



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 11:31 PM JST

PDB ID : 7DR7
EMDB ID : EMD-30825
Title : bovine 20S immunoproteasome
Authors : Xu, C.; Cong, Y.
Deposited on : 2020-12-26
Resolution : 3.30 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

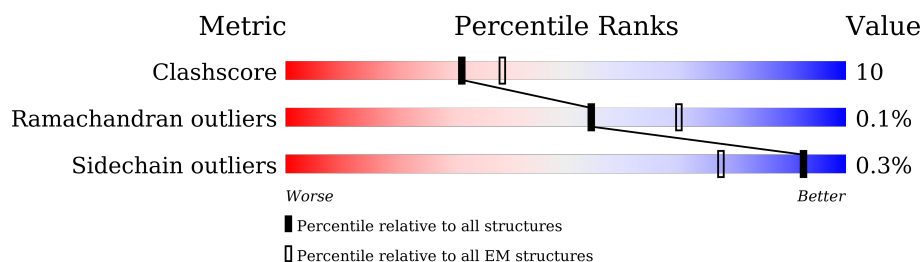
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	248	<div> <div>28%</div> <div>75%</div> <div>18%</div> <div>6%</div> </div>
1	O	248	<div> <div>27%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>
2	B	241	<div> <div>24%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
2	P	241	<div> <div>28%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
3	C	263	<div> <div>17%</div> <div>73%</div> <div>17%</div> <div>11%</div> </div>
3	Q	263	<div> <div>19%</div> <div>74%</div> <div>16%</div> <div>11%</div> </div>
4	D	255	<div> <div>24%</div> <div>76%</div> <div>18%</div> <div>6%</div> </div>
4	R	255	<div> <div>25%</div> <div>77%</div> <div>17%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	246	
5	L	246	
6	F	234	
6	M	234	
7	G	261	
7	N	261	
8	H	205	
8	S	205	
9	I	201	
9	T	201	
10	J	241	
10	U	241	
11	K	264	
11	V	264	
12	W	219	
12	Z	219	
13	1	273	
13	X	273	
14	2	276	
14	Y	276	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 48304 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-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	232	Total	C	N	O	S	0	0
			1824	1149	322	348	5		
1	O	232	Total	C	N	O	S	0	0
			1824	1149	322	348	5		

- Molecule 2 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		
2	P	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		

- Molecule 3 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	235	Total	C	N	O	S	0	0
			1846	1156	330	349	11		
3	Q	235	Total	C	N	O	S	0	0
			1846	1156	330	349	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	240	Total	C	N	O	S	0	0
			1879	1191	321	356	11		
4	R	240	Total	C	N	O	S	0	0
			1879	1191	321	356	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	244	Total	C	N	O	S	0	0
			1903	1206	320	364	13		
5	L	243	Total	C	N	O	S	0	0
			1892	1200	316	363	13		

- Molecule 6 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	231	Total	C	N	O	S	0	0
			1804	1153	306	339	6		
6	M	229	Total	C	N	O	S	0	0
			1790	1144	304	336	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	246	Total	C	N	O	S	0	0
			1936	1225	331	369	11		
7	N	246	Total	C	N	O	S	0	0
			1936	1225	331	369	11		

- Molecule 8 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		
8	S	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	198	Total	C	N	O	S	0	0
			1593	1023	270	292	8		
9	T	197	Total	C	N	O	S	0	0
			1584	1017	268	291	8		

- Molecule 10 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	213	Total	C	N	O	S	0	0
			1645	1042	282	311	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	213	Total	C	N	O	S	0	0
			1645	1042	282	311	10		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	216	Total	C	N	O	S	0	0
			1685	1065	289	319	12		
11	V	216	Total	C	N	O	S	0	0
			1682	1063	289	318	12		

- Molecule 12 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	199	Total	C	N	O	S	0	0
			1499	942	257	290	10		
12	Z	199	Total	C	N	O	S	0	0
			1500	942	257	291	10		

- Molecule 13 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	X	219	Total	C	N	O	S	0	0
			1611	1010	281	309	11		
13	1	219	Total	C	N	O	S	0	0
			1611	1010	281	309	11		

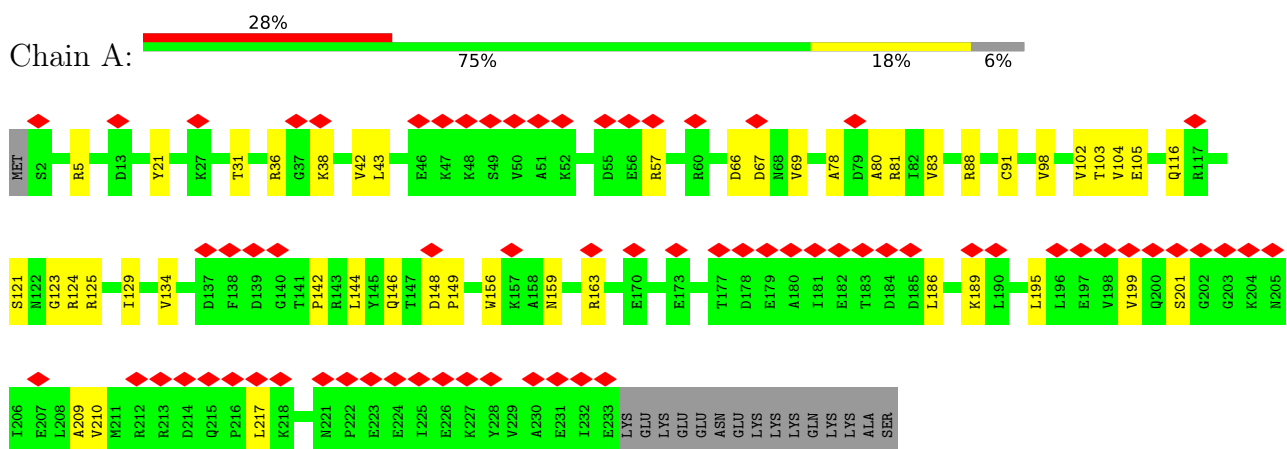
- Molecule 14 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	201	Total	C	N	O	S	0	0
			1561	975	273	297	16		
14	2	201	Total	C	N	O	S	0	0
			1561	975	273	297	16		

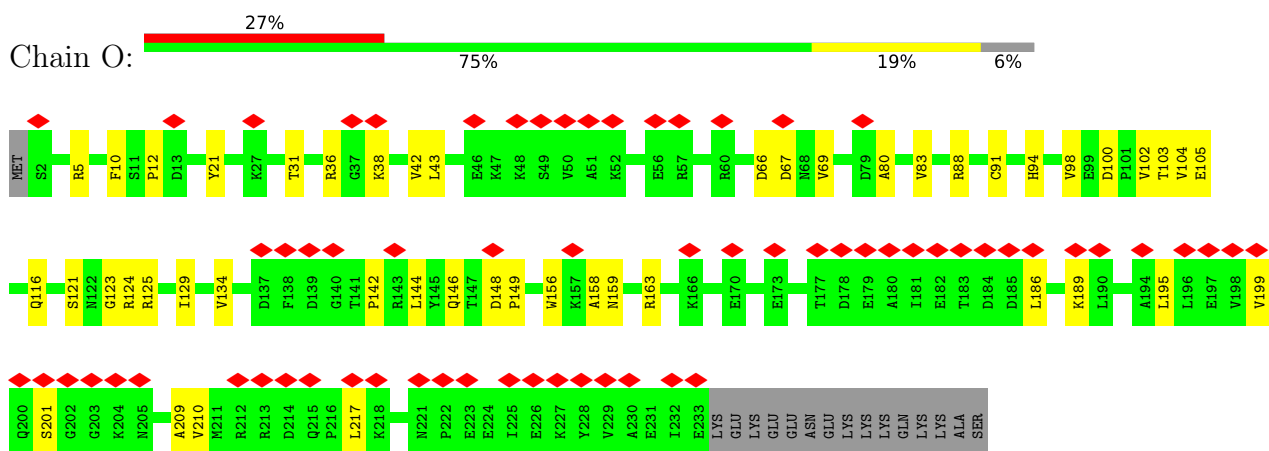
3 Residue-property plots

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

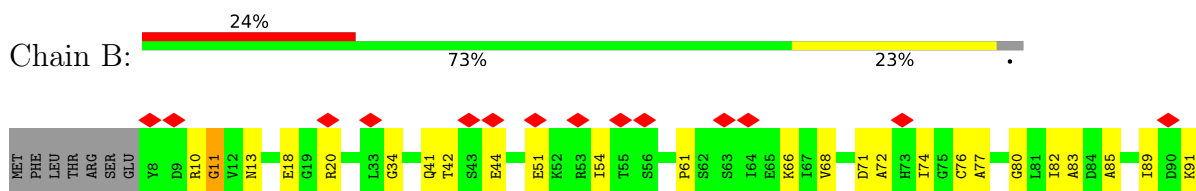
• Molecule 1: Proteasome subunit alpha type-7

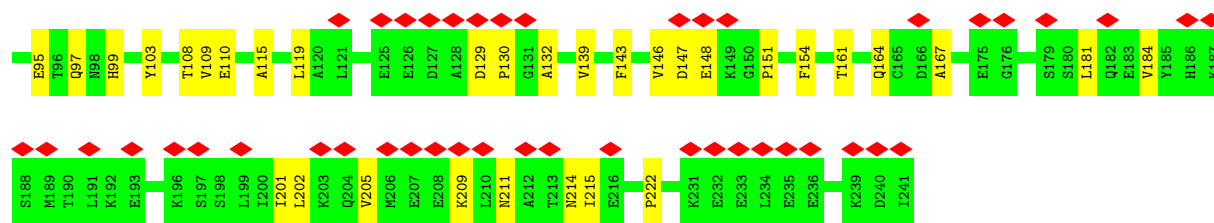


• Molecule 1: Proteasome subunit alpha type-7

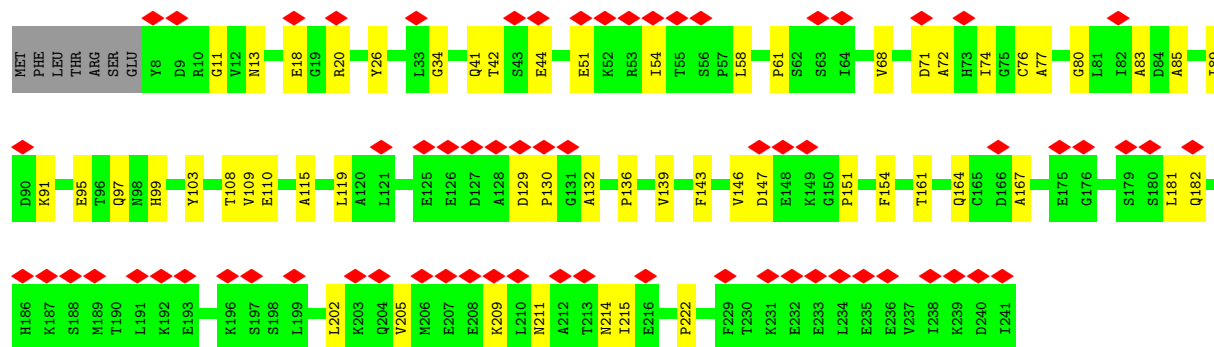
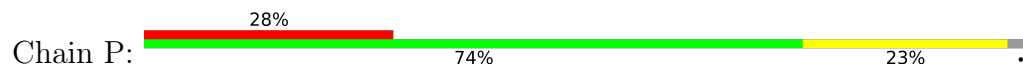


• Molecule 2: Proteasome subunit alpha type-5

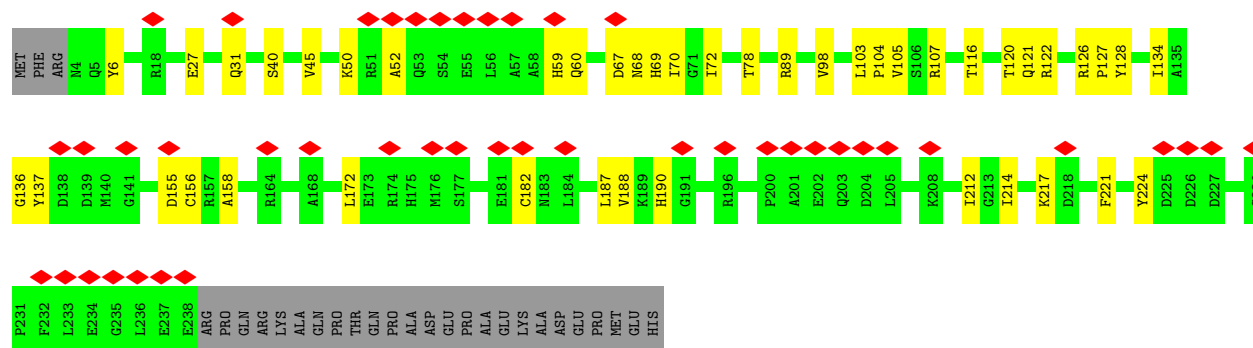
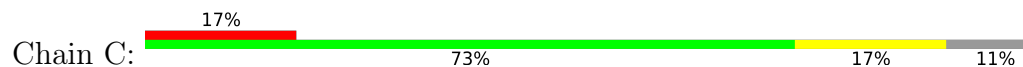




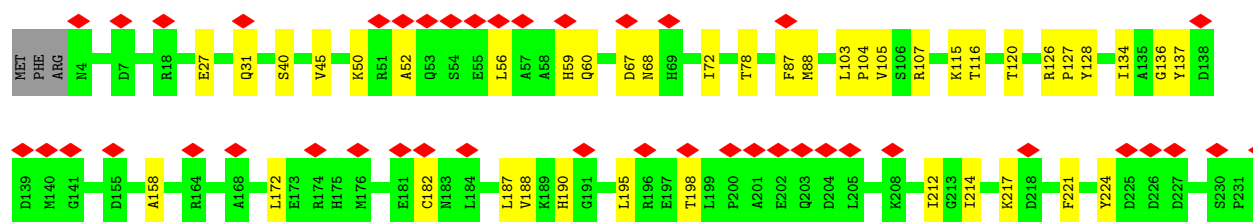
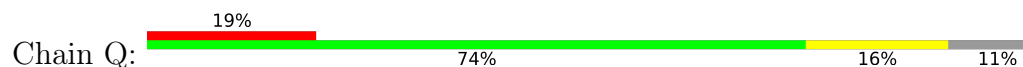
• Molecule 2: Proteasome subunit alpha type-5

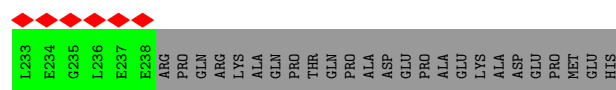


• Molecule 3: Proteasome subunit alpha type-1

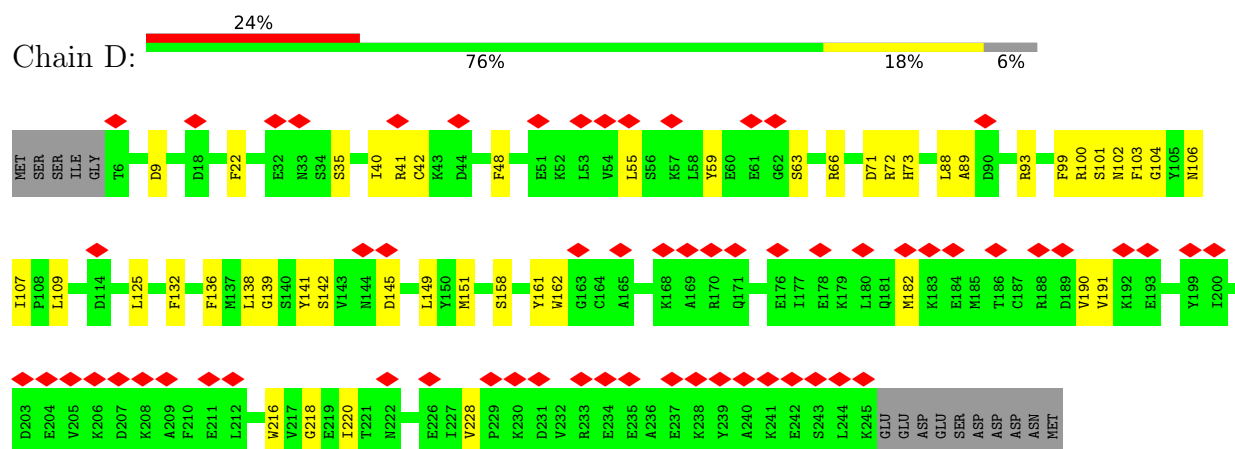


• Molecule 3: Proteasome subunit alpha type-1

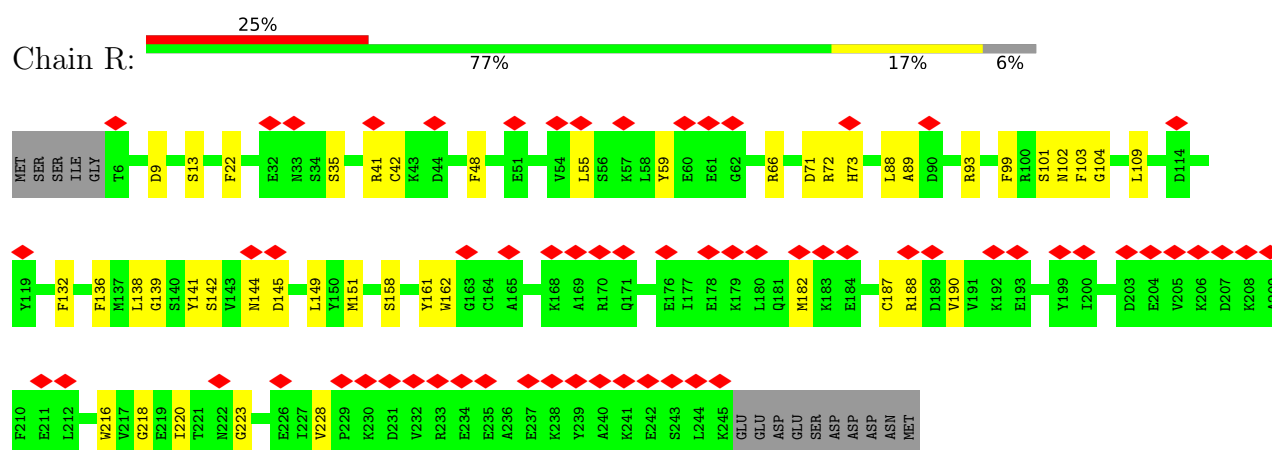




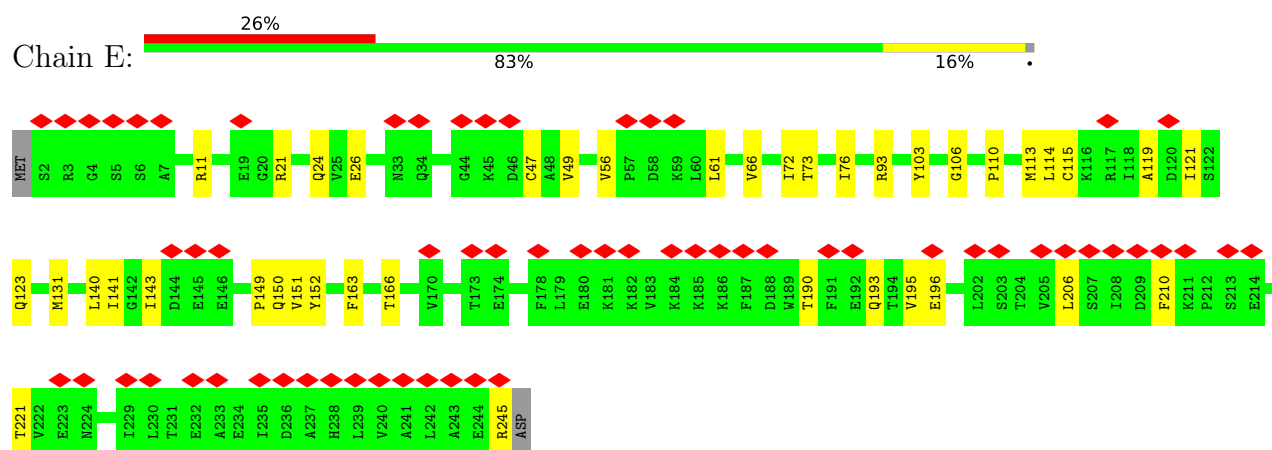
• Molecule 4: Proteasome subunit alpha type-3



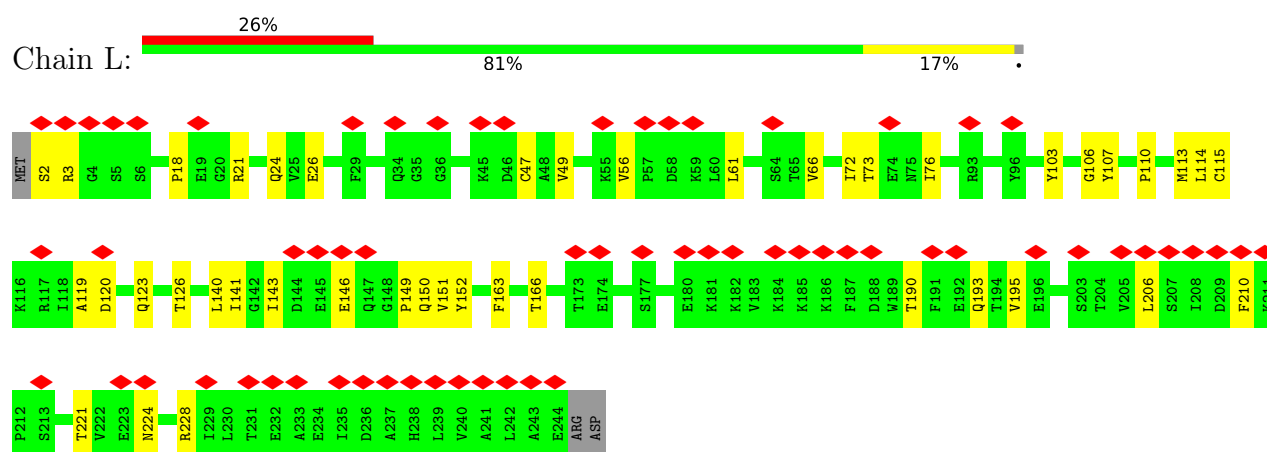
• Molecule 4: Proteasome subunit alpha type-3



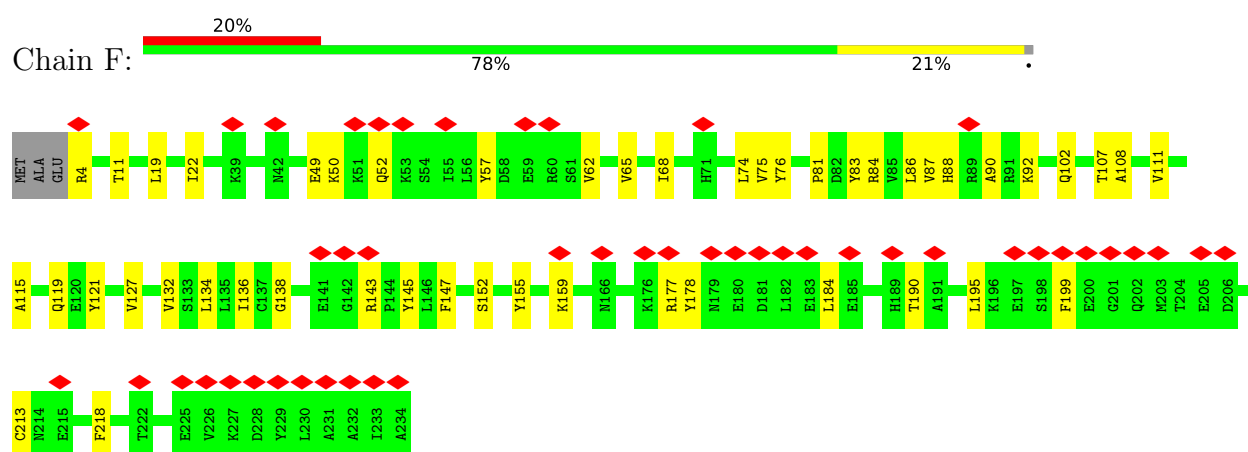
• Molecule 5: Proteasome subunit alpha type-6



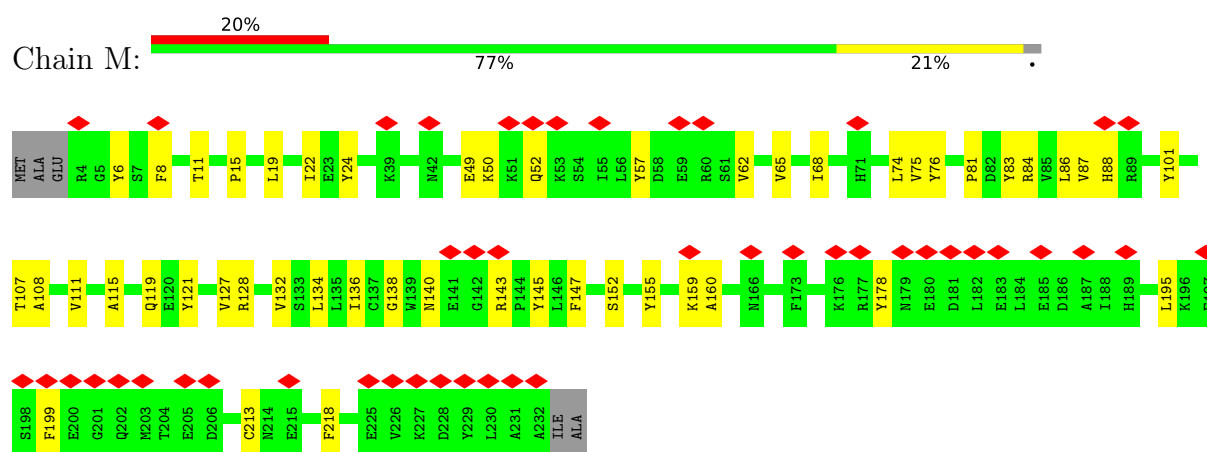
• Molecule 5: Proteasome subunit alpha type-6



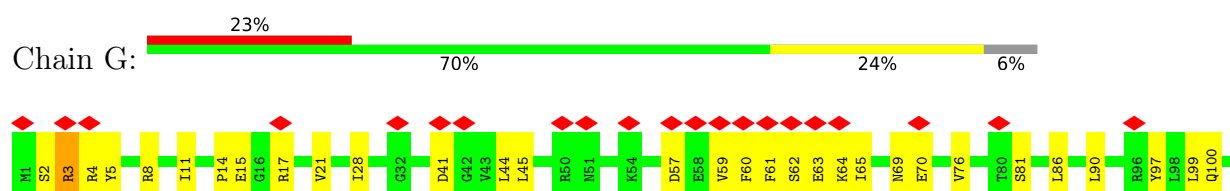
• Molecule 6: Proteasome subunit alpha type-2

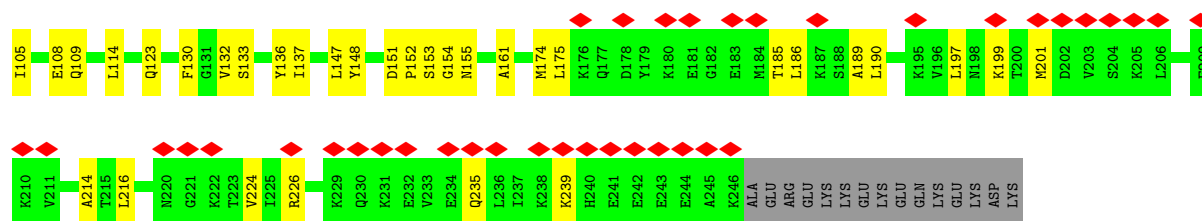


• Molecule 6: Proteasome subunit alpha type-2

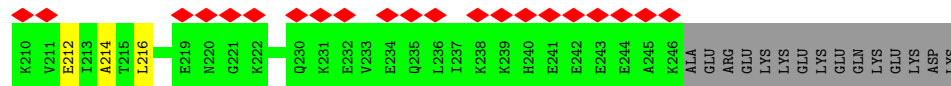
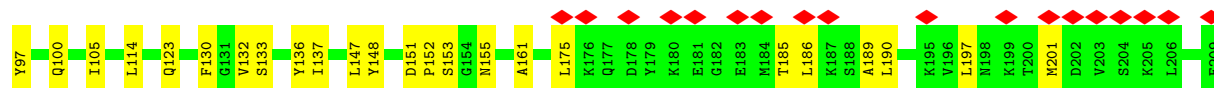
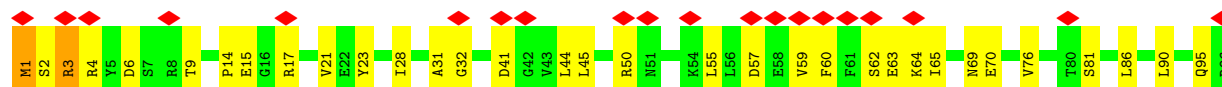


• Molecule 7: Proteasome subunit alpha type-4

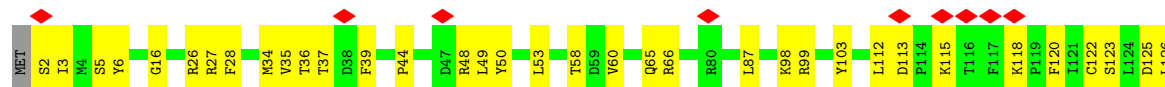




• Molecule 7: Proteasome subunit alpha type-4



• Molecule 8: Proteasome subunit beta type-3

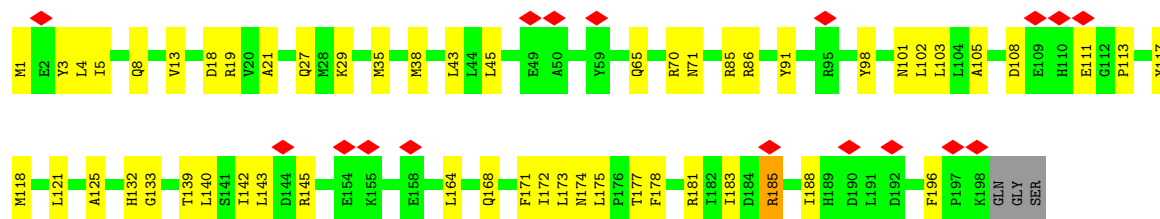


• Molecule 8: Proteasome subunit beta type-3

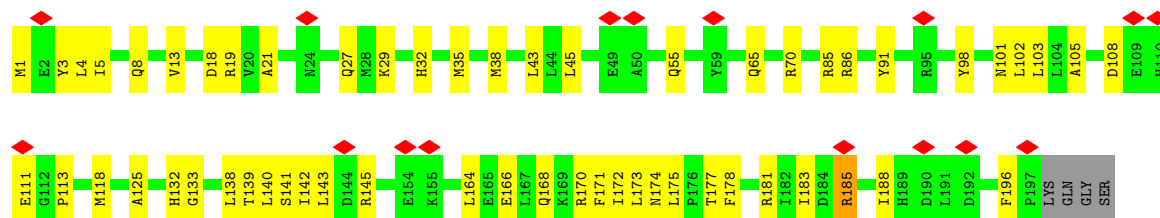


• Molecule 9: Proteasome subunit beta type-2

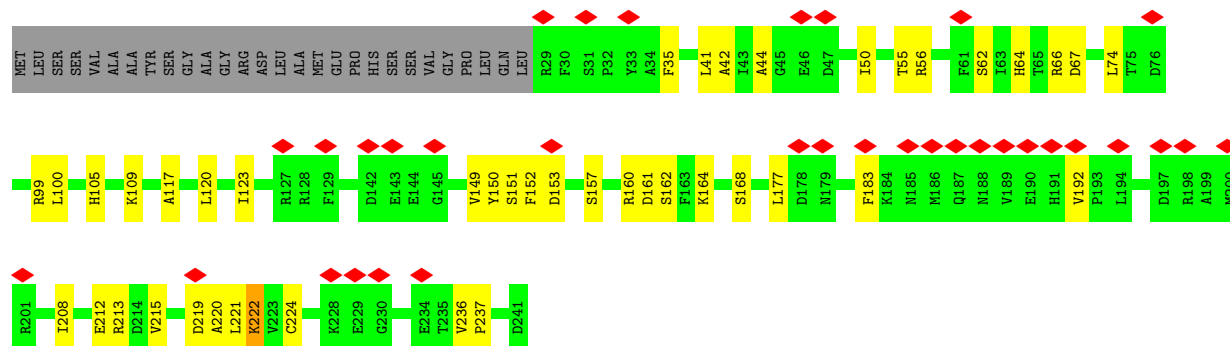




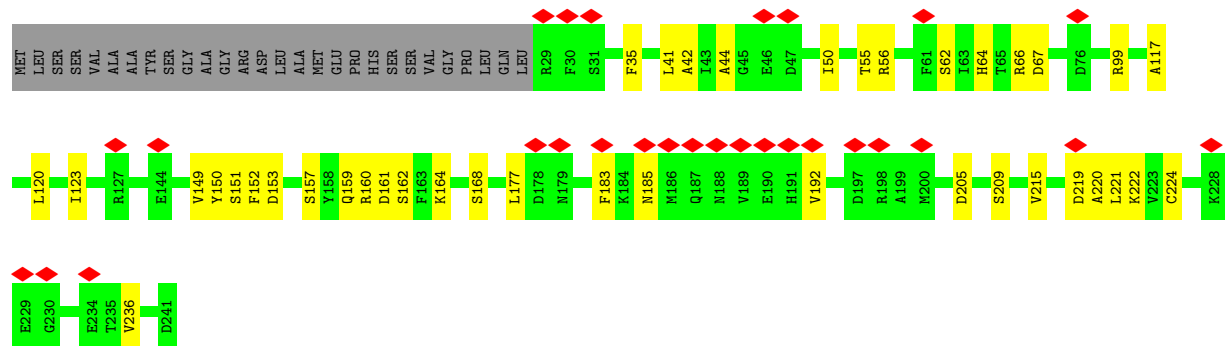
- Molecule 9: Proteasome subunit beta type-2



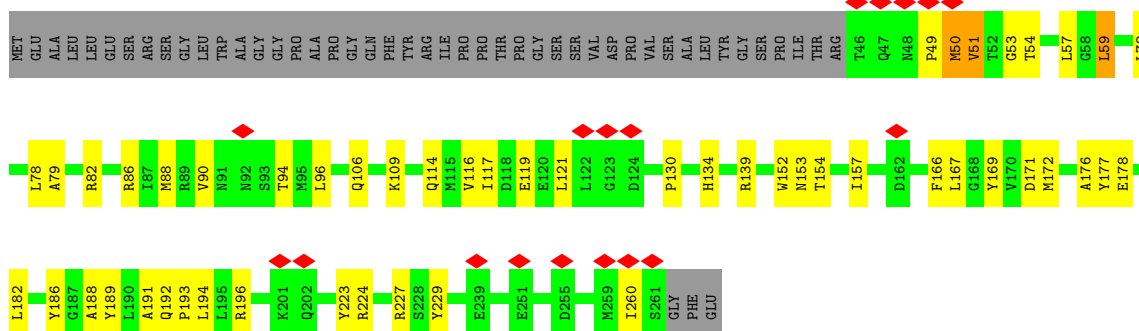
- Molecule 10: Proteasome subunit beta type-1



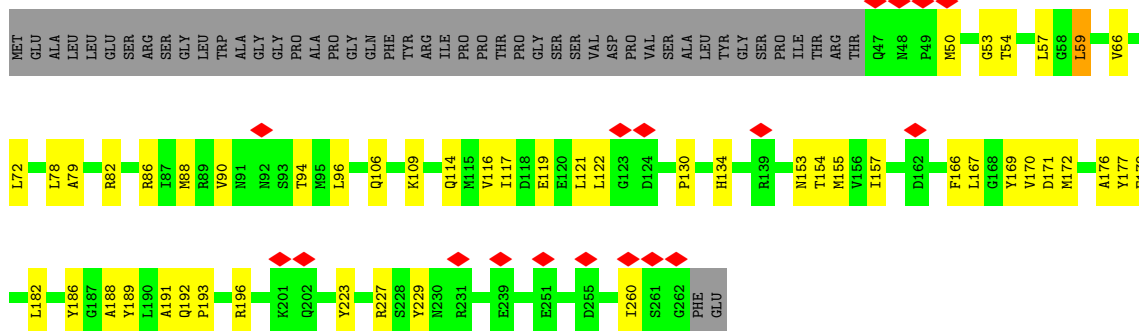
- Molecule 10: Proteasome subunit beta type-1



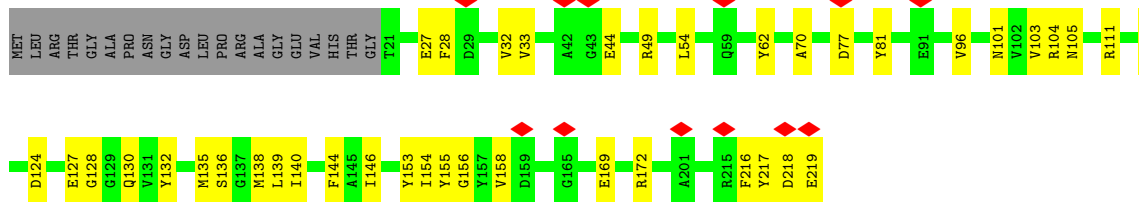
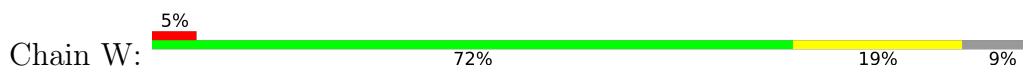
- Molecule 11: Proteasome subunit beta type-4



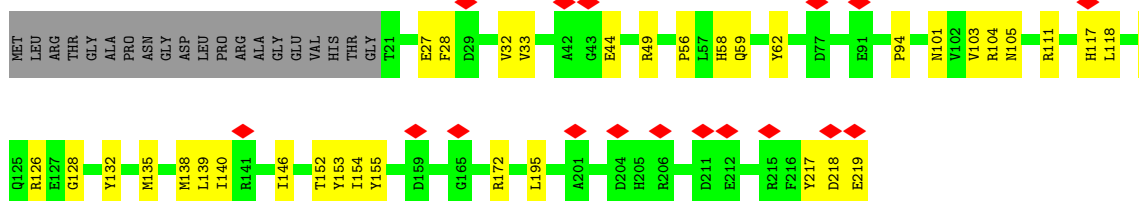
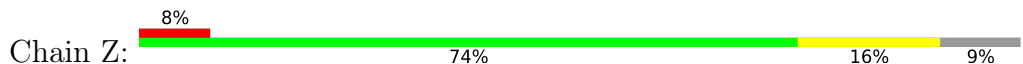
• Molecule 11: Proteasome subunit beta type-4



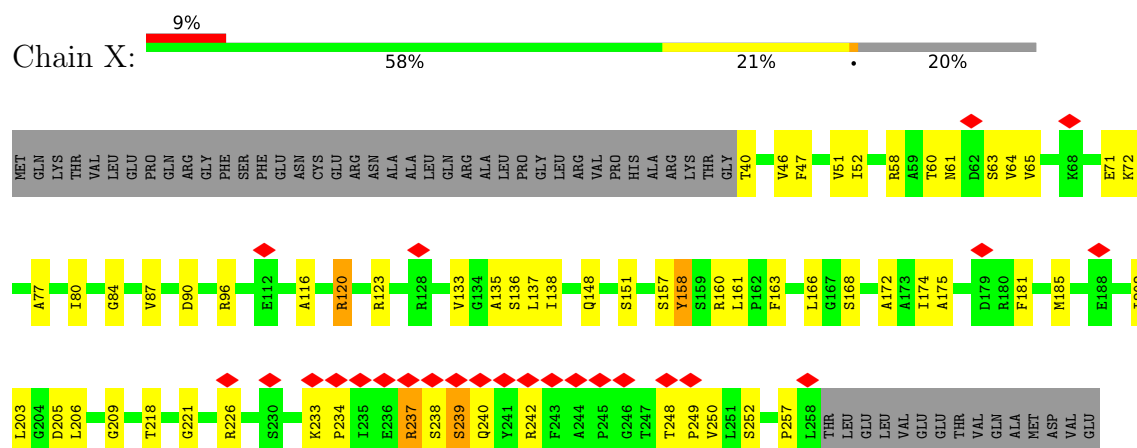
• Molecule 12: Proteasome subunit beta type-9



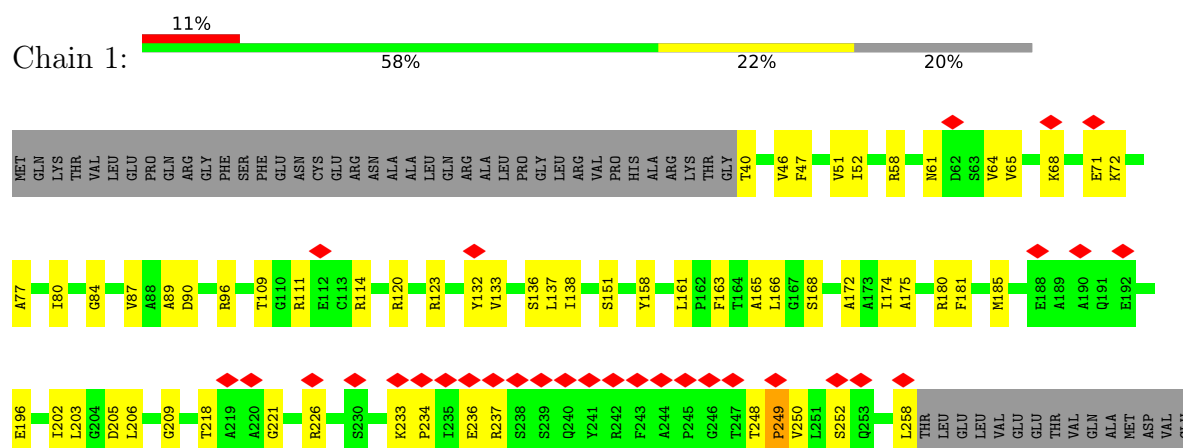
• Molecule 12: Proteasome subunit beta type-9



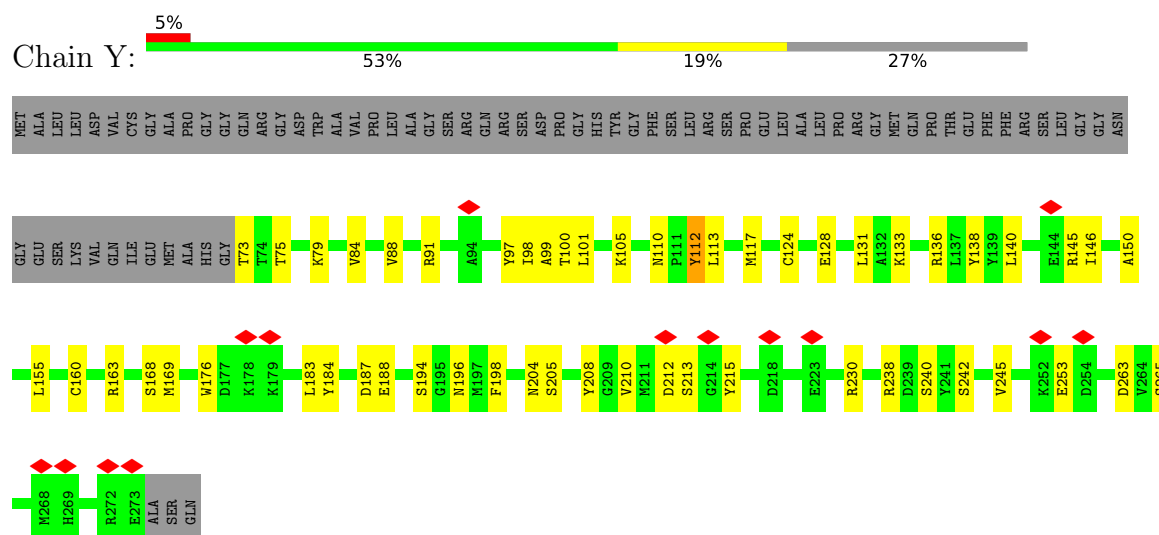
- Molecule 13: Proteasome subunit beta type-10



- Molecule 13: Proteasome subunit beta type-10

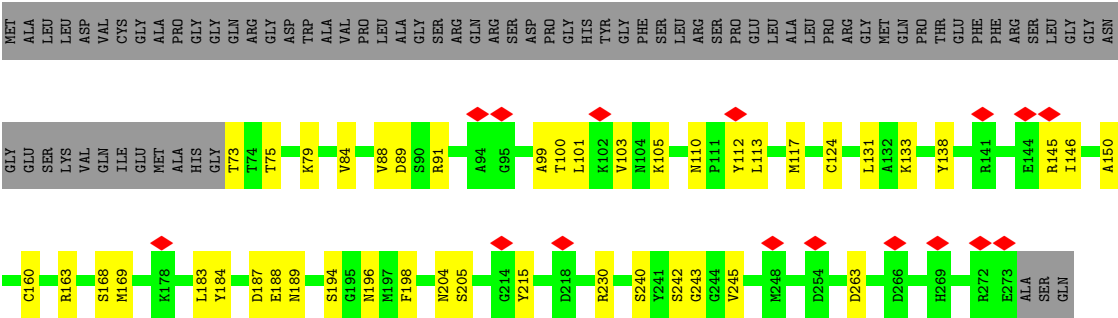


- Molecule 14: Proteasome subunit beta type-8



- Molecule 14: Proteasome subunit beta type-8





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56663	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 ($e^-/\text{\AA}^2$)	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	0.171	Depositor
Minimum map value	-0.110	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/1851	0.44	0/2501
1	O	0.26	0/1851	0.44	0/2501
2	B	0.26	0/1818	0.43	0/2455
2	P	0.26	0/1818	0.43	0/2455
3	C	0.25	0/1880	0.43	0/2541
3	Q	0.25	0/1880	0.43	0/2541
4	D	0.28	0/1914	0.42	0/2578
4	R	0.28	0/1914	0.42	0/2578
5	E	0.28	0/1937	0.43	0/2617
5	L	0.28	0/1926	0.43	0/2603
6	F	0.28	0/1843	0.42	0/2495
6	M	0.28	0/1829	0.42	0/2477
7	G	0.28	0/1966	0.45	0/2648
7	N	0.28	0/1966	0.46	0/2648
8	H	0.29	0/1623	0.46	0/2188
8	S	0.29	0/1623	0.45	0/2188
9	I	0.28	0/1627	0.44	0/2201
9	T	0.28	0/1618	0.44	0/2190
10	J	0.28	0/1676	0.44	0/2258
10	U	0.28	0/1676	0.45	0/2258
11	K	0.30	0/1718	0.45	0/2324
11	V	0.29	0/1715	0.45	0/2319
12	W	0.29	0/1528	0.44	0/2071
12	Z	0.29	0/1529	0.43	0/2071
13	1	0.27	0/1637	0.47	0/2225
13	X	0.28	0/1637	0.48	0/2225
14	2	0.29	0/1592	0.43	0/2145
14	Y	0.29	0/1592	0.44	0/2145
All	All	0.28	0/49184	0.44	0/66446

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1824	0	1851	31	0
1	O	1824	0	1851	32	0
2	B	1790	0	1773	41	0
2	P	1790	0	1773	39	0
3	C	1846	0	1832	30	0
3	Q	1846	0	1832	26	0
4	D	1879	0	1864	37	0
4	R	1879	0	1864	35	0
5	E	1903	0	1911	32	0
5	L	1892	0	1898	35	0
6	F	1804	0	1800	34	0
6	M	1790	0	1784	42	0
7	G	1936	0	1961	43	0
7	N	1936	0	1961	52	0
8	H	1594	0	1613	40	0
8	S	1594	0	1613	50	0
9	I	1593	0	1597	51	0
9	T	1584	0	1584	50	0
10	J	1645	0	1644	33	0
10	U	1645	0	1644	29	0
11	K	1685	0	1665	41	0
11	V	1682	0	1661	36	0
12	W	1499	0	1459	32	0
12	Z	1500	0	1459	28	0
13	1	1611	0	1624	54	0
13	X	1611	0	1624	69	0
14	2	1561	0	1516	35	0
14	Y	1561	0	1516	41	0
All	All	48304	0	48174	922	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 (922) 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)
8:S:100:PHE:HE1	13:1:132:TYR:CD2	1.47	1.32
8:S:100:PHE:CE1	13:1:132:TYR:CE2	2.23	1.26
8:S:100:PHE:HE1	13:1:132:TYR:CE2	1.54	1.25
8:S:100:PHE:CE1	13:1:132:TYR:CD2	2.40	1.08
13:X:123:ARG:CD	13:X:158:TYR:HD2	1.71	1.03
5:E:106:GLY:HA3	13:X:120:ARG:HD2	1.41	1.02
6:M:6:TYR:CE1	7:N:1:MET:HA	1.99	0.98
8:H:140:GLY:O	8:H:143:THR:HG23	1.68	0.92
12:W:146:ILE:HD11	12:W:155:TYR:CE1	2.05	0.91
13:X:123:ARG:CD	13:X:158:TYR:CD2	2.53	0.91
6:M:6:TYR:CD1	7:N:1:MET:HA	2.06	0.90
13:X:237:ARG:HB2	13:X:237:ARG:NH1	1.86	0.88
14:2:112:TYR:HE2	14:2:145:ARG:HD2	1.43	0.83
8:S:100:PHE:CD1	13:1:132:TYR:CE2	2.67	0.83
5:L:123:GLN:HE22	6:M:84:ARG:HB2	1.43	0.82
10:U:205:ASP:OD2	13:X:239:SER:HB2	1.78	0.82
13:X:233:LYS:HB3	13:X:234:PRO:HD3	1.59	0.82
8:S:140:GLY:O	8:S:143:THR:HG23	1.78	0.82
10:U:222:LYS:HE2	10:U:224:CYS:SG	2.21	0.81
14:Y:124:CYS:O	14:Y:128:GLU:HG3	1.81	0.80
9:I:43:LEU:HD11	9:I:188:ILE:HD12	1.63	0.79
9:T:43:LEU:HD11	9:T:188:ILE:HD12	1.63	0.79
13:X:123:ARG:NE	13:X:158:TYR:CD2	2.51	0.78
8:H:158:MET:SD	13:X:242:ARG:NH2	2.57	0.77
9:I:91:TYR:CD2	9:I:98:TYR:CD2	2.73	0.77
5:E:106:GLY:HA3	13:X:120:ARG:CD	2.15	0.77
11:V:186:TYR:HE2	12:W:44:GLU:HB2	1.52	0.75
1:A:81:ARG:NH2	7:G:154:GLY:O	2.20	0.75
4:R:216:TRP:CZ3	4:R:220:ILE:HD12	2.22	0.75
9:I:91:TYR:CE2	9:I:98:TYR:HE2	2.05	0.74
10:J:222:LYS:HE2	10:J:224:CYS:SG	2.29	0.73
13:X:71:GLU:OE1	13:X:226:ARG:NH1	2.22	0.73
13:X:123:ARG:HD3	13:X:158:TYR:CD2	2.24	0.73
4:D:101:SER:OG	11:K:114:GLN:NE2	2.22	0.73
6:M:6:TYR:CE1	7:N:1:MET:CA	2.72	0.72
10:J:222:LYS:CE	10:J:224:CYS:SG	2.77	0.72
11:K:49:PRO:HG3	11:K:152:TRP:CD1	2.24	0.72
2:B:41:GLN:NE2	2:B:151:PRO:O	2.23	0.71
5:E:93:ARG:HE	5:E:121:ILE:HD13	1.53	0.71
8:S:203:ARG:NH1	14:Y:263:ASP:OD2	2.22	0.71
2:P:41:GLN:NE2	2:P:151:PRO:O	2.23	0.71
3:Q:107:ARG:HH22	11:V:119:GLU:HG3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:123:ARG:HD2	13:X:158:TYR:HD2	1.53	0.71
1:A:125:ARG:HE	7:G:123:GLN:HA	1.55	0.71
1:A:209:ALA:HB1	1:A:217:LEU:HD11	1.72	0.71
4:R:101:SER:OG	11:V:114:GLN:NE2	2.22	0.71
1:O:209:ALA:HB1	1:O:217:LEU:HD11	1.72	0.70
9:I:91:TYR:CE2	9:I:98:TYR:CE2	2.80	0.70
5:L:21:ARG:NE	5:L:26:GLU:OE2	2.21	0.69
10:J:66:ARG:HH22	13:1:203:LEU:HB3	1.57	0.69
3:C:107:ARG:HH22	11:K:119:GLU:HG3	1.56	0.69
4:D:100:ARG:NH2	4:D:106:ASN:OD1	2.25	0.69
6:M:74:LEU:HD11	6:M:134:LEU:HD22	1.75	0.69
12:W:144:PHE:CE1	12:W:158:VAL:HB	2.27	0.69
6:F:74:LEU:HD11	6:F:134:LEU:HD22	1.74	0.69
6:M:119:GLN:NE2	7:N:81:SER:O	2.26	0.68
11:V:59:LEU:O	11:V:59:LEU:HD23	1.93	0.68
13:1:236:GLU:HA	13:1:236:GLU:OE1	1.94	0.68
8:H:140:GLY:O	8:H:143:THR:CG2	2.42	0.67
8:S:100:PHE:CE1	13:1:132:TYR:HE2	2.04	0.67
5:E:106:GLY:CA	13:X:120:ARG:HD2	2.21	0.67
9:I:181:ARG:HD3	9:I:188:ILE:HD11	1.75	0.67
4:D:40:ILE:HD11	4:D:182:MET:HG3	1.75	0.67
9:T:181:ARG:HD3	9:T:188:ILE:HD11	1.75	0.67
10:J:41:LEU:HD11	10:J:177:LEU:HD11	1.77	0.67
6:F:52:GLN:HB3	6:F:57:TYR:HD2	1.59	0.67
8:S:113:ASP:HB3	8:S:118:LYS:HB3	1.77	0.67
10:U:41:LEU:HD11	10:U:177:LEU:HD11	1.77	0.66
11:V:82:ARG:NH1	12:W:218:ASP:O	2.28	0.66
12:Z:135:MET:O	12:Z:138:MET:HG2	1.95	0.66
1:A:42:VAL:HG22	1:A:210:VAL:HG12	1.77	0.66
6:M:52:GLN:HB3	6:M:57:TYR:HD2	1.59	0.66
12:W:135:MET:O	12:W:138:MET:HG2	1.95	0.66
9:I:185:ARG:HH11	9:I:185:ARG:HB2	1.59	0.66
8:H:113:ASP:HB3	8:H:118:LYS:HB3	1.77	0.66
11:K:59:LEU:C	11:K:59:LEU:HD12	2.15	0.66
8:S:140:GLY:O	8:S:143:THR:CG2	2.44	0.66
10:U:209:SER:OG	13:X:237:ARG:NH2	2.29	0.66
13:1:218:THR:H	13:1:221:GLY:HA2	1.61	0.65
11:V:50:MET:SD	12:Z:111:ARG:NH2	2.68	0.65
1:O:42:VAL:HG22	1:O:210:VAL:HG12	1.77	0.65
13:X:237:ARG:O	13:X:237:ARG:HG3	1.96	0.65
5:L:123:GLN:NE2	6:M:81:PRO:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:77:ASP:OD2	13:X:123:ARG:NH1	2.26	0.65
11:K:50:MET:SD	12:W:111:ARG:NH2	2.69	0.65
10:U:66:ARG:NH2	13:X:203:LEU:O	2.30	0.65
4:R:188:ARG:HG3	4:R:220:ILE:HD11	1.78	0.65
12:W:169:GLU:OE1	12:W:172:ARG:NH2	2.30	0.65
2:B:10:ARG:O	2:B:11:GLY:O	2.15	0.65
5:E:21:ARG:NE	5:E:26:GLU:OE2	2.21	0.65
9:I:91:TYR:CD2	9:I:98:TYR:HD2	2.14	0.65
9:I:140:LEU:HD23	9:I:143:LEU:HD12	1.78	0.65
13:X:218:THR:H	13:X:221:GLY:HA2	1.61	0.65
12:W:138:MET:HE2	12:W:140:ILE:HD11	1.77	0.64
8:H:164:PHE:CE2	13:X:248:THR:HG21	2.32	0.64
11:K:186:TYR:HE2	12:Z:44:GLU:HB2	1.62	0.64
9:T:140:LEU:HD23	9:T:143:LEU:HD12	1.78	0.64
14:Y:73:THR:N	14:Y:242:SER:HG	1.94	0.64
8:S:164:PHE:HB2	8:S:189:ILE:HD11	1.80	0.64
14:2:73:THR:N	14:2:242:SER:HG	1.96	0.64
4:R:55:LEU:HB2	4:R:59:TYR:HE2	1.63	0.64
4:D:55:LEU:HB2	4:D:59:TYR:HE2	1.63	0.64
5:E:11:ARG:O	5:E:24:GLN:NE2	2.31	0.63
8:H:164:PHE:HB2	8:H:189:ILE:HD11	1.80	0.63
3:Q:87:PHE:HB3	3:Q:115:LYS:HE2	1.79	0.63
7:N:1:MET:CE	1:O:5:ARG:HD2	2.28	0.62
6:F:50:LYS:NZ	6:F:62:VAL:O	2.31	0.62
5:E:123:GLN:HE22	6:F:84:ARG:HB2	1.65	0.62
9:I:38:MET:O	9:I:65:GLN:NE2	2.32	0.62
13:X:40:THR:HG23	13:X:72:LYS:HE2	1.81	0.62
3:C:116:THR:HG22	3:C:128:TYR:HD2	1.64	0.62
6:M:50:LYS:NZ	6:M:62:VAL:O	2.31	0.62
4:R:187:CYS:SG	4:R:220:ILE:CD1	2.87	0.62
6:F:65:VAL:HG22	6:F:75:VAL:HG12	1.81	0.62
10:J:66:ARG:NH2	13:1:203:LEU:O	2.32	0.62
8:S:177:ARG:NH2	14:Y:99:ALA:O	2.31	0.62
8:H:177:ARG:NH2	14:2:99:ALA:O	2.31	0.62
11:K:50:MET:SD	12:W:136:SER:HB3	2.40	0.61
9:T:185:ARG:HG2	9:T:185:ARG:HH21	1.64	0.61
3:Q:45:VAL:HG11	3:Q:188:VAL:HG22	1.83	0.61
13:1:71:GLU:OE1	13:1:226:ARG:NH1	2.33	0.61
7:G:69:ASN:OD1	7:G:70:GLU:N	2.34	0.61
6:M:65:VAL:HG22	6:M:75:VAL:HG12	1.81	0.61
7:N:69:ASN:OD1	7:N:70:GLU:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:40:THR:HG23	13:1:72:LYS:HE2	1.81	0.61
5:L:146:GLU:OE1	13:1:111:ARG:NH1	2.34	0.61
7:G:44:LEU:HD22	7:G:190:LEU:HD23	1.82	0.60
3:Q:116:THR:HG22	3:Q:128:TYR:HD2	1.64	0.60
8:S:159:ASP:OD1	8:S:162:HIS:ND1	2.34	0.60
9:T:185:ARG:HH21	9:T:185:ARG:CG	2.14	0.60
8:H:159:ASP:OD1	8:H:162:HIS:ND1	2.35	0.60
1:O:116:GLN:NE2	2:P:83:ALA:O	2.35	0.60
5:E:196:GLU:OE1	5:E:245:ARG:NH2	2.34	0.60
10:J:44:ALA:HB2	10:J:149:VAL:HG23	1.82	0.60
13:X:123:ARG:NE	13:X:158:TYR:CE2	2.69	0.60
2:B:10:ARG:HH11	2:B:10:ARG:HB3	1.66	0.60
10:U:44:ALA:HB2	10:U:149:VAL:HG23	1.82	0.60
7:N:3:ARG:HH22	2:P:11:GLY:HA3	1.66	0.60
3:C:45:VAL:HG11	3:C:188:VAL:HG22	1.83	0.60
9:I:91:TYR:CD2	9:I:98:TYR:CE2	2.89	0.60
8:H:194:LYS:HG2	13:X:257:PRO:HA	1.84	0.60
10:J:208:ILE:CG2	13:1:237:ARG:HG2	2.32	0.60
1:A:116:GLN:NE2	2:B:83:ALA:O	2.35	0.59
7:G:151:ASP:HB2	7:G:152:PRO:HD2	1.83	0.59
7:N:44:LEU:HD22	7:N:190:LEU:HD23	1.82	0.59
11:K:90:VAL:HB	11:K:94:THR:HG23	1.85	0.59
13:X:237:ARG:HB2	13:X:237:ARG:CZ	2.33	0.59
13:X:237:ARG:HB2	13:X:237:ARG:HH11	1.62	0.59
14:Y:117:MET:HG3	14:Y:124:CYS:SG	2.43	0.59
7:N:151:ASP:HB2	7:N:152:PRO:HD2	1.83	0.59
9:T:43:LEU:HD13	9:T:183:ILE:HD11	1.85	0.59
14:2:79:LYS:O	14:2:215:TYR:OH	2.21	0.59
4:R:187:CYS:SG	4:R:220:ILE:HD12	2.43	0.59
12:W:154:ILE:O	12:W:154:ILE:HG13	2.02	0.59
1:A:31:THR:OG1	1:A:163:ARG:O	2.21	0.58
1:A:146:GLN:OE1	1:A:159:ASN:ND2	2.35	0.58
14:Y:79:LYS:O	14:Y:215:TYR:OH	2.21	0.58
14:2:112:TYR:CE2	14:2:145:ARG:HD2	2.31	0.58
6:F:119:GLN:NE2	7:G:81:SER:O	2.35	0.58
7:N:1:MET:HE1	1:O:5:ARG:HD2	1.85	0.58
14:2:117:MET:HG3	14:2:124:CYS:SG	2.43	0.58
14:2:124:CYS:HB3	14:2:169:MET:HB2	1.85	0.58
12:W:28:PHE:HE2	12:W:33:VAL:HG23	1.69	0.58
13:1:58:ARG:NH2	13:1:206:LEU:O	2.37	0.58
2:P:211:ASN:HB2	2:P:214:ASN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:161:LEU:HD13	13:X:163:PHE:O	2.04	0.58
13:1:90:ASP:HB3	13:1:133:VAL:HG13	1.85	0.58
2:B:211:ASN:HB2	2:B:214:ASN:HB2	1.85	0.58
14:2:75:THR:HG23	14:2:88:VAL:HG12	1.86	0.58
9:I:168:GLN:NE2	9:I:175:LEU:O	2.35	0.58
11:K:153:ASN:OD1	11:K:154:THR:N	2.37	0.58
11:V:153:ASN:OD1	11:V:154:THR:N	2.37	0.58
14:Y:100:THR:HG22	14:Y:101:LEU:H	1.69	0.58
14:2:100:THR:HG22	14:2:101:LEU:H	1.69	0.58
13:1:165:ALA:HB3	13:1:174:ILE:HG13	1.85	0.58
7:G:8:ARG:O	7:G:11:ILE:HG12	2.03	0.58
9:I:43:LEU:HD13	9:I:183:ILE:HD11	1.84	0.58
1:O:36:ARG:NH2	1:O:142:PRO:O	2.34	0.58
11:K:171:ASP:OD1	11:K:172:MET:N	2.36	0.58
6:M:6:TYR:HE1	7:N:1:MET:HA	1.63	0.58
10:U:120:LEU:HD23	10:U:152:PHE:HE2	1.69	0.58
11:V:171:ASP:OD1	11:V:172:MET:N	2.36	0.58
13:X:133:VAL:HG12	13:X:135:ALA:H	1.69	0.58
4:D:9:ASP:HB3	4:D:22:PHE:HD2	1.69	0.57
4:R:9:ASP:HB3	4:R:22:PHE:HD2	1.69	0.57
8:S:199:THR:HB	13:1:252:SER:HB2	1.87	0.57
12:Z:28:PHE:HE2	12:Z:33:VAL:HG23	1.69	0.57
11:V:90:VAL:HB	11:V:94:THR:HG23	1.85	0.57
10:J:120:LEU:HD23	10:J:152:PHE:HE2	1.69	0.57
10:J:151:SER:HB2	10:J:164:LYS:HG3	1.86	0.57
7:N:100:GLN:HG2	9:T:86:ARG:HD3	1.87	0.57
13:X:58:ARG:NH2	13:X:206:LEU:O	2.37	0.57
13:X:248:THR:O	13:X:250:VAL:N	2.37	0.57
10:U:99:ARG:HD2	10:U:123:ILE:HD11	1.87	0.57
14:Y:124:CYS:HB3	14:Y:169:MET:HB2	1.85	0.57
14:2:160:CYS:SG	14:2:163:ARG:NH2	2.73	0.57
5:L:24:GLN:NE2	4:R:13:SER:O	2.37	0.57
7:N:32:GLY:HA2	7:N:50:ARG:CZ	2.35	0.57
2:B:110:GLU:HA	2:B:154:PHE:HE2	1.70	0.57
8:S:195:ILE:HG13	13:1:258:LEU:HD11	1.87	0.57
9:T:38:MET:O	9:T:65:GLN:NE2	2.33	0.57
6:M:6:TYR:HE1	7:N:1:MET:CA	2.14	0.57
1:O:199:VAL:HG12	1:O:201:SER:H	1.70	0.57
3:Q:50:LYS:HB3	3:Q:59:HIS:HB3	1.87	0.57
10:J:99:ARG:HD2	10:J:123:ILE:HD11	1.87	0.56
14:Y:75:THR:HG23	14:Y:88:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:66:ARG:HH22	13:X:203:LEU:HB3	1.70	0.56
1:A:199:VAL:HG12	1:A:201:SER:H	1.70	0.56
6:F:52:GLN:HB3	6:F:57:TYR:CD2	2.40	0.56
9:I:185:ARG:HB2	9:I:185:ARG:NH1	2.19	0.56
1:O:146:GLN:OE1	1:O:159:ASN:ND2	2.35	0.56
13:1:248:THR:O	13:1:250:VAL:N	2.37	0.56
4:R:42:CYS:HB3	4:R:190:VAL:HG21	1.87	0.56
4:D:42:CYS:HB3	4:D:190:VAL:HG21	1.87	0.56
11:K:96:LEU:HD13	11:K:157:ILE:HG13	1.88	0.56
2:P:42:THR:HG22	2:P:44:GLU:H	1.70	0.56
6:F:86:LEU:HD13	6:F:134:LEU:HD11	1.88	0.56
10:U:151:SER:HB2	10:U:164:LYS:HG3	1.86	0.56
14:2:105:LYS:HB3	14:2:117:MET:HB3	1.88	0.56
2:B:76:CYS:SG	2:B:77:ALA:N	2.79	0.56
7:N:31:ALA:O	7:N:50:ARG:NH2	2.39	0.56
2:P:76:CYS:SG	2:P:77:ALA:N	2.79	0.56
11:V:96:LEU:HD13	11:V:157:ILE:HG13	1.88	0.56
3:C:156:CYS:HG	4:D:59:TYR:HD1	1.53	0.55
2:P:110:GLU:HA	2:P:154:PHE:HE2	1.70	0.55
13:1:180:ARG:NH1	13:1:196:GLU:OE1	2.39	0.55
7:N:123:GLN:HA	1:O:125:ARG:HE	1.71	0.55
8:S:33:GLN:HE22	14:Y:238:ARG:HB3	1.72	0.55
8:S:44:PRO:HA	8:S:50:TYR:HD1	1.71	0.55
2:B:108:THR:OG1	2:B:147:ASP:OD2	2.22	0.55
6:M:195:LEU:O	6:M:199:PHE:N	2.38	0.55
1:O:121:SER:HB2	1:O:124:ARG:HG3	1.89	0.55
2:P:108:THR:OG1	2:P:147:ASP:OD2	2.22	0.55
10:U:55:THR:HB	10:U:67:ASP:HA	1.89	0.55
7:N:3:ARG:NH2	2:P:11:GLY:HA3	2.21	0.55
9:T:168:GLN:NE2	9:T:175:LEU:O	2.35	0.55
2:B:42:THR:HG22	2:B:44:GLU:H	1.70	0.55
5:E:93:ARG:NE	5:E:121:ILE:HD13	2.21	0.55
6:M:86:LEU:HD13	6:M:134:LEU:HD11	1.88	0.55
8:S:58:THR:O	9:T:85:ARG:NH2	2.40	0.55
3:C:50:LYS:HB3	3:C:59:HIS:HB3	1.87	0.55
11:K:88:MET:SD	11:K:109:LYS:HG3	2.47	0.55
2:P:161:THR:HG1	3:Q:78:THR:HG1	1.55	0.55
2:B:13:ASN:HB3	3:C:126:ARG:HB3	1.90	0.54
2:B:74:ILE:HG12	2:B:109:VAL:HG22	1.90	0.54
12:W:156:GLY:HA3	12:Z:154:ILE:HG22	1.89	0.54
14:Y:176:TRP:CE2	14:Y:253:GLU:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:NH2	1:A:142:PRO:O	2.34	0.54
8:H:44:PRO:HA	8:H:50:TYR:HD1	1.72	0.54
1:O:31:THR:OG1	1:O:163:ARG:O	2.21	0.54
14:Y:187:ASP:OD1	14:Y:188:GLU:N	2.36	0.54
9:I:172:ILE:HG22	9:T:173:LEU:HD22	1.89	0.54
10:J:208:ILE:HG21	13:1:237:ARG:HG2	1.89	0.54
2:P:34:GLY:HA3	2:P:80:GLY:H	1.72	0.54
9:T:185:ARG:HB3	9:T:185:ARG:NH2	2.22	0.54
11:V:88:MET:SD	11:V:109:LYS:HG3	2.47	0.54
10:J:153:ASP:OD1	10:J:157:SER:N	2.41	0.54
11:K:82:ARG:NH1	12:Z:218:ASP:O	2.40	0.54
6:M:52:GLN:HB3	6:M:57:TYR:CD2	2.40	0.54
6:M:68:ILE:HD11	6:M:74:LEU:HD22	1.89	0.54
7:N:15:GLU:OE1	7:N:17:ARG:NH2	2.41	0.54
9:T:45:LEU:HB2	9:T:103:LEU:HB2	1.90	0.54
8:H:169:GLN:NE2	10:U:185:ASN:O	2.38	0.54
11:K:223:TYR:HB3	12:Z:49:ARG:HD3	1.89	0.54
1:A:121:SER:HB2	1:A:124:ARG:HG3	1.89	0.54
5:E:110:PRO:HG2	5:E:113:MET:HB2	1.90	0.54
4:R:48:PHE:HZ	4:R:139:GLY:H	1.56	0.54
8:H:2:SER:N	8:H:5:SER:HG	2.06	0.54
8:H:153:LEU:HB3	8:H:166:THR:HG23	1.90	0.53
8:S:99:ARG:NH1	13:1:132:TYR:OH	2.40	0.53
12:W:70:ALA:HB2	13:X:157:SER:OG	2.08	0.53
8:H:58:THR:O	9:I:85:ARG:NH2	2.41	0.53
10:J:55:THR:HB	10:J:67:ASP:HA	1.89	0.53
10:J:62:SER:HB2	11:K:189:TYR:HE1	1.73	0.53
2:P:74:ILE:HG12	2:P:109:VAL:HG22	1.90	0.53
13:X:237:ARG:CZ	13:X:237:ARG:CB	2.86	0.53
13:1:40:THR:N	13:1:168:SER:HG	2.06	0.53
13:X:116:ALA:O	13:X:120:ARG:HG3	2.09	0.53
6:F:68:ILE:HD11	6:F:74:LEU:HD22	1.89	0.53
9:T:185:ARG:CZ	9:T:185:ARG:CB	2.87	0.53
5:L:224:ASN:HD21	5:L:228:ARG:HE	1.56	0.53
3:Q:158:ALA:HB1	3:Q:172:LEU:HD13	1.90	0.53
10:U:153:ASP:OD1	10:U:157:SER:N	2.41	0.53
2:B:148:GLU:OE2	10:J:109:LYS:NZ	2.41	0.53
9:I:45:LEU:HB2	9:I:103:LEU:HB2	1.90	0.53
8:S:153:LEU:HB3	8:S:166:THR:HG23	1.90	0.53
12:Z:117:HIS:HB3	12:Z:135:MET:SD	2.48	0.53
4:D:216:TRP:CD1	4:D:228:VAL:HG22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:GLU:OE1	7:G:17:ARG:NH2	2.41	0.53
5:L:110:PRO:HG2	5:L:113:MET:HB2	1.90	0.53
1:O:69:VAL:HG22	1:O:104:VAL:HG22	1.90	0.53
13:1:46:VAL:HG22	13:1:51:VAL:HG12	1.91	0.53
1:A:69:VAL:HG22	1:A:104:VAL:HG22	1.90	0.53
2:B:34:GLY:HA3	2:B:80:GLY:H	1.72	0.53
6:F:111:VAL:HG22	6:F:136:ILE:HD12	1.91	0.53
6:M:111:VAL:HG22	6:M:136:ILE:HD12	1.91	0.53
2:B:54:ILE:HD11	2:B:61:PRO:HB3	1.91	0.53
7:N:3:ARG:NH2	2:P:11:GLY:CA	2.72	0.53
4:R:216:TRP:CD1	4:R:228:VAL:HG22	2.44	0.53
13:X:40:THR:N	13:X:168:SER:HG	2.06	0.53
12:Z:172:ARG:HG3	12:Z:195:LEU:HD13	1.90	0.53
7:N:151:ASP:OD1	7:N:155:ASN:N	2.36	0.52
1:A:21:TYR:CE1	7:G:14:PRO:HA	2.44	0.52
1:A:148:ASP:OD1	1:A:149:PRO:HD2	2.10	0.52
3:C:105:VAL:HG21	3:C:136:GLY:HA3	1.92	0.52
3:C:158:ALA:HB1	3:C:172:LEU:HD13	1.90	0.52
4:D:142:SER:HB3	4:D:145:ASP:HB2	1.91	0.52
6:F:111:VAL:HG21	6:F:147:PHE:HD2	1.74	0.52
4:D:48:PHE:HZ	4:D:139:GLY:H	1.56	0.52
6:F:22:ILE:HG21	6:F:152:SER:HB3	1.91	0.52
2:P:13:ASN:HB3	3:Q:126:ARG:HB3	1.91	0.52
2:P:54:ILE:HD11	2:P:61:PRO:HB3	1.91	0.52
13:X:160:ARG:HG2	13:X:160:ARG:HH11	1.74	0.52
9:I:171:PHE:CE2	9:I:173:LEU:HB2	2.44	0.52
6:M:111:VAL:HG21	6:M:147:PHE:HD2	1.74	0.52
8:S:2:SER:N	8:S:5:SER:HG	2.06	0.52
14:Y:112:TYR:CZ	14:Y:145:ARG:HD2	2.44	0.52
9:T:170:ARG:HG3	14:Y:208:TYR:HB3	1.91	0.52
9:T:171:PHE:CE2	9:T:173:LEU:HB2	2.44	0.52
9:I:185:ARG:NH1	9:I:185:ARG:CB	2.73	0.52
9:T:145:ARG:HG3	14:Y:230:ARG:HD3	1.91	0.52
10:U:64:HIS:HB3	11:V:177:TYR:CZ	2.44	0.52
14:2:187:ASP:OD1	14:2:188:GLU:N	2.36	0.52
2:B:10:ARG:NH1	2:B:10:ARG:CB	2.73	0.52
2:B:146:VAL:HG11	2:B:222:PRO:HA	1.92	0.52
8:H:123:SER:HB3	8:H:137:VAL:HB	1.92	0.52
2:B:99:HIS:CE1	2:B:103:TYR:HD2	2.28	0.52
2:P:146:VAL:HG11	2:P:222:PRO:HA	1.92	0.52
13:X:46:VAL:HG22	13:X:51:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:138:TYR:CD2	14:Y:146:ILE:HB	2.45	0.52
5:E:106:GLY:CA	13:X:120:ARG:CD	2.84	0.51
9:T:55:GLN:OE1	14:2:163:ARG:NH1	2.42	0.51
3:C:6:TYR:OH	4:D:9:ASP:OD2	2.28	0.51
7:G:3:ARG:O	7:G:4:ARG:C	2.49	0.51
4:R:216:TRP:CD1	4:R:228:VAL:HA	2.45	0.51
8:S:123:SER:HB3	8:S:137:VAL:HB	1.92	0.51
12:W:104:ARG:HD3	12:W:139:LEU:HB2	1.92	0.51
1:O:148:ASP:OD1	1:O:149:PRO:HD2	2.10	0.51
4:R:142:SER:HB3	4:R:145:ASP:HB2	1.91	0.51
8:S:2:SER:OG	8:S:3:ILE:N	2.43	0.51
9:T:164:LEU:HB3	9:T:178:PHE:CD2	2.46	0.51
11:V:72:LEU:HD11	11:V:79:ALA:HB1	1.92	0.51
13:X:84:GLY:HA2	13:X:137:LEU:HD23	1.93	0.51
12:Z:104:ARG:HD3	12:Z:139:LEU:HB2	1.92	0.51
6:M:155:TYR:HE1	7:N:60:PHE:HE2	1.56	0.51
13:X:138:ILE:HG13	13:X:166:LEU:HD12	1.93	0.51
1:A:43:LEU:HD11	1:A:134:VAL:HG21	1.93	0.51
7:N:3:ARG:O	7:N:6:ASP:HB3	2.10	0.51
2:P:99:HIS:CE1	2:P:103:TYR:HD2	2.28	0.51
13:1:84:GLY:HA2	13:1:137:LEU:HD23	1.93	0.51
13:1:138:ILE:HG13	13:1:166:LEU:HD12	1.92	0.51
14:2:138:TYR:CD2	14:2:146:ILE:HB	2.45	0.51
9:I:164:LEU:HB3	9:I:178:PHE:CD2	2.46	0.51
1:O:43:LEU:HD11	1:O:134:VAL:HG21	1.93	0.51
3:Q:105:VAL:HG21	3:Q:136:GLY:HA3	1.91	0.51
2:B:161:THR:HG1	3:C:78:THR:HG1	1.54	0.51
7:G:60:PHE:HB3	7:G:61:PHE:CD2	2.46	0.51
8:H:2:SER:OG	8:H:3:ILE:N	2.43	0.51
14:Y:73:THR:HA	14:Y:105:LYS:HE2	1.93	0.51
7:G:57:ASP:HB3	7:G:59:VAL:HG13	1.93	0.51
8:H:26:ARG:HB3	8:H:37:THR:O	2.11	0.51
6:M:22:ILE:HG21	6:M:152:SER:HB3	1.91	0.51
8:S:28:PHE:HB2	8:S:39:PHE:HB2	1.92	0.51
4:D:216:TRP:CD1	4:D:228:VAL:HA	2.45	0.51
4:D:216:TRP:HE1	4:D:228:VAL:HG13	1.76	0.51
7:N:21:VAL:HG11	7:N:153:SER:HB3	1.93	0.51
10:U:161:ASP:OD1	10:U:162:SER:N	2.44	0.51
14:Y:160:CYS:HA	14:Y:163:ARG:HG3	1.93	0.51
4:D:216:TRP:HD1	4:D:228:VAL:HA	1.76	0.50
7:G:21:VAL:HG11	7:G:153:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:198:ARG:HD3	13:X:250:VAL:HG21	1.92	0.50
11:K:72:LEU:HD11	11:K:79:ALA:HB1	1.92	0.50
8:S:26:ARG:HB3	8:S:37:THR:O	2.11	0.50
9:I:8:GLN:HE21	9:I:113:PRO:HG2	1.76	0.50
7:N:57:ASP:HB3	7:N:59:VAL:HG13	1.93	0.50
7:N:76:VAL:HG13	7:N:132:VAL:HG13	1.94	0.50
3:Q:72:ILE:HG22	3:Q:134:ILE:HG13	1.94	0.50
12:W:103:VAL:HG13	12:W:118:LEU:HD12	1.93	0.50
1:A:5:ARG:HH12	7:G:8:ARG:HD3	1.75	0.50
3:C:45:VAL:HG22	3:C:214:ILE:HG12	1.93	0.50
6:F:74:LEU:HD13	6:F:136:ILE:HG12	1.94	0.50
7:G:151:ASP:OD1	7:G:155:ASN:N	2.36	0.50
7:N:62:SER:OG	7:N:212:GLU:OE1	2.22	0.50
9:T:185:ARG:CG	9:T:185:ARG:NH2	2.73	0.50
10:U:215:VAL:HG22	13:X:63:SER:HB2	1.94	0.50
2:B:129:ASP:HB2	2:B:130:PRO:HD2	1.94	0.50
3:C:72:ILE:HG22	3:C:134:ILE:HG13	1.94	0.50
8:H:28:PHE:HB2	8:H:39:PHE:HB2	1.92	0.50
11:K:72:LEU:HD22	11:K:229:TYR:HB2	1.94	0.50
11:K:78:LEU:HD13	12:Z:153:TYR:CE1	2.47	0.50
5:L:56:VAL:HG13	5:L:61:LEU:HD23	1.94	0.50
1:O:5:ARG:O	1:O:123:GLY:N	2.44	0.50
9:I:145:ARG:NE	14:2:230:ARG:CD	2.75	0.50
13:X:151:SER:O	13:X:158:TYR:HA	2.11	0.50
13:X:60:THR:HB	13:X:64:VAL:O	2.12	0.50
14:2:79:LYS:HE2	14:2:196:ASN:HA	1.94	0.50
1:A:195:LEU:O	1:A:199:VAL:HG23	2.12	0.50
2:B:97:GLN:HB3	14:Y:133:LYS:HG3	1.94	0.50
7:G:235:GLN:HE21	7:G:239:LYS:HE3	1.77	0.50
5:L:115:CYS:SG	5:L:140:LEU:HD12	2.52	0.50
14:Y:79:LYS:HE2	14:Y:196:ASN:HA	1.94	0.50
11:V:72:LEU:HD22	11:V:229:TYR:HB2	1.94	0.49
3:C:67:ASP:OD1	3:C:68:ASN:N	2.42	0.49
5:E:115:CYS:SG	5:E:140:LEU:HD12	2.52	0.49
5:E:163:PHE:HB2	5:E:166:THR:HG22	1.94	0.49
1:O:195:LEU:O	1:O:199:VAL:HG23	2.12	0.49
3:Q:45:VAL:HG22	3:Q:214:ILE:HG12	1.93	0.49
4:R:216:TRP:HD1	4:R:228:VAL:HA	1.76	0.49
2:B:167:ALA:HB3	2:B:181:LEU:HD21	1.94	0.49
2:P:76:CYS:HG	2:P:143:PHE:HE1	1.59	0.49
2:P:167:ALA:HB3	2:P:181:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:216:PHE:O	12:W:217:TYR:C	2.50	0.49
14:Y:110:ASN:OD1	14:Y:113:LEU:HD12	2.13	0.49
5:E:56:VAL:HG13	5:E:61:LEU:HD23	1.94	0.49
5:L:163:PHE:HB2	5:L:166:THR:HG22	1.94	0.49
3:Q:120:THR:HG22	3:Q:127:PRO:HB3	1.94	0.49
12:Z:103:VAL:HG13	12:Z:118:LEU:HD12	1.93	0.49
3:C:122:ARG:HH21	6:F:4:ARG:HH22	1.60	0.49
4:D:73:HIS:HE1	4:D:107:ILE:O	1.94	0.49
13:X:158:TYR:CD1	13:X:158:TYR:C	2.85	0.49
14:2:110:ASN:OD1	14:2:113:LEU:HD12	2.13	0.49
1:O:83:VAL:HG21	1:O:129:ILE:HD11	1.95	0.49
4:R:73:HIS:ND1	4:R:223:GLY:O	2.39	0.49
4:R:216:TRP:HE1	4:R:228:VAL:HG13	1.76	0.49
14:Y:169:MET:H	14:Y:188:GLU:HB3	1.78	0.49
6:F:195:LEU:O	6:F:199:PHE:N	2.38	0.49
7:G:76:VAL:HG13	7:G:132:VAL:HG13	1.94	0.49
9:T:8:GLN:HE21	9:T:113:PRO:HG2	1.76	0.49
13:X:163:PHE:C	13:X:163:PHE:CD1	2.85	0.49
7:G:3:ARG:O	7:G:5:TYR:N	2.46	0.49
6:M:74:LEU:HD13	6:M:136:ILE:HG12	1.94	0.49
8:S:130:PRO:HG3	13:1:96:ARG:HH22	1.78	0.49
12:W:146:ILE:HD11	12:W:155:TYR:CD1	2.46	0.49
13:X:87:VAL:HB	13:X:90:ASP:HB2	1.93	0.49
14:Y:91:ARG:HH11	14:Y:98:ILE:HD13	1.77	0.49
13:1:161:LEU:HD13	13:1:163:PHE:O	2.12	0.49
2:P:129:ASP:HB2	2:P:130:PRO:HD2	1.94	0.49
9:T:166:GLU:OE1	14:Y:212:ASP:HB3	2.11	0.49
3:C:121:GLN:NE2	4:D:132:PHE:HE1	2.11	0.49
6:F:177:ARG:HE	6:F:190:THR:HG22	1.78	0.49
7:G:161:ALA:HB1	7:G:175:LEU:HD13	1.95	0.49
9:I:145:ARG:HG3	14:2:230:ARG:HD3	1.95	0.49
10:J:161:ASP:OD1	10:J:162:SER:N	2.44	0.49
14:2:169:MET:H	14:2:188:GLU:HB3	1.78	0.49
1:A:5:ARG:O	1:A:123:GLY:N	2.44	0.48
1:A:81:ARG:CZ	7:G:154:GLY:O	2.61	0.48
2:B:85:ALA:HB2	2:B:139:VAL:HG21	1.94	0.48
2:P:85:ALA:HB2	2:P:139:VAL:HG21	1.94	0.48
9:T:145:ARG:NH1	14:Y:213:SER:OG	2.46	0.48
10:U:55:THR:OG1	10:U:220:ALA:HB3	2.13	0.48
13:X:238:SER:O	13:X:240:GLN:N	2.46	0.48
7:G:100:GLN:HG2	9:I:86:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:5:ILE:HD12	9:I:139:THR:HG21	1.95	0.48
11:K:169:TYR:HB2	11:K:182:LEU:HD13	1.95	0.48
9:T:175:LEU:HB3	9:T:178:PHE:CE1	2.49	0.48
12:Z:58:HIS:CG	12:Z:59:GLN:H	2.31	0.48
13:1:61:ASN:O	13:1:64:VAL:HG22	2.13	0.48
3:C:107:ARG:NH2	11:K:119:GLU:HG3	2.26	0.48
7:G:3:ARG:H	7:G:3:ARG:HD2	1.78	0.48
8:S:16:GLY:HA3	8:S:163:LEU:HD11	1.95	0.48
9:T:185:ARG:NH2	9:T:185:ARG:CB	2.76	0.48
10:U:205:ASP:OD2	13:X:239:SER:CB	2.57	0.48
13:1:87:VAL:HB	13:1:90:ASP:HB2	1.93	0.48
7:G:185:THR:O	7:G:189:ALA:N	2.45	0.48
2:P:71:ASP:OD1	2:P:72:ALA:N	2.43	0.48
8:S:101:GLY:N	8:S:102:PRO:HD3	2.29	0.48
3:C:120:THR:HG22	3:C:127:PRO:HB3	1.94	0.48
5:L:143:ILE:HG12	5:L:149:PRO:HA	1.95	0.48
3:Q:182:CYS:SG	3:Q:190:HIS:NE2	2.86	0.48
11:V:59:LEU:HD23	11:V:66:VAL:CG1	2.44	0.48
11:V:223:TYR:HB3	12:W:49:ARG:HD3	1.96	0.48
11:V:169:TYR:HB2	11:V:182:LEU:HD13	1.95	0.48
1:A:83:VAL:HG21	1:A:129:ILE:HD11	1.95	0.48
2:B:91:LYS:HG2	2:B:119:LEU:HD11	1.95	0.48
9:I:175:LEU:HB3	9:I:178:PHE:CE1	2.49	0.48
2:P:91:LYS:HG2	2:P:119:LEU:HD11	1.95	0.48
13:X:61:ASN:O	13:X:64:VAL:HG22	2.13	0.48
5:E:143:ILE:HG12	5:E:149:PRO:HA	1.95	0.48
5:L:224:ASN:HD21	5:L:228:ARG:NE	2.12	0.48
7:N:185:THR:O	7:N:189:ALA:N	2.45	0.48
12:W:54:LEU:HD12	12:W:54:LEU:N	2.29	0.48
13:X:174:ILE:HG23	13:X:175:ALA:N	2.28	0.48
12:Z:217:TYR:CZ	12:Z:219:GLU:HB2	2.49	0.48
8:H:44:PRO:HA	8:H:50:TYR:CD1	2.49	0.47
8:H:125:ASP:OD1	8:H:126:LEU:N	2.44	0.47
10:J:55:THR:OG1	10:J:220:ALA:HB3	2.13	0.47
12:W:124:ASP:OD1	12:W:128:GLY:N	2.46	0.47
13:X:90:ASP:HB3	13:X:133:VAL:HG13	1.95	0.47
4:D:149:LEU:HD22	4:D:161:TYR:HB2	1.96	0.47
8:H:16:GLY:HA3	8:H:163:LEU:HD11	1.95	0.47
8:S:44:PRO:HA	8:S:50:TYR:CD1	2.48	0.47
5:E:206:LEU:HD12	5:E:210:PHE:HZ	1.79	0.47
8:H:120:PHE:HE2	8:H:122:CYS:HG	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:CYS:SG	3:C:190:HIS:NE2	2.86	0.47
4:D:71:ASP:OD1	4:D:72:ARG:N	2.45	0.47
5:E:93:ARG:HE	5:E:121:ILE:HG21	1.79	0.47
1:O:144:LEU:HD22	1:O:156:TRP:HB2	1.97	0.47
9:T:141:SER:HB3	14:Y:210:VAL:HG23	1.96	0.47
12:Z:152:THR:HA	12:Z:155:TYR:HE2	1.79	0.47
8:H:199:THR:HB	13:X:252:SER:HB2	1.97	0.47
7:N:161:ALA:HB1	7:N:175:LEU:HD13	1.95	0.47
8:S:125:ASP:OD1	8:S:126:LEU:N	2.44	0.47
8:S:145:GLN:NE2	14:Y:97:TYR:HD1	2.12	0.47
12:Z:124:ASP:OD1	12:Z:128:GLY:N	2.46	0.47
5:E:47:CYS:HB3	5:E:221:THR:HG22	1.97	0.47
6:F:143:ARG:NH2	6:F:145:TYR:OH	2.32	0.47
3:Q:52:ALA:HB2	3:Q:59:HIS:NE2	2.30	0.47
8:S:129:CYS:HB2	13:I:89:ALA:HB2	1.97	0.47
9:T:5:ILE:HD12	9:T:139:THR:HG21	1.95	0.47
10:U:120:LEU:HD23	10:U:152:PHE:CE2	2.49	0.47
14:Y:131:LEU:HD22	14:Y:155:LEU:HB2	1.96	0.47
14:2:91:ARG:NH2	14:2:240:SER:O	2.48	0.47
11:K:106:GLN:HA	11:K:109:LYS:HB3	1.97	0.47
13:X:148:GLN:HG2	13:X:160:ARG:HH21	1.80	0.47
2:P:97:GLN:HB3	14:2:133:LYS:HG3	1.95	0.47
12:W:96:VAL:HB	12:W:130:GLN:OE1	2.14	0.47
12:W:217:TYR:CZ	12:W:219:GLU:HB2	2.49	0.47
4:D:41:ARG:HE	4:D:162:TRP:HA	1.80	0.47
4:D:88:LEU:HD13	4:D:136:PHE:CE2	2.50	0.47
9:I:4:LEU:HD22	9:I:45:LEU:HB3	1.97	0.47
3:Q:67:ASP:OD1	3:Q:68:ASN:N	2.42	0.47
8:H:98:LYS:HG3	8:H:103:TYR:CE2	2.50	0.46
8:S:98:LYS:HG3	8:S:103:TYR:CE2	2.51	0.46
8:S:120:PHE:HE2	8:S:122:CYS:HG	1.63	0.46
9:T:27:GLN:HE22	9:T:174:ASN:HB3	1.81	0.46
4:R:144:ASN:ND2	12:Z:126:ARG:HH21	2.13	0.46
4:R:149:LEU:HD22	4:R:161:TYR:HB2	1.96	0.46
8:S:32:ALA:HA	14:Y:240:SER:OG	2.16	0.46
9:T:19:ARG:HD3	9:T:177:THR:HG22	1.97	0.46
12:Z:56:PRO:HB3	12:Z:62:TYR:CE1	2.49	0.46
9:I:19:ARG:HD3	9:I:177:THR:HG22	1.97	0.46
9:T:4:LEU:HD22	9:T:45:LEU:HB3	1.97	0.46
12:Z:154:ILE:HG13	12:Z:154:ILE:O	2.15	0.46
14:2:131:LEU:HD22	14:2:155:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:HA	1:A:81:ARG:CZ	2.45	0.46
3:C:52:ALA:HB2	3:C:59:HIS:NE2	2.30	0.46
4:D:104:GLY:HA3	12:W:101:ASN:ND2	2.31	0.46
7:G:2:SER:O	7:G:3:ARG:C	2.54	0.46
11:K:260:ILE:HG12	13:1:161:LEU:HA	1.98	0.46
5:L:47:CYS:HB3	5:L:221:THR:HG22	1.97	0.46
7:N:137:ILE:HD12	7:N:216:LEU:HB2	1.97	0.46
4:R:88:LEU:HD13	4:R:136:PHE:CE2	2.50	0.46
10:U:150:TYR:HE1	10:U:160:ARG:HB2	1.81	0.46
11:V:117:ILE:O	11:V:121:LEU:HG	2.16	0.46
5:E:141:ILE:HG22	5:E:151:VAL:HG22	1.98	0.46
11:K:82:ARG:NH2	12:Z:219:GLU:O	2.48	0.46
5:L:106:GLY:HA3	13:1:120:ARG:HD3	1.97	0.46
5:L:206:LEU:HD12	5:L:210:PHE:HZ	1.79	0.46
6:M:108:ALA:HA	6:M:147:PHE:HE2	1.80	0.46
2:P:95:GLU:HG3	2:P:115:ALA:HB1	1.98	0.46
13:X:136:SER:OG	13:X:166:LEU:HD13	2.16	0.46
14:2:163:ARG:NH2	14:2:189:ASN:O	2.42	0.46
6:F:11:THR:HG22	6:F:19:LEU:HD22	1.97	0.46
7:G:28:ILE:HD13	7:G:133:SER:HB2	1.97	0.46
7:G:90:LEU:HD21	7:G:114:LEU:HB2	1.98	0.46
10:J:64:HIS:HB3	11:K:177:TYR:CZ	2.50	0.46
10:J:221:LEU:HB3	10:J:236:VAL:HB	1.98	0.46
5:L:126:THR:HG22	6:M:128:ARG:HH21	1.81	0.46
6:M:11:THR:HG22	6:M:19:LEU:HD22	1.97	0.46
2:P:51:GLU:HA	2:P:215:ILE:HG22	1.97	0.46
2:B:51:GLU:HA	2:B:215:ILE:HG22	1.97	0.46
6:F:108:ALA:HA	6:F:147:PHE:HE2	1.80	0.46
7:G:86:LEU:HD21	7:G:130:PHE:CD2	2.51	0.46
5:L:141:ILE:HG22	5:L:151:VAL:HG22	1.98	0.46
7:N:86:LEU:HD21	7:N:130:PHE:CD2	2.50	0.46
10:U:117:ALA:HA	10:U:152:PHE:HZ	1.81	0.46
12:W:54:LEU:N	12:W:54:LEU:CD1	2.78	0.46
2:B:10:ARG:HB3	2:B:10:ARG:NH1	2.29	0.46
7:G:62:SER:HB3	7:G:65:ILE:HB	1.98	0.46
8:H:162:HIS:HD2	13:X:242:ARG:HD2	1.81	0.46
2:P:129:ASP:OD1	2:P:132:ALA:N	2.49	0.46
13:X:202:ILE:HG23	13:X:209:GLY:HA2	1.98	0.46
1:A:144:LEU:HD22	1:A:156:TRP:HB2	1.97	0.46
2:B:95:GLU:HG3	2:B:115:ALA:HB1	1.98	0.46
1:O:88:ARG:HH11	9:T:70:ARG:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:HG13	14:Y:150:ALA:HB2	1.98	0.45
2:B:18:GLU:OE1	2:B:20:ARG:NH2	2.46	0.45
2:B:129:ASP:OD1	2:B:132:ALA:N	2.49	0.45
9:I:145:ARG:NE	14:2:230:ARG:HD2	2.31	0.45
4:R:41:ARG:HE	4:R:162:TRP:HA	1.80	0.45
11:V:260:ILE:HG12	13:X:161:LEU:HA	1.98	0.45
13:1:136:SER:OG	13:1:166:LEU:HD13	2.16	0.45
14:2:79:LYS:HB3	14:2:84:VAL:HG22	1.99	0.45
5:E:61:LEU:HD11	5:E:66:VAL:HG21	1.99	0.45
6:F:102:GLN:HE22	13:X:96:ARG:HD3	1.81	0.45
9:I:27:GLN:HE22	9:I:174:ASN:HB3	1.81	0.45
10:J:150:TYR:HE1	10:J:160:ARG:HB2	1.81	0.45
7:N:62:SER:HB3	7:N:65:ILE:HB	1.98	0.45
7:N:197:LEU:O	7:N:201:MET:HG2	2.16	0.45
5:E:163:PHE:CD2	5:E:166:THR:HG22	2.52	0.45
6:F:155:TYR:HE1	7:G:60:PHE:HE2	1.63	0.45
9:I:91:TYR:CZ	9:I:98:TYR:HE2	2.34	0.45
11:V:106:GLN:HA	11:V:109:LYS:HB3	1.97	0.45
13:1:58:ARG:HD2	13:1:65:VAL:HG22	1.98	0.45
6:F:115:ALA:O	6:F:119:GLN:HG3	2.17	0.45
11:K:117:ILE:O	11:K:121:LEU:HG	2.16	0.45
5:L:163:PHE:CD2	5:L:166:THR:HG22	2.52	0.45
6:M:115:ALA:O	6:M:119:GLN:HG3	2.17	0.45
4:R:109:LEU:HD11	4:R:138:LEU:HB3	1.98	0.45
8:S:99:ARG:HD3	8:S:127:ILE:HG23	1.99	0.45
10:U:62:SER:HB2	11:V:189:TYR:HE1	1.82	0.45
1:A:88:ARG:HH11	9:I:70:ARG:HA	1.80	0.45
4:D:9:ASP:HB3	4:D:22:PHE:CD2	2.51	0.45
7:G:137:ILE:HD12	7:G:216:LEU:HB2	1.97	0.45
6:M:121:TYR:CD1	6:M:127:VAL:HG21	2.52	0.45
4:R:35:SER:HB3	4:R:66:ARG:HH12	1.82	0.45
13:1:202:ILE:HG23	13:1:209:GLY:HA2	1.98	0.45
1:A:88:ARG:NH1	9:I:70:ARG:HA	2.32	0.45
6:F:121:TYR:HD1	6:F:127:VAL:HG21	1.82	0.45
5:L:150:GLN:HB3	5:L:152:TYR:HE2	1.82	0.45
7:N:28:ILE:HD13	7:N:133:SER:HB2	1.97	0.45
11:V:167:LEU:HG	11:V:182:LEU:HD12	1.99	0.45
12:Z:27:GLU:HA	12:Z:32:VAL:HG12	1.98	0.45
8:H:138:VAL:HB	8:H:146:MET:HE3	1.98	0.45
9:I:21:ALA:HB3	9:I:29:LYS:HB3	1.98	0.45
10:J:117:ALA:HA	10:J:152:PHE:HZ	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:159:GLN:HG3	14:2:103:VAL:HG22	1.99	0.45
13:X:58:ARG:HD2	13:X:65:VAL:HG22	1.98	0.45
9:I:145:ARG:NE	14:2:230:ARG:HD3	2.32	0.45
11:K:57:LEU:HD21	11:K:191:ALA:HB3	1.99	0.45
11:K:167:LEU:HG	11:K:182:LEU:HD12	1.99	0.45
5:L:113:MET:SD	13:1:109:THR:HA	2.57	0.45
4:D:109:LEU:HD11	4:D:138:LEU:HB3	1.98	0.45
4:D:141:TYR:CG	4:D:218:GLY:HA2	2.52	0.45
6:F:88:HIS:CE1	6:F:92:LYS:HE3	2.52	0.45
9:I:18:ASP:HB2	9:I:175:LEU:HD22	1.99	0.45
7:N:90:LEU:HD21	7:N:114:LEU:HB2	1.98	0.45
11:V:57:LEU:HD21	11:V:191:ALA:HB3	1.99	0.45
12:W:27:GLU:HA	12:W:32:VAL:HG12	1.98	0.45
5:E:190:THR:H	5:E:193:GLN:HB3	1.82	0.45
5:L:113:MET:HG3	13:1:109:THR:HG22	1.99	0.45
6:M:121:TYR:HD1	6:M:127:VAL:HG21	1.82	0.45
7:N:14:PRO:HA	1:O:21:TYR:CE1	2.52	0.45
4:R:99:PHE:CE1	4:R:103:PHE:HD2	2.35	0.45
13:X:233:LYS:CB	13:X:234:PRO:HD3	2.39	0.45
14:2:184:TYR:CE1	14:2:194:SER:HB3	2.52	0.45
5:L:73:THR:HG22	5:L:76:ILE:HB	1.98	0.44
9:T:21:ALA:HB3	9:T:29:LYS:HB3	1.98	0.44
10:U:221:LEU:HB3	10:U:236:VAL:HB	1.98	0.44
8:H:99:ARG:HD3	8:H:127:ILE:HG23	1.98	0.44
10:J:183:PHE:HE2	10:J:192:VAL:H	1.64	0.44
11:K:53:GLY:O	11:K:227:ARG:NH1	2.49	0.44
4:R:141:TYR:CG	4:R:218:GLY:HA2	2.52	0.44
9:T:18:ASP:HB2	9:T:175:LEU:HD22	1.98	0.44
14:Y:136:ARG:NH2	14:Y:140:LEU:HD21	2.33	0.44
3:C:69:HIS:CD2	3:C:70:ILE:HG13	2.52	0.44
4:D:125:LEU:HD23	5:E:131:MET:HE1	1.98	0.44
6:F:121:TYR:CD1	6:F:127:VAL:HG21	2.52	0.44
2:P:209:LYS:O	2:P:214:ASN:ND2	2.51	0.44
3:Q:40:SER:HB3	3:Q:187:LEU:HD12	2.00	0.44
11:V:155:MET:HE3	11:V:170:VAL:HG21	1.99	0.44
14:Y:79:LYS:HB3	14:Y:84:VAL:HG22	1.98	0.44
14:Y:100:THR:HG22	14:Y:101:LEU:N	2.31	0.44
7:G:197:LEU:O	7:G:201:MET:HG2	2.16	0.44
8:H:34:MET:HG2	8:H:35:VAL:N	2.33	0.44
5:L:103:TYR:C	13:1:120:ARG:HH12	2.20	0.44
8:S:203:ARG:HA	14:Y:265:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:233:LYS:HB3	13:X:234:PRO:CD	2.41	0.44
2:B:76:CYS:HG	2:B:143:PHE:HE1	1.64	0.44
5:E:72:ILE:HG21	5:E:114:LEU:HD21	2.00	0.44
5:E:123:GLN:NE2	6:F:81:PRO:O	2.50	0.44
5:E:150:GLN:HB3	5:E:152:TYR:HE2	1.82	0.44
5:L:190:THR:H	5:L:193:GLN:HB3	1.82	0.44
1:O:158:ALA:HB3	2:P:58:LEU:HD13	1.99	0.44
1:A:80:ALA:HA	1:A:129:ILE:HD13	2.00	0.44
4:D:35:SER:HB3	4:D:66:ARG:HH12	1.82	0.44
4:D:99:PHE:CE1	4:D:103:PHE:HD2	2.35	0.44
7:G:41:ASP:O	7:G:186:LEU:HB2	2.18	0.44
11:K:54:THR:H	11:K:86:ARG:NH2	2.15	0.44
5:L:61:LEU:HD11	5:L:66:VAL:HG21	1.99	0.44
4:R:9:ASP:HB3	4:R:22:PHE:CD2	2.51	0.44
10:U:183:PHE:HE2	10:U:192:VAL:H	1.64	0.44
11:V:130:PRO:HB2	11:V:166:PHE:CD2	2.53	0.44
11:V:167:LEU:O	11:V:178:GLU:HG3	2.18	0.44
14:Y:184:TYR:CE1	14:Y:194:SER:HB3	2.52	0.44
4:D:191:VAL:HG21	4:D:216:TRP:CZ2	2.53	0.44
8:H:49:LEU:HD21	8:H:87:LEU:HD22	2.00	0.44
8:H:140:GLY:N	8:H:143:THR:HG22	2.33	0.44
10:J:212:GLU:HB3	13:1:68:LYS:HE3	2.00	0.44
12:Z:58:HIS:CD2	12:Z:94:PRO:HD2	2.53	0.44
12:Z:152:THR:HA	12:Z:155:TYR:CE2	2.53	0.44
10:J:120:LEU:HD23	10:J:152:PHE:CE2	2.49	0.44
8:S:34:MET:HG2	8:S:35:VAL:N	2.33	0.44
2:B:71:ASP:OD1	2:B:72:ALA:N	2.43	0.44
3:C:40:SER:HB3	3:C:187:LEU:HD12	1.99	0.44
5:E:73:THR:HG22	5:E:76:ILE:HB	1.98	0.44
7:N:41:ASP:O	7:N:186:LEU:HB2	2.18	0.44
2:P:68:VAL:HG21	2:P:89:ILE:HD13	1.99	0.44
11:V:54:THR:H	11:V:86:ARG:NH2	2.15	0.44
14:Y:124:CYS:O	14:Y:128:GLU:CG	2.61	0.44
3:C:89:ARG:NH1	10:J:105:HIS:HB3	2.31	0.43
11:K:130:PRO:HB2	11:K:166:PHE:CD2	2.53	0.43
11:K:167:LEU:O	11:K:178:GLU:HG3	2.18	0.43
4:R:151:MET:O	4:R:158:SER:HA	2.18	0.43
11:V:53:GLY:O	11:V:227:ARG:NH1	2.49	0.43
14:2:204:ASN:OD1	14:2:205:SER:N	2.52	0.43
1:A:57:ARG:NH1	7:G:108:GLU:OE2	2.41	0.43
2:B:161:THR:HG21	3:C:60:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:174:MET:SD	7:G:199:LYS:HD3	2.58	0.43
13:X:77:ALA:HB3	13:X:80:ILE:HB	2.00	0.43
13:1:77:ALA:HB3	13:1:80:ILE:HB	2.01	0.43
13:1:181:PHE:HA	13:1:185:MET:HE1	2.00	0.43
3:C:103:LEU:HD12	3:C:104:PRO:HD2	2.00	0.43
8:H:53:LEU:HB2	8:H:60:VAL:HG13	2.00	0.43
11:K:192:GLN:HE21	11:K:196:ARG:HG3	1.84	0.43
6:M:15:PRO:HA	7:N:23:TYR:CE1	2.54	0.43
11:V:78:LEU:HG	12:W:153:TYR:CE1	2.53	0.43
14:Y:204:ASN:OD1	14:Y:205:SER:N	2.52	0.43
1:O:10:PHE:HE2	2:P:136:PRO:HG2	1.83	0.43
1:O:98:VAL:HG13	14:2:150:ALA:HB2	2.01	0.43
9:T:139:THR:O	9:T:142:ILE:N	2.50	0.43
13:X:158:TYR:O	13:X:158:TYR:CG	2.70	0.43
13:X:181:PHE:HA	13:X:185:MET:HE1	2.00	0.43
4:D:35:SER:HB3	4:D:66:ARG:NH1	2.33	0.43
4:D:88:LEU:HD21	4:D:132:PHE:CE2	2.54	0.43
4:D:151:MET:O	4:D:158:SER:HA	2.17	0.43
6:M:8:PHE:CZ	7:N:9:THR:HG23	2.53	0.43
7:N:136:TYR:HB2	7:N:148:TYR:HB2	2.00	0.43
7:N:136:TYR:O	7:N:147:LEU:HD12	2.19	0.43
9:T:13:VAL:HG11	9:T:105:ALA:HB1	2.01	0.43
14:2:100:THR:HG22	14:2:101:LEU:N	2.32	0.43
2:B:209:LYS:O	2:B:214:ASN:ND2	2.51	0.43
7:G:136:TYR:O	7:G:147:LEU:HD12	2.19	0.43
5:L:72:ILE:HG21	5:L:114:LEU:HD21	2.00	0.43
2:P:18:GLU:OE1	2:P:20:ARG:NH2	2.47	0.43
4:R:71:ASP:OD1	4:R:72:ARG:N	2.46	0.43
4:R:88:LEU:HD21	4:R:132:PHE:CE2	2.54	0.43
8:S:49:LEU:HD21	8:S:87:LEU:HD22	2.00	0.43
12:W:132:TYR:HA	12:W:140:ILE:O	2.18	0.43
2:B:68:VAL:HG21	2:B:89:ILE:HD13	1.99	0.43
10:J:222:LYS:HE3	10:J:224:CYS:SG	2.57	0.43
1:O:66:ASP:OD1	1:O:67:ASP:N	2.45	0.43
1:O:80:ALA:HA	1:O:129:ILE:HD13	2.00	0.43
1:O:103:THR:HG22	1:O:105:GLU:H	1.84	0.43
13:X:47:PHE:HE2	13:X:52:ILE:HG13	1.84	0.43
12:Z:146:ILE:HD11	12:Z:155:TYR:CE1	2.54	0.43
1:A:66:ASP:OD1	1:A:67:ASP:N	2.45	0.43
7:G:136:TYR:HB2	7:G:148:TYR:HB2	2.00	0.43
7:G:224:VAL:HG12	7:G:226:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:159:LYS:HB3	6:M:178:TYR:CZ	2.53	0.43
4:R:89:ALA:O	4:R:93:ARG:HG3	2.19	0.43
14:Y:183:LEU:HD22	14:Y:198:PHE:HD2	1.84	0.43
3:C:155:ASP:HB3	4:D:63:SER:HB2	2.00	0.43
4:D:89:ALA:O	4:D:93:ARG:HG3	2.19	0.43
6:F:107:THR:OG1	6:F:138:GLY:HA3	2.19	0.43
6:F:159:LYS:HB3	6:F:178:TYR:CZ	2.54	0.43
7:G:63:GLU:O	7:G:64:LYS:HB2	2.19	0.43
11:K:50:MET:O	11:K:51:VAL:HB	2.18	0.43
5:L:224:ASN:HD21	5:L:228:ARG:HD2	1.84	0.43
7:N:97:TYR:CE2	7:N:105:ILE:HA	2.54	0.43
11:V:134:HIS:CE1	11:V:176:ALA:HB1	2.54	0.43
1:A:103:THR:HG22	1:A:105:GLU:H	1.84	0.43
2:B:154:PHE:CD1	2:B:164:GLN:HA	2.54	0.43
11:K:134:HIS:CE1	11:K:176:ALA:HB1	2.54	0.43
5:L:49:VAL:HG11	5:L:195:VAL:HG22	2.00	0.43
5:L:224:ASN:HD21	5:L:228:ARG:CD	2.31	0.43
3:Q:137:TYR:CZ	3:Q:217:LYS:HA	2.54	0.43
13:1:47:PHE:HE2	13:1:52:ILE:HG13	1.84	0.43
6:M:107:THR:OG1	6:M:138:GLY:HA3	2.19	0.42
7:N:100:GLN:HE21	9:T:86:ARG:NH1	2.17	0.42
13:1:123:ARG:HD3	13:1:158:TYR:CD2	2.53	0.42
2:B:110:GLU:HA	2:B:154:PHE:CE2	2.53	0.42
3:C:98:VAL:HA	11:K:139:ARG:HG3	2.01	0.42
3:C:137:TYR:CZ	3:C:217:LYS:HA	2.54	0.42
4:D:40:ILE:HD11	4:D:182:MET:CG	2.47	0.42
8:H:66:ARG:NE	8:H:103:TYR:OH	2.52	0.42
4:R:35:SER:HB3	4:R:66:ARG:NH1	2.34	0.42
9:T:138:LEU:HD23	14:Y:205:SER:O	2.19	0.42
1:A:78:ALA:HA	1:A:81:ARG:NH1	2.35	0.42
4:D:102:ASN:HA	12:W:105:ASN:ND2	2.34	0.42
11:K:193:PRO:HG3	13:1:172:ALA:HA	2.01	0.42
8:S:53:LEU:HB2	8:S:60:VAL:HG13	2.00	0.42
10:U:35:PHE:HZ	10:U:168:SER:HB3	1.84	0.42
13:X:174:ILE:CG2	13:X:175:ALA:N	2.82	0.42
5:E:49:VAL:HG11	5:E:195:VAL:HG22	2.00	0.42
5:E:119:ALA:O	5:E:123:GLN:HG3	2.19	0.42
14:Y:245:VAL:HG12	14:Y:263:ASP:HA	2.00	0.42
13:1:233:LYS:HB3	13:1:234:PRO:HD3	2.01	0.42
7:G:97:TYR:CE2	7:G:105:ILE:HA	2.54	0.42
5:L:18:PRO:HA	6:M:24:TYR:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:90:LEU:HD21	7:N:114:LEU:HD22	2.01	0.42
2:P:91:LYS:HG2	2:P:119:LEU:CD1	2.50	0.42
9:T:168:GLN:HG3	9:T:196:PHE:HD2	1.85	0.42
14:2:245:VAL:HG12	14:2:263:ASP:HA	2.00	0.42
6:F:76:TYR:HB2	6:F:132:VAL:HG13	2.01	0.42
3:Q:103:LEU:HD12	3:Q:104:PRO:HD2	2.00	0.42
4:R:73:HIS:HD1	4:R:223:GLY:C	2.22	0.42
8:S:66:ARG:NE	8:S:103:TYR:OH	2.52	0.42
4:D:73:HIS:NE2	4:D:106:ASN:HB3	2.34	0.42
2:P:154:PHE:CD1	2:P:164:GLN:HA	2.54	0.42
7:N:123:GLN:HG3	1:O:125:ARG:HB3	2.01	0.42
3:Q:214:ILE:O	3:Q:221:PHE:HA	2.20	0.42
4:R:187:CYS:SG	4:R:220:ILE:HD11	2.59	0.42
8:S:183:MET:SD	8:S:204:MET:HE3	2.59	0.42
10:U:42:ALA:HA	10:U:50:ILE:O	2.20	0.42
14:Y:168:SER:HA	14:Y:188:GLU:OE1	2.20	0.42
12:Z:28:PHE:CE2	12:Z:33:VAL:HG23	2.53	0.42
13:1:205:ASP:OD1	13:1:206:LEU:N	2.53	0.42
5:E:163:PHE:HD2	5:E:166:THR:HG22	1.85	0.42
6:F:76:TYR:HB3	6:F:83:TYR:CD1	2.55	0.42
9:I:13:VAL:HG11	9:I:105:ALA:HB1	2.01	0.42
9:I:168:GLN:HG3	9:I:196:PHE:HD2	1.85	0.42
5:L:163:PHE:HD2	5:L:166:THR:HG22	1.85	0.42
6:M:49:GLU:HB2	6:M:195:LEU:HD23	2.01	0.42
6:M:76:TYR:HB3	6:M:83:TYR:CD1	2.55	0.42
4:R:104:GLY:HA3	12:Z:101:ASN:ND2	2.35	0.42
8:S:201:LYS:HB3	13:1:249:PRO:O	2.19	0.42
10:U:56:ARG:HH21	10:U:219:ASP:CG	2.23	0.42
9:I:35:MET:HG2	9:I:45:LEU:CD2	2.50	0.42
10:J:56:ARG:NH1	10:J:215:VAL:O	2.53	0.42
5:L:119:ALA:O	5:L:123:GLN:HG3	2.19	0.42
7:N:63:GLU:O	7:N:64:LYS:HB2	2.19	0.42
3:Q:27:GLU:O	3:Q:31:GLN:HG2	2.20	0.42
2:B:91:LYS:HG2	2:B:119:LEU:CD1	2.50	0.41
6:F:49:GLU:HB2	6:F:195:LEU:HD23	2.01	0.41
9:I:108:ASP:OD2	9:I:111:GLU:N	2.45	0.41
7:N:2:SER:O	7:N:4:ARG:N	2.53	0.41
7:N:4:ARG:C	7:N:6:ASP:H	2.23	0.41
9:T:35:MET:HG2	9:T:45:LEU:CD2	2.50	0.41
1:A:91:CYS:HA	1:A:102:VAL:HG21	2.02	0.41
9:I:101:ASN:HB3	9:I:132:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:167:ALA:CB	2:P:181:LEU:HD21	2.51	0.41
9:T:91:TYR:CD2	9:T:98:TYR:CE2	3.08	0.41
11:V:192:GLN:HE21	11:V:196:ARG:HG3	1.83	0.41
8:H:50:TYR:CD2	8:H:190:ILE:HD11	2.55	0.41
9:I:139:THR:O	9:I:142:ILE:N	2.50	0.41
11:K:139:ARG:HA	11:K:139:ARG:HD3	1.77	0.41
6:M:143:ARG:NH2	7:N:59:VAL:HG12	2.35	0.41
3:Q:88:MET:HE1	3:Q:134:ILE:HG12	2.02	0.41
3:Q:107:ARG:HE	11:V:122:LEU:HD23	1.85	0.41
11:V:59:LEU:HD23	11:V:66:VAL:HG12	2.02	0.41
1:A:186:LEU:HA	1:A:189:LYS:HB2	2.02	0.41
3:C:27:GLU:O	3:C:31:GLN:HG2	2.20	0.41
6:M:213:CYS:HB2	6:M:218:PHE:HD1	1.85	0.41
7:N:45:LEU:N	7:N:214:ALA:O	2.48	0.41
3:Q:212:ILE:HD11	3:Q:224:TYR:HD2	1.86	0.41
4:R:162:TRP:HB3	4:R:182:MET:SD	2.60	0.41
10:U:56:ARG:NH1	10:U:215:VAL:O	2.53	0.41
13:X:205:ASP:OD1	13:X:206:LEU:N	2.53	0.41
13:1:151:SER:O	13:1:158:TYR:HA	2.20	0.41
9:I:173:LEU:HD22	9:T:172:ILE:HG22	2.01	0.41
11:K:188:ALA:HA	11:K:192:GLN:HB2	2.03	0.41
12:W:127:GLU:HB2	12:W:130:GLN:NE2	2.35	0.41
13:X:158:TYR:CD1	13:X:158:TYR:O	2.74	0.41
12:Z:132:TYR:HA	12:Z:140:ILE:O	2.21	0.41
8:S:50:TYR:CD2	8:S:190:ILE:HD11	2.55	0.41
9:T:5:ILE:HD11	9:T:143:LEU:HD11	2.02	0.41
9:T:29:LYS:HD3	9:T:32:HIS:HB2	2.03	0.41
2:B:66:LYS:HE2	2:B:82:ILE:HD11	2.03	0.41
2:B:167:ALA:CB	2:B:181:LEU:HD21	2.51	0.41
7:G:45:LEU:N	7:G:214:ALA:O	2.48	0.41
7:G:99:LEU:HD12	8:H:65:GLN:HB3	2.03	0.41
8:S:36:THR:HG21	9:T:125:ALA:HB1	2.01	0.41
9:T:3:TYR:OH	9:T:139:THR:HG21	2.21	0.41
11:V:193:PRO:HG3	13:X:172:ALA:HA	2.02	0.41
2:B:10:ARG:HH11	2:B:10:ARG:CB	2.30	0.41
3:C:214:ILE:O	3:C:221:PHE:HA	2.20	0.41
6:F:213:CYS:HB2	6:F:218:PHE:HD1	1.85	0.41
9:I:102:LEU:HD12	9:I:118:MET:SD	2.60	0.41
6:M:76:TYR:HB2	6:M:132:VAL:HG13	2.01	0.41
2:P:202:LEU:HA	2:P:205:VAL:HG22	2.03	0.41
9:T:102:LEU:HD12	9:T:118:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:108:ASP:OD2	9:T:111:GLU:N	2.45	0.41
14:2:168:SER:HA	14:2:188:GLU:OE1	2.19	0.41
2:B:184:VAL:HG21	2:B:201:ILE:HD11	2.03	0.41
2:B:202:LEU:HA	2:B:205:VAL:HG22	2.03	0.41
8:H:27:ARG:NH1	8:H:180:VAL:O	2.54	0.41
8:H:36:THR:HG21	9:I:125:ALA:HB1	2.03	0.41
8:H:48:ARG:NH2	8:H:192:LYS:O	2.48	0.41
9:I:1:MET:SD	9:I:133:GLY:HA2	2.61	0.41
9:I:185:ARG:H	9:I:185:ARG:HG3	1.59	0.41
10:J:35:PHE:HZ	10:J:168:SER:HB3	1.84	0.41
10:J:236:VAL:HG13	10:J:237:PRO:HD2	2.03	0.41
11:K:224:ARG:CZ	13:1:174:ILE:HG21	2.51	0.41
1:O:186:LEU:HA	1:O:189:LYS:HB2	2.02	0.41
9:T:101:ASN:HB3	9:T:132:HIS:ND1	2.36	0.41
13:X:123:ARG:HH21	13:X:123:ARG:HG2	1.86	0.41
7:G:90:LEU:HD21	7:G:114:LEU:HD22	2.01	0.41
7:G:109:GLN:OE1	9:I:71:ASN:ND2	2.44	0.41
8:H:6:TYR:CE2	9:I:121:LEU:HD12	2.55	0.41
8:H:48:ARG:HD3	8:H:112:LEU:HD12	2.02	0.41
5:L:2:SER:OG	5:L:3:ARG:N	2.53	0.41
7:N:95:GLN:HB3	8:S:69:PHE:CD1	2.55	0.41
3:Q:195:LEU:O	3:Q:198:THR:OG1	2.30	0.41
4:R:102:ASN:HA	12:Z:105:ASN:ND2	2.35	0.41
8:S:109:ILE:HB	8:S:122:CYS:SG	2.62	0.41
12:W:54:LEU:HB3	12:W:62:TYR:HD1	1.86	0.41
3:C:212:ILE:HD11	3:C:224:TYR:HD2	1.86	0.40
6:F:74:LEU:HD23	6:F:87:VAL:HG22	2.03	0.40
9:I:117:TYR:CE1	9:I:132:HIS:CE1	3.09	0.40
5:L:107:TYR:CD2	13:1:114:ARG:HD2	2.56	0.40
7:N:4:ARG:C	7:N:6:ASP:N	2.74	0.40
1:O:12:PRO:HA	2:P:26:TYR:CE1	2.57	0.40
8:S:27:ARG:NH1	8:S:180:VAL:O	2.54	0.40
5:E:103:TYR:HB2	12:W:81:TYR:CD1	2.56	0.40
9:I:168:GLN:HG3	9:I:196:PHE:CD2	2.56	0.40
5:L:120:ASP:OD2	6:M:88:HIS:HE1	2.04	0.40
6:M:74:LEU:HD23	6:M:87:VAL:HG22	2.03	0.40
6:M:140:ASN:HB2	6:M:145:TYR:HE2	1.86	0.40
6:M:160:ALA:O	7:N:55:LEU:HD13	2.21	0.40
6:F:86:LEU:O	6:F:90:ALA:N	2.41	0.40
10:J:56:ARG:HH21	10:J:219:ASP:CG	2.23	0.40
11:K:90:VAL:HG13	11:K:116:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:194:LEU:HD21	13:1:175:ALA:O	2.21	0.40
1:O:94:HIS:CD2	1:O:102:VAL:HG22	2.56	0.40
8:S:48:ARG:HD3	8:S:112:LEU:HD12	2.02	0.40
11:V:90:VAL:HG13	11:V:116:VAL:HG21	2.03	0.40
14:2:183:LEU:HD22	14:2:198:PHE:HD2	1.84	0.40
4:D:125:LEU:HB3	5:E:131:MET:HE3	2.01	0.40
10:J:42:ALA:HA	10:J:50:ILE:O	2.20	0.40
10:J:74:LEU:HB3	10:J:100:LEU:HD11	2.04	0.40
6:M:101:TYR:HE1	8:S:90:MET:HG2	1.86	0.40
1:O:91:CYS:HA	1:O:102:VAL:HG21	2.02	0.40
2:P:182:GLN:HG2	3:Q:56:LEU:HD22	2.03	0.40
9:T:171:PHE:HE2	9:T:173:LEU:HB2	1.86	0.40
14:2:89:ASP:HB2	14:2:243:GLY:O	2.22	0.40
9:I:3:TYR:OH	9:I:139:THR:HG21	2.21	0.40
10:J:213:ARG:HA	13:1:65:VAL:HB	2.03	0.40
1:O:98:VAL:HG12	1:O:100:ASP:H	1.87	0.40
2:P:161:THR:HG21	3:Q:60:GLN:HE21	1.86	0.40
9:T:1:MET:SD	9:T:133:GLY:HA2	2.61	0.40
11:V:188:ALA:HA	11:V:192:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/248 (93%)	221 (96%)	9 (4%)	0	100	100
1	O	230/248 (93%)	220 (96%)	10 (4%)	0	100	100
2	B	232/241 (96%)	221 (95%)	10 (4%)	1 (0%)	34	66
2	P	232/241 (96%)	225 (97%)	7 (3%)	0	100	100
3	C	233/263 (89%)	225 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	233/263 (89%)	225 (97%)	8 (3%)	0	100	100
4	D	238/255 (93%)	229 (96%)	9 (4%)	0	100	100
4	R	238/255 (93%)	229 (96%)	9 (4%)	0	100	100
5	E	242/246 (98%)	231 (96%)	11 (4%)	0	100	100
5	L	241/246 (98%)	231 (96%)	10 (4%)	0	100	100
6	F	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	M	227/234 (97%)	220 (97%)	7 (3%)	0	100	100
7	G	244/261 (94%)	232 (95%)	12 (5%)	0	100	100
7	N	244/261 (94%)	231 (95%)	12 (5%)	1 (0%)	34	66
8	H	202/205 (98%)	193 (96%)	8 (4%)	1 (0%)	29	61
8	S	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	29	61
9	I	196/201 (98%)	189 (96%)	7 (4%)	0	100	100
9	T	195/201 (97%)	189 (97%)	6 (3%)	0	100	100
10	J	211/241 (88%)	206 (98%)	5 (2%)	0	100	100
10	U	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
11	K	214/264 (81%)	207 (97%)	6 (3%)	1 (0%)	29	61
11	V	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
12	W	197/219 (90%)	187 (95%)	10 (5%)	0	100	100
12	Z	197/219 (90%)	189 (96%)	8 (4%)	0	100	100
13	1	217/273 (80%)	205 (94%)	11 (5%)	1 (0%)	29	61
13	X	217/273 (80%)	205 (94%)	10 (5%)	2 (1%)	17	48
14	2	199/276 (72%)	191 (96%)	8 (4%)	0	100	100
14	Y	199/276 (72%)	192 (96%)	7 (4%)	0	100	100
All	All	6164/6854 (90%)	5919 (96%)	237 (4%)	8 (0%)	54	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	N	3	ARG
13	X	239	SER
2	B	11	GLY
8	H	115	LYS
8	S	115	LYS
11	K	51	VAL

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Mol	Chain	Res	Type
13	X	249	PRO
13	1	249	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/211 (93%)	195 (100%)	1 (0%)	88	93
1	O	196/211 (93%)	195 (100%)	1 (0%)	88	93
2	B	196/203 (97%)	196 (100%)	0	100	100
2	P	196/203 (97%)	196 (100%)	0	100	100
3	C	201/225 (89%)	201 (100%)	0	100	100
3	Q	201/225 (89%)	201 (100%)	0	100	100
4	D	198/212 (93%)	197 (100%)	1 (0%)	88	93
4	R	198/212 (93%)	198 (100%)	0	100	100
5	E	208/210 (99%)	208 (100%)	0	100	100
5	L	207/210 (99%)	207 (100%)	0	100	100
6	F	189/191 (99%)	188 (100%)	1 (0%)	88	93
6	M	188/191 (98%)	188 (100%)	0	100	100
7	G	207/221 (94%)	206 (100%)	1 (0%)	88	93
7	N	207/221 (94%)	206 (100%)	1 (0%)	88	93
8	H	174/175 (99%)	174 (100%)	0	100	100
8	S	174/175 (99%)	174 (100%)	0	100	100
9	I	169/171 (99%)	168 (99%)	1 (1%)	86	91
9	T	168/171 (98%)	167 (99%)	1 (1%)	86	91
10	J	177/198 (89%)	176 (99%)	1 (1%)	86	91
10	U	177/198 (89%)	177 (100%)	0	100	100
11	K	178/215 (83%)	176 (99%)	2 (1%)	73	85
11	V	177/215 (82%)	176 (99%)	1 (1%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	W	153/167 (92%)	153 (100%)	0	100	100
12	Z	153/167 (92%)	153 (100%)	0	100	100
13	1	170/216 (79%)	170 (100%)	0	100	100
13	X	170/216 (79%)	167 (98%)	3 (2%)	59	78
14	2	166/222 (75%)	166 (100%)	0	100	100
14	Y	166/222 (75%)	165 (99%)	1 (1%)	86	91
All	All	5160/5674 (91%)	5144 (100%)	16 (0%)	92	96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
4	D	220	ILE
6	F	184	LEU
7	G	3	ARG
9	I	185	ARG
10	J	222	LYS
11	K	50	MET
11	K	59	LEU
7	N	1	MET
1	O	38	LYS
9	T	185	ARG
11	V	59	LEU
13	X	120	ARG
13	X	158	TYR
13	X	237	ARG
14	Y	112	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	116	GLN
1	A	122	ASN
2	B	73	HIS
2	B	155	HIS
2	B	227	HIS
3	C	68	ASN
3	C	121	GLN

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Mol	Chain	Res	Type
4	D	73	HIS
4	D	144	ASN
5	E	90	GLN
5	E	123	GLN
6	F	52	GLN
6	F	102	GLN
6	F	109	GLN
7	G	235	GLN
7	G	240	HIS
8	H	33	GLN
9	I	8	GLN
9	I	27	GLN
11	K	110	GLN
11	K	114	GLN
11	K	126	HIS
11	K	192	GLN
5	L	123	GLN
5	L	224	ASN
6	M	52	GLN
6	M	88	HIS
6	M	102	GLN
6	M	109	GLN
6	M	119	GLN
6	M	207	ASN
7	N	100	GLN
7	N	102	GLN
7	N	240	HIS
1	O	94	HIS
1	O	116	GLN
2	P	73	HIS
2	P	155	HIS
2	P	227	HIS
3	Q	68	ASN
4	R	144	ASN
8	S	33	GLN
9	T	8	GLN
9	T	27	GLN
11	V	114	GLN
11	V	192	GLN
12	W	58	HIS
14	Y	234	HIS
14	Y	237	HIS

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Mol	Chain	Res	Type
14	2	234	HIS
14	2	237	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

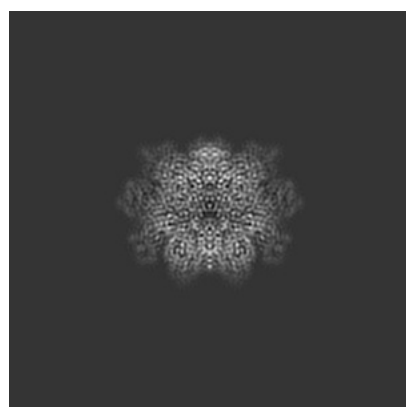
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30825. These allow visual inspection of the internal detail of the map and identification of artifacts.

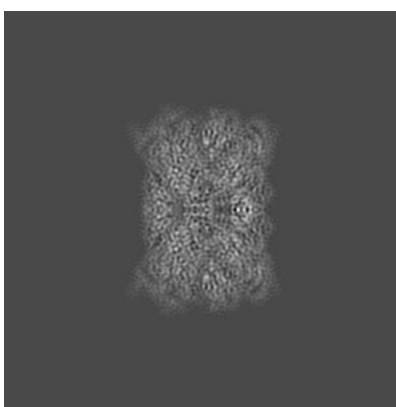
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

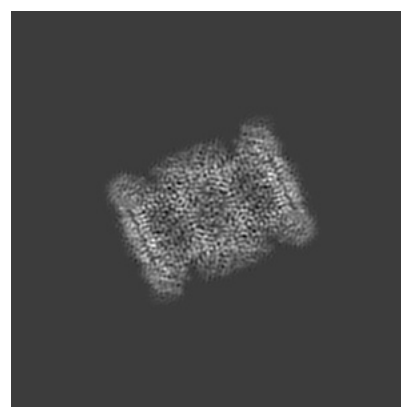
6.1.1 Primary map



X



Y

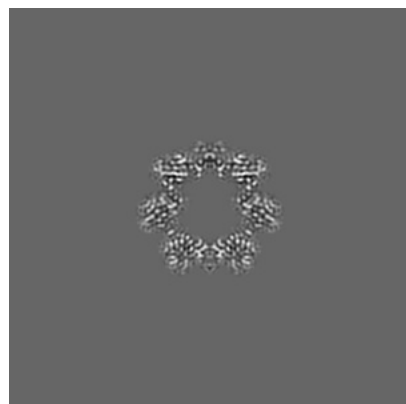


Z

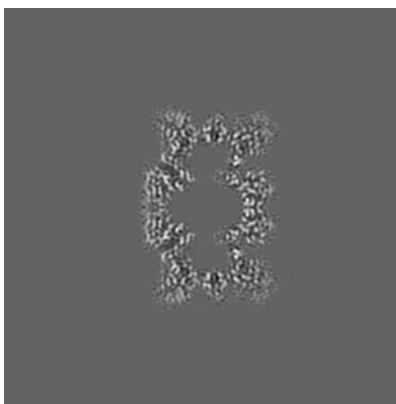
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

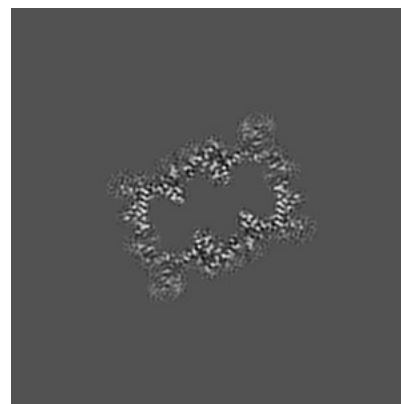
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

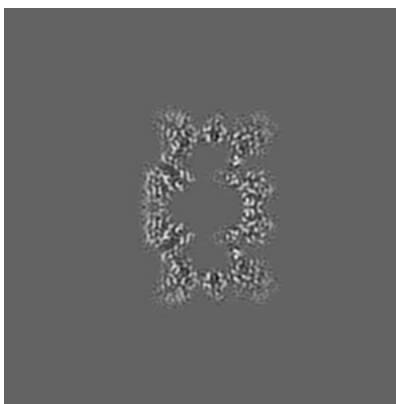
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

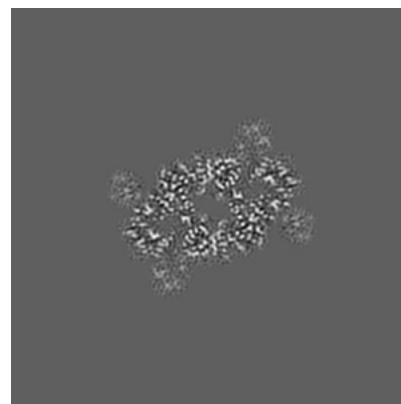
6.3.1 Primary map



X Index: 131



Y Index: 128



Z Index: 146

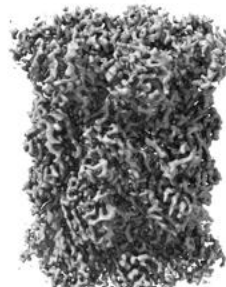
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

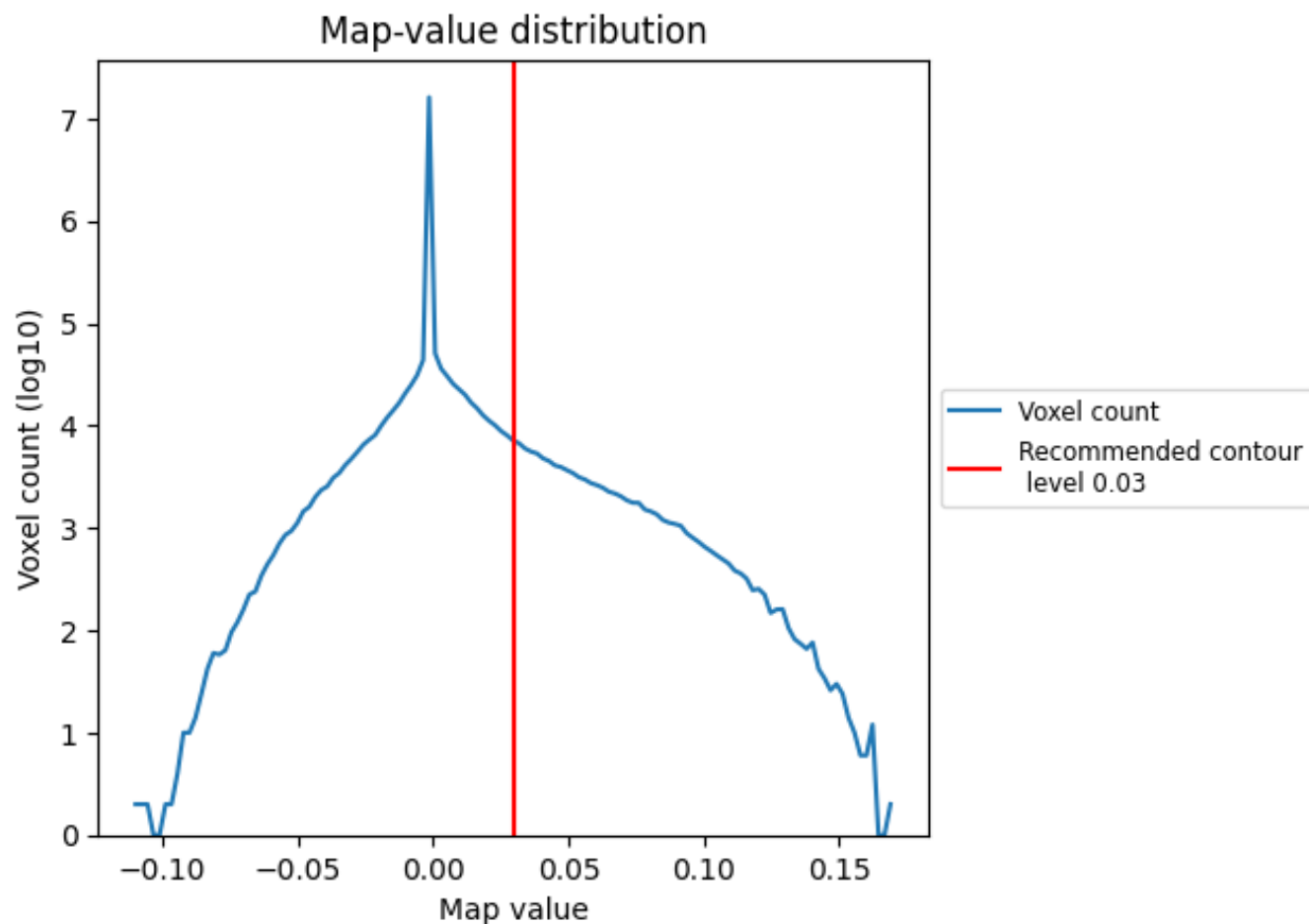
6.5 Mask visualisation

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

7 Map analysis [i](#)

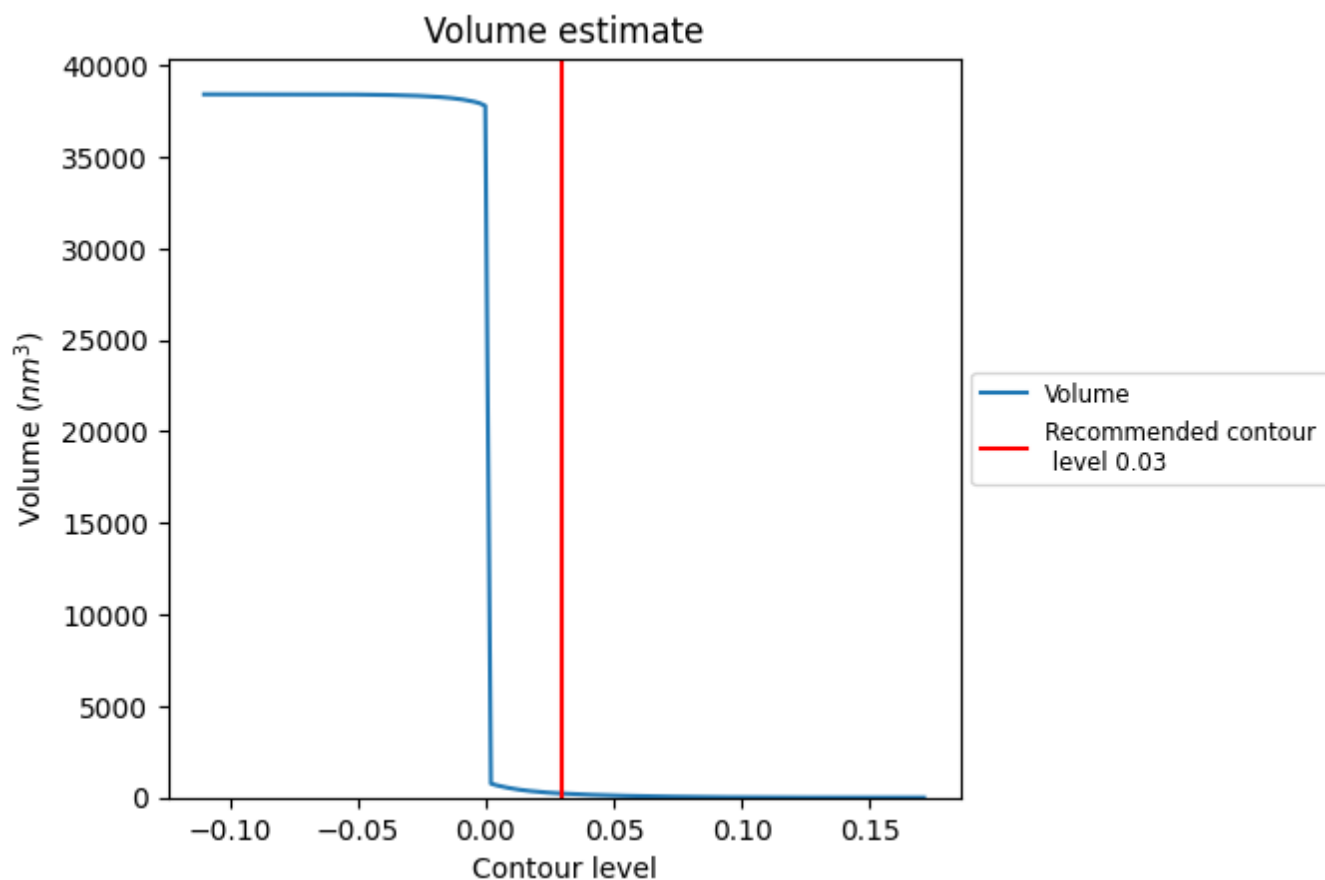
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

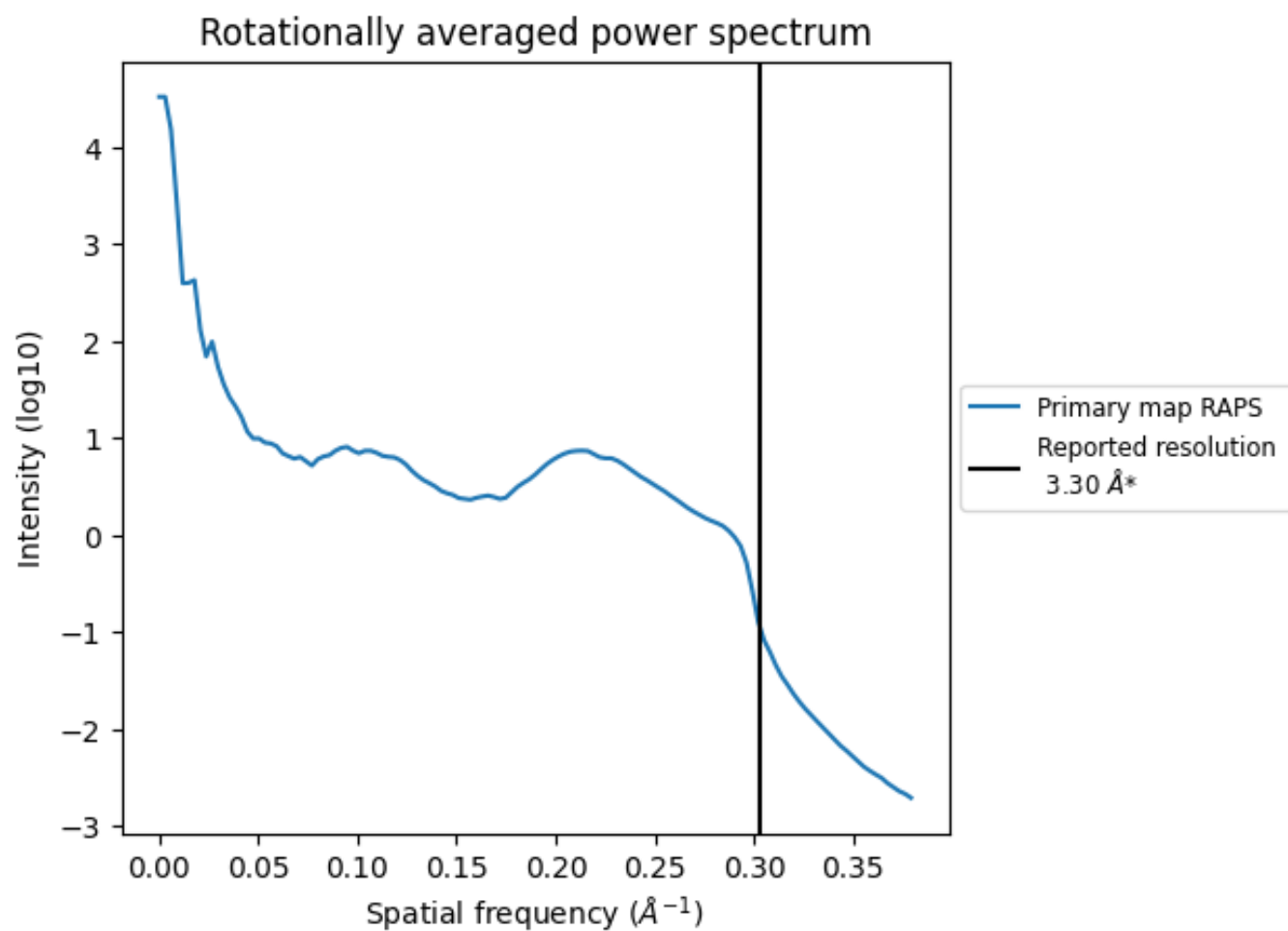
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221 nm³; this corresponds to an approximate mass of 199 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

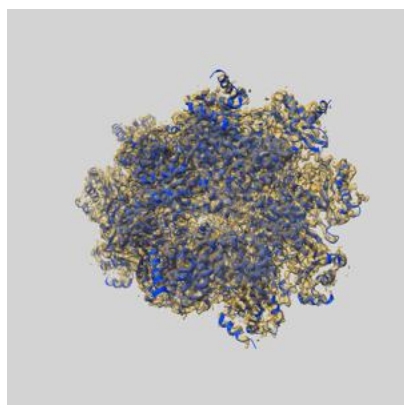
8 Fourier-Shell correlation

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

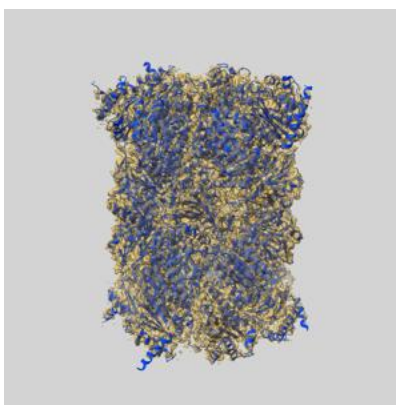
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30825 and PDB model 7DR7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

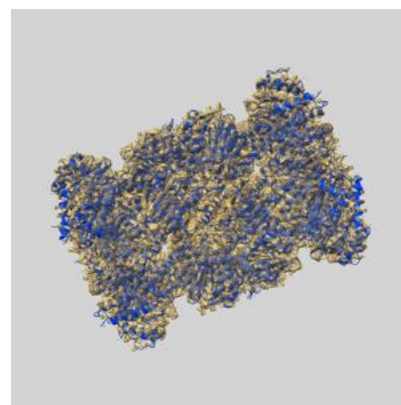
9.1 Map-model overlay [i](#)



X



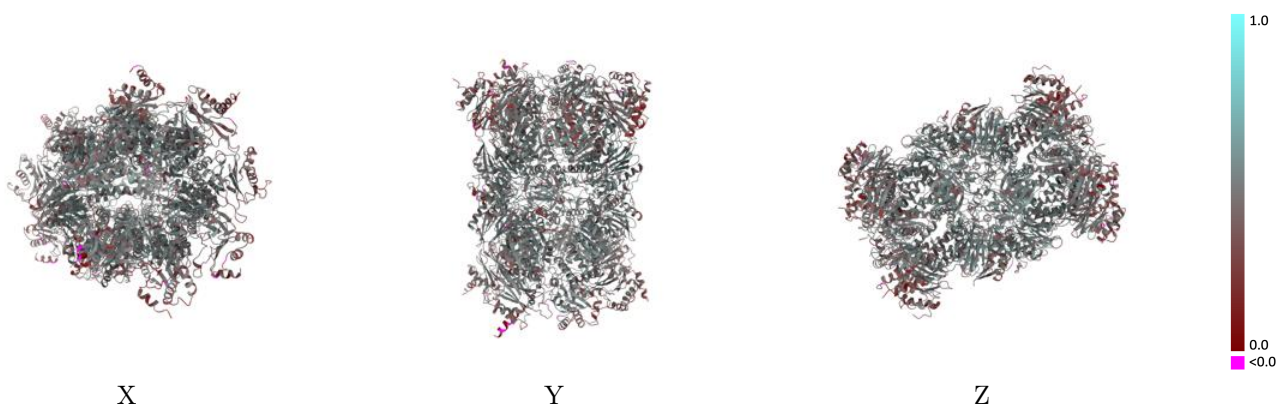
Y



Z

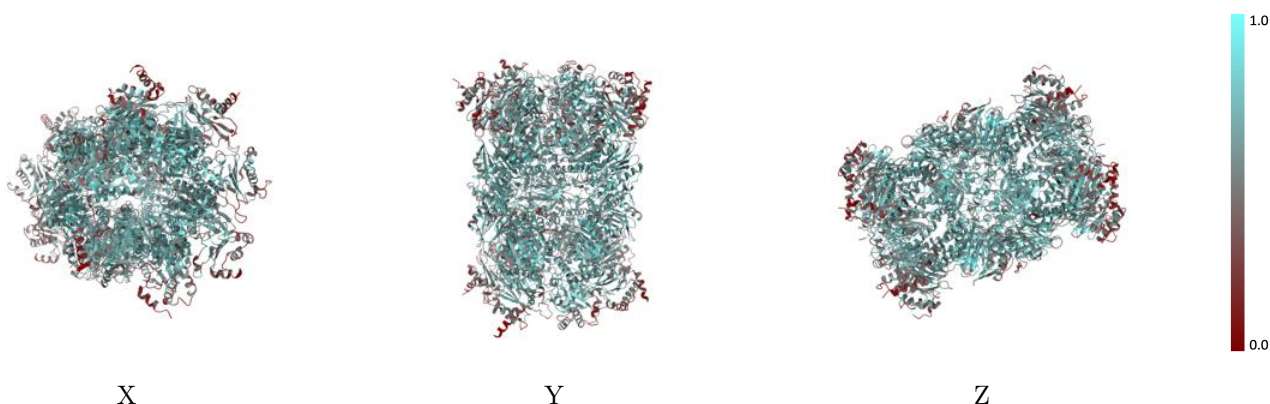
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



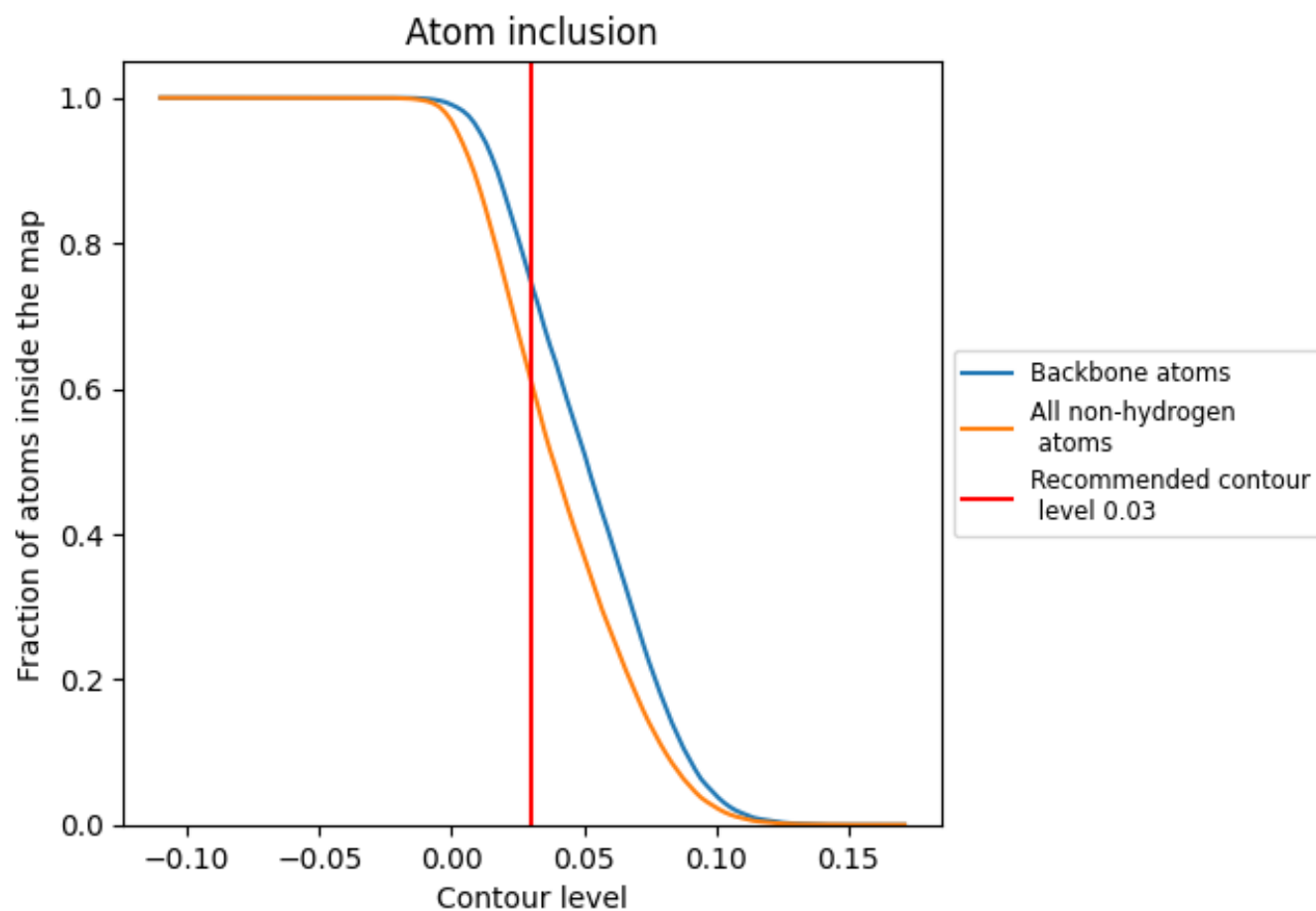
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 61% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6105	 0.4480
1	 0.6369	 0.4720
2	 0.6770	 0.4750
A	 0.5315	 0.4120
B	 0.5290	 0.4200
C	 0.5773	 0.4330
D	 0.5762	 0.4170
E	 0.5425	 0.4130
F	 0.5929	 0.4470
G	 0.5637	 0.4250
H	 0.6984	 0.4910
I	 0.6746	 0.4760
J	 0.6189	 0.4600
K	 0.6770	 0.4630
L	 0.5441	 0.4170
M	 0.5908	 0.4390
N	 0.5658	 0.4270
O	 0.5348	 0.4080
P	 0.5228	 0.4150
Q	 0.5695	 0.4300
R	 0.5707	 0.4160
S	 0.6927	 0.4870
T	 0.6766	 0.4830
U	 0.6276	 0.4660
V	 0.6813	 0.4630
W	 0.7174	 0.5010
X	 0.6458	 0.4820
Y	 0.6855	 0.4840
Z	 0.6992	 0.4890

