



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:55 PM UTC

PDB ID : 6ZIU / pdb_00006ziu
EMDB ID : EMD-11230
Title : bovine ATP synthase stator domain, state 3
Authors : Spikes, T.E.; Montgomery, M.G.; Walker, J.E.
Deposited on : 2020-06-26
Resolution : 6.02 Å (reported)
Based on initial models : 2CLY, 2WSS, 2V7Q

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

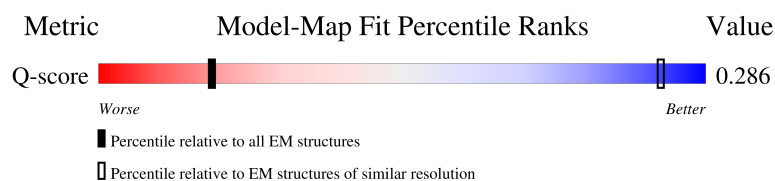
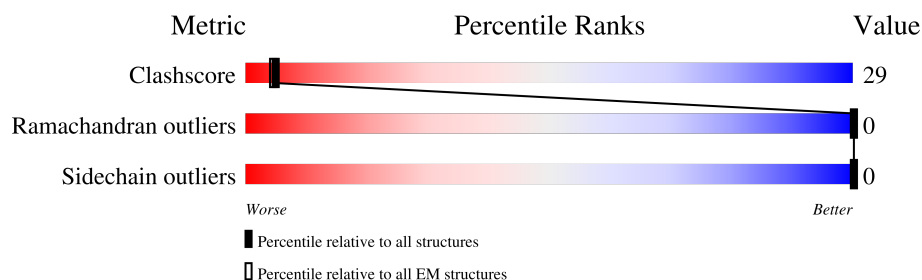
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.02 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	486 (5.57 - 6.52)

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	8	66	38% 29% 33% 38%
2	a	226	55% 45% 55%
3	d	160	38% 48% 49% .
4	e	70	37% 41% 17% 41%

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Mol	Chain	Length	Quality of chain
5	f	87	
6	g	102	
7	j	60	
8	b	214	
9	h	76	
10	S	190	
11	C	510	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 18919 atoms, of which 9636 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 ATP synthase protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	8	41	Total	C	H	N	O	S	0	0
			696	231	352	52	58	3		

- Molecule 2 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	a	226	Total	C	H	N	O	S	0	0
			3611	1155	1870	276	298	12		

- Molecule 3 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	155	Total	C	H	N	O	S	0	0
			2549	821	1276	207	242	3		

- Molecule 4 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	e	41	Total	C	H	N	O	S	0	0
			687	218	352	61	55	1		

- Molecule 5 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	f	83	Total	C	H	N	O	S	0	0
			1411	456	718	120	114	3		

- Molecule 6 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	g	79	Total	C	H	N	O	S	0	0
			1291	420	662	100	108	1		

- Molecule 7 is a protein called ATP synthase subunit ATP5MPL, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	j	48	Total	C	H	N	O	S	0	0
			828	267	428	66	65	2		

- Molecule 8 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	b	209	Total	C	H	N	O	S	0	0
			3456	1095	1755	292	308	6		

- Molecule 9 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	62	Total	C	H	N	O	S	0	0
			1009	326	495	87	99	2		

- Molecule 10 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	S	129	Total	C	H	N	O	S	0	0
			2048	627	1057	171	186	7		

- Molecule 11 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	C	89	Total	C	H	N	O	S	0	0
			1333	409	671	115	136	2		

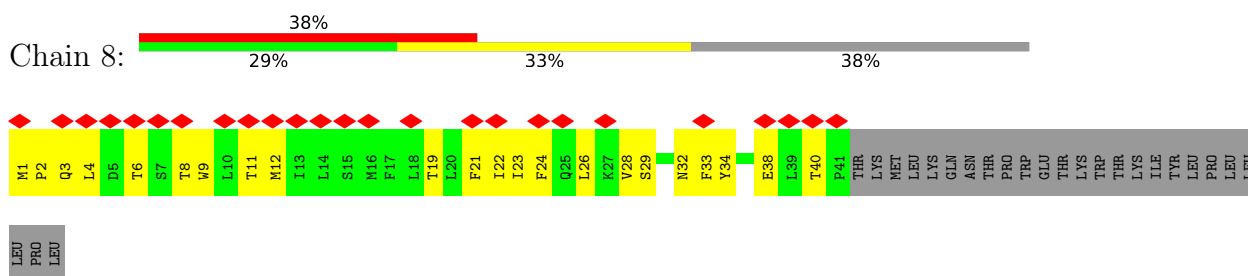
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLU	GLN	variant	UNP P19483

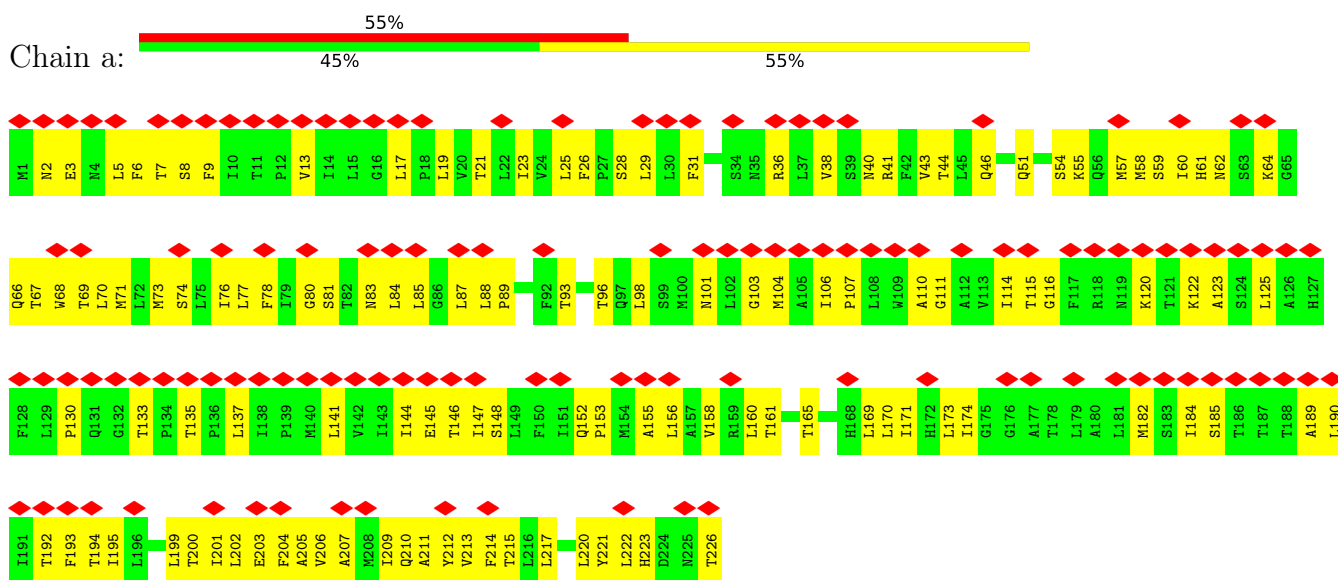
3 Residue-property plots [i](#)

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.

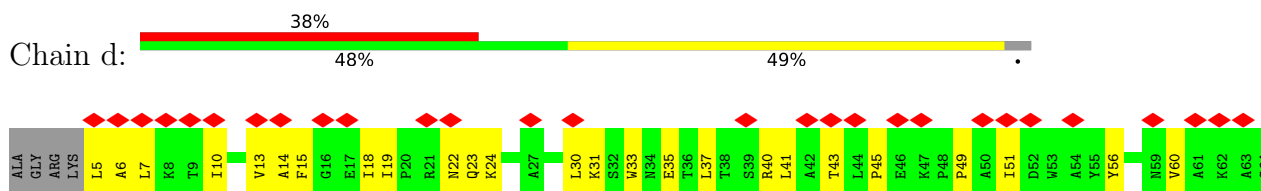
- Molecule 1: ATP synthase protein 8

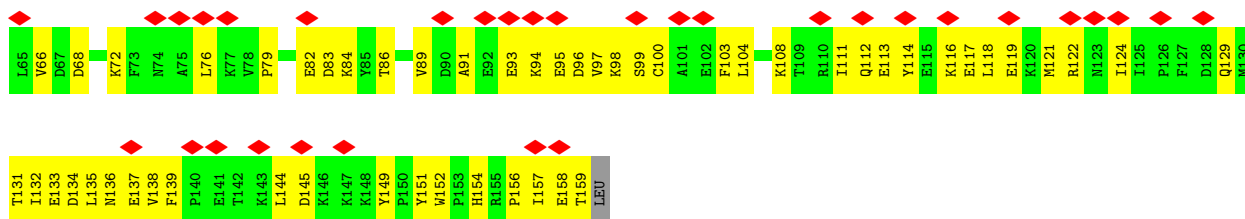


- Molecule 2: ATP synthase subunit a

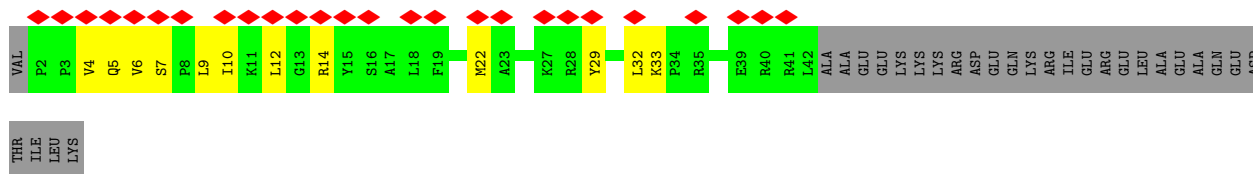


- Molecule 3: ATP synthase subunit d, mitochondrial

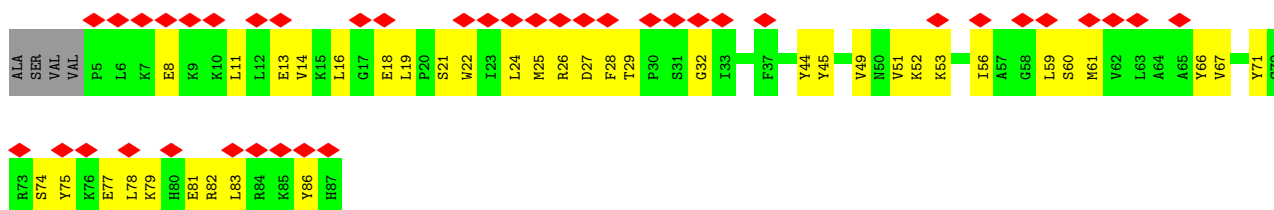




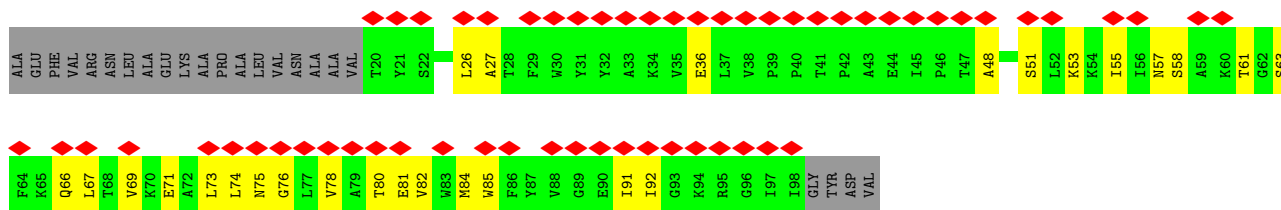
• Molecule 4: ATP synthase subunit e, mitochondrial



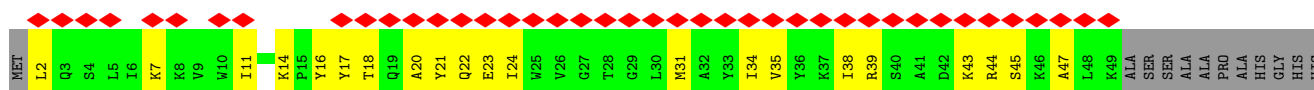
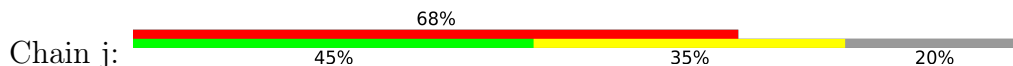
• Molecule 5: ATP synthase subunit f, mitochondrial



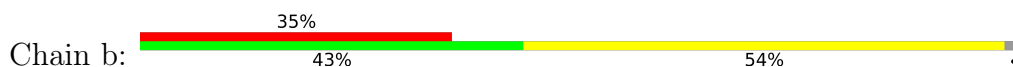
• Molecule 6: ATP synthase subunit g, mitochondrial

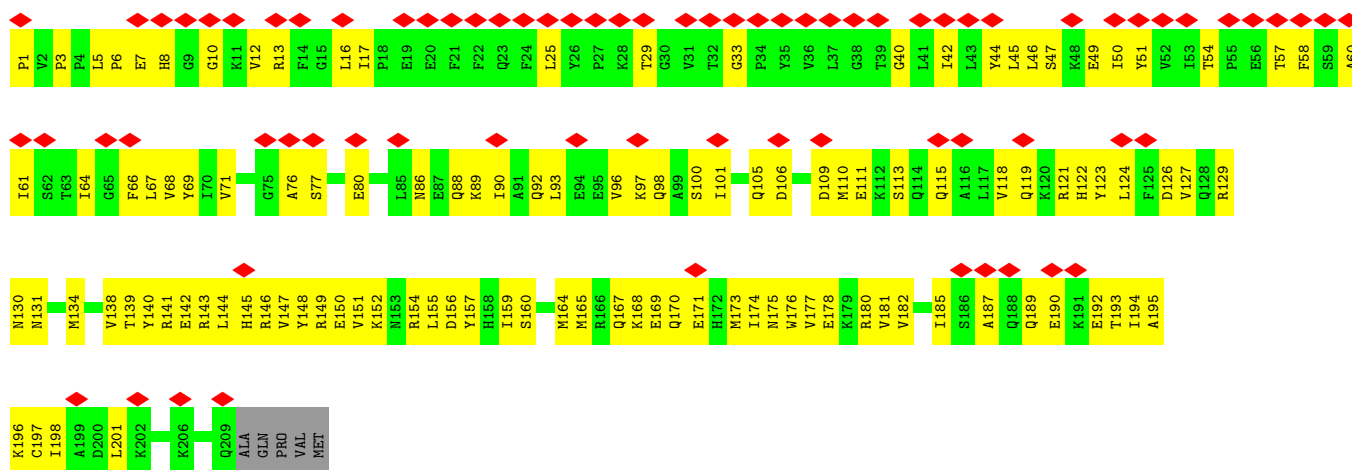


• Molecule 7: ATP synthase subunit ATP5MPL, mitochondrial

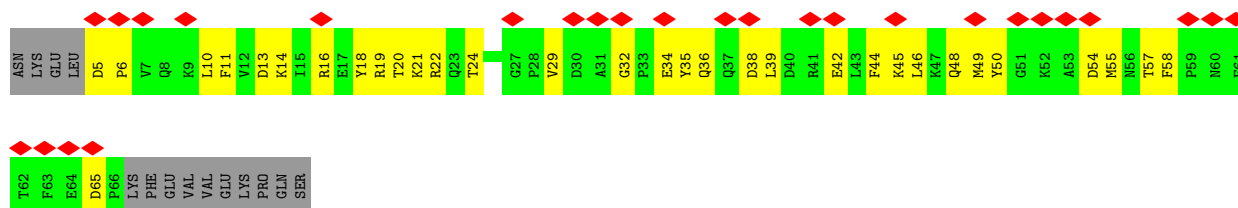


• Molecule 8: ATP synthase F(0) complex subunit B1, mitochondrial

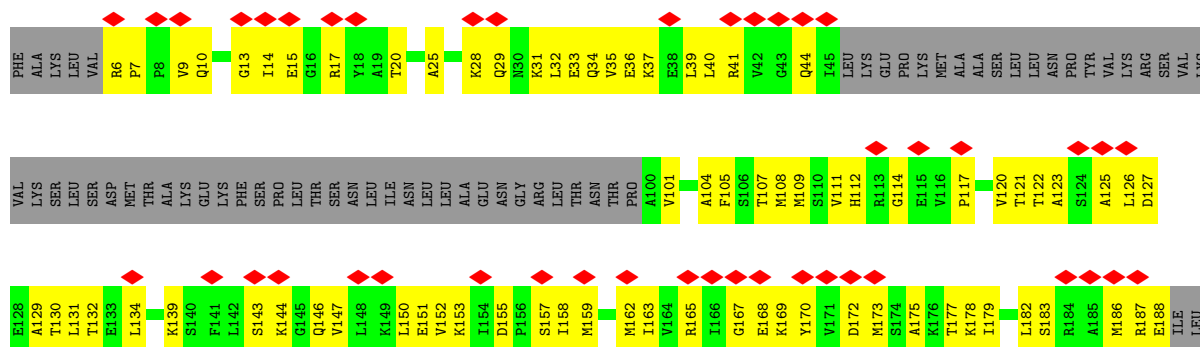




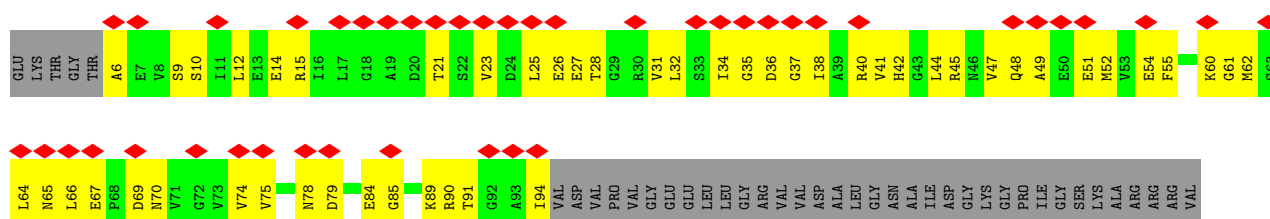
- Molecule 9: ATP synthase-coupling factor 6, mitochondrial



- Molecule 10: ATP synthase subunit O, mitochondrial



- Molecule 11: ATP synthase subunit alpha, mitochondrial



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	61458	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 ($e^-/\text{\AA}^2$)	4.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0171	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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	8	0.22	0/355	0.42	0/483
2	a	0.24	0/1779	0.46	0/2433
3	d	0.21	0/1304	0.43	0/1768
4	e	0.20	0/343	0.43	0/460
5	f	0.24	0/711	0.46	0/952
6	g	0.20	0/646	0.44	0/879
7	j	0.17	0/410	0.38	0/552
8	b	0.24	0/1733	0.49	0/2334
9	h	0.25	0/526	0.57	0/707
10	S	0.20	0/1000	0.43	0/1341
11	C	0.19	0/665	0.50	0/894
All	All	0.22	0/9472	0.46	0/12803

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	8	344	352	352	25	0
2	a	1741	1870	1870	132	0
3	d	1273	1276	1275	90	0
4	e	335	352	352	19	0
5	f	693	718	718	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	g	629	662	662	34	0
7	j	400	428	428	21	0
8	b	1701	1755	1755	142	0
9	h	514	495	495	40	0
10	S	991	1057	1055	78	0
11	C	662	671	671	57	0
All	All	9283	9636	9633	557	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 29.

All (557) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:14:ARG:NH1	6:g:82:VAL:O	1.91	1.03
5:f:71:TYR:OH	8:b:50:ILE:O	1.78	1.00
2:a:69:THR:HG22	2:a:73:MET:HE2	1.43	0.99
2:a:55:LYS:NZ	3:d:157:ILE:O	1.98	0.95
2:a:64:LYS:O	2:a:67:THR:OG1	1.88	0.92
10:S:158:ILE:HG21	10:S:163:ILE:HD11	1.52	0.90
10:S:183:SER:O	10:S:187:ARG:NH1	2.10	0.85
2:a:26:PHE:HE2	2:a:29:LEU:HD11	1.41	0.85
1:8:8:THR:O	1:8:11:THR:OG1	1.94	0.84
2:a:101:ASN:OD1	2:a:161:THR:OG1	1.93	0.83
3:d:131:THR:N	3:d:134:ASP:OD2	2.11	0.82
3:d:40:ARG:O	3:d:43:THR:OG1	1.98	0.82
3:d:22:ASN:OD1	3:d:23:GLN:N	2.14	0.80
6:g:53:LYS:O	6:g:57:ASN:ND2	2.14	0.80
9:h:21:LYS:O	9:h:24:THR:N	2.15	0.80
3:d:68:ASP:OD1	3:d:72:LYS:NZ	2.14	0.79
3:d:82:GLU:OE1	3:d:82:GLU:N	2.15	0.79
5:f:8:GLU:N	5:f:8:GLU:OE1	2.16	0.79
5:f:53:LYS:NZ	8:b:7:GLU:OE2	2.17	0.78
3:d:96:ASP:O	3:d:100:CYS:N	2.13	0.77
8:b:169:GLU:OE1	9:h:35:TYR:OH	2.00	0.77
1:8:3:GLN:O	1:8:9:TRP:NE1	2.17	0.77
3:d:83:ASP:OD1	3:d:86:THR:OG1	2.03	0.77
8:b:157:TYR:HB3	9:h:55:MET:HE2	1.67	0.77
6:g:66:GLN:N	6:g:66:GLN:OE1	2.18	0.76
2:a:40:ASN:OD1	2:a:41:ARG:N	2.18	0.76
10:S:114:GLY:O	10:S:147:VAL:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:122:HIS:ND1	8:b:126:ASP:OD2	2.19	0.75
10:S:120:VAL:O	10:S:153:LYS:N	2.20	0.75
3:d:82:GLU:O	3:d:84:LYS:NZ	2.19	0.74
8:b:110:MET:HE1	8:b:111:GLU:OE2	1.87	0.74
8:b:154:ARG:NH2	9:h:57:THR:O	2.20	0.74
8:b:101:ILE:O	8:b:105:GLN:NE2	2.20	0.74
5:f:82:ARG:NH1	8:b:49:GLU:OE1	2.21	0.73
10:S:139:LYS:NZ	10:S:146:GLN:O	2.20	0.73
5:f:52:LYS:NZ	8:b:5:LEU:O	2.21	0.73
10:S:169:LYS:HB3	11:C:25:LEU:HD11	1.68	0.73
2:a:87:LEU:HD11	2:a:203:GLU:HB3	1.69	0.72
3:d:40:ARG:HH21	8:b:138:VAL:HG22	1.53	0.72
3:d:86:THR:HG23	8:b:129:ARG:NH2	2.05	0.72
3:d:158:GLU:OE1	3:d:158:GLU:N	2.22	0.72
2:a:213:VAL:O	2:a:217:LEU:HD23	1.90	0.72
11:C:44:LEU:O	11:C:47:VAL:HG12	1.89	0.72
7:j:44:ARG:NH1	7:j:45:SER:OG	2.22	0.72
1:8:32:ASN:OD1	1:8:33:PHE:N	2.22	0.72
3:d:129:GLN:O	8:b:1:PRO:N	2.23	0.71
7:j:43:LYS:O	7:j:47:ALA:N	2.23	0.71
2:a:43:VAL:O	2:a:46:GLN:NE2	2.24	0.71
8:b:154:ARG:HA	9:h:55:MET:HE1	1.72	0.71
2:a:120:LYS:NZ	2:a:123:ALA:HB3	2.05	0.71
11:C:48:GLN:N	11:C:51:GLU:OE1	2.23	0.71
10:S:158:ILE:HD13	10:S:163:ILE:CD1	2.20	0.70
11:C:31:VAL:O	11:C:85:GLY:N	2.24	0.70
3:d:37:LEU:HB3	8:b:134:MET:HE1	1.74	0.70
6:g:71:GLU:O	6:g:75:ASN:ND2	2.25	0.70
2:a:211:ALA:O	2:a:215:THR:HG23	1.91	0.69
5:f:77:GLU:N	5:f:77:GLU:OE1	2.25	0.69
2:a:36:ARG:NH1	8:b:3:PRO:O	2.24	0.69
10:S:31:LYS:O	10:S:35:VAL:N	2.24	0.69
10:S:127:ASP:O	10:S:130:THR:OG1	2.10	0.69
11:C:32:LEU:HD21	11:C:42:HIS:HB2	1.75	0.69
8:b:185:ILE:HD13	10:S:159:MET:HB2	1.73	0.68
2:a:58:MET:HE2	2:a:66:GLN:HA	1.74	0.68
5:f:51:VAL:HG11	8:b:8:HIS:C	2.19	0.68
2:a:103:GLY:HA2	7:j:31:MET:HE1	1.73	0.68
1:8:3:GLN:HG2	2:a:98:LEU:HD13	1.76	0.68
5:f:27:ASP:OD2	5:f:28:PHE:N	2.26	0.68
10:S:169:LYS:HD2	11:C:25:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:51:GLU:OE2	11:C:90:ARG:NE	2.27	0.67
8:b:165:MET:SD	8:b:168:LYS:NZ	2.67	0.67
6:g:58:SER:O	6:g:63:SER:OG	2.09	0.66
2:a:55:LYS:NZ	3:d:159:THR:O	2.27	0.66
10:S:188:GLU:N	10:S:188:GLU:OE1	2.28	0.66
2:a:76:ILE:HB	2:a:215:THR:HG21	1.78	0.66
3:d:131:THR:OG1	3:d:134:ASP:OD2	2.11	0.66
8:b:134:MET:O	8:b:138:VAL:HG23	1.95	0.66
2:a:199:LEU:O	2:a:202:LEU:N	2.27	0.66
6:g:91:ILE:HD11	8:b:47:SER:CB	2.25	0.66
1:8:21:PHE:O	7:j:17:TYR:OH	2.14	0.66
3:d:40:ARG:NH2	8:b:138:VAL:HG22	2.10	0.66
2:a:26:PHE:CE2	2:a:29:LEU:HD11	2.28	0.66
11:C:28:THR:HG22	11:C:89:LYS:HG3	1.77	0.66
2:a:195:ILE:O	2:a:199:LEU:HD23	1.96	0.65
5:f:11:LEU:HD11	5:f:22:TRP:CH2	2.32	0.65
10:S:7:PRO:HG3	10:S:20:THR:HG23	1.78	0.65
2:a:40:ASN:ND2	5:f:49:VAL:O	2.30	0.64
11:C:54:GLU:OE1	11:C:91:THR:HG23	1.97	0.64
5:f:51:VAL:HG11	8:b:8:HIS:O	1.97	0.64
2:a:161:THR:O	2:a:165:THR:HG22	1.98	0.63
3:d:98:LYS:O	3:d:103:PHE:N	2.32	0.63
8:b:143:ARG:NH2	9:h:65:ASP:OD2	2.31	0.63
3:d:156:PRO:O	3:d:159:THR:OG1	2.13	0.63
2:a:182:MET:HE3	2:a:182:MET:O	1.98	0.63
2:a:2:ASN:OD1	2:a:3:GLU:N	2.32	0.63
10:S:120:VAL:N	10:S:151:GLU:O	2.30	0.63
10:S:169:LYS:CD	11:C:25:LEU:HD21	2.29	0.63
2:a:120:LYS:HZ3	2:a:123:ALA:HB3	1.63	0.63
9:h:21:LYS:HE2	9:h:29:VAL:HG12	1.80	0.63
2:a:70:LEU:HD13	3:d:152:TRP:CG	2.33	0.62
5:f:61:MET:HE1	8:b:16:LEU:C	2.24	0.62
11:C:62:MET:HE3	11:C:74:VAL:CG2	2.30	0.62
1:8:6:THR:HG22	7:j:39:ARG:HE	1.64	0.62
2:a:130:PRO:O	2:a:133:THR:OG1	2.16	0.62
4:e:22:MET:HE1	6:g:92:ILE:CG2	2.30	0.62
8:b:170:GLN:OE1	11:C:12:LEU:HD21	1.99	0.62
3:d:18:ILE:HD11	8:b:121:ARG:HD2	1.81	0.62
2:a:31:PHE:HE2	2:a:77:LEU:HD12	1.65	0.62
3:d:134:ASP:O	3:d:138:VAL:HG23	2.00	0.62
6:g:71:GLU:OE1	6:g:74:LEU:HD23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:75:VAL:HG11	11:C:79:ASP:OD1	1.99	0.61
10:S:33:GLU:OE1	10:S:33:GLU:N	2.28	0.61
2:a:203:GLU:HA	2:a:206:VAL:HG22	1.83	0.61
2:a:80:GLY:O	2:a:84:LEU:HD23	2.00	0.61
8:b:157:TYR:CB	9:h:55:MET:HE2	2.30	0.61
8:b:173:MET:SD	9:h:21:LYS:HE3	2.40	0.61
3:d:18:ILE:HG23	3:d:19:ILE:N	2.16	0.61
2:a:71:MET:O	2:a:74:SER:OG	2.16	0.61
2:a:71:MET:SD	7:j:21:TYR:OH	2.55	0.60
2:a:111:GLY:O	2:a:115:THR:OG1	2.17	0.60
6:g:76:GLY:O	6:g:80:THR:HG23	2.02	0.60
5:f:79:LYS:O	5:f:82:ARG:NE	2.35	0.60
8:b:170:GLN:OE1	8:b:174:ILE:HD11	2.01	0.60
11:C:6:ALA:O	11:C:9:SER:OG	2.05	0.60
11:C:62:MET:HE3	11:C:74:VAL:HG22	1.84	0.60
3:d:72:LYS:O	3:d:76:LEU:HD23	2.02	0.59
3:d:149:TYR:O	3:d:154:HIS:ND1	2.34	0.59
8:b:89:LYS:O	8:b:93:LEU:HD23	2.02	0.59
9:h:34:GLU:N	9:h:34:GLU:OE1	2.35	0.59
3:d:113:GLU:O	3:d:117:GLU:OE1	2.20	0.59
6:g:91:ILE:HD11	8:b:47:SER:HB3	1.82	0.59
8:b:25:LEU:O	8:b:29:THR:HG22	2.03	0.59
11:C:54:GLU:OE1	11:C:54:GLU:N	2.35	0.59
10:S:170:TYR:HB3	11:C:28:THR:HG21	1.85	0.59
1:8:19:THR:HG21	2:a:78:PHE:CE1	2.38	0.59
2:a:87:LEU:HD11	2:a:203:GLU:CB	2.32	0.59
9:h:45:LYS:HA	9:h:48:GLN:OE1	2.02	0.59
2:a:210:GLN:HA	2:a:213:VAL:HG22	1.84	0.59
11:C:49:ALA:N	11:C:66:LEU:HD11	2.18	0.59
11:C:40:ARG:NH2	11:C:70:ASN:OD1	2.35	0.58
1:8:26:LEU:O	1:8:29:SER:OG	2.18	0.58
8:b:185:ILE:HD11	10:S:175:ALA:CB	2.32	0.58
2:a:98:LEU:HD12	2:a:161:THR:HG21	1.85	0.58
3:d:93:GLU:OE1	3:d:93:GLU:N	2.36	0.58
6:g:69:VAL:O	6:g:73:LEU:HD13	2.03	0.57
6:g:78:VAL:O	6:g:82:VAL:HG23	2.04	0.57
6:g:84:MET:HE1	8:b:44:TYR:N	2.18	0.57
2:a:103:GLY:CA	7:j:31:MET:HE1	2.34	0.57
2:a:222:LEU:O	2:a:226:THR:N	2.36	0.57
3:d:10:ILE:CD1	8:b:127:VAL:HG22	2.34	0.57
2:a:57:MET:CE	2:a:212:TYR:CE1	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:10:SER:O	11:C:14:GLU:OE1	2.22	0.57
2:a:23:ILE:HG23	5:f:66:TYR:OH	2.03	0.57
2:a:67:THR:HG22	3:d:151:TYR:CD2	2.39	0.57
4:e:32:LEU:HD12	4:e:33:LYS:N	2.20	0.57
11:C:34:ILE:HD12	11:C:38:ILE:O	2.03	0.57
1:8:28:VAL:HG13	2:a:70:LEU:HD11	1.85	0.57
2:a:174:ILE:HD11	2:a:192:THR:OG1	2.04	0.57
11:C:26:GLU:O	11:C:28:THR:HG23	2.05	0.57
2:a:76:ILE:CB	2:a:215:THR:HG21	2.35	0.57
8:b:150:GLU:O	8:b:154:ARG:HG2	2.04	0.57
9:h:36:GLN:OE1	9:h:36:GLN:N	2.34	0.57
4:e:14:ARG:HA	4:e:14:ARG:NE	2.19	0.56
8:b:185:ILE:HD11	10:S:175:ALA:HB1	1.87	0.56
11:C:38:ILE:CD1	11:C:74:VAL:HG12	2.34	0.56
9:h:24:THR:HG22	9:h:24:THR:O	2.04	0.56
1:8:1:MET:HE3	1:8:2:PRO:HD2	1.87	0.56
3:d:118:LEU:O	3:d:121:MET:N	2.35	0.56
10:S:126:LEU:HB2	10:S:131:LEU:HD21	1.87	0.56
11:C:52:MET:HE2	11:C:52:MET:HA	1.86	0.56
2:a:206:VAL:O	2:a:207:ALA:C	2.48	0.56
8:b:58:PHE:HA	8:b:61:ILE:HD12	1.87	0.56
11:C:78:ASN:OD1	11:C:79:ASP:N	2.38	0.56
11:C:67:GLU:OE1	11:C:70:ASN:N	2.39	0.56
1:8:9:TRP:HA	1:8:12:MET:HE2	1.87	0.56
3:d:10:ILE:HD13	8:b:127:VAL:HG22	1.87	0.56
8:b:45:LEU:O	8:b:51:TYR:N	2.38	0.56
2:a:184:ILE:HG22	2:a:185:SER:N	2.21	0.55
6:g:91:ILE:HD11	8:b:47:SER:HB2	1.88	0.55
8:b:170:GLN:O	8:b:174:ILE:HG12	2.06	0.55
10:S:7:PRO:CG	10:S:20:THR:HG23	2.36	0.55
3:d:111:ILE:O	3:d:114:TYR:N	2.39	0.55
8:b:110:MET:O	8:b:113:SER:OG	2.20	0.55
8:b:174:ILE:HD12	10:S:186:MET:SD	2.46	0.55
2:a:31:PHE:CE2	2:a:77:LEU:HD12	2.41	0.55
11:C:27:GLU:HG2	11:C:44:LEU:HD23	1.88	0.55
11:C:37:GLY:O	11:C:38:ILE:HD13	2.06	0.55
8:b:76:ALA:O	8:b:80:GLU:OE1	2.24	0.55
8:b:92:GLN:OE1	8:b:93:LEU:HD22	2.06	0.55
2:a:160:LEU:HD21	2:a:214:PHE:CD2	2.42	0.55
8:b:197:CYS:O	8:b:201:LEU:HD23	2.07	0.55
2:a:199:LEU:O	2:a:203:GLU:OE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:148:TYR:CZ	8:b:152:LYS:HD2	2.41	0.54
1:8:19:THR:HG21	2:a:78:PHE:HE1	1.71	0.54
2:a:81:SER:O	2:a:85:LEU:HD23	2.08	0.54
3:d:56:TYR:O	3:d:60:VAL:N	2.30	0.54
7:j:14:LYS:O	7:j:18:THR:N	2.40	0.54
8:b:164:MET:SD	8:b:165:MET:N	2.81	0.54
2:a:148:SER:O	2:a:152:GLN:NE2	2.38	0.54
8:b:10:GLY:O	8:b:12:VAL:HG23	2.07	0.54
3:d:56:TYR:CD2	8:b:155:LEU:HD13	2.43	0.53
8:b:126:ASP:O	8:b:130:ASN:ND2	2.41	0.53
10:S:28:LYS:O	10:S:29:GLN:HB2	2.08	0.53
3:d:132:ILE:O	3:d:136:ASN:ND2	2.38	0.53
8:b:150:GLU:HG3	8:b:151:VAL:N	2.23	0.53
8:b:167:GLN:O	8:b:171:GLU:OE1	2.27	0.53
10:S:37:LYS:O	10:S:41:ARG:HD3	2.08	0.53
2:a:152:GLN:O	2:a:155:ALA:N	2.42	0.53
8:b:29:THR:OG1	8:b:33:GLY:N	2.42	0.53
8:b:46:LEU:HD22	8:b:51:TYR:HB2	1.90	0.53
10:S:168:GLU:OE2	11:C:28:THR:N	2.37	0.53
2:a:26:PHE:CD1	5:f:66:TYR:CD1	2.97	0.53
2:a:184:ILE:HG22	2:a:185:SER:H	1.74	0.53
2:a:206:VAL:O	2:a:210:GLN:OE1	2.27	0.53
6:g:84:MET:O	6:g:84:MET:HG2	2.08	0.53
8:b:49:GLU:CD	8:b:49:GLU:O	2.52	0.53
10:S:186:MET:SD	10:S:187:ARG:NH2	2.81	0.52
4:e:14:ARG:NE	4:e:14:ARG:CA	2.72	0.52
8:b:106:ASP:O	8:b:109:ASP:OD1	2.27	0.52
8:b:174:ILE:HD12	10:S:187:ARG:NH2	2.25	0.52
8:b:189:GLN:O	8:b:193:THR:HG23	2.09	0.52
10:S:125:ALA:C	10:S:126:LEU:HD22	2.34	0.52
5:f:13:GLU:N	5:f:13:GLU:OE1	2.42	0.52
2:a:98:LEU:CD1	2:a:161:THR:HG21	2.40	0.52
2:a:104:MET:HE2	2:a:104:MET:HA	1.91	0.52
2:a:5:LEU:HD12	2:a:6:PHE:CD1	2.45	0.52
5:f:79:LYS:HA	5:f:82:ARG:HE	1.74	0.52
6:g:67:LEU:HD11	6:g:71:GLU:HB3	1.92	0.52
2:a:76:ILE:HG23	2:a:77:LEU:HD22	1.92	0.52
3:d:41:LEU:HD23	3:d:41:LEU:C	2.35	0.52
1:8:23:ILE:HG21	2:a:28:SER:HB2	1.93	0.51
11:C:67:GLU:OE1	11:C:69:ASP:N	2.43	0.51
9:h:44:PHE:O	9:h:48:GLN:OE1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:57:MET:HE2	2:a:212:TYR:CE1	2.46	0.51
2:a:170:LEU:O	2:a:170:LEU:HD23	2.10	0.51
7:j:16:TYR:HA	7:j:20:ALA:HB3	1.92	0.51
7:j:34:ILE:HG13	7:j:38:ILE:HD11	1.93	0.51
7:j:14:LYS:O	7:j:18:THR:HG23	2.10	0.51
1:8:38:GLU:OE1	1:8:40:THR:N	2.43	0.51
8:b:185:ILE:HD12	10:S:179:ILE:HD11	1.92	0.51
9:h:35:TYR:O	9:h:39:LEU:HG	2.10	0.51
9:h:49:MET:HE1	9:h:50:TYR:CE2	2.45	0.51
2:a:217:LEU:O	2:a:221:TYR:CD2	2.63	0.51
9:h:18:TYR:CE1	11:C:9:SER:HB2	2.46	0.51
10:S:15:GLU:CB	10:S:101:VAL:HG22	2.41	0.50
11:C:64:LEU:HD23	11:C:64:LEU:H	1.76	0.50
2:a:160:LEU:HD21	2:a:214:PHE:HD2	1.76	0.50
8:b:190:GLU:OE1	8:b:190:GLU:N	2.41	0.50
10:S:122:THR:HA	10:S:158:ILE:HD11	1.91	0.50
4:e:14:ARG:NE	6:g:82:VAL:HG13	2.26	0.50
8:b:144:LEU:O	8:b:147:VAL:HG12	2.10	0.50
2:a:96:THR:O	2:a:161:THR:HG23	2.12	0.50
2:a:173:LEU:C	2:a:173:LEU:HD23	2.37	0.50
8:b:110:MET:SD	8:b:110:MET:C	2.95	0.50
3:d:19:ILE:HG21	3:d:24:LYS:HA	1.92	0.50
8:b:123:TYR:O	8:b:127:VAL:HG23	2.12	0.50
3:d:99:SER:HB2	8:b:118:VAL:HG13	1.93	0.50
10:S:158:ILE:HD13	10:S:163:ILE:HD12	1.91	0.50
3:d:133:GLU:O	3:d:137:GLU:OE1	2.30	0.50
3:d:111:ILE:O	3:d:112:GLN:C	2.55	0.49
10:S:35:VAL:O	10:S:39:LEU:HD13	2.12	0.49
3:d:118:LEU:C	3:d:118:LEU:HD23	2.37	0.49
9:h:11:PHE:CZ	11:C:21:THR:HG22	2.48	0.49
10:S:117:PRO:O	10:S:167:GLY:N	2.43	0.49
8:b:29:THR:HG21	8:b:33:GLY:HA3	1.93	0.49
2:a:26:PHE:HD1	5:f:66:TYR:CD1	2.30	0.49
8:b:64:ILE:O	8:b:68:VAL:HG12	2.13	0.49
1:8:23:ILE:HG21	2:a:28:SER:CB	2.43	0.49
3:d:135:LEU:O	3:d:139:PHE:N	2.34	0.49
4:e:9:LEU:HD11	6:g:51:SER:OG	2.12	0.49
5:f:59:LEU:O	5:f:60:SER:C	2.55	0.49
2:a:85:LEU:O	2:a:88:LEU:HD13	2.12	0.49
2:a:171:ILE:HD11	2:a:199:LEU:HB3	1.95	0.49
11:C:45:ARG:O	11:C:45:ARG:NE	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:86:THR:CG2	8:b:129:ARG:NH2	2.76	0.49
8:b:167:GLN:O	8:b:170:GLN:HB3	2.13	0.49
10:S:9:VAL:HG13	10:S:9:VAL:O	2.12	0.49
4:e:14:ARG:CZ	6:g:82:VAL:HG13	2.43	0.48
5:f:44:TYR:OH	5:f:61:MET:HG3	2.13	0.48
6:g:67:LEU:HD21	6:g:71:GLU:HG3	1.95	0.48
6:g:84:MET:HE1	8:b:40:GLY:O	2.13	0.48
4:e:4:VAL:N	6:g:36:GLU:OE2	2.42	0.48
8:b:174:ILE:O	8:b:175:ASN:C	2.56	0.48
9:h:38:ASP:O	9:h:39:LEU:C	2.56	0.48
5:f:74:SER:O	5:f:74:SER:OG	2.26	0.48
11:C:55:PHE:CZ	11:C:75:VAL:HG22	2.48	0.48
3:d:15:PHE:O	3:d:18:ILE:HG22	2.13	0.48
8:b:155:LEU:CD2	8:b:159:ILE:HD11	2.43	0.48
11:C:34:ILE:HG22	11:C:84:GLU:CD	2.39	0.48
2:a:26:PHE:HD1	5:f:66:TYR:CE1	2.30	0.48
5:f:22:TRP:HA	5:f:25:MET:HE3	1.95	0.48
10:S:187:ARG:CZ	10:S:187:ARG:HA	2.44	0.48
8:b:97:LYS:O	8:b:100:SER:OG	2.26	0.48
8:b:146:ARG:HH22	8:b:147:VAL:HB	1.79	0.48
10:S:107:THR:O	10:S:111:VAL:HG23	2.13	0.48
2:a:122:LYS:O	2:a:125:LEU:N	2.45	0.48
3:d:97:VAL:O	3:d:98:LYS:C	2.57	0.48
5:f:51:VAL:HG12	8:b:6:PRO:HB2	1.95	0.48
8:b:177:VAL:O	8:b:181:VAL:HG23	2.14	0.48
10:S:36:GLU:O	10:S:40:LEU:HD23	2.13	0.48
6:g:84:MET:SD	8:b:40:GLY:O	2.72	0.47
9:h:54:ASP:OD1	9:h:54:ASP:O	2.32	0.47
10:S:39:LEU:HD22	10:S:105:PHE:CD2	2.49	0.47
1:8:32:ASN:HB2	3:d:132:ILE:HD12	1.95	0.47
2:a:189:ALA:O	2:a:193:PHE:HD1	1.98	0.47
8:b:109:ASP:OD1	8:b:110:MET:N	2.48	0.47
8:b:182:VAL:O	8:b:185:ILE:HG22	2.14	0.47
10:S:187:ARG:HA	10:S:187:ARG:NE	2.29	0.47
2:a:135:THR:O	2:a:137:LEU:N	2.47	0.47
4:e:14:ARG:HA	4:e:14:ARG:CZ	2.44	0.47
10:S:131:LEU:HA	10:S:134:LEU:HD12	1.97	0.47
10:S:15:GLU:HB2	10:S:101:VAL:HG22	1.95	0.47
10:S:31:LYS:O	10:S:35:VAL:HG12	2.15	0.47
2:a:13:VAL:O	2:a:13:VAL:HG23	2.15	0.47
2:a:21:THR:O	2:a:25:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:33:TRP:O	3:d:37:LEU:HD13	2.15	0.47
4:e:10:ILE:O	4:e:14:ARG:HG2	2.14	0.47
8:b:140:TYR:CE2	8:b:144:LEU:HD11	2.49	0.47
9:h:32:GLY:O	9:h:36:GLN:OE1	2.32	0.47
10:S:109:MET:O	10:S:112:HIS:HB3	2.15	0.47
8:b:42:ILE:O	8:b:46:LEU:HD23	2.14	0.47
2:a:51:GLN:O	2:a:55:LYS:HG2	2.15	0.47
2:a:152:GLN:O	2:a:153:PRO:C	2.58	0.47
5:f:21:SER:O	5:f:24:LEU:HG	2.15	0.47
10:S:155:ASP:OD2	10:S:157:SER:N	2.41	0.47
3:d:89:VAL:N	8:b:129:ARG:NH1	2.62	0.47
10:S:104:ALA:O	10:S:107:THR:OG1	2.29	0.47
1:8:3:GLN:OE1	2:a:9:PHE:CZ	2.69	0.46
3:d:72:LYS:HB2	9:h:58:PHE:CE2	2.50	0.46
8:b:160:SER:OG	9:h:46:LEU:HD11	2.15	0.46
9:h:19:ARG:HE	9:h:19:ARG:HA	1.79	0.46
2:a:146:THR:HG23	2:a:147:ILE:N	2.31	0.46
10:S:150:LEU:C	10:S:150:LEU:HD12	2.41	0.46
5:f:29:THR:HG23	5:f:32:GLY:H	1.80	0.46
11:C:41:VAL:O	11:C:70:ASN:HB2	2.16	0.46
3:d:18:ILE:CG2	3:d:19:ILE:N	2.79	0.46
7:j:7:LYS:HA	7:j:11:ILE:HG12	1.98	0.46
11:C:38:ILE:HD12	11:C:74:VAL:HG12	1.97	0.46
2:a:201:ILE:HD12	8:b:66:PHE:CE1	2.50	0.46
3:d:89:VAL:N	8:b:129:ARG:HH12	2.12	0.46
3:d:133:GLU:HG2	3:d:134:ASP:N	2.31	0.46
10:S:186:MET:HA	11:C:15:ARG:HD2	1.98	0.46
4:e:22:MET:HE1	6:g:92:ILE:HG23	1.97	0.46
1:8:21:PHE:CE2	7:j:24:ILE:HG21	2.51	0.46
5:f:86:TYR:O	5:f:86:TYR:CD2	2.69	0.46
2:a:19:LEU:HD23	2:a:19:LEU:C	2.41	0.45
5:f:61:MET:CE	8:b:16:LEU:HA	2.46	0.45
5:f:81:GLU:N	5:f:81:GLU:OE1	2.49	0.45
9:h:19:ARG:O	9:h:22:ARG:N	2.49	0.45
10:S:158:ILE:HD13	10:S:163:ILE:HD11	1.98	0.45
6:g:84:MET:SD	8:b:40:GLY:CA	3.04	0.45
9:h:21:LYS:O	9:h:22:ARG:C	2.59	0.45
11:C:94:ILE:O	11:C:94:ILE:HG22	2.17	0.45
2:a:85:LEU:HA	2:a:88:LEU:HD13	1.98	0.45
3:d:83:ASP:OD1	3:d:86:THR:CB	2.64	0.45
5:f:60:SER:O	5:f:61:MET:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:51:GLN:O	2:a:54:SER:OG	2.34	0.45
2:a:199:LEU:C	2:a:203:GLU:OE1	2.59	0.45
8:b:173:MET:SD	9:h:21:LYS:CE	3.04	0.45
1:8:4:LEU:O	1:8:6:THR:N	2.49	0.45
2:a:141:LEU:O	2:a:145:GLU:OE1	2.33	0.45
5:f:45:TYR:CD2	5:f:49:VAL:HB	2.51	0.45
11:C:54:GLU:CD	11:C:91:THR:HG23	2.42	0.45
2:a:89:PRO:HB3	8:b:60:ALA:HB2	1.97	0.45
3:d:31:LYS:O	3:d:35:GLU:OE1	2.35	0.45
8:b:174:ILE:O	8:b:178:GLU:OE1	2.33	0.45
2:a:106:ILE:HD11	7:j:31:MET:HA	1.99	0.45
2:a:144:ILE:O	2:a:145:GLU:C	2.58	0.45
7:j:35:VAL:HA	7:j:38:ILE:HD12	1.99	0.45
8:b:138:VAL:O	8:b:142:GLU:HG3	2.16	0.45
10:S:7:PRO:HB3	10:S:108:MET:SD	2.56	0.45
3:d:99:SER:HA	3:d:103:PHE:HB3	1.98	0.45
7:j:2:LEU:C	7:j:2:LEU:HD12	2.42	0.45
7:j:22:GLN:HG3	7:j:23:GLU:N	2.32	0.45
8:b:139:THR:O	8:b:143:ARG:HG3	2.16	0.45
10:S:14:ILE:HG23	10:S:15:GLU:N	2.32	0.45
2:a:93:THR:HB	2:a:96:THR:HG23	1.99	0.45
3:d:113:GLU:O	3:d:116:LYS:N	2.50	0.45
4:e:4:VAL:HG12	4:e:5:GLN:N	2.32	0.45
5:f:16:LEU:HD22	6:g:67:LEU:O	2.17	0.45
8:b:115:GLN:O	8:b:119:GLN:NE2	2.46	0.45
10:S:165:ARG:NE	10:S:167:GLY:O	2.42	0.45
2:a:116:GLY:O	2:a:120:LYS:N	2.46	0.44
8:b:123:TYR:HA	8:b:126:ASP:OD2	2.16	0.44
10:S:13:GLY:O	10:S:17:ARG:N	2.39	0.44
2:a:111:GLY:HA2	7:j:23:GLU:HB3	1.98	0.44
8:b:101:ILE:C	8:b:105:GLN:HE22	2.26	0.44
10:S:31:LYS:O	10:S:32:LEU:C	2.60	0.44
2:a:83:ASN:CB	2:a:207:ALA:HB1	2.47	0.44
5:f:22:TRP:HA	5:f:25:MET:CE	2.47	0.44
8:b:45:LEU:HA	8:b:50:ILE:HB	1.99	0.44
8:b:77:SER:HA	8:b:80:GLU:OE2	2.17	0.44
9:h:13:ASP:OD1	9:h:16:ARG:NH2	2.51	0.44
10:S:122:THR:HG22	10:S:123:ALA:N	2.33	0.44
11:C:47:VAL:HG13	11:C:47:VAL:O	2.18	0.44
2:a:40:ASN:HD22	5:f:49:VAL:HG12	1.83	0.44
9:h:38:ASP:O	9:h:42:GLU:OE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:62:MET:SD	11:C:62:MET:C	3.00	0.44
8:b:152:LYS:O	8:b:156:ASP:CG	2.60	0.44
2:a:223:HIS:O	2:a:226:THR:HG22	2.18	0.44
3:d:95:GLU:O	3:d:96:ASP:C	2.61	0.44
9:h:44:PHE:CE1	9:h:48:GLN:NE2	2.86	0.44
2:a:7:THR:HG23	2:a:8:SER:N	2.33	0.43
2:a:38:VAL:O	8:b:5:LEU:HD11	2.18	0.43
2:a:199:LEU:O	2:a:200:THR:C	2.61	0.43
4:e:9:LEU:HD12	4:e:9:LEU:H	1.82	0.43
10:S:173:MET:HG2	11:C:23:VAL:HG21	2.00	0.43
3:d:100:CYS:O	3:d:104:LEU:HB3	2.18	0.43
3:d:104:LEU:O	3:d:108:LYS:HG2	2.18	0.43
3:d:158:GLU:CD	3:d:159:THR:HG23	2.43	0.43
5:f:56:ILE:O	5:f:56:ILE:HG22	2.17	0.43
10:S:33:GLU:OE2	10:S:34:GLN:NE2	2.51	0.43
11:C:54:GLU:HG2	11:C:89:LYS:HB2	1.99	0.43
2:a:189:ALA:O	2:a:192:THR:HG22	2.18	0.43
5:f:22:TRP:CH2	5:f:26:ARG:HB2	2.53	0.43
10:S:178:LYS:O	10:S:182:LEU:HD23	2.18	0.43
10:S:186:MET:SD	11:C:12:LEU:HD22	2.58	0.43
1:8:22:ILE:O	1:8:26:LEU:HG	2.18	0.43
5:f:61:MET:HE1	8:b:16:LEU:O	2.18	0.43
2:a:5:LEU:HD12	2:a:6:PHE:N	2.33	0.43
2:a:114:ILE:CG2	7:j:23:GLU:HB3	2.48	0.43
5:f:44:TYR:OH	5:f:61:MET:CG	2.66	0.43
2:a:58:MET:HE3	2:a:61:HIS:HB2	2.01	0.43
2:a:60:ILE:HG13	2:a:61:HIS:N	2.33	0.43
3:d:18:ILE:CD1	8:b:121:ARG:HA	2.48	0.43
3:d:45:PRO:O	8:b:141:ARG:HD3	2.18	0.43
3:d:51:ILE:HD11	8:b:151:VAL:CG1	2.48	0.43
3:d:138:VAL:HG12	3:d:139:PHE:CE2	2.54	0.43
8:b:195:ALA:O	8:b:198:ILE:HG22	2.19	0.43
3:d:30:LEU:HD21	8:b:131:ASN:ND2	2.33	0.43
3:d:51:ILE:HD11	8:b:151:VAL:HG11	2.00	0.43
6:g:81:GLU:C	6:g:81:GLU:CD	2.86	0.43
10:S:25:ALA:O	10:S:28:LYS:O	2.36	0.43
2:a:106:ILE:HG13	2:a:107:PRO:N	2.33	0.42
2:a:170:LEU:HD23	2:a:170:LEU:C	2.44	0.42
8:b:93:LEU:O	8:b:96:VAL:HG12	2.18	0.42
10:S:168:GLU:OE2	11:C:28:THR:O	2.37	0.42
2:a:190:LEU:O	2:a:194:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:98:GLN:OE1	8:b:101:ILE:HD11	2.18	0.42
2:a:155:ALA:O	2:a:158:VAL:HG12	2.19	0.42
10:S:31:LYS:HA	10:S:34:GLN:OE1	2.19	0.42
2:a:66:GLN:OE1	3:d:157:ILE:HG12	2.19	0.42
3:d:89:VAL:HB	8:b:129:ARG:HH22	1.84	0.42
3:d:131:THR:O	3:d:134:ASP:N	2.52	0.42
5:f:27:ASP:OD1	5:f:29:THR:HG22	2.19	0.42
8:b:154:ARG:HA	9:h:55:MET:CE	2.47	0.42
3:d:144:LEU:O	3:d:145:ASP:OD1	2.38	0.42
6:g:84:MET:SD	8:b:40:GLY:C	3.02	0.42
8:b:68:VAL:HG13	8:b:69:TYR:N	2.33	0.42
10:S:32:LEU:HB3	10:S:109:MET:HE2	2.01	0.42
5:f:53:LYS:O	5:f:53:LYS:HG3	2.20	0.42
10:S:129:ALA:O	10:S:130:THR:C	2.63	0.42
1:8:24:PHE:O	1:8:28:VAL:HG12	2.19	0.42
2:a:59:SER:HA	3:d:157:ILE:HD11	2.02	0.42
2:a:217:LEU:O	2:a:220:LEU:HG	2.20	0.42
3:d:49:PRO:HG2	8:b:148:TYR:CZ	2.55	0.42
3:d:91:ALA:O	3:d:94:LYS:HG2	2.18	0.42
3:d:144:LEU:O	3:d:145:ASP:C	2.63	0.42
4:e:14:ARG:HH11	6:g:85:TRP:HB2	1.84	0.42
8:b:124:LEU:C	8:b:124:LEU:HD23	2.45	0.42
9:h:10:LEU:O	9:h:14:LYS:HG2	2.19	0.42
10:S:109:MET:O	10:S:112:HIS:N	2.52	0.42
3:d:6:ALA:C	3:d:7:LEU:HD22	2.45	0.42
3:d:122:ARG:CZ	3:d:122:ARG:HA	2.50	0.42
6:g:26:LEU:HD12	6:g:27:ALA:N	2.35	0.42
8:b:164:MET:HA	8:b:167:GLN:HG3	2.02	0.42
8:b:176:TRP:O	8:b:180:ARG:HG2	2.20	0.42
8:b:192:GLU:C	8:b:196:LYS:HZ2	2.27	0.42
2:a:62:ASN:O	2:a:66:GLN:HG3	2.19	0.42
2:a:68:TRP:HA	2:a:71:MET:HE2	2.01	0.42
3:d:118:LEU:HD23	3:d:119:GLU:N	2.35	0.42
9:h:55:MET:O	9:h:55:MET:HG3	2.19	0.42
2:a:110:ALA:O	2:a:114:ILE:HG22	2.20	0.42
4:e:6:VAL:HG12	4:e:7:SER:N	2.35	0.42
8:b:157:TYR:C	8:b:157:TYR:CD2	2.98	0.42
2:a:58:MET:HE3	2:a:61:HIS:CG	2.56	0.41
3:d:96:ASP:O	3:d:97:VAL:C	2.62	0.41
4:e:29:TYR:HD1	4:e:32:LEU:HD11	1.85	0.41
5:f:83:LEU:HD12	5:f:83:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:7:PRO:CB	10:S:108:MET:SD	3.08	0.41
3:d:133:GLU:O	3:d:134:ASP:C	2.61	0.41
4:e:5:GLN:HA	4:e:5:GLN:NE2	2.35	0.41
5:f:14:VAL:HG13	5:f:18:GLU:OE2	2.20	0.41
8:b:16:LEU:HB2	8:b:17:ILE:HD12	2.02	0.41
8:b:194:ILE:HA	8:b:197:CYS:SG	2.60	0.41
9:h:19:ARG:O	9:h:20:THR:C	2.62	0.41
11:C:35:GLY:O	11:C:36:ASP:OD1	2.38	0.41
6:g:61:THR:O	6:g:61:THR:HG22	2.20	0.41
6:g:74:LEU:O	6:g:78:VAL:HG23	2.20	0.41
9:h:21:LYS:O	9:h:24:THR:CA	2.67	0.41
10:S:143:SER:OG	10:S:144:LYS:N	2.53	0.41
10:S:172:ASP:OD1	10:S:172:ASP:C	2.62	0.41
1:8:2:PRO:HB2	2:a:9:PHE:CD2	2.56	0.41
3:d:60:VAL:HG11	3:d:66:VAL:CG2	2.50	0.41
3:d:121:MET:O	3:d:124:ILE:HG12	2.20	0.41
8:b:190:GLU:O	8:b:194:ILE:HG12	2.20	0.41
10:S:168:GLU:OE2	11:C:27:GLU:HG3	2.20	0.41
10:S:177:THR:HG23	10:S:178:LYS:N	2.35	0.41
11:C:25:LEU:HD12	11:C:26:GLU:H	1.85	0.41
2:a:38:VAL:CG2	8:b:90:ILE:HD11	2.51	0.41
2:a:156:LEU:O	2:a:160:LEU:HD13	2.19	0.41
3:d:40:ARG:CZ	8:b:138:VAL:HG13	2.50	0.41
10:S:6:ARG:NE	10:S:10:GLN:OE1	2.51	0.41
10:S:170:TYR:CB	11:C:28:THR:HG21	2.50	0.41
2:a:17:LEU:C	2:a:17:LEU:HD12	2.45	0.41
5:f:75:TYR:HD2	5:f:78:LEU:HD11	1.85	0.41
2:a:58:MET:O	2:a:59:SER:C	2.63	0.41
10:S:159:MET:HE3	10:S:159:MET:HA	2.02	0.41
11:C:60:LYS:HG3	11:C:61:GLY:N	2.36	0.41
1:8:23:ILE:CG2	2:a:28:SER:OG	2.69	0.41
3:d:121:MET:O	3:d:124:ILE:HG23	2.20	0.41
4:e:12:LEU:HD22	6:g:48:ALA:CB	2.51	0.41
11:C:28:THR:C	11:C:44:LEU:HD21	2.46	0.41
1:8:19:THR:HG1	2:a:25:LEU:HD22	1.86	0.41
2:a:44:THR:HG21	8:b:86:ASN:OD1	2.20	0.41
2:a:169:LEU:HD12	2:a:170:LEU:N	2.36	0.41
2:a:205:ALA:O	2:a:209:ILE:HG13	2.20	0.41
3:d:5:LEU:HD12	3:d:5:LEU:O	2.20	0.41
3:d:49:PRO:O	8:b:148:TYR:CE1	2.74	0.41
8:b:12:VAL:HG12	8:b:13:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:54:THR:O	8:b:57:THR:HB	2.20	0.41
8:b:88:GLN:C	8:b:88:GLN:CD	2.88	0.41
8:b:168:LYS:HE3	9:h:39:LEU:HD21	2.03	0.41
8:b:192:GLU:O	8:b:196:LYS:HG2	2.21	0.41
10:S:150:LEU:HD13	10:S:152:VAL:HG23	2.03	0.41
11:C:64:LEU:HG	11:C:65:ASN:N	2.35	0.41
2:a:116:GLY:O	2:a:120:LYS:O	2.39	0.41
3:d:152:TRP:CD1	3:d:152:TRP:C	2.99	0.41
10:S:129:ALA:O	10:S:132:THR:N	2.54	0.41
10:S:158:ILE:HG13	10:S:158:ILE:O	2.21	0.41
3:d:79:PRO:O	8:b:143:ARG:NH1	2.54	0.40
11:C:35:GLY:O	11:C:36:ASP:C	2.64	0.40
1:8:34:TYR:HA	3:d:144:LEU:HD11	2.03	0.40
2:a:87:LEU:HB3	2:a:204:PHE:HE1	1.86	0.40
2:a:104:MET:HE2	2:a:104:MET:CA	2.52	0.40
2:a:115:THR:OG1	7:j:23:GLU:HG2	2.22	0.40
3:d:37:LEU:HB3	8:b:134:MET:CE	2.47	0.40
6:g:55:ILE:O	6:g:58:SER:OG	2.32	0.40
7:j:21:TYR:O	7:j:22:GLN:C	2.62	0.40
8:b:98:GLN:OE1	8:b:98:GLN:HA	2.21	0.40
8:b:145:HIS:O	8:b:149:ARG:HG3	2.21	0.40
8:b:170:GLN:CD	11:C:12:LEU:HD21	2.44	0.40
9:h:34:GLU:HG2	9:h:35:TYR:N	2.35	0.40
2:a:58:MET:HG2	2:a:69:THR:OG1	2.22	0.40
3:d:13:VAL:HG13	3:d:14:ALA:N	2.37	0.40
5:f:14:VAL:CG1	5:f:19:LEU:HD13	2.50	0.40
5:f:51:VAL:HG12	8:b:6:PRO:O	2.21	0.40
8:b:67:LEU:O	8:b:71:VAL:HG12	2.21	0.40
8:b:157:TYR:HB3	9:h:55:MET:CE	2.46	0.40
9:h:10:LEU:H	9:h:10:LEU:HD23	1.86	0.40
10:S:40:LEU:O	10:S:44:GLN:NE2	2.54	0.40
10:S:121:THR:O	10:S:162:MET:HB2	2.21	0.40
2:a:83:ASN:O	2:a:87:LEU:HD23	2.22	0.40
8:b:187:ALA:HB1	8:b:189:GLN:HE22	1.87	0.40
9:h:5:ASP:HB2	9:h:6:PRO:HD3	2.04	0.40
5:f:66:TYR:O	5:f:67:VAL:C	2.64	0.40
8:b:165:MET:SD	8:b:168:LYS:CE	3.10	0.40
11:C:45:ARG:HE	11:C:45:ARG:C	2.29	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	8	39/66 (59%)	28 (72%)	11 (28%)	0	100	100
2	a	224/226 (99%)	204 (91%)	20 (9%)	0	100	100
3	d	153/160 (96%)	129 (84%)	24 (16%)	0	100	100
4	e	39/70 (56%)	37 (95%)	2 (5%)	0	100	100
5	f	81/87 (93%)	72 (89%)	9 (11%)	0	100	100
6	g	77/102 (76%)	72 (94%)	5 (6%)	0	100	100
7	j	46/60 (77%)	45 (98%)	1 (2%)	0	100	100
8	b	207/214 (97%)	196 (95%)	11 (5%)	0	100	100
9	h	60/76 (79%)	47 (78%)	13 (22%)	0	100	100
10	S	125/190 (66%)	109 (87%)	16 (13%)	0	100	100
11	C	87/510 (17%)	80 (92%)	7 (8%)	0	100	100
All	All	1138/1761 (65%)	1019 (90%)	119 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8	41/66 (62%)	41 (100%)	0	100	100
2	a	200/200 (100%)	200 (100%)	0	100	100
3	d	139/142 (98%)	139 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	e	34/59 (58%)	34 (100%)	0	100	100
5	f	72/75 (96%)	72 (100%)	0	100	100
6	g	67/83 (81%)	67 (100%)	0	100	100
7	j	42/49 (86%)	42 (100%)	0	100	100
8	b	186/190 (98%)	186 (100%)	0	100	100
9	h	56/70 (80%)	56 (100%)	0	100	100
10	S	110/165 (67%)	110 (100%)	0	100	100
11	C	73/413 (18%)	73 (100%)	0	100	100
All	All	1020/1512 (68%)	1020 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	8	3	GLN
1	8	31	HIS
1	8	35	HIS
1	8	36	ASN
5	f	46	ASN
6	g	75	ASN
8	b	86	ASN
8	b	105	GLN
8	b	130	ASN
8	b	145	HIS
10	S	112	HIS

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 [i](#)

There are no oligosaccharides 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.

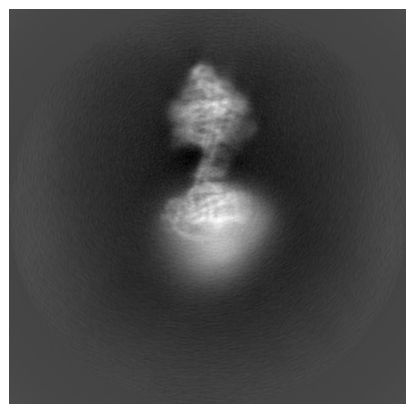
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11230. These allow visual inspection of the internal detail of the map and identification of artifacts.

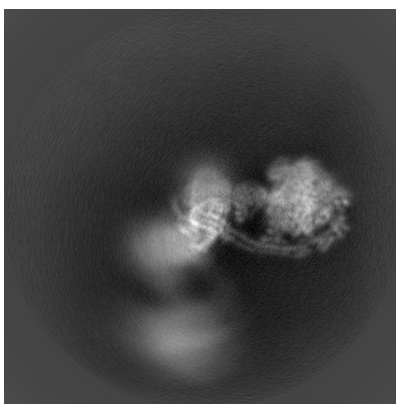
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

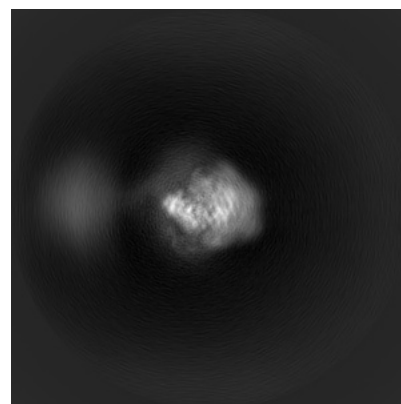
6.1.1 Primary map



X

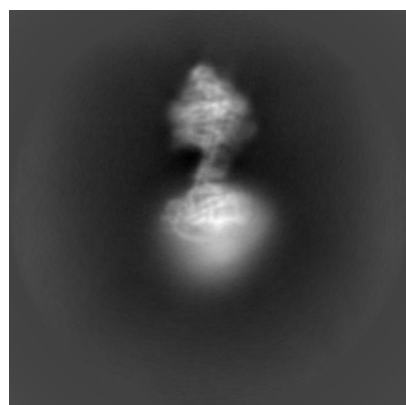


Y

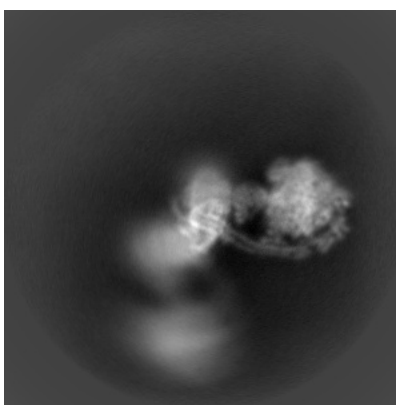


Z

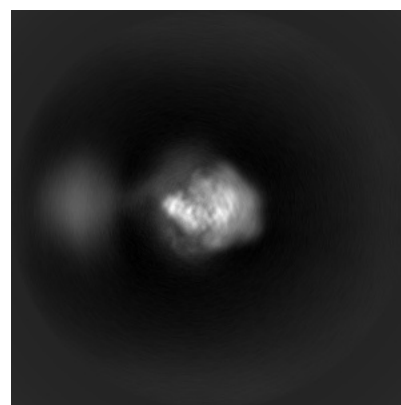
6.1.2 Raw map



X



Y

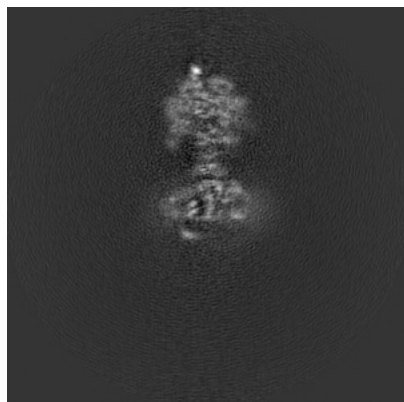


Z

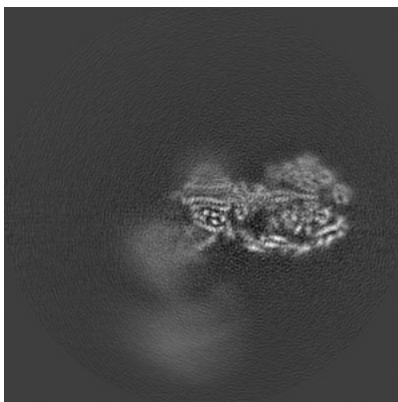
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

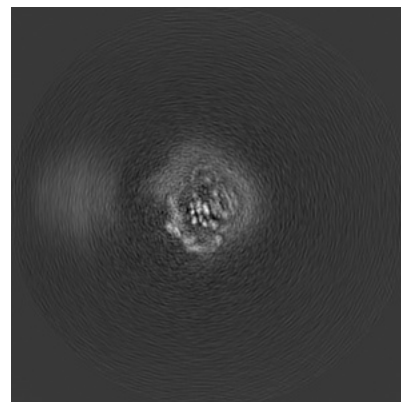
6.2.1 Primary map



X Index: 250

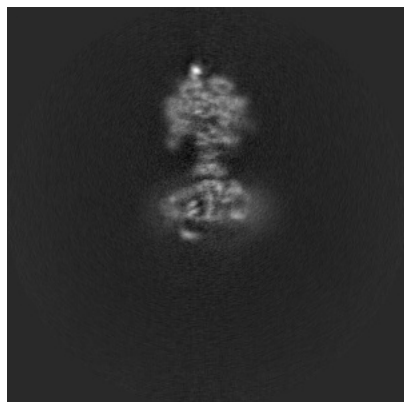


Y Index: 250

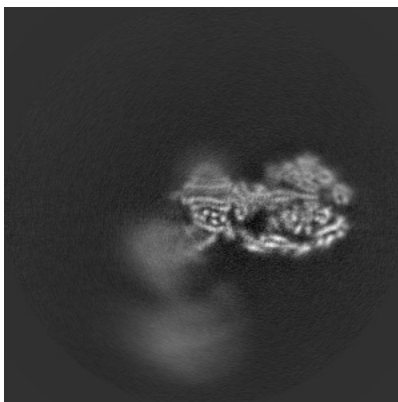


Z Index: 250

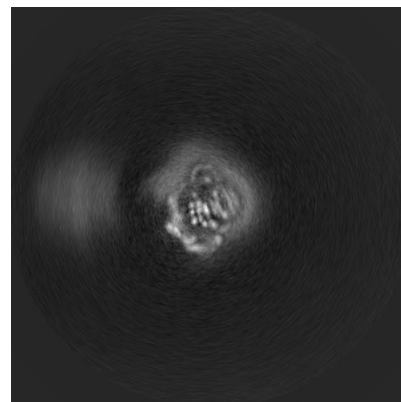
6.2.2 Raw map



X Index: 250



Y Index: 250

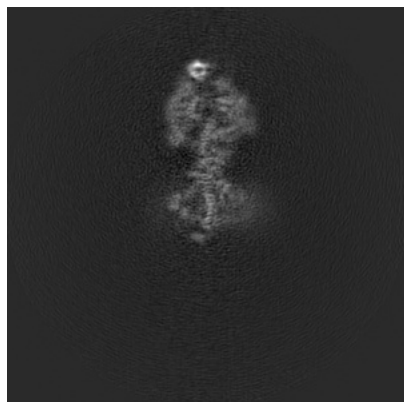


Z Index: 250

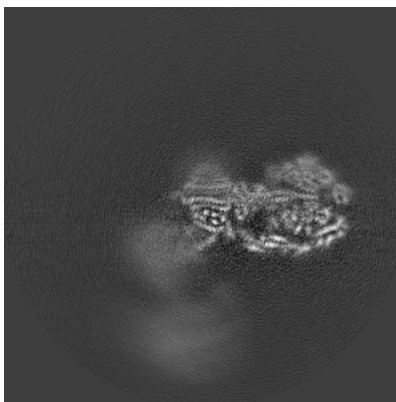
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

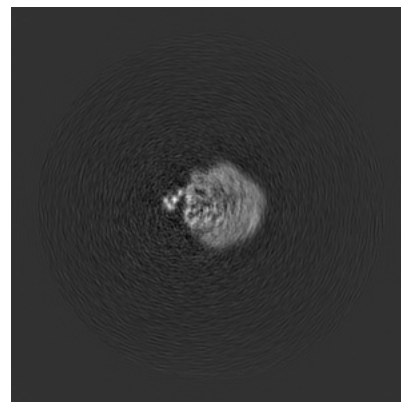
6.3.1 Primary map



X Index: 258

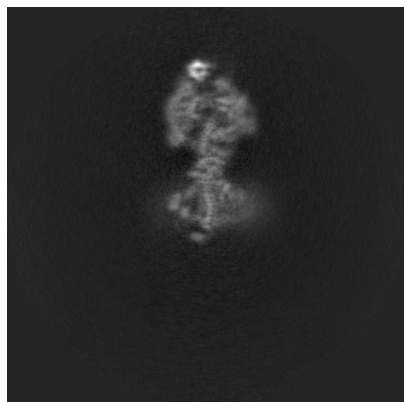


Y Index: 250

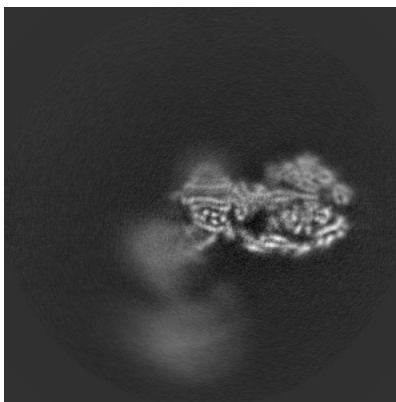


Z Index: 377

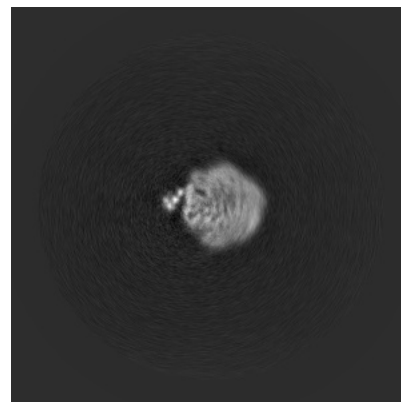
6.3.2 Raw map



X Index: 258



Y Index: 250

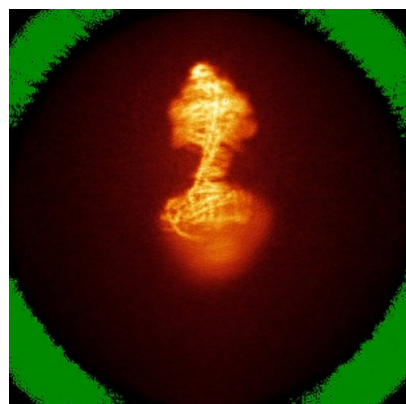


Z Index: 378

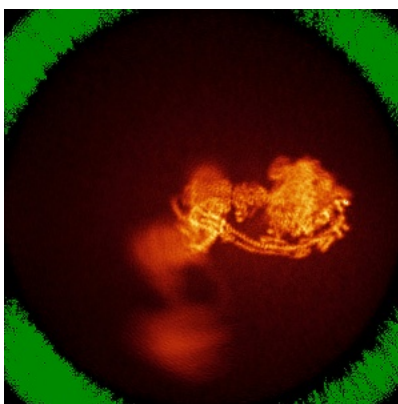
The images above show the largest variance slices of the map in three orthogonal directions.

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

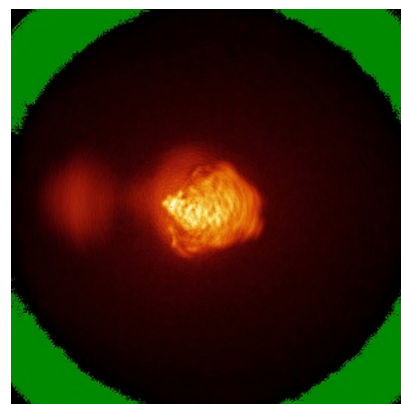
6.4.1 Primary map



X



Y



Z

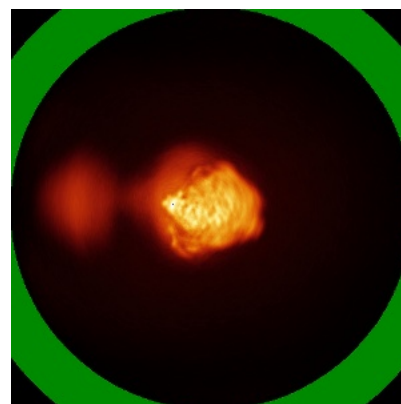
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0171. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

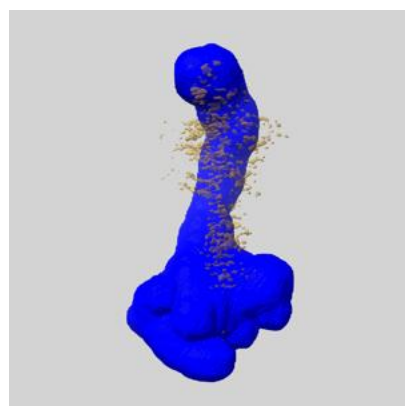
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

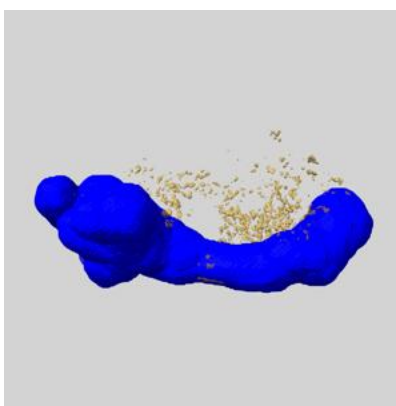
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

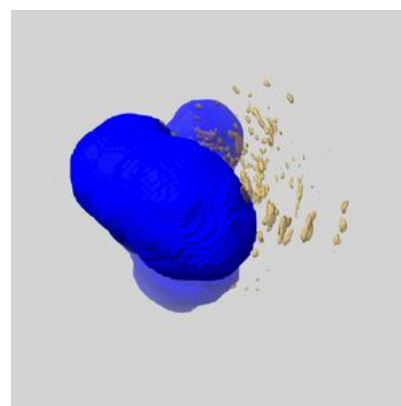
6.6.1 emd_11230_msk_1.map [i](#)



X



Y

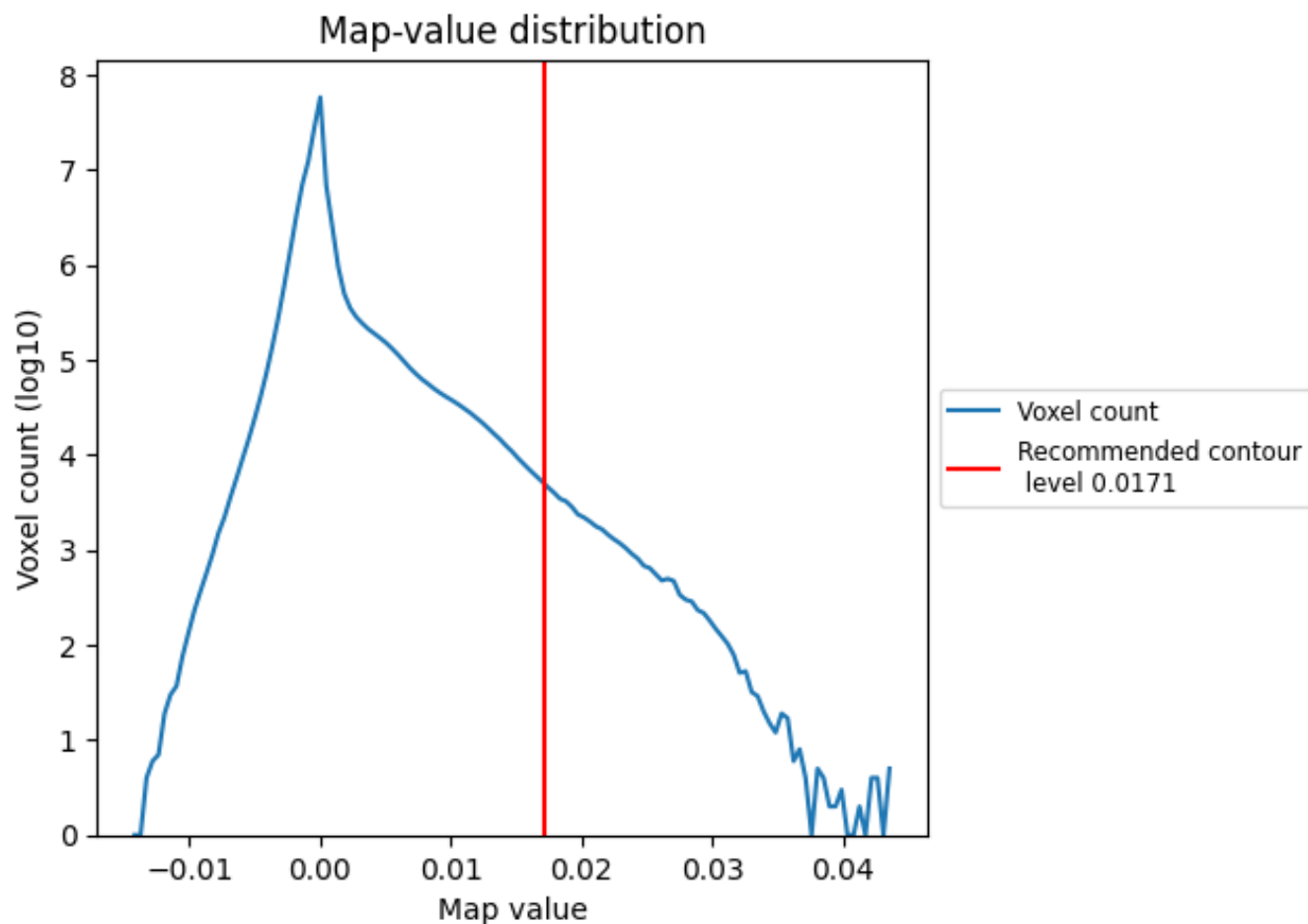


Z

7 Map analysis [i](#)

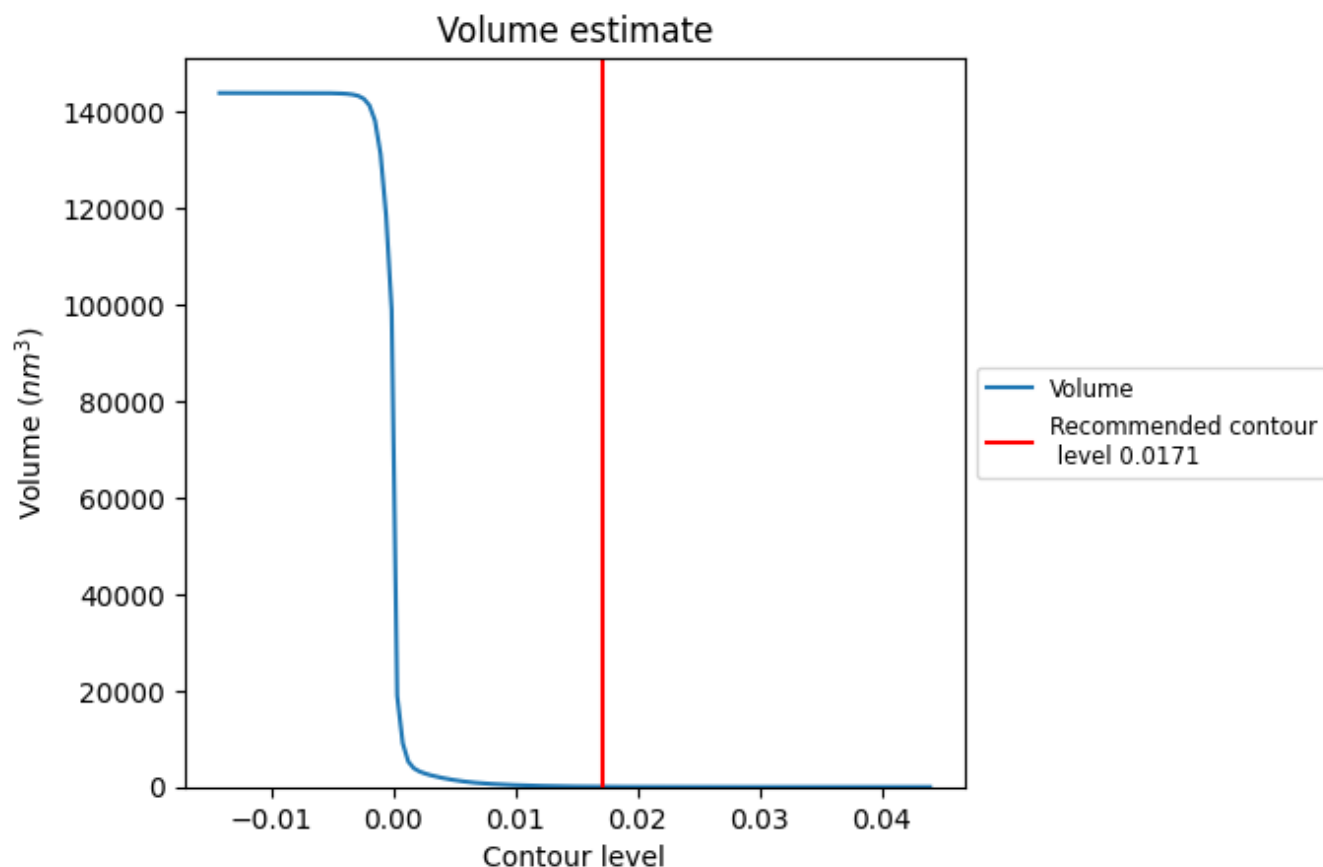
This section contains the results of statistical analysis of the map.

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.

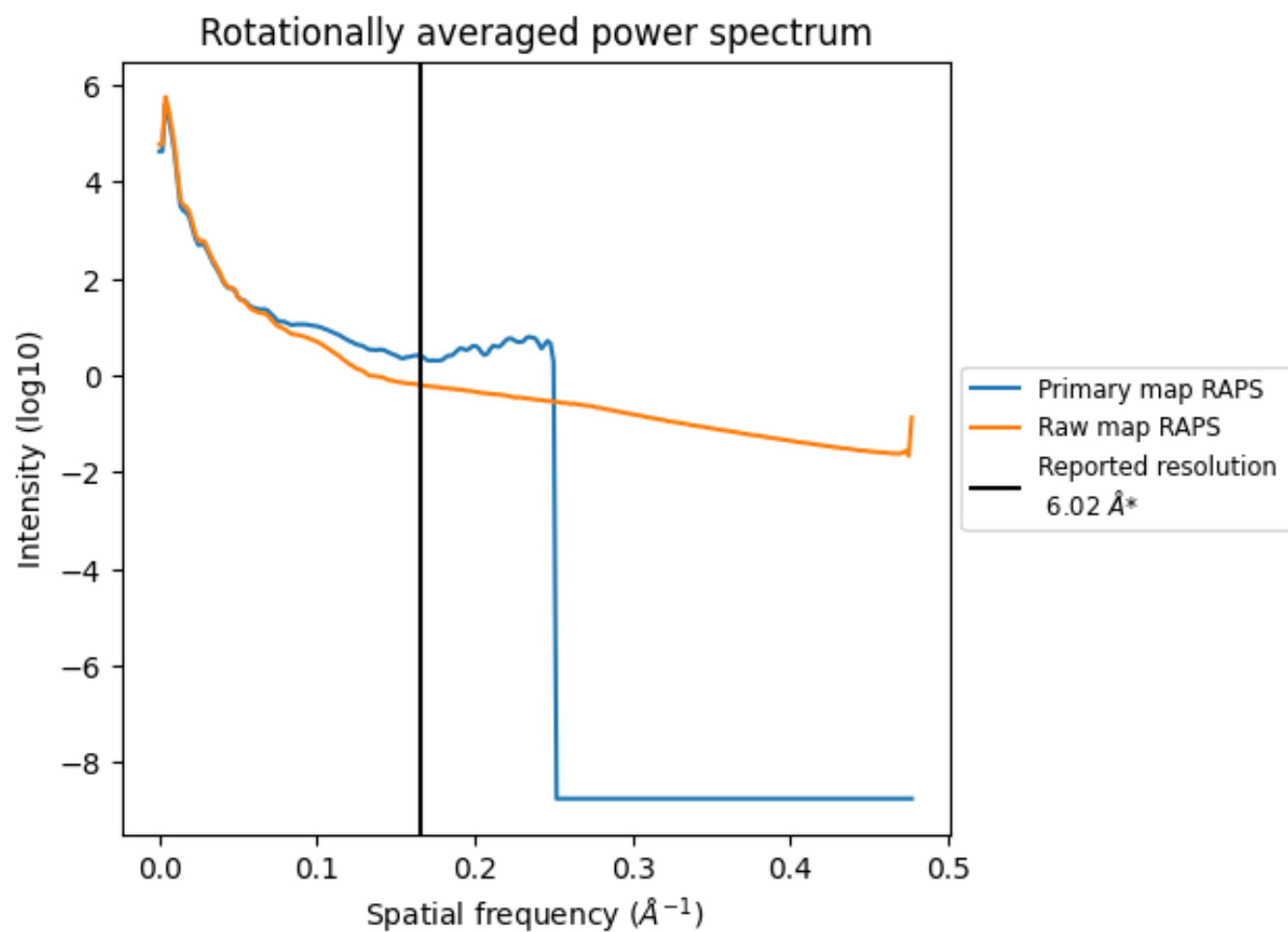
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51 nm^3 ; this corresponds to an approximate mass of 46 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 ⓘ

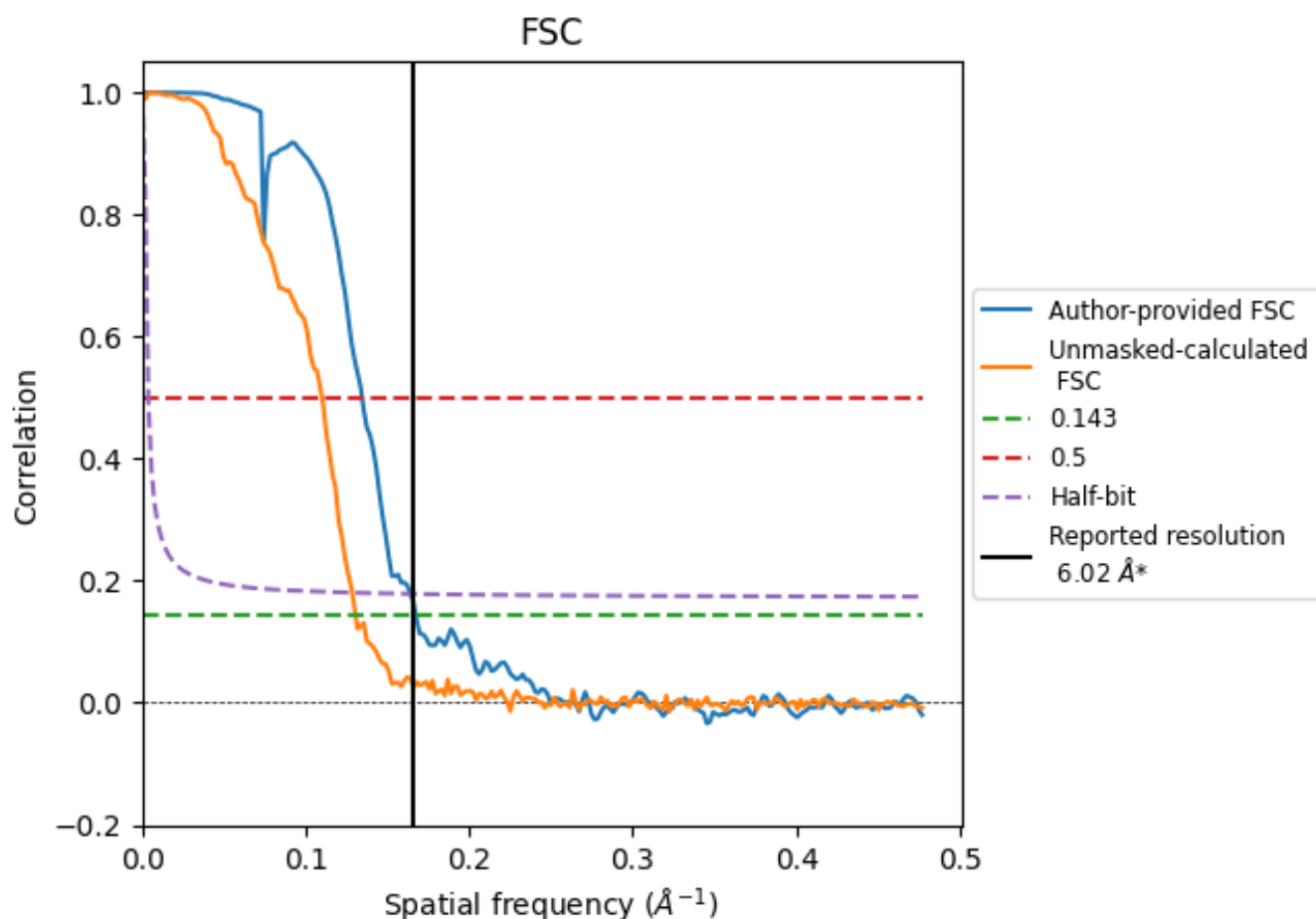


*Reported resolution corresponds to spatial frequency of $0.166 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.166 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.02	-	-
Author-provided FSC curve	5.97	7.43	6.09
Unmasked-calculated*	7.66	9.09	7.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.66 differs from the reported value 6.02 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11230 and PDB model 6ZIU. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



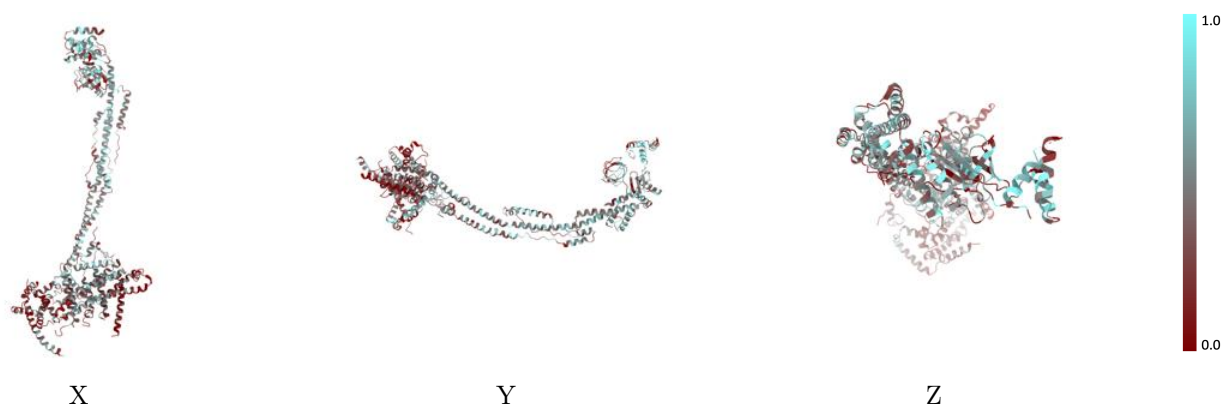
The images above show the 3D surface view of the map at the recommended contour level 0.0171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



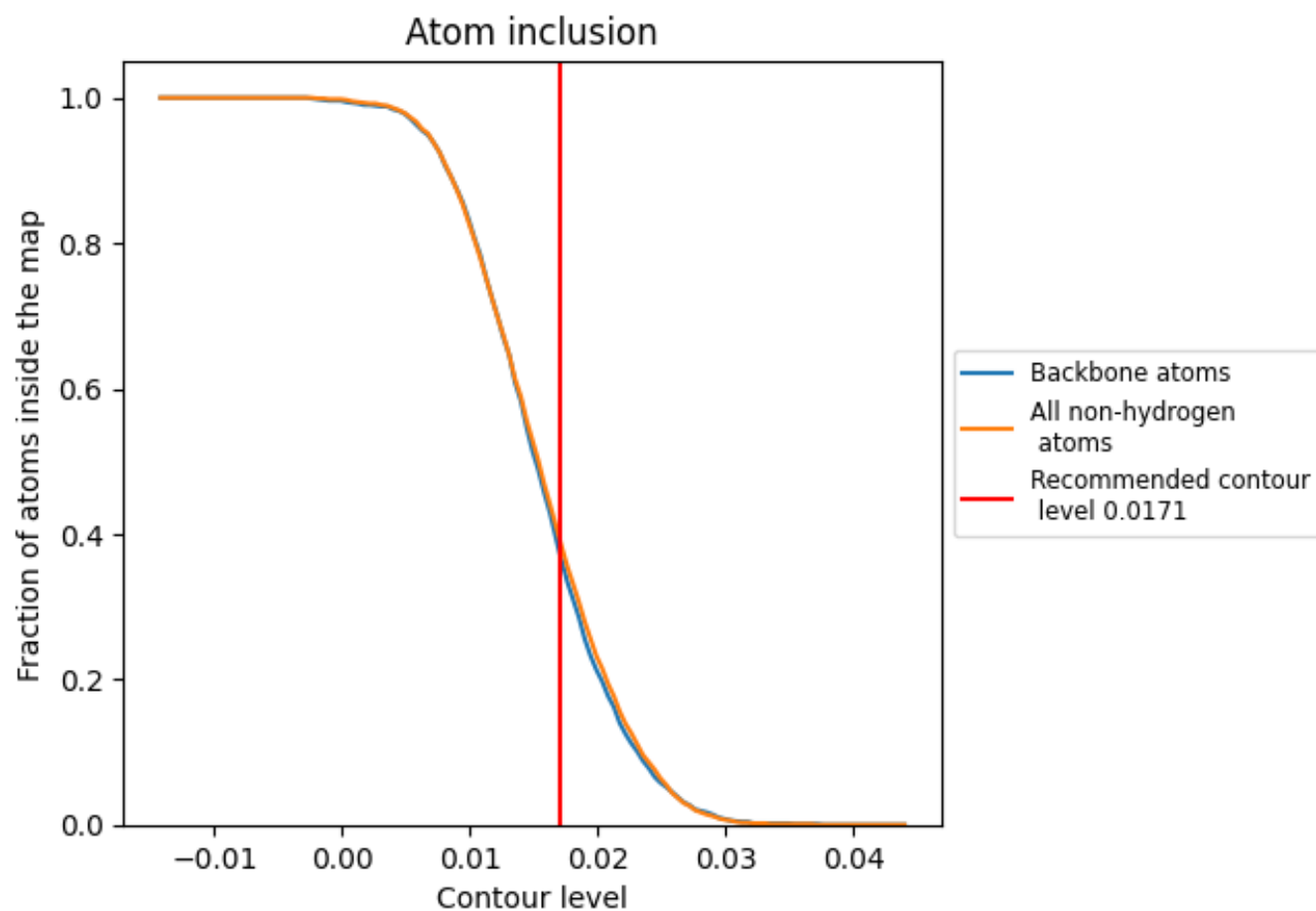
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0171).

9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 39% 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 (0.0171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3870	0.2860
8	0.3510	0.3570
C	0.4020	0.2910
S	0.4720	0.2440
a	0.3480	0.3040
b	0.4670	0.2930
d	0.4500	0.3120
e	0.3020	0.2450
f	0.3930	0.3180
g	0.2510	0.2340
h	0.4310	0.2480
j	0.1720	0.2530

1.0

0.0

<0.0