23	2.00	0.44
9:P:151:SER:O	10:Q:81:SER:OG	2.22	0.44
10:Q:72:MET:HB2	10:Q:137:ILE:O	2.17	0.44
14:U:94:GLU:HA	14:U:97:ASN:HB2	1.98	0.44
2:B:114:TYR:HD2	2:B:118:SER:HB3	1.82	0.44
4:D:48:GLY:HA3	4:D:100:VAL:HA	1.99	0.44
2:I:75:ARG:HH22	2:I:105:VAL:HB	1.83	0.44
11:Y:146:GLN:OE1	11:Y:159:ASN:ND2	2.50	0.44
10:Q:148:TYR:HD1	10:Q:158:GLY:HA2	1.83	0.44
2:B:214:GLU:HG3	3:C:197:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:ASP:HB2	3:C:161:HIS:CD2	2.51	0.44
4:D:6:GLY:HA2	4:D:15:VAL:HA	1.99	0.44
1:H:77:HIS:CE1	14:U:104:TYR:HE1	2.35	0.44
2:I:114:TYR:HD2	2:I:118:SER:HB3	1.81	0.44
4:K:13:VAL:HG22	4:K:183:ILE:HB	2.00	0.44
10:Q:135:LEU:HG	10:Q:164:ILE:HD13	1.99	0.44
11:R:76:LEU:HD21	11:R:78:ALA:HB3	1.99	0.44
1:A:77:HIS:HB3	1:A:112:TYR:CE2	2.52	0.44
8:V:128:GLN:HA	9:W:127:ARG:HG2	2.00	0.44
1:A:7:GLN:HB2	1:A:111:VAL:HG23	2.00	0.44
2:B:44:CYS:HB2	2:B:99:VAL:HB	1.98	0.44
2:B:140:ASP:OD2	7:N:171:ARG:HD3	2.17	0.44
4:D:38:MET:HG2	4:D:61:GLN:HG2	2.00	0.44
11:Y:45:VAL:HG21	11:Y:61:LYS:HB2	1.99	0.44
8:O:144:ASP:OD1	8:O:145:GLU:N	2.50	0.44
10:Q:2:SER:HA	13:T:123:TYR:CE2	2.52	0.44
14:U:75:MET:HE2	14:U:137:LEU:HD21	1.99	0.44
3:C:52:LEU:HD13	3:C:59:VAL:HA	2.00	0.44
6:F:35:ILE:HB	7:G:151:ARG:HH12	1.83	0.44
10:X:218:ARG:HA	10:X:223:THR:HA	2.00	0.44
9:P:183:LEU:HD21	9:P:211:ILE:HD12	2.00	0.44
3:C:69:ARG:NH2	3:C:92:ASN:HD22	2.13	0.44
3:J:85:THR:OG1	9:P:102:GLU:OE2	2.27	0.44
8:O:13:ILE:N	8:O:24:GLN:HE21	2.15	0.44
8:O:18:PRO:HA	9:P:23:TYR:CD1	2.53	0.44
10:Q:45:LEU:HD23	10:Q:137:ILE:HD13	1.99	0.44
5:E:76:VAL:HG13	5:E:101:ILE:HG22	2.00	0.44
3:J:73:TYR:OH	3:J:79:ARG:NE	2.47	0.44
12:Z:41:GLN:N	12:Z:166:ASP:O	2.49	0.44
9:P:38:LYS:HA	9:P:43:VAL:HG22	2.00	0.44
11:R:50:VAL:HG13	11:R:54:GLN:HB3	1.99	0.44
13:T:67:ASP:OD1	13:T:68:ASN:N	2.47	0.44
14:U:21:PHE:HB3	14:U:25:TYR:CE2	2.53	0.44
5:L:62:GLN:HA	5:L:65:ILE:HD12	2.00	0.43
6:M:125:ASP:OD1	6:M:129:SER:N	2.32	0.43
8:O:17:SER:N	8:O:20:GLY:HA2	2.33	0.43
9:P:45:LEU:HD12	9:P:217:PHE:HE1	1.83	0.43
4:D:172:ILE:HG12	4:K:27:GLN:HB3	2.00	0.43
6:F:18:GLU:O	6:F:118:LYS:HA	2.18	0.43
9:W:120:TYR:HD1	9:W:126:VAL:HG21	1.83	0.43
12:Z:110:GLU:HA	12:Z:154:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:146:VAL:HG22	12:Z:151:PRO:HB3	2.00	0.43
8:O:161:CYS:SG	9:P:61:VAL:HG21	2.58	0.43
9:P:45:LEU:HD21	9:P:136:CYS:SG	2.58	0.43
3:J:105:GLU:HB3	3:J:138:SER:HB3	1.99	0.43
5:L:1:THR:N	5:L:169:TYR:O	2.51	0.43
8:O:157:ALA:O	9:P:80:PRO:HG3	2.17	0.43
11:R:83:VAL:HG21	11:R:129:ILE:HD11	2.00	0.43
13:T:37:GLY:HA2	13:T:46:LEU:HA	2.00	0.43
13:T:92:CYS:O	13:T:95:SER:OG	2.27	0.43
4:D:65:GLN:HB2	11:Y:92:GLN:HE21	1.84	0.43
6:F:124:PHE:CE1	6:F:130:TYR:HA	2.53	0.43
1:H:7:GLN:HB2	1:H:111:VAL:HG23	1.99	0.43
1:H:65:PHE:CE1	8:O:95:ARG:HB3	2.54	0.43
8:V:68:THR:HG22	8:V:69:HIS:N	2.32	0.43
11:Y:10:PHE:CE2	12:Z:135:ARG:HB2	2.53	0.43
12:Z:77:ALA:HB3	12:Z:142:LEU:HB2	1.99	0.43
8:O:123:GLN:HE22	9:P:81:ASP:HA	1.83	0.43
3:C:69:ARG:HH21	9:W:99:VAL:HG13	1.83	0.43
7:G:126:ASP:OD1	7:G:127:MET:N	2.42	0.43
3:J:14:LYS:HE3	3:J:120:ILE:HG12	2.00	0.43
5:L:113:TYR:CE2	5:L:115:ASP:HB2	2.54	0.43
9:W:203:THR:H	9:W:206:ASN:HB2	1.84	0.43
10:X:97:TYR:HB2	10:X:105:ILE:HD12	1.99	0.43
11:Y:76:LEU:HD21	11:Y:78:ALA:HB3	2.01	0.43
8:O:141:ILE:HD12	8:O:220:VAL:HG22	2.00	0.43
9:P:107:ALA:HA	9:P:146:PHE:HE2	1.84	0.43
10:Q:104:PRO:HD2	10:Q:141:LYS:HE3	1.99	0.43
11:R:155:ALA:HB3	12:S:60:GLU:HB3	2.01	0.43
7:G:166:ARG:NH1	7:G:200:GLU:OE2	2.51	0.43
7:G:171:ARG:HD3	2:I:140:ASP:OD2	2.19	0.43
1:H:61:TYR:HA	8:O:103:TYR:CE2	2.53	0.43
8:V:151:GLN:NE2	8:V:153:TYR:OH	2.52	0.43
12:Z:110:GLU:HA	12:Z:154:PHE:CE2	2.54	0.43
13:T:80:ASP:HA	13:T:83:LEU:HB3	2.00	0.43
4:K:9:GLY:HA3	4:K:12:TYR:CZ	2.54	0.43
10:Q:12:PHE:CE2	11:R:125:ARG:HB2	2.53	0.43
1:A:190:LEU:H	1:A:193:GLN:HB2	1.84	0.43
6:F:37:THR:HB	7:G:132:TYR:CD1	2.54	0.43
9:W:22:GLU:OE1	9:W:22:GLU:HA	2.19	0.43
11:R:188:ILE:HG23	11:R:208:LEU:HD21	2.00	0.43
7:G:25:ASP:OD1	7:G:187:PHE:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:50:ALA:O	5:L:91:LYS:NZ	2.48	0.43
8:O:51:VAL:HG12	8:O:202:LEU:HD12	2.00	0.43
9:P:7:PHE:O	9:P:124:GLY:HA3	2.18	0.43
9:P:121:THR:HG22	9:P:128:PRO:HB3	2.00	0.43
6:M:125:ASP:OD1	6:M:128:GLY:N	2.52	0.42
9:W:70:HIS:CD2	9:W:71:ILE:HG13	2.53	0.42
8:O:187:PHE:O	8:O:190:THR:OG1	2.28	0.42
1:H:77:HIS:HB3	1:H:112:TYR:CE2	2.54	0.42
3:J:83:PRO:HG2	3:J:119:PHE:HB2	2.01	0.42
11:R:104:VAL:HG21	11:R:143:ARG:HB2	2.00	0.42
11:R:121:SER:HA	12:S:132:ALA:O	2.19	0.42
2:B:21:THR:HG22	2:B:26:VAL:HA	2.01	0.42
4:D:38:MET:HB3	4:D:64:VAL:HG11	2.01	0.42
7:G:35:ARG:HG2	7:G:36:PHE:CD1	2.55	0.42
12:Z:16:SER:HB2	12:Z:17:PRO:CD	2.44	0.42
8:O:16:PHE:N	8:O:16:PHE:HD1	2.18	0.42
9:P:85:LEU:HD13	9:P:133:LEU:HD11	2.00	0.42
9:P:178:ASN:HB2	9:P:181:LEU:HG	2.01	0.42
12:S:54:ILE:HD11	12:S:61:PRO:HB3	2.01	0.42
14:U:35:THR:HG22	14:U:166:GLY:HA3	2.02	0.42
2:B:7:VAL:HG13	2:B:108:PRO:HB2	2.01	0.42
5:E:177:TYR:CD1	5:E:186:ARG:HA	2.55	0.42
3:J:100:GLY:O	4:K:93:ARG:NH1	2.52	0.42
4:K:13:VAL:O	4:K:15:VAL:HG13	2.19	0.42
13:T:82:ARG:HA	13:T:85:CYS:HB3	2.01	0.42
3:C:204:ASP:HB2	5:L:171:GLY:HA2	2.01	0.42
4:D:162:LYS:HB3	5:L:141:ARG:NH1	2.34	0.42
5:E:141:ARG:NH2	4:K:162:LYS:O	2.48	0.42
7:G:186:ARG:HH12	1:H:199:VAL:HG21	1.84	0.42
7:G:210:ASP:HB3	1:H:190:LEU:HD22	2.01	0.42
3:J:52:LEU:HB2	3:J:59:VAL:HG13	2.02	0.42
5:L:87:VAL:HG21	5:L:116:SER:HA	2.02	0.42
8:O:125:TYR:HD1	8:O:131:MET:HG3	1.84	0.42
13:T:45:VAL:HG22	13:T:214:ILE:HG12	2.01	0.42
5:E:3:THR:OG1	5:E:128:VAL:HB	2.20	0.42
6:F:55:SER:O	6:F:107:TYR:N	2.43	0.42
2:I:81:ARG:HG2	2:I:84:LYS:HE2	2.01	0.42
9:W:146:PHE:CZ	10:X:59:VAL:HG21	2.55	0.42
10:X:166:ASN:OD1	10:X:167:ASN:N	2.53	0.42
11:R:42:VAL:HG22	11:R:210:VAL:HG12	2.00	0.42
12:S:182:GLN:HA	13:T:56:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:156:CYS:HG	14:U:58:TYR:HD1	1.67	0.42
2:B:177:VAL:HB	2:B:184:ASP:HB3	2.02	0.42
5:E:81:LYS:NZ	11:Y:96:LEU:O	2.36	0.42
8:V:59:ASP:HB3	8:V:62:LEU:HG	2.01	0.42
7:N:122:LEU:HG	7:N:137:LEU:HD12	2.02	0.42
8:O:17:SER:HB2	8:O:18:PRO:HD2	2.02	0.42
1:H:63:LEU:HD23	1:H:66:HIS:ND1	2.34	0.42
8:O:165:ALA:O	9:P:55:LEU:HD23	2.20	0.42
12:S:117:SER:O	13:T:82:ARG:NH2	2.42	0.42
14:U:67:PHE:O	14:U:75:MET:N	2.48	0.42
4:K:23:SER:OG	4:K:27:GLN:HA	2.20	0.42
4:K:70:ARG:HA	11:R:88:ARG:NH1	2.34	0.42
9:W:51:GLN:HB3	9:W:56:TYR:HD2	1.84	0.42
11:Y:116:GLN:HE22	12:Z:86:LYS:HD2	1.85	0.42
14:U:70:ASP:OD1	14:U:71:ARG:N	2.46	0.42
1:A:77:HIS:HB3	1:A:112:TYR:CD2	2.54	0.41
8:O:150:GLN:NE2	8:O:152:TYR:OH	2.53	0.41
10:Q:115:CYS:O	10:Q:119:GLN:HG3	2.20	0.41
12:S:24:VAL:HG11	12:S:159:SER:HB3	2.01	0.41
2:I:94:ILE:HG22	2:I:96:ALA:H	1.84	0.41
4:K:4:LEU:HD22	4:K:45:LEU:HD13	2.03	0.41
4:K:33:ASP:OD1	4:K:35:MET:HB3	2.20	0.41
9:W:107:ALA:HA	9:W:146:PHE:HE2	1.85	0.41
10:X:119:GLN:HE22	11:Y:79:ASP:CA	2.31	0.41
7:G:210:ASP:OD1	7:G:211:ILE:N	2.53	0.41
2:I:137:VAL:HG21	2:I:158:ALA:HA	2.03	0.41
7:N:4:PRO:HB3	7:N:56:ASP:HB2	2.02	0.41
11:Y:121:SER:HA	12:Z:132:ALA:O	2.20	0.41
12:Z:16:SER:HB3	12:Z:22:PHE:CZ	2.48	0.41
8:O:17:SER:OG	8:O:20:GLY:N	2.53	0.41
14:U:54:LEU:HB3	14:U:58:TYR:HE2	1.85	0.41
2:B:170:GLY:O	2:B:171:SER:OG	2.30	0.41
3:C:27:PHE:HD2	3:C:34:VAL:HB	1.85	0.41
4:D:104:LEU:HB3	4:D:116:TYR:HB2	2.02	0.41
7:N:126:ASP:OD1	7:N:127:MET:N	2.43	0.41
11:Y:104:VAL:HG13	11:Y:133:ILE:HG22	2.01	0.41
14:U:118:TYR:HH	14:U:122:TYR:HH	1.61	0.41
2:I:11:GLY:HA2	2:I:103:VAL:HG21	2.01	0.41
3:J:47:ARG:HD3	3:J:111:LEU:HD12	2.02	0.41
3:J:90:VAL:HG21	3:J:108:ILE:HD11	2.01	0.41
3:J:112:ASP:HB3	3:J:117:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:46:ASN:OD1	7:N:49:THR:N	2.54	0.41
7:N:72:ILE:O	7:N:76:LEU:HB2	2.20	0.41
9:W:73:LEU:HD13	9:W:135:ILE:HG12	2.01	0.41
8:O:165:ALA:HB1	8:O:179:LEU:HD22	2.03	0.41
1:A:59:VAL:HG21	1:A:83:PHE:CE1	2.56	0.41
1:H:77:HIS:HB3	1:H:112:TYR:CD2	2.56	0.41
9:W:7:PHE:O	9:W:124:GLY:HA3	2.21	0.41
11:Y:180:ALA:O	11:Y:187:THR:OG1	2.27	0.41
9:P:183:LEU:HD11	9:P:211:ILE:HB	2.03	0.41
11:R:36:ARG:HG3	11:R:142:PRO:HB2	2.03	0.41
13:T:146:GLN:OE1	13:T:159:MET:HG2	2.21	0.41
2:I:42:TYR:CD2	2:I:178:ILE:HD11	2.56	0.41
5:L:45:MET:HG3	5:L:52:CYS:HB2	2.01	0.41
7:N:89:HIS:NE2	7:N:124:TYR:O	2.51	0.41
8:V:142:ILE:HD12	8:V:221:VAL:HG22	2.03	0.41
12:Z:14:THR:O	12:Z:21:LEU:HA	2.20	0.41
11:R:63:CYS:HB3	11:R:88:ARG:NH2	2.36	0.41
12:S:129:ASP:OD1	12:S:130:PRO:HD2	2.21	0.41
13:T:13:TRP:NE1	14:U:129:ARG:HB2	2.35	0.41
5:E:191:ASN:HD21	3:J:202:ARG:HH12	1.69	0.41
7:G:33:LEU:HD12	1:H:166:ARG:O	2.21	0.41
4:K:48:GLY:HA3	4:K:100:VAL:HA	2.02	0.41
5:L:40:TYR:HE1	5:L:74:ILE:HG22	1.85	0.41
7:N:35:ARG:HG2	7:N:36:PHE:CD1	2.55	0.41
10:X:122:THR:HG22	10:X:129:PRO:HB3	2.03	0.41
13:T:176:MET:HA	13:T:179:PHE:CD2	2.55	0.41
3:C:31:ALA:O	3:C:32:GLN:HB2	2.21	0.41
4:K:14:LEU:HD12	4:K:181:ARG:O	2.20	0.41
4:K:103:LEU:HB2	4:K:132:HIS:NE2	2.36	0.41
5:L:20:ALA:HB2	5:L:33:LYS:NZ	2.36	0.41
6:M:7:PHE:HZ	6:M:140:SER:HB3	1.85	0.41
9:W:35:VAL:HG11	9:W:193:THR:HG21	2.02	0.41
9:W:41:ASN:HD21	9:W:183:LEU:H	1.68	0.41
9:W:129:PHE:O	9:W:150:PRO:HB3	2.21	0.41
10:X:86:LEU:HD21	10:X:130:PHE:CD2	2.56	0.41
9:P:120:TYR:HD1	9:P:126:VAL:HG21	1.86	0.41
10:Q:86:LEU:HD21	10:Q:130:PHE:CD2	2.55	0.41
13:T:69:HIS:CD2	13:T:70:ILE:HG13	2.56	0.41
14:U:51:LYS:NZ	14:U:212:GLU:OE2	2.47	0.41
3:C:105:GLU:OE1	3:C:139:GLY:N	2.40	0.41
7:G:29:SER:HA	7:G:33:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:30:TYR:O	7:G:33:LEU:HB3	2.21	0.41
7:G:138:ALA:HB3	7:G:147:GLN:HG3	2.03	0.41
11:Y:120:GLN:O	12:Z:134:SER:OG	2.27	0.41
8:O:16:PHE:HZ	9:P:127:ARG:CD	2.29	0.41
8:O:19:GLU:CD	8:O:19:GLU:N	2.72	0.41
10:Q:3:ARG:NH2	13:T:9:ASP:HB2	2.33	0.41
10:Q:90:LEU:HD21	10:Q:114:LEU:HD22	2.03	0.41
3:C:52:LEU:HB2	3:C:59:VAL:HG13	2.03	0.40
7:G:8:GLY:HA3	7:G:41:ARG:HH12	1.86	0.40
1:H:104:ASP:OD1	1:H:108:GLY:N	2.54	0.40
2:I:1:THR:HG21	2:I:46:ALA:HA	2.03	0.40
2:I:7:VAL:HG13	2:I:108:PRO:HB2	2.02	0.40
5:L:71:LYS:NZ	12:S:65:GLU:OE1	2.36	0.40
8:O:88:ARG:HA	8:O:91:VAL:HG23	2.03	0.40
8:O:132:ARG:NH1	14:U:14:PHE:CZ	2.69	0.40
10:Q:118:LYS:NZ	10:Q:150:SER:OG	2.46	0.40
11:R:50:VAL:HG12	11:R:52:LYS:H	1.85	0.40
1:H:66:HIS:CE1	14:U:102:PHE:HZ	2.40	0.40
3:J:27:PHE:HD2	3:J:34:VAL:HB	1.86	0.40
7:N:25:ASP:OD1	7:N:187:PHE:HB3	2.21	0.40
9:W:43:VAL:HG11	9:W:136:CYS:SG	2.62	0.40
10:X:60:PHE:O	10:X:60:PHE:CG	2.74	0.40
12:S:85:ALA:HB2	12:S:139:VAL:HG21	2.03	0.40
14:U:108:LEU:HG	14:U:149:TYR:CD2	2.55	0.40
9:W:183:LEU:HD21	9:W:211:ILE:HD12	2.03	0.40
11:Y:94:HIS:HB2	11:Y:102:VAL:HG12	2.04	0.40
10:Q:3:ARG:HG3	10:Q:4:ARG:N	2.36	0.40
12:S:34:GLY:O	12:S:53:ARG:NH1	2.54	0.40
12:S:99:HIS:HE1	12:S:105:GLU:HB2	1.86	0.40
14:U:173:LYS:HA	14:U:176:ILE:HB	2.02	0.40
3:C:57:THR:HG23	3:C:58:ASP:H	1.87	0.40
1:H:133:SER:HA	1:H:136:TYR:CE2	2.56	0.40
11:Y:17:PHE:HB3	11:Y:21:TYR:CE2	2.57	0.40
9:P:164:LYS:NZ	9:P:199:GLU:OE2	2.36	0.40
14:U:164:ALA:HB2	14:U:176:ILE:HD12	2.03	0.40
5:E:113:TYR:O	5:E:120:ARG:HA	2.21	0.40
6:F:11:THR:HG21	6:F:141:ALA:HB3	2.02	0.40
6:F:71:ARG:HD2	6:F:95:ILE:HD11	2.04	0.40
8:O:153:LYS:HD3	8:O:163:PHE:HE2	1.86	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	200/205 (98%)	195 (98%)	5 (2%)	0	100	100
1	H	200/205 (98%)	194 (97%)	6 (3%)	0	100	100
2	B	218/234 (93%)	200 (92%)	18 (8%)	0	100	100
2	I	218/234 (93%)	200 (92%)	18 (8%)	0	100	100
3	C	202/205 (98%)	186 (92%)	16 (8%)	0	100	100
3	J	202/205 (98%)	187 (93%)	15 (7%)	0	100	100
4	D	194/201 (96%)	184 (95%)	10 (5%)	0	100	100
4	K	194/201 (96%)	185 (95%)	9 (5%)	0	100	100
5	E	198/204 (97%)	185 (93%)	13 (7%)	0	100	100
5	L	198/204 (97%)	184 (93%)	14 (7%)	0	100	100
6	F	210/213 (99%)	197 (94%)	12 (6%)	1 (0%)	29	68
6	M	210/213 (99%)	195 (93%)	15 (7%)	0	100	100
7	G	210/219 (96%)	203 (97%)	7 (3%)	0	100	100
7	N	210/219 (96%)	203 (97%)	7 (3%)	0	100	100
8	O	236/246 (96%)	217 (92%)	18 (8%)	1 (0%)	34	72
8	V	236/246 (96%)	219 (93%)	17 (7%)	0	100	100
9	P	226/234 (97%)	218 (96%)	8 (4%)	0	100	100
9	W	226/234 (97%)	218 (96%)	8 (4%)	0	100	100
10	Q	246/261 (94%)	227 (92%)	18 (7%)	1 (0%)	34	72
10	X	245/261 (94%)	229 (94%)	15 (6%)	1 (0%)	34	72
11	R	230/248 (93%)	216 (94%)	13 (6%)	1 (0%)	34	72
11	Y	230/248 (93%)	218 (95%)	11 (5%)	1 (0%)	34	72
12	S	231/241 (96%)	219 (95%)	12 (5%)	0	100	100
12	Z	231/241 (96%)	219 (95%)	10 (4%)	2 (1%)	17	56
13	T	231/263 (88%)	219 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/263 (88%)	218 (94%)	13 (6%)	0	100	100
14	U	237/255 (93%)	222 (94%)	15 (6%)	0	100	100
14	b	237/255 (93%)	223 (94%)	14 (6%)	0	100	100
All	All	6137/6458 (95%)	5780 (94%)	349 (6%)	8 (0%)	54	85

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	Y	216	SER
12	Z	21	LEU
12	Z	22	PHE
11	R	216	SER
10	Q	61	PHE
10	X	61	PHE
8	O	24	GLN
6	F	106	VAL

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	157/159 (99%)	157 (100%)	0	100	100
1	H	157/159 (99%)	157 (100%)	0	100	100
2	B	181/195 (93%)	181 (100%)	0	100	100
2	I	181/195 (93%)	181 (100%)	0	100	100
3	C	173/174 (99%)	173 (100%)	0	100	100
3	J	173/174 (99%)	173 (100%)	0	100	100
4	D	167/171 (98%)	167 (100%)	0	100	100
4	K	167/171 (98%)	167 (100%)	0	100	100
5	E	156/159 (98%)	156 (100%)	0	100	100
5	L	156/159 (98%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	177/178 (99%)	177 (100%)	0	100 100
6	M	177/178 (99%)	177 (100%)	0	100 100
7	G	175/181 (97%)	175 (100%)	0	100 100
7	N	175/181 (97%)	175 (100%)	0	100 100
8	O	204/210 (97%)	203 (100%)	1 (0%)	88 93
8	V	204/210 (97%)	204 (100%)	0	100 100
9	P	187/191 (98%)	187 (100%)	0	100 100
9	W	187/191 (98%)	185 (99%)	2 (1%)	73 85
10	Q	208/221 (94%)	208 (100%)	0	100 100
10	X	207/221 (94%)	207 (100%)	0	100 100
11	R	196/211 (93%)	196 (100%)	0	100 100
11	Y	196/211 (93%)	196 (100%)	0	100 100
12	S	195/203 (96%)	195 (100%)	0	100 100
12	Z	195/203 (96%)	195 (100%)	0	100 100
13	T	199/224 (89%)	199 (100%)	0	100 100
13	a	199/224 (89%)	199 (100%)	0	100 100
14	U	197/212 (93%)	196 (100%)	1 (0%)	88 93
14	b	197/212 (93%)	197 (100%)	0	100 100
All	All	5143/5378 (96%)	5139 (100%)	4 (0%)	93 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	W	19	VAL
9	W	20	GLN
8	O	16	PHE
14	U	13	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	77	HIS
1	A	106	GLN
2	B	66	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	64	GLN
3	C	92	ASN
3	C	161	HIS
3	C	172	ASN
4	D	8	GLN
4	D	61	GLN
6	F	79	ASN
1	H	7	GLN
1	H	77	HIS
1	H	106	GLN
2	I	193	ASN
3	J	64	GLN
3	J	92	ASN
3	J	161	HIS
3	J	172	ASN
4	K	8	GLN
7	N	147	GLN
8	V	91	GLN
8	V	151	GLN
8	V	239	HIS
9	W	51	GLN
9	W	94	GLN
9	W	118	GLN
9	W	206	ASN
10	X	119	GLN
11	Y	116	GLN
11	Y	205	ASN
12	Z	114	GLN
13	a	21	GLN
8	O	12	HIS
8	O	24	GLN
8	O	90	GLN
8	O	150	GLN
9	P	94	GLN
9	P	118	GLN
9	P	206	ASN
11	R	54	GLN
11	R	116	GLN
12	S	98	ASN
12	S	99	HIS
14	U	22	GLN
14	U	143	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

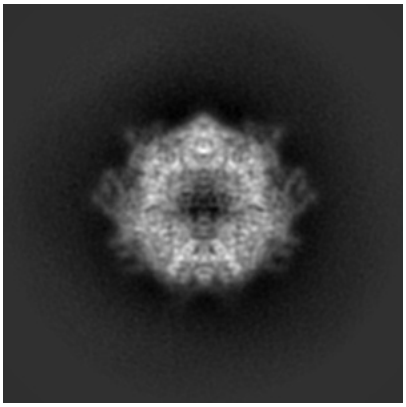
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31724. These allow visual inspection of the internal detail of the map and identification of artifacts.

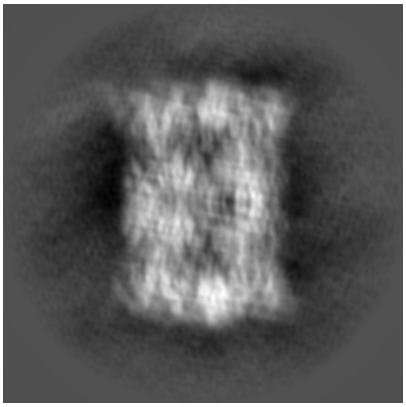
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

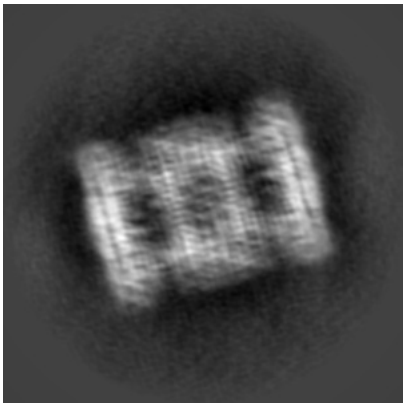
6.1.1 Primary map



X



Y

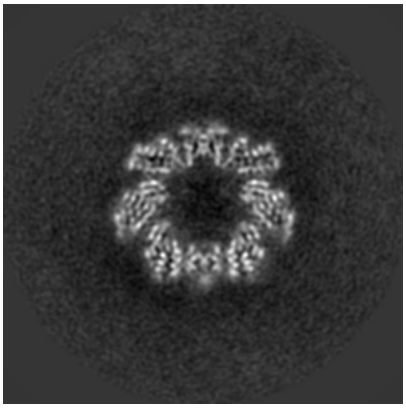


Z

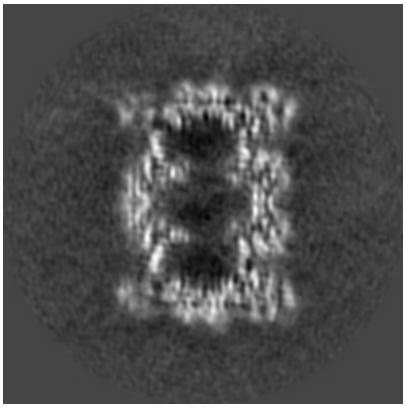
The images above show the map projected in three orthogonal directions.

6.2 Central slices

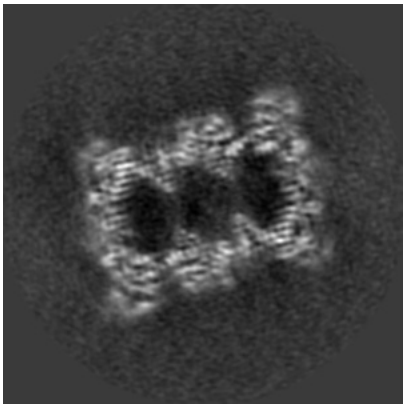
6.2.1 Primary map



X Index: 100



Y Index: 100

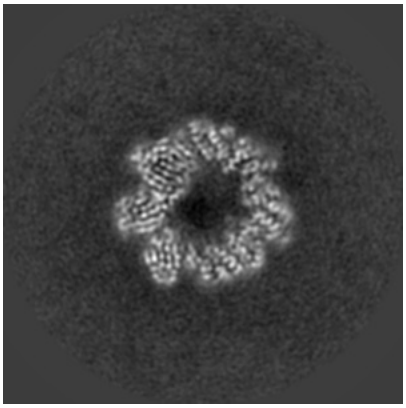


Z Index: 100

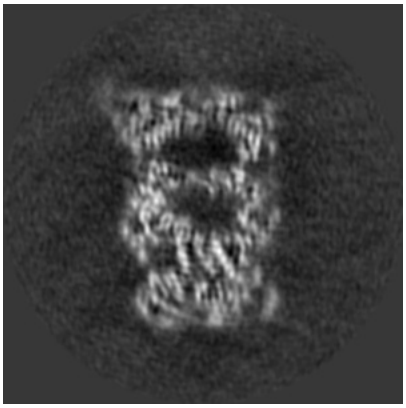
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

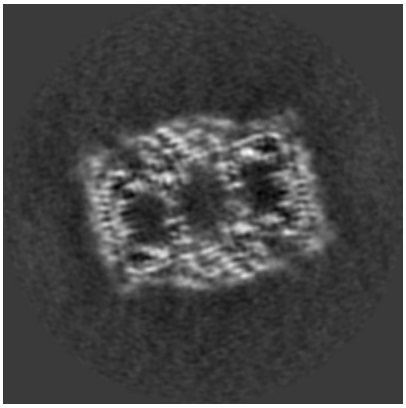
6.3.1 Primary map



X Index: 94



Y Index: 114

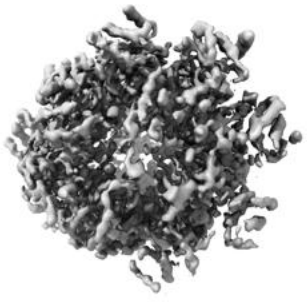


Z Index: 87

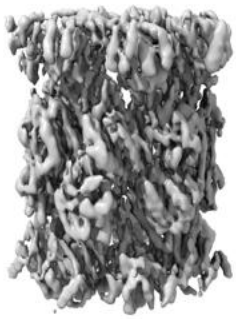
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

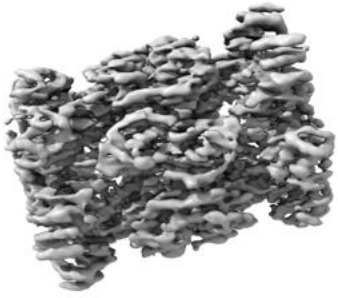
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

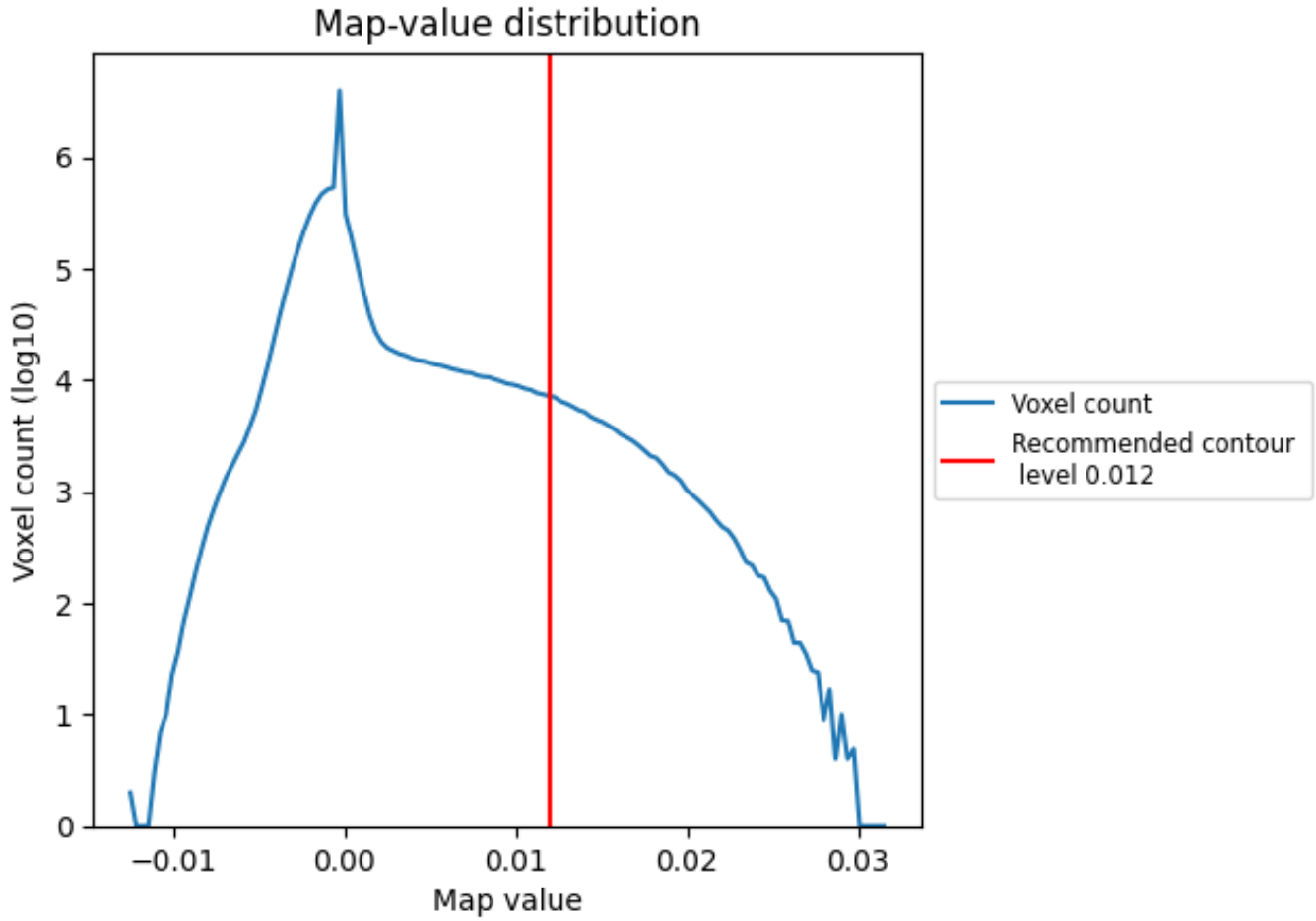
6.5 Mask visualisation (i)

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

7 Map analysis

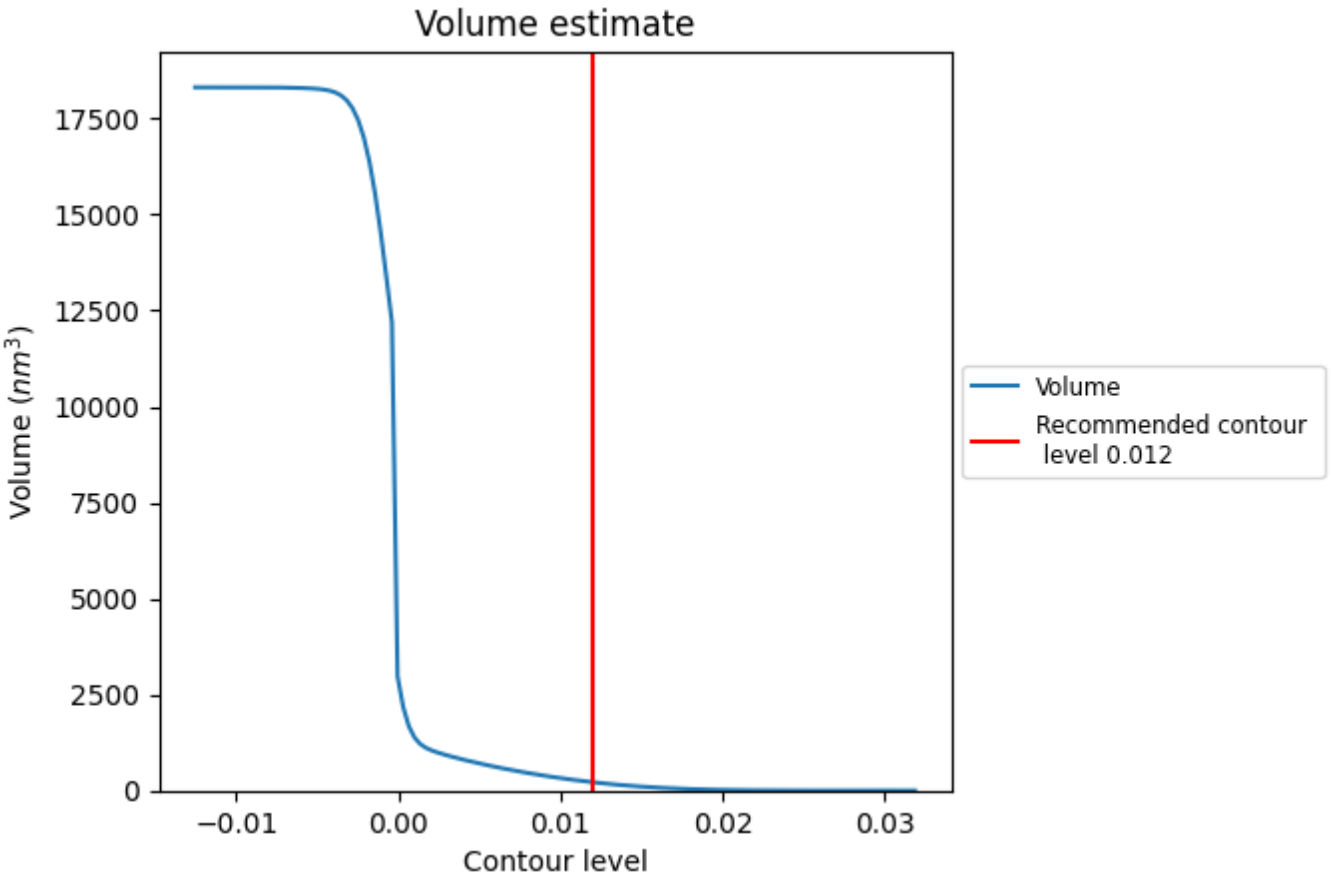
This section contains the results of statistical analysis of the map.

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.

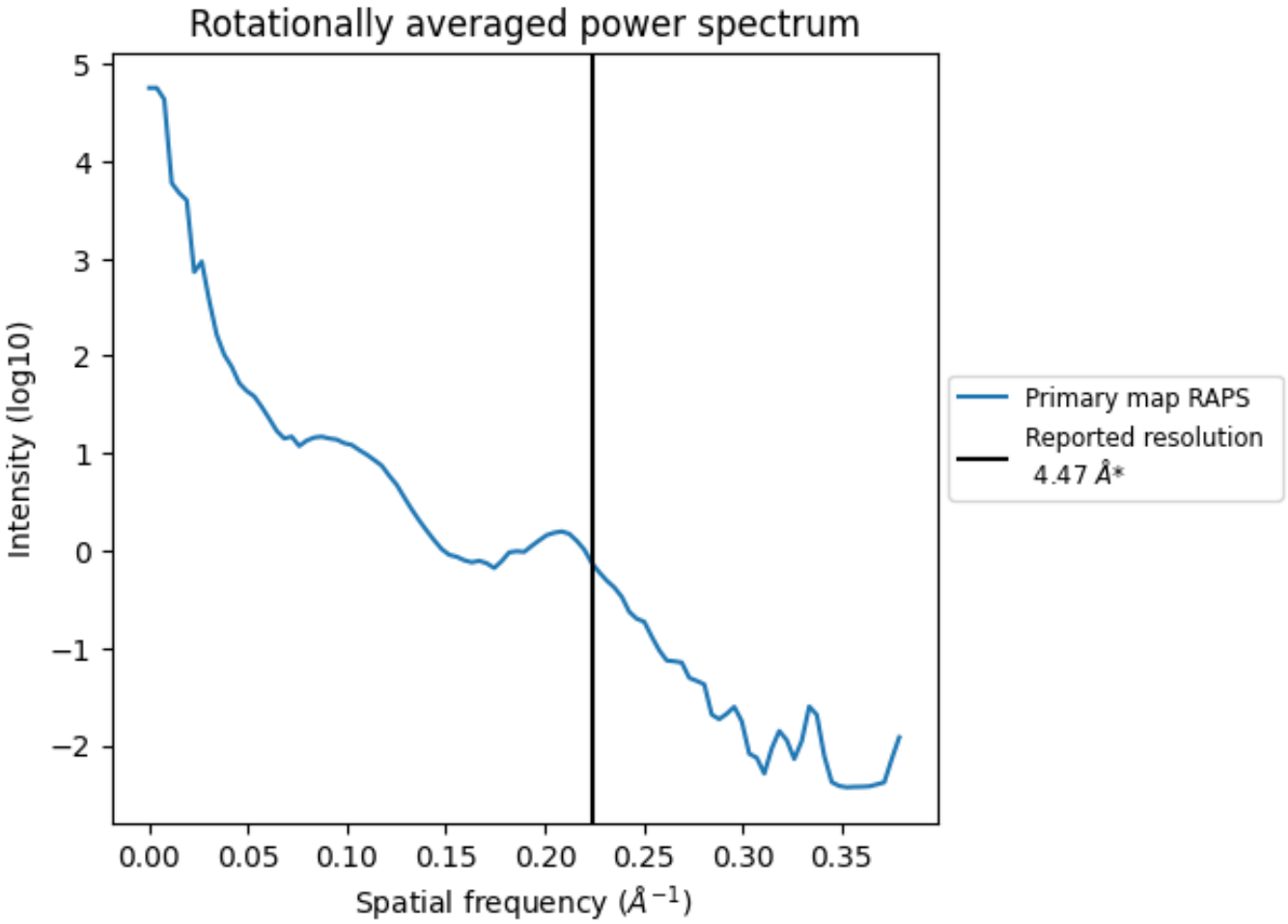
7.2 Volume estimate



The volume at the recommended contour level is 217 nm^3; this corresponds to an approximate mass of 196 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 0.224 Å^{-1}

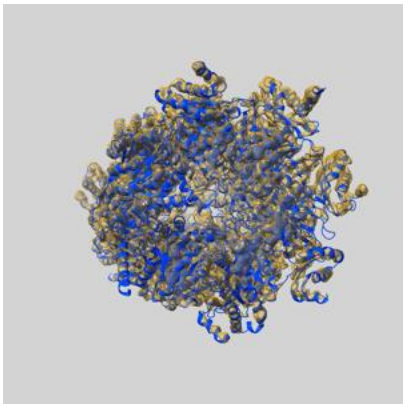
8 Fourier-Shell correlation (i)

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

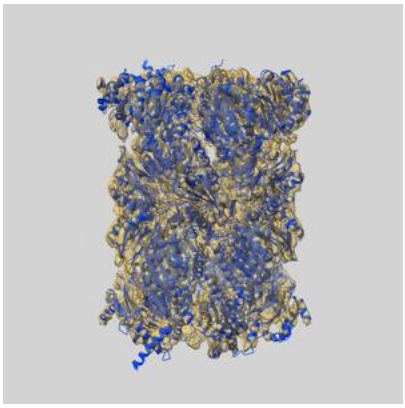
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31724 and PDB model 7V5G. Per-residue inclusion information can be found in section 3 on page 7.

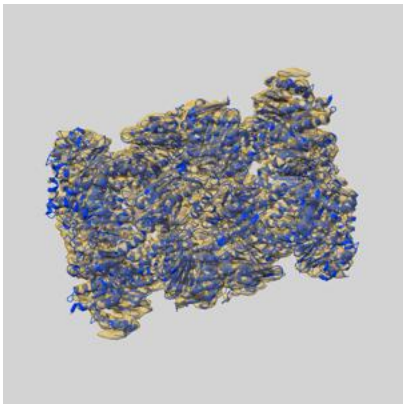
9.1 Map-model overlay



X



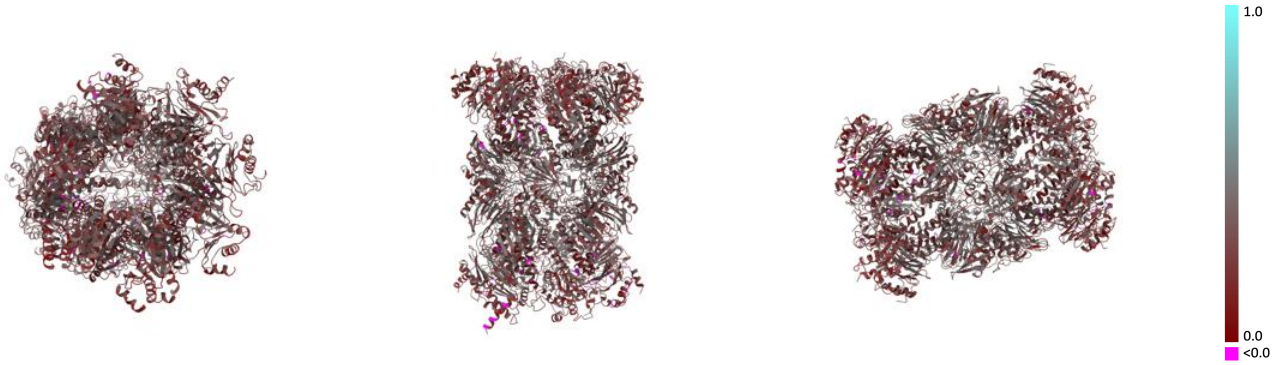
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

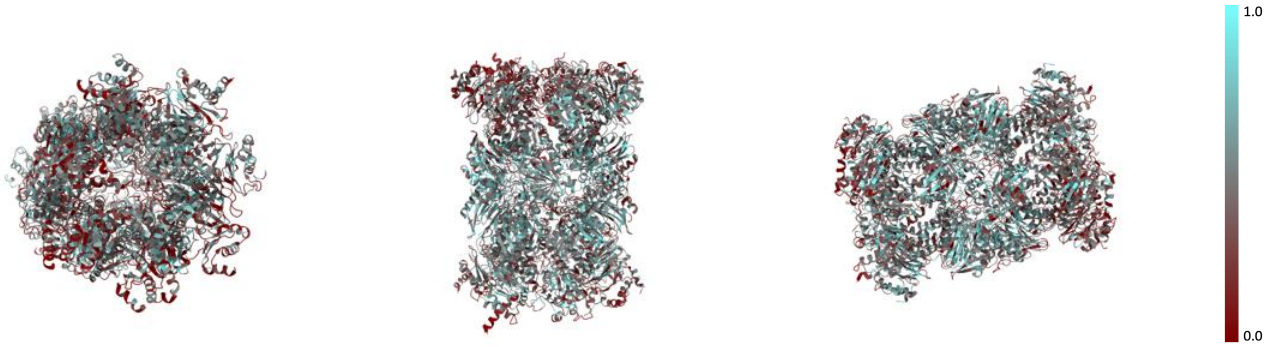
9.2 Q-score mapped to coordinate model (i)



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.

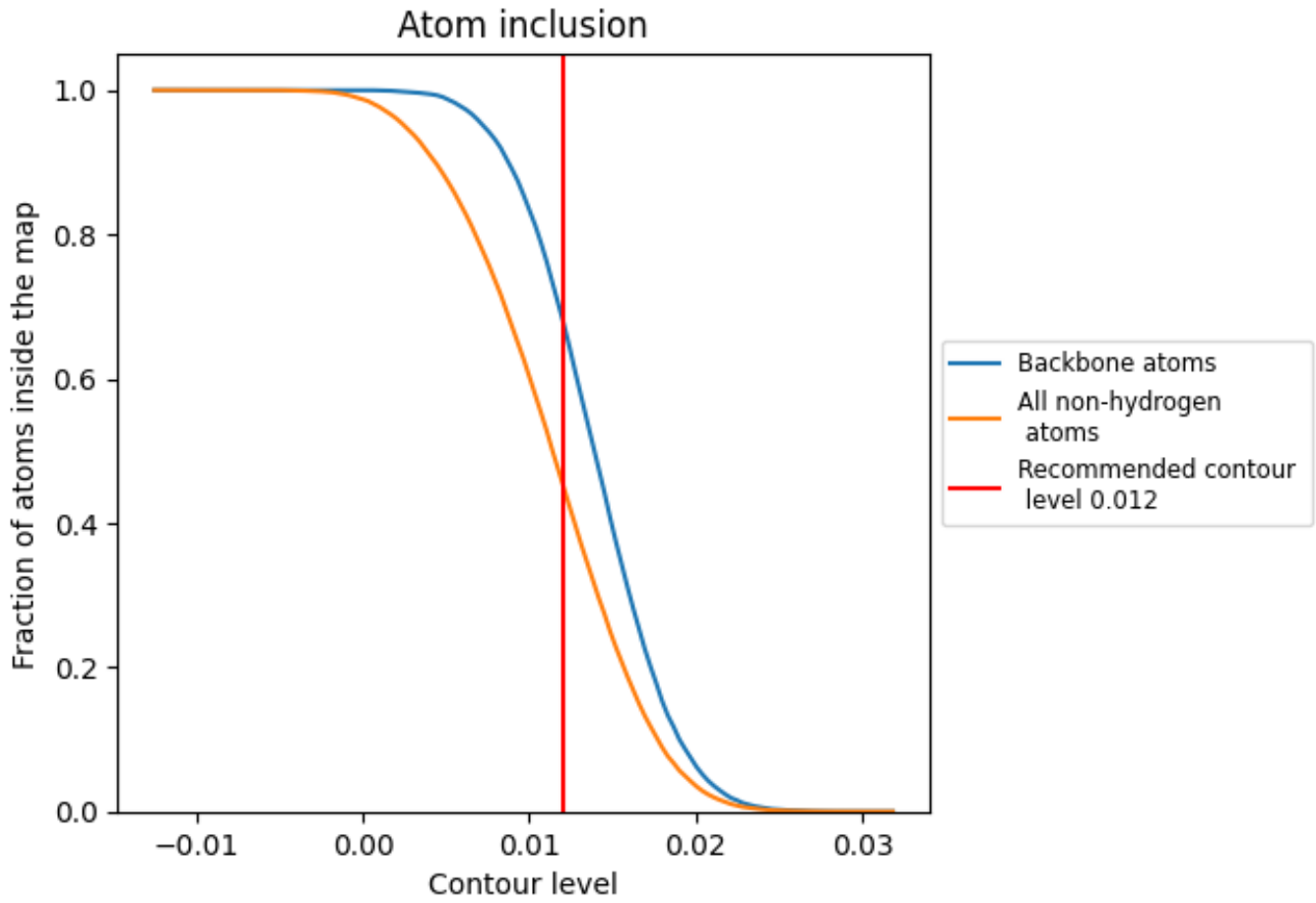
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4545	0.3050
A	0.5162	0.3410
B	0.5092	0.3400
C	0.4609	0.3130
D	0.4850	0.3200
E	0.5641	0.3340
F	0.5258	0.3300
G	0.5258	0.3390
H	0.4912	0.3290
I	0.5025	0.3260
J	0.5230	0.3240
K	0.5326	0.3280
L	0.5794	0.3410
M	0.5202	0.3450
N	0.5152	0.3440
O	0.3996	0.2630
P	0.4601	0.2760
Q	0.4352	0.2810
R	0.4441	0.2920
S	0.4154	0.3000
T	0.4617	0.2850
U	0.4539	0.2790
V	0.3733	0.2850
W	0.3259	0.2810
X	0.3148	0.2540
Y	0.3249	0.2580
Z	0.3314	0.2790
a	0.4102	0.2940
b	0.4463	0.3000