



Full wwPDB EM Validation Report ⓘ

Nov 12, 2025 – 10:18 AM EST

PDB ID : 9NDY / pdb_00009ndy
EMDB ID : EMD-49281
Title : Composite baseplate asymmetric unit of JohannRWettstein (Bas63)
Authors : Hodgkinson-Bean, J.
Deposited on : 2025-02-18
Resolution : 3.83 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

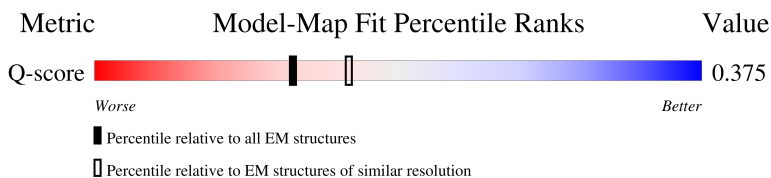
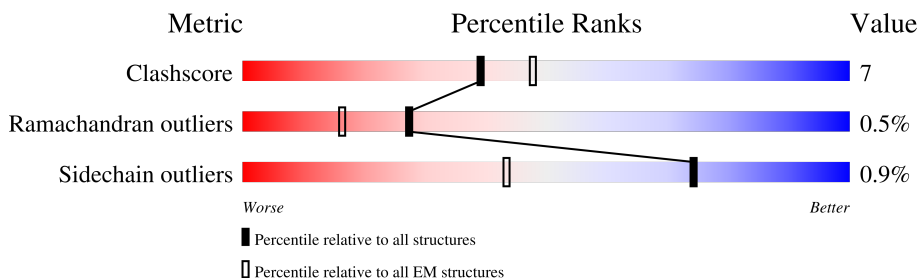
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.83 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.




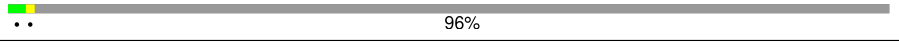
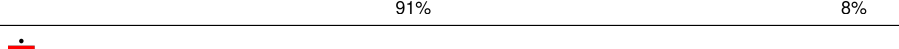
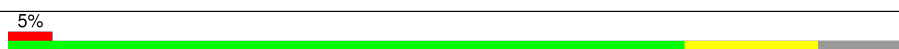


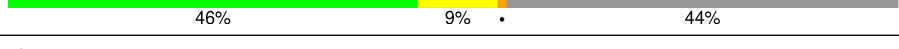
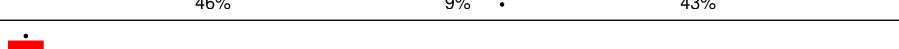

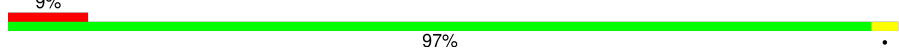
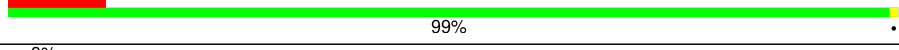
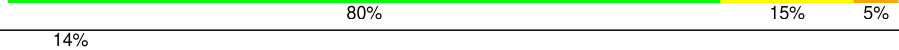
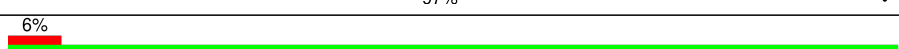
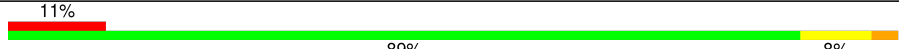



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	9087 (3.33 - 4.33)

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	265	<div> <div>8%</div> <div>64%</div> <div>12%</div> <div>24%</div> </div>
1	B	265	<div> <div>13%</div> <div>67%</div> <div>9%</div> <div>24%</div> </div>
2	C	139	<div> <div>10%</div> <div>86%</div> <div>•</div> <div>9%</div> </div>
2	D	139	<div> <div>9%</div> <div>78%</div> <div>12%</div> <div>•</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	325	
4	F	742	
5	G	207	
6	H	489	
6	I	489	
6	K	489	
6	L	489	
7	J	285	
7	M	285	
8	N	113	
8	O	113	
9	P	100	
9	Q	100	
9	R	100	
9	S	100	
9	T	100	
9	U	100	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 30166 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 Tube initiator protein (gp018).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	202	Total	C	N	O	S	0	0
			1519	933	262	317	7		
1	B	201	Total	C	N	O	S	0	0
			1513	930	261	315	7		

- Molecule 2 is a protein called Sheath initiator (gp022).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	126	Total	C	N	O	S	0	0
			995	628	170	194	3		
2	D	126	Total	C	N	O	S	0	0
			995	628	170	194	3		

- Molecule 3 is a protein called Hub protein (gp020).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	305	Total	C	N	O	S	0	0
			2463	1558	421	472	12		

- Molecule 4 is a protein called Tape measure protein (gp017).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	26	Total	C	N	O	S	0	0
			206	127	31	47	1		

- Molecule 5 is a protein called Puncture apparatus (gp021).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	206	Total	C	N	O	S	0	0
			1619	1021	269	319	10		

- Molecule 6 is a protein called Wedge protein 2 (gp023).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	459	Total	C	N	O	S	0	0
			3541	2234	581	724	2		
6	I	442	Total	C	N	O	S	0	0
			3398	2140	564	692	2		
6	K	446	Total	C	N	O	S	0	0
			3436	2162	572	700	2		
6	L	476	Total	C	N	O	S	0	0
			3656	2304	604	746	2		

- Molecule 7 is a protein called Wedge protein 1 (gp024).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	160	Total	C	N	O	S	0	0
			1289	821	220	244	4		
7	M	162	Total	C	N	O	S	0	0
			1306	833	222	247	4		

- Molecule 8 is a protein called Spacer protein (gp019).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	112	Total	C	N	O	S	0	0
			919	584	150	180	5		
8	O	111	Total	C	N	O	S	0	0
			911	579	149	179	4		

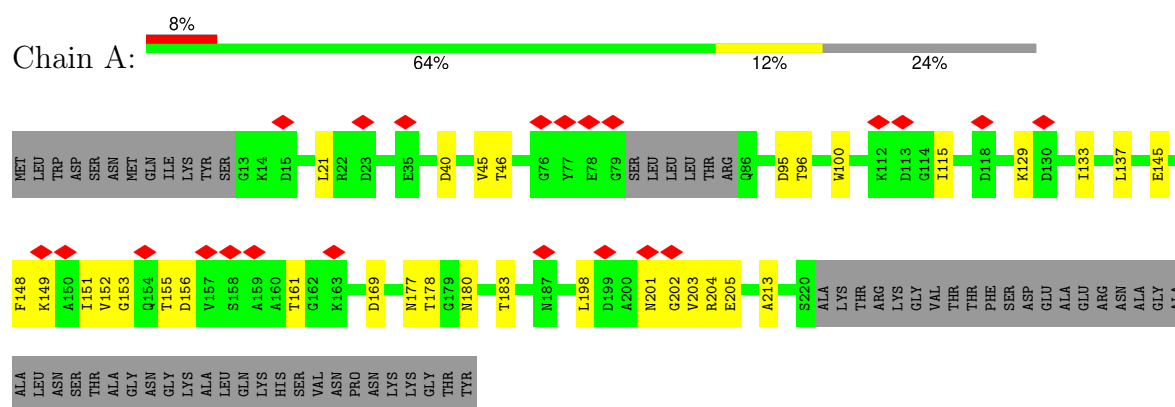
- Molecule 9 is a protein called LTF platform protein (gp025).

Mol	Chain	Residues	Atoms				AltConf	Trace
9	S	100	Total	C	N	O	0	0
			400	200	100	100		
9	T	100	Total	C	N	O	0	0
			400	200	100	100		
9	U	100	Total	C	N	O	0	0
			400	200	100	100		
9	P	100	Total	C	N	O	0	0
			400	200	100	100		
9	Q	100	Total	C	N	O	0	0
			400	200	100	100		
9	R	100	Total	C	N	O	0	0
			400	200	100	100		

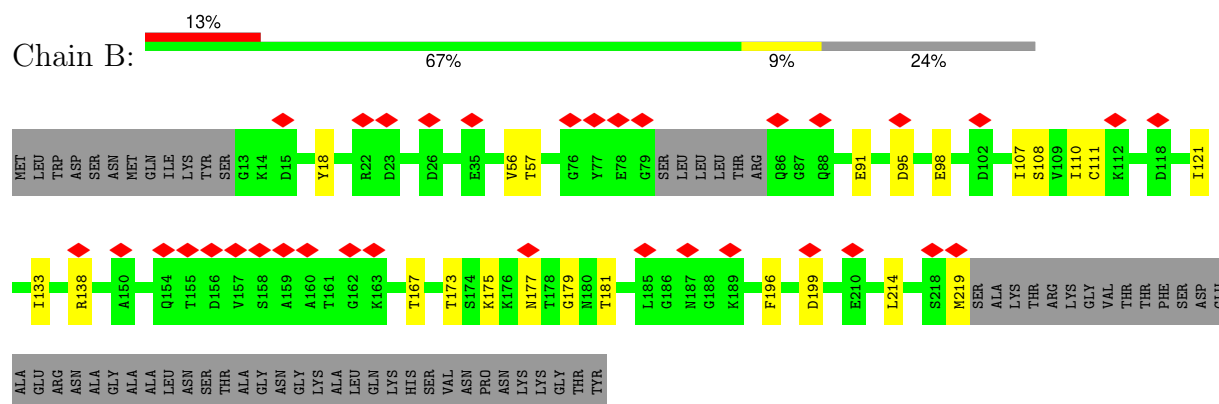
3 Residue-property plots [i](#)

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.

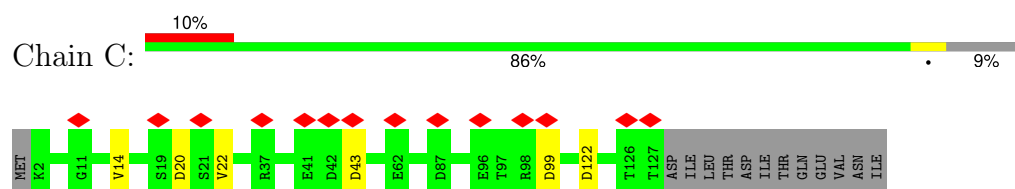
• Molecule 1: Tube initiator protein (gp018)



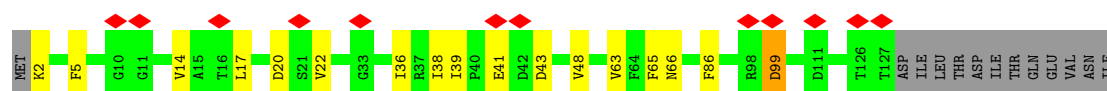
• Molecule 1: Tube initiator protein (gp018)

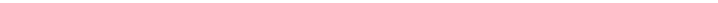


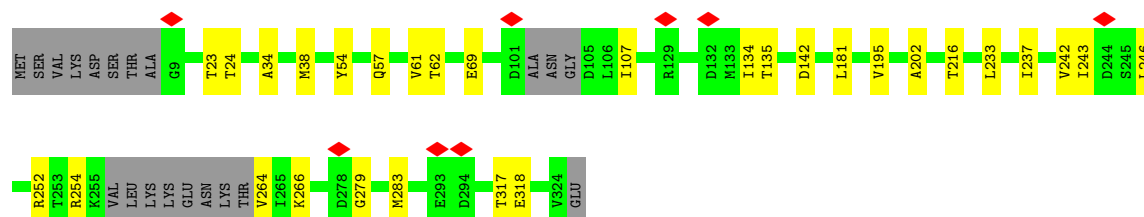
• Molecule 2: Sheath initiator (gp022)



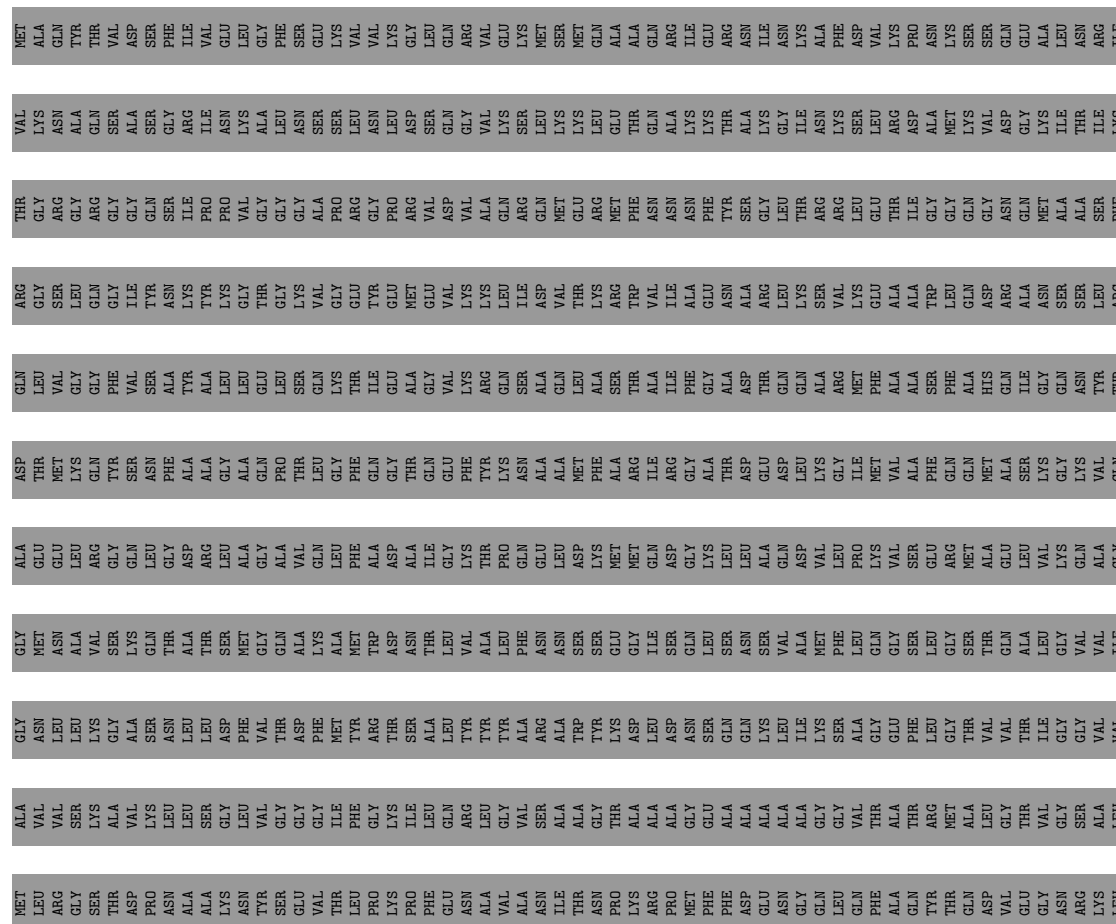
• Molecule 2: Sheath initiator (gp022)

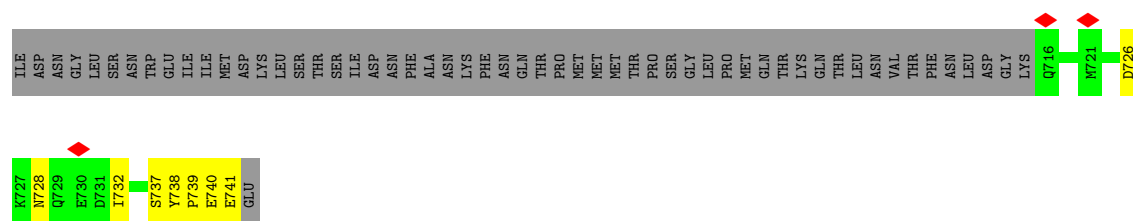


- Chain E:  85% 9% 6%

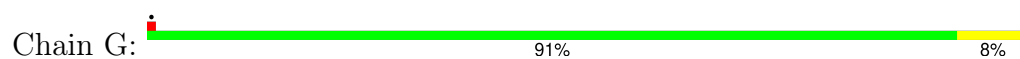


- Chain F:  96%

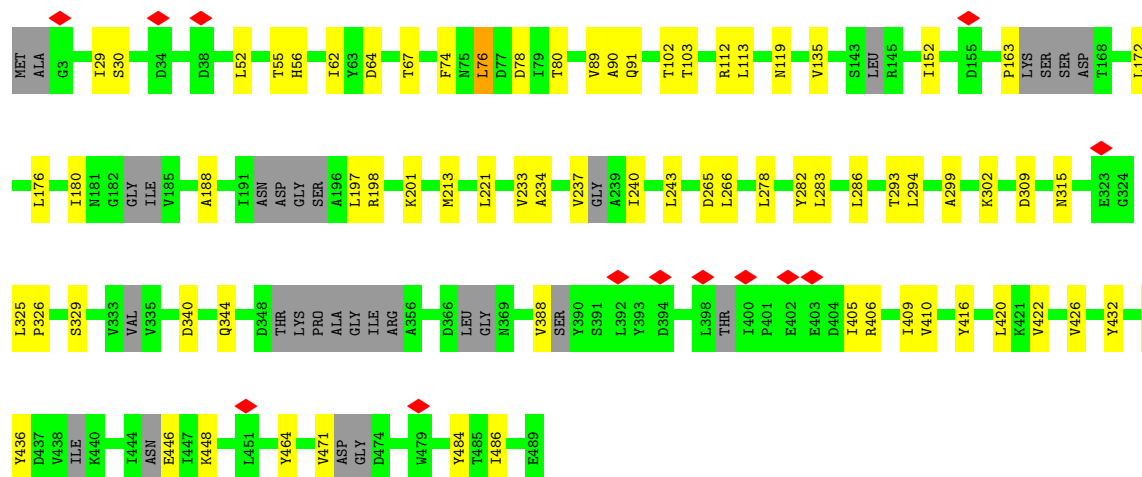
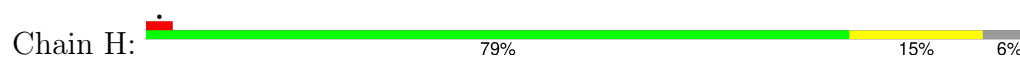




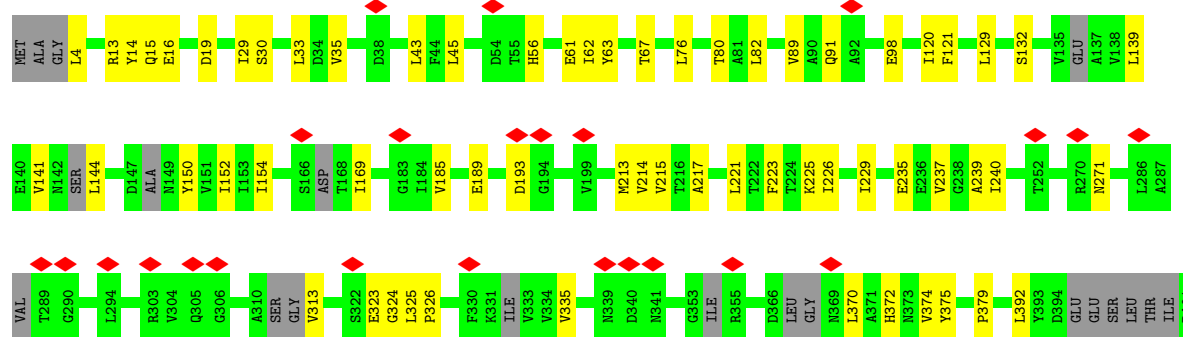
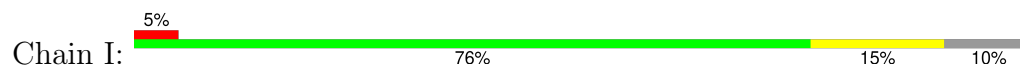
- Molecule 5: Puncture apparatus (gp021)

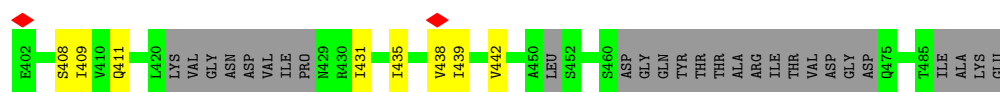


- Molecule 6: Wedge protein 2 (gp023)



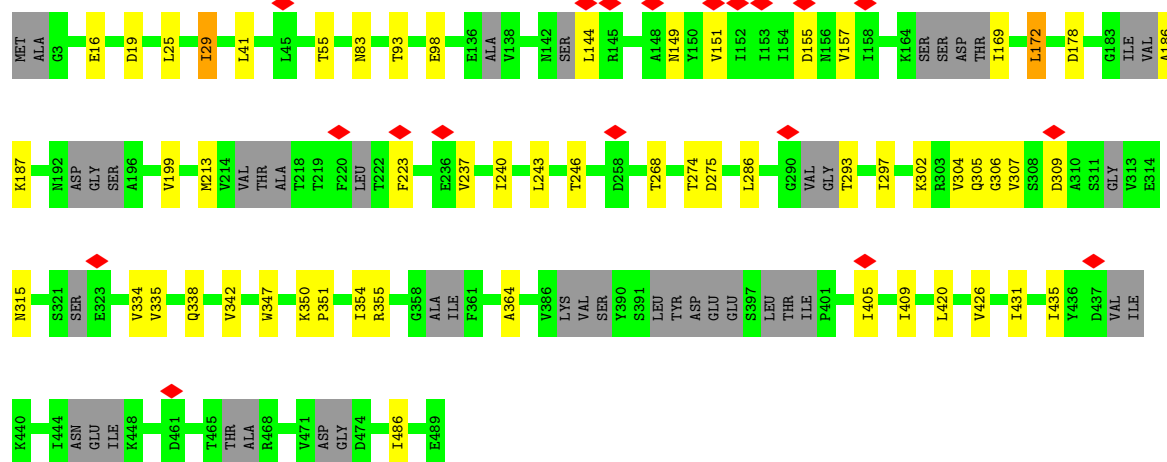
- Molecule 6: Wedge protein 2 (gp023)





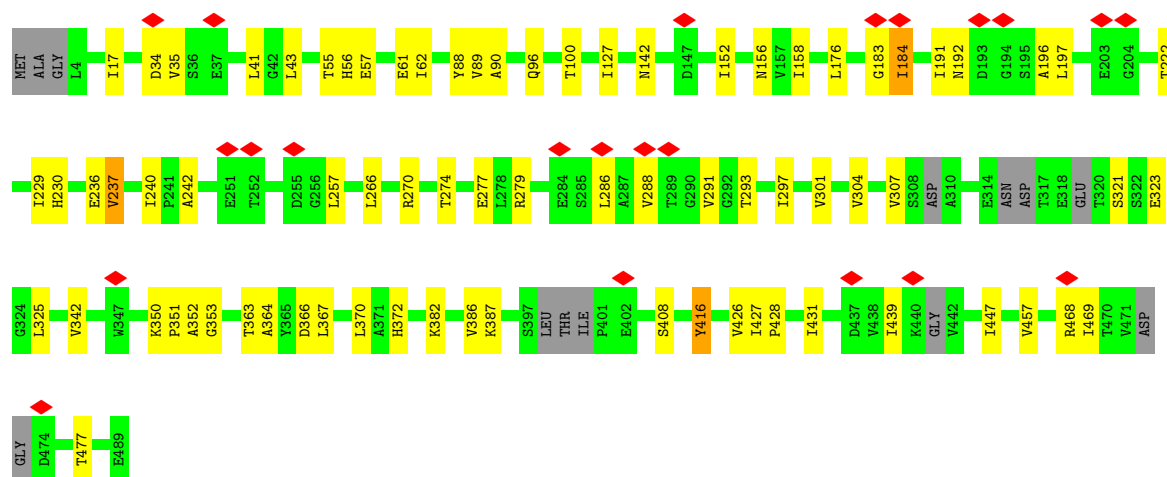
• Molecule 6: Wedge protein 2 (gp023)

Chain K: 80% 11% 9%



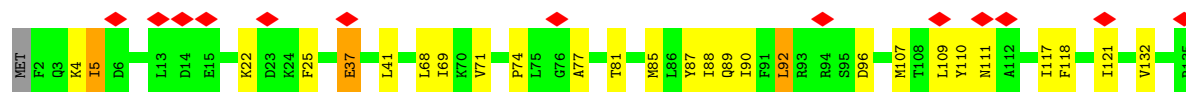
• Molecule 6: Wedge protein 2 (gp023)

Chain L: 82% 15% 3%

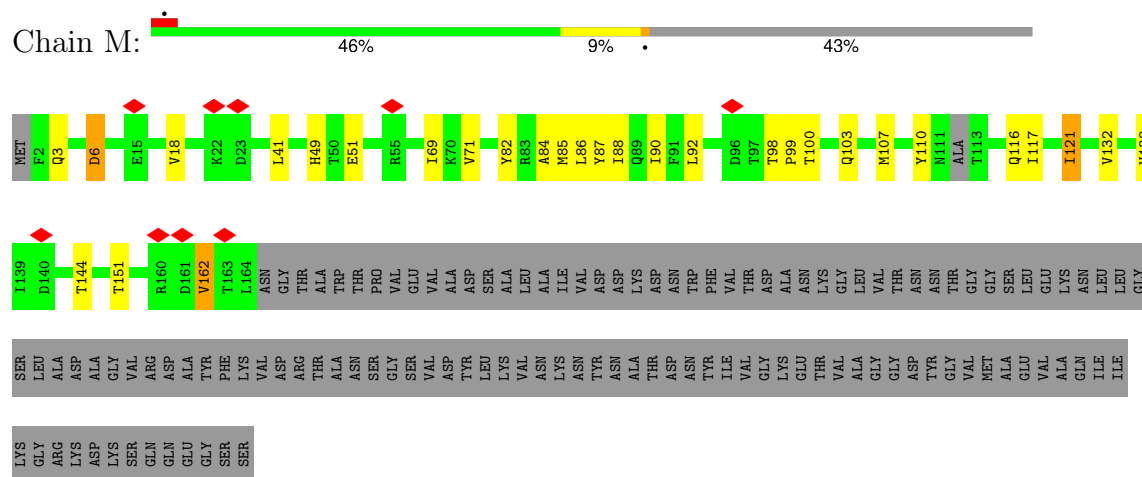


• Molecule 7: Wedge protein 1 (gp024)

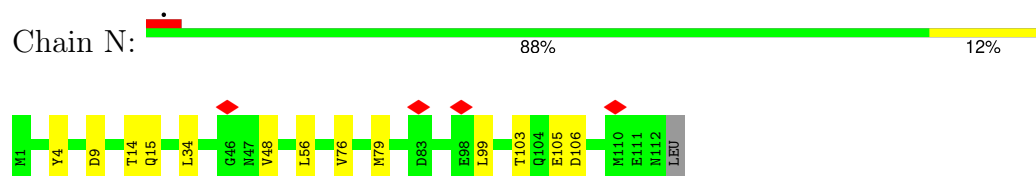
Chain J: 5% 46% 9% 44%



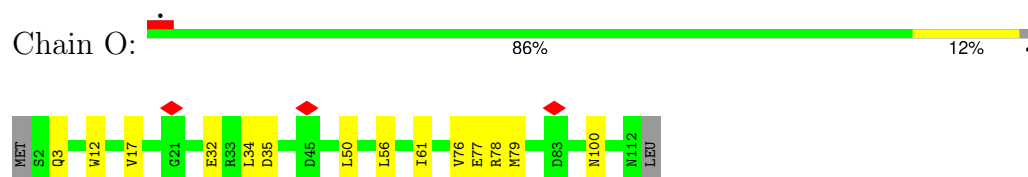
- Molecule 7: Wedge protein 1 (gp024)



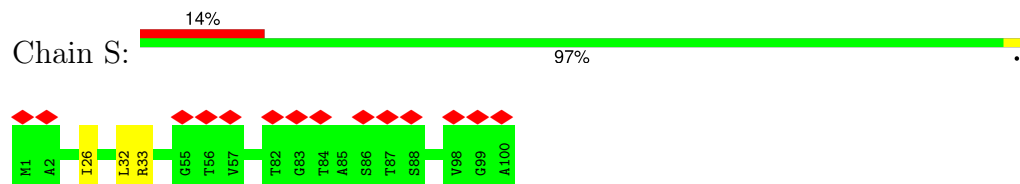
- Molecule 8: Spacer protein (gp019)



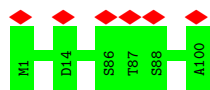
- Molecule 8: Spacer protein (gp019)



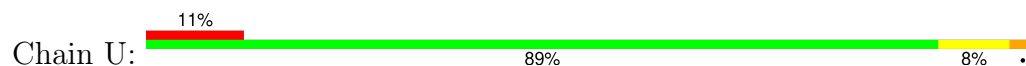
- Molecule 9: LTF platform protein (gp025)



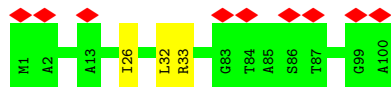
- Molecule 9: LTF platform protein (gp025)



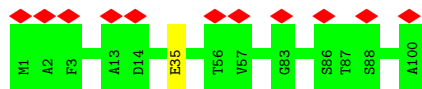
- Molecule 9: LTF platform protein (gp025)



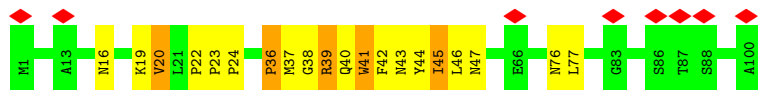
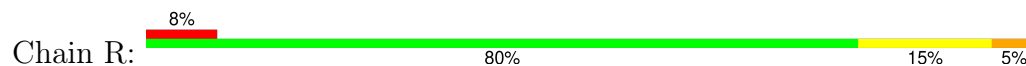
- Molecule 9: LTF platform protein (gp025)



- Molecule 9: LTF platform protein (gp025)



- Molecule 9: LTF platform protein (gp025)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14390	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	31.048	Depositor
Minimum map value	-8.973	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.044	Depositor
Recommended contour level	4.78	Depositor
Map size (\AA)	554.8, 554.8, 554.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.387, 1.387, 1.387	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	0.13	0/1532	0.36	0/2069
1	B	0.12	0/1526	0.30	0/2061
2	C	0.12	0/1012	0.32	0/1369
2	D	0.12	0/1012	0.31	0/1369
3	E	0.11	0/2507	0.29	0/3378
4	F	0.19	0/207	0.47	0/279
5	G	0.12	0/1661	0.29	0/2260
6	H	0.10	0/3586	0.27	0/4877
6	I	0.12	0/3441	0.30	1/4676 (0.0%)
6	K	0.11	0/3474	0.29	0/4708
6	L	0.11	0/3709	0.28	0/5051
7	J	0.13	0/1310	0.35	0/1779
7	M	0.15	0/1326	0.36	0/1800
8	N	0.14	0/937	0.31	0/1269
8	O	0.13	0/929	0.31	0/1259
9	P	0.21	0/399	0.57	0/497
9	Q	0.23	0/399	0.54	0/497
9	R	0.62	0/399	0.97	1/497 (0.2%)
9	S	0.20	0/399	0.56	0/497
9	T	0.23	0/399	0.54	0/497
9	U	0.49	0/399	0.93	3/497 (0.6%)
All	All	0.15	0/30563	0.35	5/41186 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	36	PRO	N-CA-C	6.92	126.72	112.47
6	I	185	VAL	N-CA-C	-6.29	106.80	111.90
9	U	44	TYR	N-CA-C	-6.00	104.75	111.28
9	U	43	ASN	N-CA-C	-5.25	105.46	111.07
9	U	39	ARG	N-CA-C	-5.12	106.72	112.87

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	1519	0	1500	25	0
1	B	1513	0	1495	16	0
2	C	995	0	980	4	0
2	D	995	0	980	13	0
3	E	2463	0	2441	26	0
4	F	206	0	200	23	0
5	G	1619	0	1540	23	0
6	H	3541	0	3479	50	0
6	I	3398	0	3340	61	0
6	K	3436	0	3373	39	0
6	L	3656	0	3616	69	0
7	J	1289	0	1310	27	0
7	M	1306	0	1331	33	0
8	N	919	0	900	10	0
8	O	911	0	888	16	0
9	P	400	0	115	1	0
9	Q	400	0	115	3	0
9	R	400	0	115	14	0
9	S	400	0	115	1	0
9	T	400	0	115	0	0
9	U	400	0	115	7	0
All	All	30166	0	28063	405	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 7.

All (405) 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)
7:J:118:PHE:CE2	9:Q:35:GLU:CA	1.85	1.41
7:J:118:PHE:HE2	9:Q:35:GLU:CA	1.28	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:738:TYR:CD2	5:G:18:GLU:OE1	1.83	1.29
4:F:738:TYR:CG	5:G:18:GLU:OE1	1.84	1.28
9:R:19:LYS:CA	9:R:40:GLN:CA	2.25	1.14
3:E:254:ARG:NH2	4:F:738:TYR:HB3	1.73	1.04
4:F:726:ASP:OD2	5:G:2:LYS:O	1.76	1.03
3:E:254:ARG:HH21	4:F:738:TYR:HB3	1.21	0.97
3:E:254:ARG:HG3	4:F:740:GLU:O	1.67	0.94
4:F:738:TYR:CD1	5:G:18:GLU:OE1	1.98	0.92
7:J:118:PHE:CD2	9:Q:35:GLU:CA	2.52	0.92
4:F:738:TYR:CE2	5:G:18:GLU:OE1	2.02	0.90
4:F:728:ASN:O	4:F:732:ILE:HD12	1.76	0.84
1:A:45:VAL:HG22	1:B:121:ILE:HD11	1.60	0.83
4:F:726:ASP:OD2	5:G:2:LYS:C	2.24	0.81
7:J:138:VAL:HG12	7:J:138:VAL:O	1.84	0.75
7:M:88:ILE:HD12	7:M:144:THR:CG2	2.16	0.75
4:F:726:ASP:CG	5:G:2:LYS:O	2.33	0.72
6:L:426:VAL:HG21	6:L:468:ARG:HA	1.70	0.72
6:H:76:LEU:O	6:H:80:THR:HG23	1.90	0.71
9:R:44:TYR:C	9:R:46:LEU:N	2.42	0.71
1:A:183:THR:CG2	3:E:34:ALA:HB1	2.20	0.71
7:M:69:ILE:HG23	7:M:71:VAL:HG22	1.72	0.71
6:I:213:MET:HE1	6:I:215:VAL:HG23	1.74	0.70
6:K:409:ILE:HG23	6:K:435:ILE:HD12	1.73	0.69
6:L:426:VAL:HG12	6:L:428:PRO:HD2	1.72	0.69
4:F:726:ASP:OD2	5:G:2:LYS:HB3	1.93	0.69
6:K:297:ILE:HG23	6:K:350:LYS:HE3	1.75	0.68
9:R:44:TYR:C	9:R:46:LEU:H	2.02	0.68
9:R:44:TYR:O	9:R:46:LEU:N	2.27	0.68
6:H:90:ALA:HB1	6:H:237:VAL:HG11	1.77	0.67
6:L:55:THR:HG21	7:M:41:LEU:HD23	1.77	0.67
1:A:133:ILE:O	1:A:133:ILE:HG22	1.94	0.67
1:A:149:LYS:HA	1:A:161:THR:HG21	1.76	0.66
6:I:392:LEU:CD2	6:I:442:VAL:HG12	2.25	0.66
2:D:48:VAL:HG22	2:D:99:ASP:OD1	1.94	0.66
6:I:91:GLN:CG	6:I:237:VAL:HG13	2.26	0.65
6:L:370:LEU:HB2	6:L:372:HIS:NE2	2.10	0.65
7:M:71:VAL:HG21	7:M:86:LEU:HD13	1.78	0.65
9:U:46:LEU:O	9:U:47:ASN:C	2.38	0.65
6:L:291:VAL:HG21	7:M:98:THR:CG2	2.27	0.65
6:I:408:SER:HB2	6:I:439:ILE:HD11	1.78	0.65
6:I:82:LEU:HD21	7:J:69:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:370:LEU:HB2	6:L:372:HIS:CD2	2.32	0.64
6:L:370:LEU:CB	6:L:372:HIS:NE2	2.61	0.64
6:I:435:ILE:HD11	6:I:439:ILE:HD12	1.80	0.64
6:L:370:LEU:HD11	7:M:116:GLN:HB3	1.78	0.64
8:N:103:THR:HG22	8:N:106:ASP:OD1	1.98	0.64
6:I:438:VAL:HG23	6:I:439:ILE:HG13	1.79	0.64
3:E:61:VAL:HG13	3:E:62:THR:HG22	1.80	0.63
6:I:91:GLN:HG3	6:I:237:VAL:HG13	1.79	0.63
6:L:353:GLY:O	7:M:121:ILE:HD12	1.98	0.63
7:M:162:VAL:HG12	7:M:162:VAL:O	1.99	0.62
2:C:20:ASP:O	2:C:20:ASP:OD2	2.19	0.61
7:M:110:TYR:CE1	7:M:138:VAL:HG12	2.36	0.61
6:I:335:VAL:HG22	6:I:379:PRO:HG3	1.83	0.61
3:E:254:ARG:HE	4:F:739:PRO:HG2	1.66	0.61
6:L:304:VAL:HG11	6:L:342:VAL:HG22	1.83	0.60
7:J:87:TYR:HA	7:J:90:ILE:HD12	1.82	0.60
6:K:93:THR:HG22	6:K:268:THR:HA	1.82	0.60
3:E:195:VAL:HG21	3:E:202:ALA:HB2	1.84	0.60
6:I:144:LEU:N	6:I:150:TYR:HH	1.99	0.59
6:H:325:LEU:HD21	6:H:329:SER:O	2.03	0.59
6:I:225:LYS:O	6:I:226:ILE:HD13	2.02	0.59
6:L:43:LEU:HD13	7:M:18:VAL:HG21	1.84	0.59
7:J:138:VAL:O	7:J:138:VAL:CG1	2.50	0.59
6:I:139:LEU:HD22	6:I:221:LEU:HD13	1.85	0.58
6:I:132:SER:O	6:I:214:VAL:HG22	2.03	0.58
1:B:91:GLU:O	1:B:95:ASP:OD1	2.20	0.58
6:H:410:VAL:HG13	6:H:484:TYR:CD2	2.39	0.58
6:L:96:GLN:HB3	6:L:229:ILE:HD11	1.85	0.58
6:L:236:GLU:O	6:L:237:VAL:HG12	2.03	0.58
6:H:315:ASN:HB2	6:H:325:LEU:HD22	1.86	0.57
6:I:374:VAL:HG12	6:I:375:TYR:H	1.69	0.57
7:M:107:MET:HE1	7:M:132:VAL:HG23	1.84	0.57
9:U:40:GLN:O	9:U:43:ASN:N	2.37	0.57
6:K:293:THR:CA	7:M:151:THR:HG22	2.35	0.57
6:K:55:THR:HG23	6:L:56:HIS:CE1	2.39	0.57
6:K:199:VAL:HG12	6:K:213:MET:HE1	1.87	0.57
6:L:382:LYS:HB3	6:L:477:THR:HG22	1.86	0.57
6:H:197:LEU:HD23	6:H:198:ARG:N	2.19	0.57
6:H:201:LYS:HG3	6:H:213:MET:HE2	1.86	0.57
6:I:154:ILE:HG23	6:I:213:MET:HE3	1.87	0.57
6:I:392:LEU:HD23	6:I:442:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:366:ASP:OD2	6:L:372:HIS:NE2	2.38	0.56
6:L:416:TYR:CD1	6:L:427:ILE:HD13	2.40	0.56
4:F:726:ASP:OD2	5:G:2:LYS:CA	2.53	0.56
6:I:372:HIS:HE1	7:J:117:ILE:O	1.89	0.56
6:K:93:THR:HG21	6:K:240:ILE:O	2.06	0.56
7:M:71:VAL:HG23	7:M:71:VAL:O	2.07	0.55
7:M:88:ILE:HD12	7:M:144:THR:HG23	1.88	0.55
1:A:45:VAL:HG12	1:A:46:THR:H	1.71	0.55
6:H:293:THR:HG22	6:H:294:LEU:H	1.71	0.55
6:H:286:LEU:N	6:H:286:LEU:HD12	2.22	0.55
9:R:44:TYR:O	9:R:45:ILE:C	2.48	0.55
8:N:9:ASP:C	8:N:9:ASP:OD1	2.49	0.54
6:H:188:ALA:HB1	6:H:197:LEU:HD21	1.89	0.54
8:O:79:MET:HA	8:O:79:MET:HE2	1.89	0.54
9:R:44:TYR:O	9:R:47:ASN:N	2.41	0.54
6:I:129:LEU:HD11	6:I:226:ILE:HB	1.89	0.54
6:K:274:THR:HG22	6:K:275:ASP:H	1.73	0.54
7:M:3:GLN:OE1	7:M:3:GLN:N	2.40	0.54
5:G:22:GLU:N	5:G:22:GLU:OE2	2.39	0.54
6:H:406:ARG:O	6:H:410:VAL:HG23	2.08	0.54
6:L:301:VAL:O	6:L:304:VAL:HG12	2.07	0.54
8:O:32:GLU:N	8:O:32:GLU:OE1	2.39	0.54
4:F:726:ASP:OD2	5:G:2:LYS:CB	2.55	0.54
6:H:293:THR:HG22	6:H:294:LEU:N	2.22	0.54
6:L:279:ARG:NH1	8:O:56:LEU:HD13	2.23	0.54
5:G:181:THR:OG1	5:G:183:VAL:HG22	2.08	0.54
6:H:78:ASP:C	6:H:78:ASP:OD1	2.51	0.54
5:G:183:VAL:HG23	5:G:183:VAL:O	2.08	0.54
6:L:366:ASP:OD2	6:L:372:HIS:CD2	2.61	0.53
6:H:416:TYR:CE1	6:H:420:LEU:HD11	2.42	0.53
7:J:88:ILE:O	7:J:92:LEU:HD22	2.09	0.53
8:O:79:MET:HE2	8:O:79:MET:N	2.24	0.53
2:C:14:VAL:HG23	2:C:22:VAL:O	2.07	0.53
7:J:109:LEU:HD22	7:J:141:THR:HG22	1.91	0.53
6:L:274:THR:HG22	6:L:277:GLU:OE2	2.09	0.53
1:A:169:ASP:C	1:A:169:ASP:OD2	2.52	0.52
7:J:121:ILE:HG23	7:J:121:ILE:O	2.09	0.52
7:J:89:GLN:HA	7:J:92:LEU:HD23	1.92	0.52
7:J:110:TYR:HD2	7:J:132:VAL:HG11	1.75	0.52
6:L:34:ASP:OD1	6:L:34:ASP:O	2.28	0.52
1:A:45:VAL:HG12	1:A:46:THR:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:370:LEU:HD23	6:I:372:HIS:CE1	2.44	0.52
6:K:351:PRO:HA	6:L:293:THR:HG21	1.92	0.52
6:L:416:TYR:CE1	6:L:427:ILE:HG21	2.45	0.52
6:K:302:LYS:HZ1	6:K:309:ASP:C	2.18	0.52
6:L:386:VAL:HG12	6:L:387:LYS:N	2.25	0.52
1:A:152:VAL:HG12	1:A:153:GLY:N	2.24	0.52
1:B:177:ASN:C	1:B:177:ASN:OD1	2.53	0.52
5:G:29:ALA:O	5:G:30:ILE:HD13	2.09	0.52
6:L:408:SER:HB2	6:L:439:ILE:HD11	1.91	0.52
9:R:23:PRO:O	9:R:24:PRO:C	2.53	0.52
2:D:36:ILE:HD11	6:K:41:LEU:HD22	1.93	0.51
6:L:240:ILE:HG23	6:L:240:ILE:O	2.10	0.51
7:M:84:ALA:O	7:M:88:ILE:HG12	2.10	0.51
8:O:79:MET:HE2	8:O:79:MET:CA	2.40	0.51
6:H:388:VAL:HG22	6:H:446:GLU:O	2.10	0.51
6:I:89:VAL:HG13	6:I:91:GLN:HE22	1.75	0.51
6:K:169:ILE:O	6:K:172:LEU:HD23	2.10	0.51
5:G:104:GLU:N	5:G:104:GLU:OE1	2.43	0.51
6:K:293:THR:C	7:M:151:THR:HG22	2.35	0.51
8:N:48:VAL:O	8:N:48:VAL:HG13	2.10	0.51
9:U:40:GLN:O	9:U:41:TRP:C	2.52	0.51
3:E:252:ARG:O	4:F:740:GLU:OE2	2.27	0.51
6:H:56:HIS:CD2	7:J:41:LEU:HD11	2.45	0.51
1:B:167:THR:HG22	2:D:65:PHE:O	2.11	0.51
6:H:282:TYR:O	6:H:286:LEU:HD11	2.10	0.51
6:I:61:GLU:HB2	8:N:34:LEU:HD21	1.91	0.51
6:I:193:ASP:O	6:I:193:ASP:OD2	2.29	0.51
2:C:43:ASP:OD1	2:C:43:ASP:C	2.54	0.51
8:N:56:LEU:O	8:N:76:VAL:HG21	2.11	0.51
6:K:335:VAL:HG22	6:K:335:VAL:O	2.10	0.51
6:L:191:ILE:HG22	6:L:192:ASN:N	2.26	0.51
6:K:420:LEU:HD21	6:K:426:VAL:HG22	1.93	0.51
6:L:286:LEU:HD23	6:L:286:LEU:N	2.25	0.51
1:A:198:LEU:HD11	1:A:205:GLU:HG2	1.94	0.50
3:E:61:VAL:CG1	3:E:62:THR:HG22	2.42	0.50
6:H:243:LEU:HD23	6:H:265:ASP:OD2	2.12	0.50
6:L:142:ASN:OD1	6:L:222:THR:HG23	2.11	0.50
6:I:374:VAL:HG12	6:I:375:TYR:N	2.26	0.50
6:K:409:ILE:HD12	6:K:435:ILE:HG23	1.93	0.50
6:L:297:ILE:O	6:L:301:VAL:HG23	2.12	0.50
8:O:35:ASP:CG	8:O:35:ASP:O	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:144:LEU:HD22	6:K:169:ILE:HD11	1.94	0.49
6:K:304:VAL:HG22	6:K:305:GLN:N	2.27	0.49
6:K:354:ILE:HG23	6:K:355:ARG:H	1.76	0.49
6:I:141:VAL:HG21	6:I:169:ILE:HG21	1.94	0.49
9:R:39:ARG:O	9:R:40:GLN:C	2.54	0.49
1:A:156:ASP:C	1:A:156:ASP:OD2	2.55	0.49
6:H:325:LEU:HD23	6:H:326:PRO:O	2.12	0.49
6:I:154:ILE:HG23	6:I:213:MET:CE	2.43	0.49
6:I:323:GLU:CG	6:I:325:LEU:HD12	2.43	0.49
5:G:77:LYS:O	5:G:78:THR:HG22	2.12	0.49
6:K:149:ASN:O	6:K:151:VAL:HG23	2.12	0.49
3:E:252:ARG:O	4:F:740:GLU:CD	2.45	0.49
7:J:109:LEU:HD13	7:J:141:THR:HG22	1.93	0.49
6:H:135:VAL:O	6:H:213:MET:HE3	2.13	0.49
6:L:61:GLU:HB2	8:O:34:LEU:HD21	1.93	0.49
6:L:367:LEU:HD11	7:M:100:THR:HG23	1.93	0.49
6:L:17:ILE:HD11	6:L:56:HIS:HD2	1.78	0.49
7:M:103:GLN:HG2	7:M:117:ILE:HD11	1.95	0.49
6:K:186:ALA:N	6:K:187:LYS:HZ3	2.10	0.49
6:K:237:VAL:O	6:K:237:VAL:HG23	2.12	0.48
1:A:148:PHE:O	1:A:148:PHE:CD2	2.66	0.48
6:H:152:ILE:HD11	6:H:221:LEU:HD12	1.94	0.48
3:E:57:GLN:O	3:E:57:GLN:HG3	2.12	0.48
7:J:81:THR:C	7:J:85:MET:HE3	2.38	0.48
6:H:410:VAL:HG13	6:H:484:TYR:CE2	2.48	0.48
6:I:16:GLU:O	6:I:19:ASP:OD1	2.31	0.48
3:E:317:THR:HG22	3:E:318:GLU:N	2.29	0.48
8:O:77:GLU:OE2	8:O:77:GLU:N	2.46	0.48
3:E:242:VAL:HG11	3:E:246:LEU:HD11	1.95	0.48
6:I:82:LEU:O	6:I:82:LEU:HD23	2.13	0.48
6:I:372:HIS:CE1	7:J:117:ILE:O	2.66	0.48
6:K:243:LEU:HB2	6:K:246:THR:HG21	1.96	0.48
1:A:201:ASN:OD1	1:A:202:GLY:N	2.47	0.48
2:D:2:LYS:HE3	2:D:2:LYS:HA	1.95	0.47
3:E:254:ARG:NH1	4:F:741:GLU:OE1	2.47	0.47
6:I:411:GLN:HG2	6:I:438:VAL:HG11	1.96	0.47
8:O:100:ASN:OD1	8:O:100:ASN:C	2.57	0.47
3:E:254:ARG:NH2	4:F:738:TYR:CB	2.61	0.47
6:L:152:ILE:CD1	6:L:176:LEU:HD21	2.45	0.47
8:N:105:GLU:OE2	8:N:105:GLU:HA	2.14	0.47
6:H:265:ASP:C	6:H:266:LEU:HD23	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:29:ILE:HG22	6:I:30:SER:N	2.29	0.47
6:H:299:ALA:HA	6:H:302:LYS:HG2	1.96	0.47
8:N:99:LEU:C	8:N:99:LEU:HD23	2.39	0.47
1:B:133:ILE:HD11	1:B:138:ARG:HH12	1.80	0.47
7:J:81:THR:O	7:J:85:MET:HE3	2.15	0.47
6:I:324:GLY:O	6:I:325:LEU:C	2.57	0.47
9:P:32:LEU:O	9:P:33:ARG:C	2.58	0.47
6:L:156:ASN:C	6:L:156:ASN:OD1	2.57	0.47
7:M:162:VAL:O	7:M:162:VAL:CG1	2.62	0.47
9:R:40:GLN:O	9:R:41:TRP:C	2.57	0.47
6:L:197:LEU:O	6:L:197:LEU:HD23	2.15	0.46
6:H:176:LEU:O	6:H:180:ILE:HG12	2.15	0.46
6:I:392:LEU:HD21	6:I:442:VAL:HG12	1.94	0.46
6:I:431:ILE:HG22	6:I:431:ILE:O	2.13	0.46
5:G:1:MET:HE2	5:G:1:MET:HA	1.96	0.46
6:K:405:ILE:HG22	6:K:405:ILE:O	2.15	0.46
9:S:32:LEU:O	9:S:33:ARG:C	2.58	0.46
1:A:151:ILE:HG23	1:A:152:VAL:N	2.30	0.46
1:B:56:VAL:HG22	1:B:57:THR:N	2.31	0.46
7:M:107:MET:HA	7:M:107:MET:HE2	1.96	0.46
9:U:38:GLY:C	9:U:40:GLN:N	2.72	0.46
1:B:98:GLU:OE2	1:B:98:GLU:HA	2.15	0.46
3:E:54:TYR:HB3	3:E:283:MET:HE2	1.97	0.46
6:H:240:ILE:HG13	6:H:240:ILE:O	2.15	0.46
6:L:351:PRO:O	6:L:352:ALA:C	2.59	0.46
6:I:13:ARG:O	6:I:15:GLN:N	2.49	0.46
6:I:223:PHE:HB3	6:I:226:ILE:HD11	1.96	0.46
7:J:96:ASP:OD1	7:J:96:ASP:C	2.59	0.46
6:I:35:VAL:HG12	6:I:35:VAL:O	2.15	0.46
6:L:304:VAL:HG13	6:L:307:VAL:CG2	2.46	0.46
6:L:428:PRO:HA	6:L:431:ILE:HG12	1.98	0.46
4:F:732:ILE:HD12	4:F:732:ILE:H	1.81	0.46
6:H:89:VAL:HG22	6:H:90:ALA:N	2.31	0.46
6:I:141:VAL:HG21	6:I:169:ILE:CG2	2.46	0.46
1:B:175:LYS:HD3	1:B:175:LYS:C	2.41	0.46
1:B:199:ASP:HB2	1:B:214:LEU:HD21	1.98	0.46
6:H:426:VAL:HG23	6:H:471:VAL:HG21	1.98	0.46
6:L:288:VAL:HG13	6:L:288:VAL:O	2.16	0.46
8:N:4:TYR:HE1	8:N:79:MET:HE1	1.81	0.46
8:O:61:ILE:O	8:O:61:ILE:HG22	2.16	0.46
1:B:173:THR:HG23	8:O:12:TRP:CE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:HG21	8:O:3:GLN:OE1	2.16	0.45
2:D:41:GLU:N	2:D:41:GLU:OE1	2.49	0.45
4:F:726:ASP:OD1	5:G:2:LYS:O	2.33	0.45
6:L:426:VAL:HG12	6:L:428:PRO:CD	2.44	0.45
7:M:85:MET:HA	7:M:88:ILE:HG12	1.98	0.45
6:I:313:VAL:HG23	6:I:313:VAL:O	2.17	0.45
3:E:233:LEU:C	3:E:233:LEU:HD13	2.42	0.45
5:G:60:VAL:O	5:G:60:VAL:HG23	2.17	0.45
9:R:22:PRO:O	9:R:23:PRO:C	2.59	0.45
6:H:405:ILE:O	6:H:409:ILE:HG23	2.17	0.45
6:I:213:MET:HE2	6:I:214:VAL:N	2.32	0.45
6:K:55:THR:HG23	6:L:56:HIS:HE1	1.81	0.45
2:D:14:VAL:HG23	2:D:22:VAL:O	2.16	0.45
6:I:325:LEU:O	6:I:326:PRO:C	2.60	0.45
1:A:203:VAL:O	1:A:204:ARG:C	2.60	0.45
6:I:62:ILE:HD12	6:I:62:ILE:H	1.80	0.45
2:D:36:ILE:HD11	6:K:41:LEU:HD13	1.99	0.45
8:O:50:LEU:HD12	8:O:50:LEU:O	2.17	0.45
7:M:87:TYR:HA	7:M:90:ILE:HG22	1.99	0.45
2:D:17:LEU:H	2:D:20:ASP:HB3	1.82	0.44
6:H:74:PHE:CD1	6:H:74:PHE:C	2.95	0.44
6:H:163:PRO:HG3	6:H:172:LEU:HD13	1.99	0.44
6:H:91:GLN:C	6:H:237:VAL:HG13	2.43	0.44
6:H:432:TYR:O	6:H:435:ILE:HG22	2.17	0.44
7:J:117:ILE:O	7:J:117:ILE:HG23	2.16	0.44
6:K:334:VAL:HG12	6:K:335:VAL:N	2.33	0.44
2:C:99:ASP:OD1	2:C:99:ASP:N	2.49	0.44
6:H:112:ARG:C	6:H:113:LEU:HD23	2.42	0.44
3:E:38:MET:HE2	3:E:38:MET:N	2.33	0.44
1:A:155:THR:HG23	1:A:161:THR:HA	1.99	0.44
6:H:102:THR:HG22	6:H:103:THR:N	2.33	0.44
6:L:447:ILE:HG23	6:L:447:ILE:O	2.18	0.44
5:G:93:ASP:OD2	5:G:93:ASP:C	2.61	0.44
6:H:64:ASP:O	6:H:67:THR:HG22	2.18	0.44
6:I:4:LEU:HD12	6:I:4:LEU:O	2.18	0.44
6:I:120:ILE:HG21	6:I:235:GLU:OE1	2.18	0.44
6:L:416:TYR:CE1	6:L:427:ILE:HD13	2.53	0.44
1:B:110:ILE:HG22	1:B:111:CYS:N	2.33	0.43
3:E:23:THR:C	3:E:24:THR:HG23	2.42	0.43
3:E:69:GLU:HG2	3:E:134:ILE:HG23	2.00	0.43
5:G:138:LEU:C	5:G:138:LEU:HD23	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:291:VAL:HG11	7:M:98:THR:HG21	1.99	0.43
6:L:416:TYR:HD1	6:L:427:ILE:HD13	1.83	0.43
6:K:16:GLU:O	6:K:19:ASP:OD1	2.36	0.43
7:M:85:MET:HA	7:M:85:MET:HE2	2.00	0.43
2:D:5:PHE:CE2	6:L:41:LEU:HD21	2.54	0.43
6:H:76:LEU:CD2	6:H:278:LEU:HD23	2.48	0.43
6:I:82:LEU:HD23	6:I:82:LEU:C	2.43	0.43
6:I:409:ILE:HA	6:I:435:ILE:HD13	1.99	0.43
6:L:370:LEU:HB3	6:L:372:HIS:NE2	2.32	0.43
3:E:142:ASP:HB3	3:E:216:THR:HG21	2.00	0.43
6:H:410:VAL:HG13	6:H:484:TYR:HD2	1.81	0.43
4:F:726:ASP:OD1	4:F:726:ASP:C	2.61	0.43
6:H:29:ILE:HG22	6:H:30:SER:N	2.33	0.43
6:L:127:ILE:HD11	6:L:230:HIS:CG	2.53	0.43
6:L:321:SER:HB2	6:L:325:LEU:HD22	2.00	0.43
9:U:45:ILE:O	9:U:46:LEU:C	2.60	0.43
9:R:76:ASN:O	9:R:77:LEU:C	2.61	0.43
6:I:76:LEU:O	6:I:80:THR:HG22	2.18	0.43
6:I:129:LEU:HD11	6:I:226:ILE:CG2	2.49	0.43
6:K:315:ASN:OD1	6:K:315:ASN:C	2.62	0.43
1:A:21:LEU:HD21	1:A:100:TRP:CE2	2.54	0.43
3:E:242:VAL:HG22	3:E:243:ILE:N	2.34	0.43
5:G:49:ILE:HG13	5:G:50:ASN:OD1	2.19	0.43
6:H:309:ASP:OD2	6:H:422:VAL:HG23	2.18	0.43
6:K:83:ASN:ND2	6:K:286:LEU:HD23	2.33	0.43
6:L:34:ASP:OD1	6:L:34:ASP:C	2.61	0.43
6:L:323:GLU:O	6:L:323:GLU:HG3	2.18	0.43
7:M:82:TYR:O	7:M:86:LEU:HD23	2.19	0.43
8:N:76:VAL:O	8:N:76:VAL:HG23	2.18	0.43
1:A:151:ILE:CG2	1:A:152:VAL:N	2.82	0.42
2:D:86:PHE:CD2	2:D:86:PHE:C	2.97	0.42
6:H:409:ILE:CD1	6:H:486:ILE:HG21	2.50	0.42
6:I:35:VAL:O	6:I:35:VAL:CG1	2.66	0.42
6:L:363:THR:HG22	6:L:364:ALA:N	2.34	0.42
9:R:42:PHE:O	9:R:43:ASN:C	2.63	0.42
1:A:21:LEU:HD21	1:A:100:TRP:CD2	2.54	0.42
1:B:196:PHE:CD2	1:B:196:PHE:C	2.98	0.42
6:H:283:LEU:O	6:H:286:LEU:HD13	2.19	0.42
6:I:91:GLN:HG2	6:I:237:VAL:HG13	2.00	0.42
6:I:98:GLU:HG2	6:I:229:ILE:HG22	2.01	0.42
6:I:225:LYS:C	6:I:226:ILE:HD13	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:109:LEU:O	7:J:109:LEU:HD23	2.19	0.42
7:M:51:GLU:C	7:M:51:GLU:OE1	2.62	0.42
3:E:181:LEU:HD23	3:E:181:LEU:H	1.84	0.42
1:B:219:MET:HE2	1:B:219:MET:C	2.45	0.42
6:H:340:ASP:O	6:H:344:GLN:HG2	2.19	0.42
6:H:388:VAL:HB	6:H:486:ILE:HG23	2.01	0.42
6:L:62:ILE:HG22	7:M:49:HIS:HB2	2.00	0.42
9:U:76:ASN:O	9:U:77:LEU:C	2.61	0.42
7:J:107:MET:O	7:J:111:ASN:N	2.52	0.42
6:L:183:GLY:O	6:L:184:ILE:HB	2.20	0.42
6:L:191:ILE:HG22	6:L:192:ASN:H	1.85	0.42
6:L:291:VAL:HG21	7:M:98:THR:HG23	1.99	0.42
6:L:457:VAL:O	6:L:457:VAL:HG12	2.18	0.42
7:M:92:LEU:HD12	7:M:92:LEU:O	2.19	0.42
6:L:35:VAL:O	6:L:35:VAL:HG13	2.19	0.42
6:L:370:LEU:CB	6:L:372:HIS:CD2	3.02	0.42
3:E:134:ILE:HG22	3:E:135:THR:N	2.35	0.42
1:A:177:ASN:ND2	3:E:279:GLY:C	2.78	0.42
6:H:62:ILE:HD11	6:I:63:TYR:HB2	2.02	0.42
6:K:240:ILE:O	6:K:240:ILE:HG23	2.20	0.42
1:A:180:ASN:O	1:A:180:ASN:ND2	2.53	0.41
6:L:426:VAL:HG21	6:L:469:ILE:N	2.35	0.41
6:K:347:TRP:CB	6:K:364:ALA:HB1	2.50	0.41
6:L:90:ALA:HB1	6:L:270:ARG:O	2.20	0.41
7:M:88:ILE:HG23	7:M:144:THR:HG22	2.02	0.41
8:O:56:LEU:O	8:O:76:VAL:HG21	2.21	0.41
9:U:43:ASN:O	9:U:44:TYR:C	2.62	0.41
6:I:30:SER:O	6:I:33:LEU:HD23	2.20	0.41
6:I:120:ILE:HG22	6:I:121:PHE:N	2.35	0.41
8:O:78:ARG:C	8:O:79:MET:HE2	2.46	0.41
2:D:22:VAL:O	2:D:22:VAL:HG13	2.20	0.41
2:D:63:VAL:HG12	2:D:66:ASN:H	1.86	0.41
4:F:737:SER:HA	5:G:11:TYR:HE1	1.86	0.41
6:H:448:LYS:HB3	6:H:464:TYR:HB3	2.03	0.41
6:K:25:LEU:O	6:K:29:ILE:HG22	2.21	0.41
7:M:132:VAL:O	7:M:132:VAL:HG13	2.21	0.41
6:H:52:LEU:HA	6:H:55:THR:HG22	2.02	0.41
6:I:215:VAL:HG11	6:I:223:PHE:CZ	2.56	0.41
6:K:155:ASP:O	6:K:157:VAL:HG23	2.21	0.41
6:L:89:VAL:HG22	6:L:90:ALA:H	1.86	0.41
1:A:40:ASP:OD2	1:A:40:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:233:VAL:HG22	6:H:234:ALA:N	2.35	0.41
6:L:158:ILE:HG23	6:L:158:ILE:O	2.20	0.41
6:L:191:ILE:O	6:L:196:ALA:HB3	2.21	0.41
1:B:179:GLY:O	8:O:17:VAL:HG12	2.21	0.41
3:E:264:VAL:O	3:E:264:VAL:HG13	2.21	0.41
6:K:338:GLN:O	6:K:342:VAL:HG23	2.20	0.41
6:L:100:THR:O	6:L:257:LEU:HD12	2.20	0.41
6:L:350:LYS:NZ	7:M:99:PRO:HG2	2.36	0.41
8:N:14:THR:HG22	8:N:15:GLN:N	2.36	0.41
9:R:20:VAL:H	9:R:40:GLN:C	2.29	0.41
1:A:145:GLU:OE2	1:A:145:GLU:C	2.64	0.41
1:B:107:ILE:HG22	1:B:108:SER:N	2.36	0.41
6:K:178:ASP:OD1	6:K:178:ASP:C	2.64	0.41
9:R:38:GLY:O	9:R:39:ARG:O	2.39	0.41
1:A:95:ASP:OD2	1:A:96:THR:N	2.54	0.40
6:I:43:LEU:N	6:I:43:LEU:HD12	2.35	0.40
6:I:239:ALA:HB2	6:I:271:ASN:HB3	2.03	0.40
7:J:74:PRO:HG2	7:J:77:ALA:HB3	2.04	0.40
6:K:306:GLY:C	6:K:307:VAL:HG22	2.46	0.40
6:H:119:ASN:CG	6:H:240:ILE:HD13	2.46	0.40
6:I:29:ILE:CG2	6:I:30:SER:N	2.84	0.40
6:K:431:ILE:O	6:K:435:ILE:HG12	2.21	0.40
6:I:193:ASP:OD2	6:I:193:ASP:C	2.64	0.40
7:J:4:LYS:O	7:J:5:ILE:CB	2.69	0.40
7:J:68:LEU:HD23	7:J:68:LEU:C	2.46	0.40
7:J:69:ILE:HG22	7:J:71:VAL:HG23	2.02	0.40
6:L:242:ALA:HB3	6:L:266:LEU:HD12	2.03	0.40
6:H:435:ILE:HG23	6:H:436:TYR:N	2.36	0.40
6:I:152:ILE:HD12	6:I:217:ALA:HA	2.03	0.40
7:J:37:GLU:O	7:J:37:GLU:HG2	2.22	0.40
6:K:297:ILE:HG23	6:K:350:LYS:CE	2.48	0.40
1:A:129:LYS:HG2	1:A:137:LEU:HD21	2.02	0.40
1:A:177:ASN:CG	1:A:178:THR:H	2.30	0.40
2:D:43:ASP:OD1	2:D:43:ASP:C	2.63	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	198/265 (75%)	175 (88%)	21 (11%)	2 (1%)	13	46
1	B	197/265 (74%)	186 (94%)	11 (6%)	0	100	100
2	C	124/139 (89%)	119 (96%)	5 (4%)	0	100	100
2	D	124/139 (89%)	116 (94%)	8 (6%)	0	100	100
3	E	299/325 (92%)	287 (96%)	12 (4%)	0	100	100
4	F	24/742 (3%)	24 (100%)	0	0	100	100
5	G	204/207 (99%)	189 (93%)	15 (7%)	0	100	100
6	H	431/489 (88%)	407 (94%)	24 (6%)	0	100	100
6	I	414/489 (85%)	383 (92%)	30 (7%)	1 (0%)	44	75
6	K	409/489 (84%)	382 (93%)	26 (6%)	1 (0%)	44	75
6	L	462/489 (94%)	426 (92%)	34 (7%)	2 (0%)	30	65
7	J	158/285 (55%)	139 (88%)	16 (10%)	3 (2%)	6	35
7	M	158/285 (55%)	147 (93%)	9 (6%)	2 (1%)	10	41
8	N	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
8	O	109/113 (96%)	102 (94%)	7 (6%)	0	100	100
9	P	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	13	46
9	Q	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
9	R	98/100 (98%)	80 (82%)	11 (11%)	7 (7%)	1	14
9	S	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	13	46
9	T	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
9	U	98/100 (98%)	85 (87%)	12 (12%)	1 (1%)	13	46
All	All	4009/5434 (74%)	3703 (92%)	285 (7%)	21 (0%)	27	60

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	I	14	TYR
7	J	5	ILE
9	S	26	ILE
9	P	26	ILE
9	R	36	PRO
9	R	37	MET
1	A	213	ALA
7	J	22	LYS
9	R	20	VAL
9	R	39	ARG
7	J	25	PHE
9	R	41	TRP
9	R	45	ILE
7	M	6	ASP
9	R	16	ASN
7	M	162	VAL
9	U	45	ILE
6	L	184	ILE
6	L	237	VAL
6	K	486	ILE
1	A	115	ILE

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	171/222 (77%)	171 (100%)	0	100	100
1	B	170/222 (77%)	169 (99%)	1 (1%)	84	88
2	C	109/122 (89%)	108 (99%)	1 (1%)	75	83
2	D	109/122 (89%)	106 (97%)	3 (3%)	38	60
3	E	271/288 (94%)	268 (99%)	3 (1%)	70	79
4	F	25/590 (4%)	25 (100%)	0	100	100
5	G	183/184 (100%)	181 (99%)	2 (1%)	70	79
6	H	389/411 (95%)	388 (100%)	1 (0%)	91	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	I	373/411 (91%)	368 (99%)	5 (1%)	65	76
6	K	376/411 (92%)	372 (99%)	4 (1%)	70	79
6	L	402/411 (98%)	399 (99%)	3 (1%)	81	86
7	J	143/242 (59%)	141 (99%)	2 (1%)	62	75
7	M	146/242 (60%)	144 (99%)	2 (1%)	62	75
8	N	103/104 (99%)	103 (100%)	0	100	100
8	O	102/104 (98%)	102 (100%)	0	100	100
All	All	3072/4086 (75%)	3045 (99%)	27 (1%)	74	83

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	TYR
2	C	122	ASP
2	D	38	ILE
2	D	39	ILE
2	D	99	ASP
3	E	107	ILE
3	E	237	ILE
3	E	266	LYS
5	G	49	ILE
5	G	123	CYS
6	H	76	LEU
6	I	45	LEU
6	I	56	HIS
6	I	67	THR
6	I	189	GLU
6	I	240	ILE
7	J	37	GLU
7	J	92	LEU
6	K	29	ILE
6	K	98	GLU
6	K	172	LEU
6	K	223	PHE
6	L	57	GLU
6	L	88	TYR
6	L	416	TYR
7	M	6	ASP
7	M	121	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	54	GLN
2	D	34	ASN
2	D	114	GLN
6	H	315	ASN
6	H	372	HIS
6	I	372	HIS
6	I	429	ASN
6	I	453	ASN
7	J	103	GLN
6	L	56	HIS
8	N	15	GLN
8	N	85	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

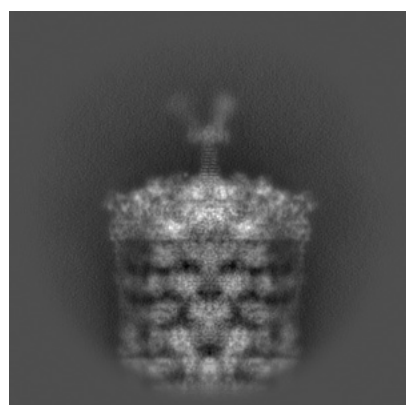
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49281. These allow visual inspection of the internal detail of the map and identification of artifacts.

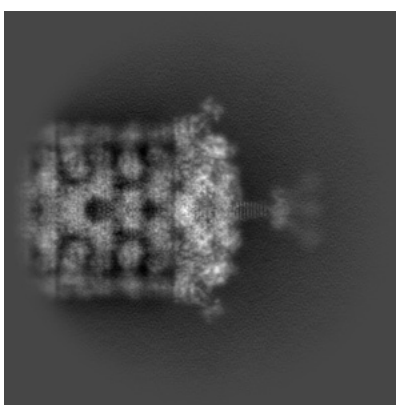
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

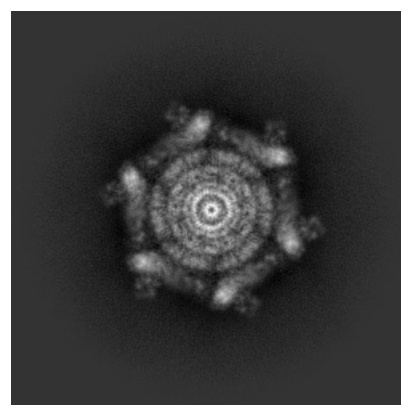
6.1.1 Primary map



X



Y

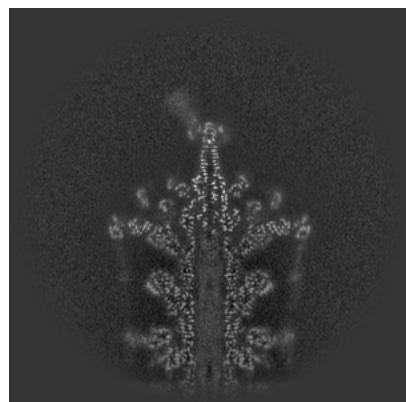


Z

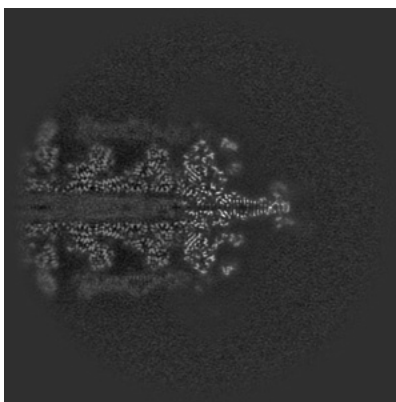
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

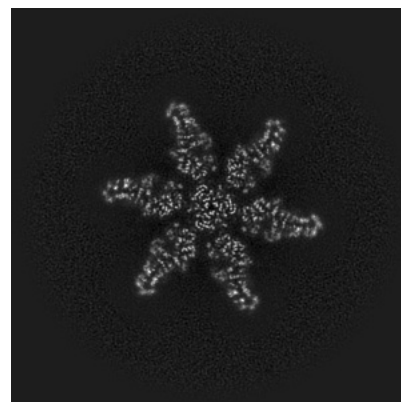
6.2.1 Primary map



X Index: 200



Y Index: 200

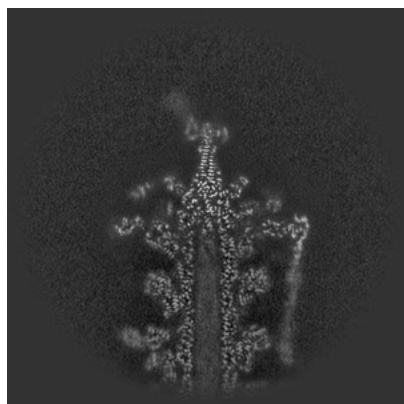


Z Index: 200

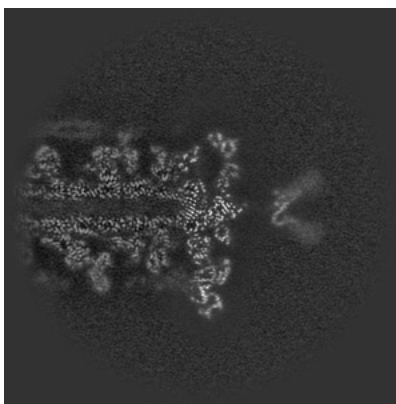
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

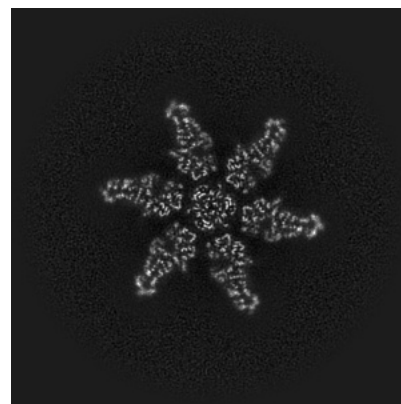
6.3.1 Primary map



X Index: 196



Y Index: 212

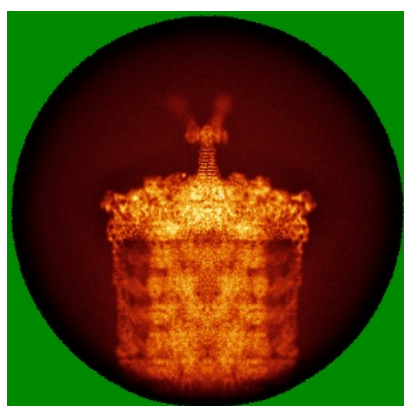


Z Index: 201

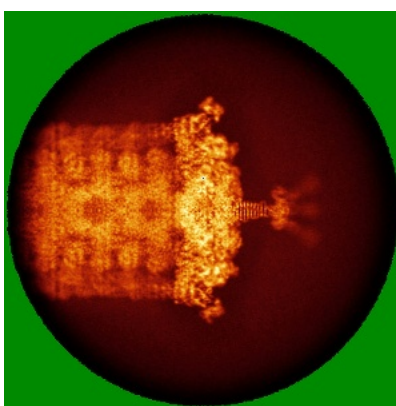
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

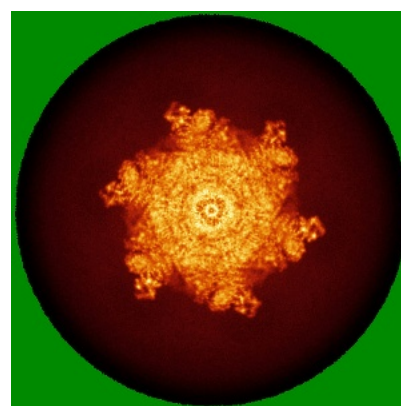
6.4.1 Primary map



X



Y

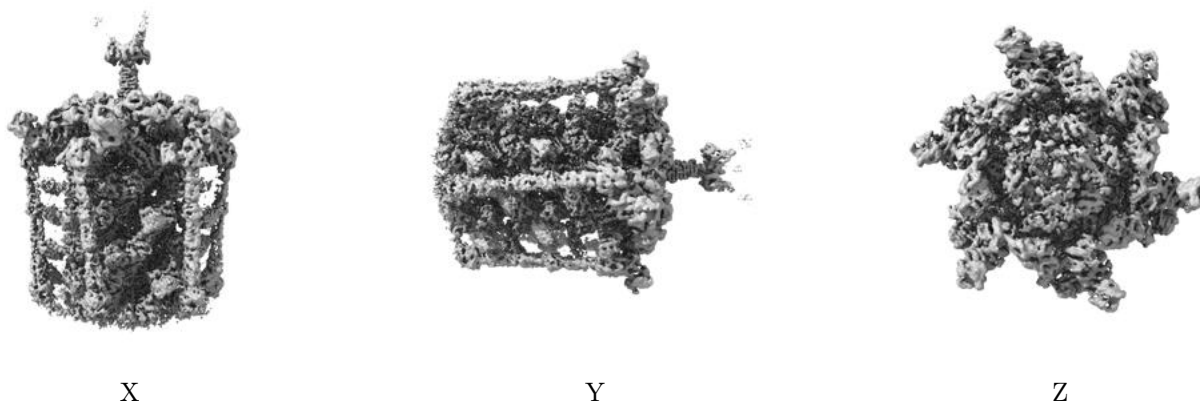


Z

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

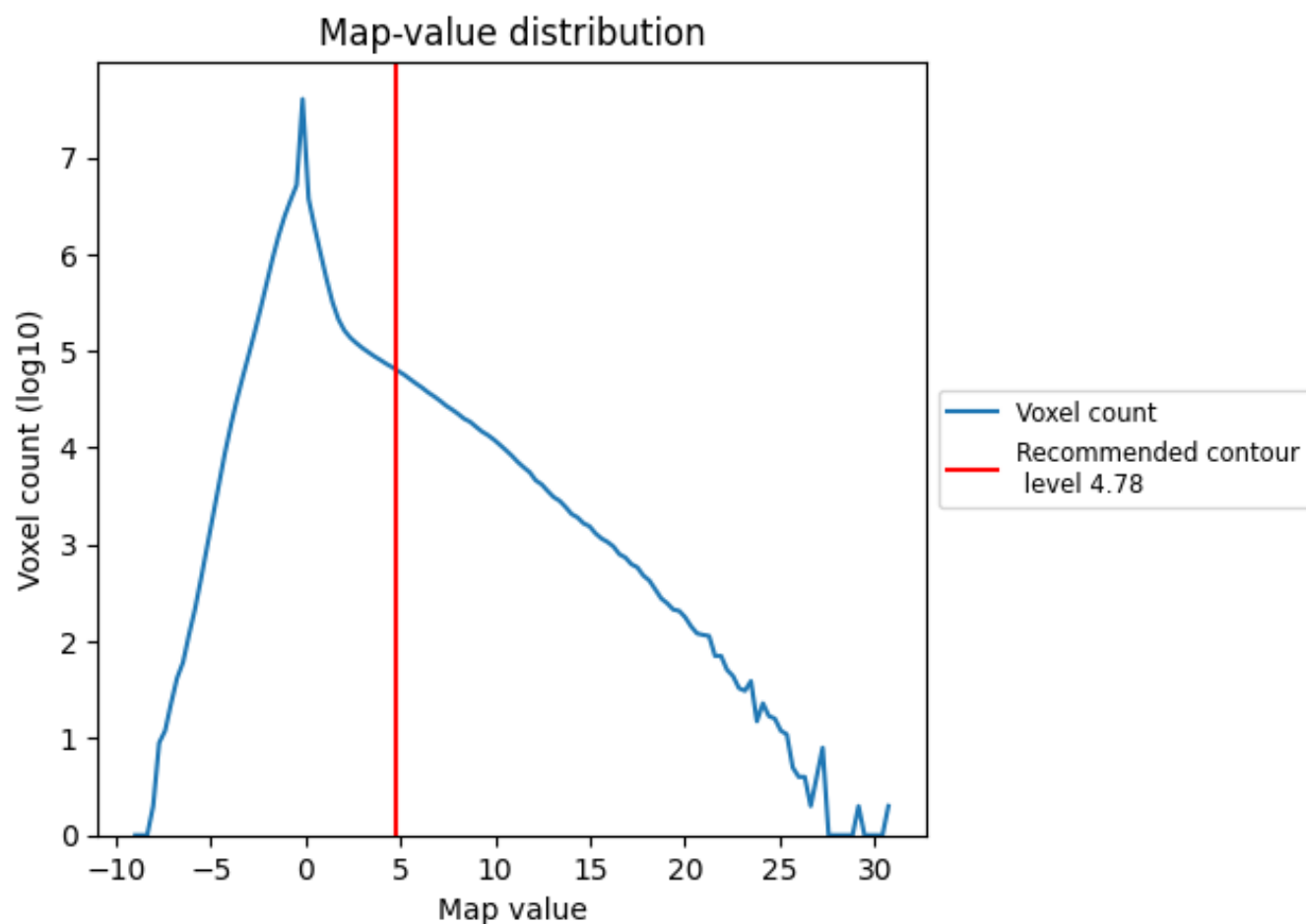
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

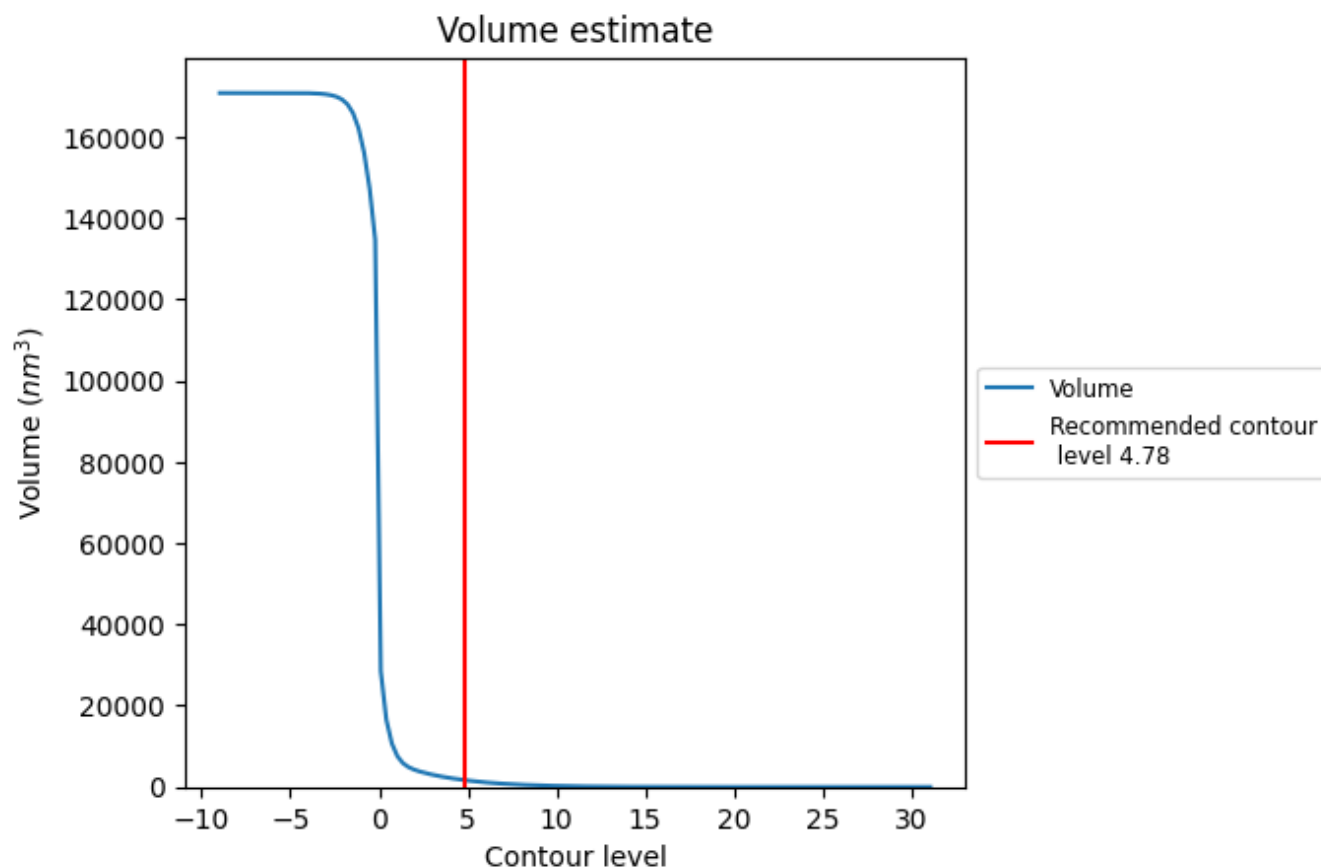
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

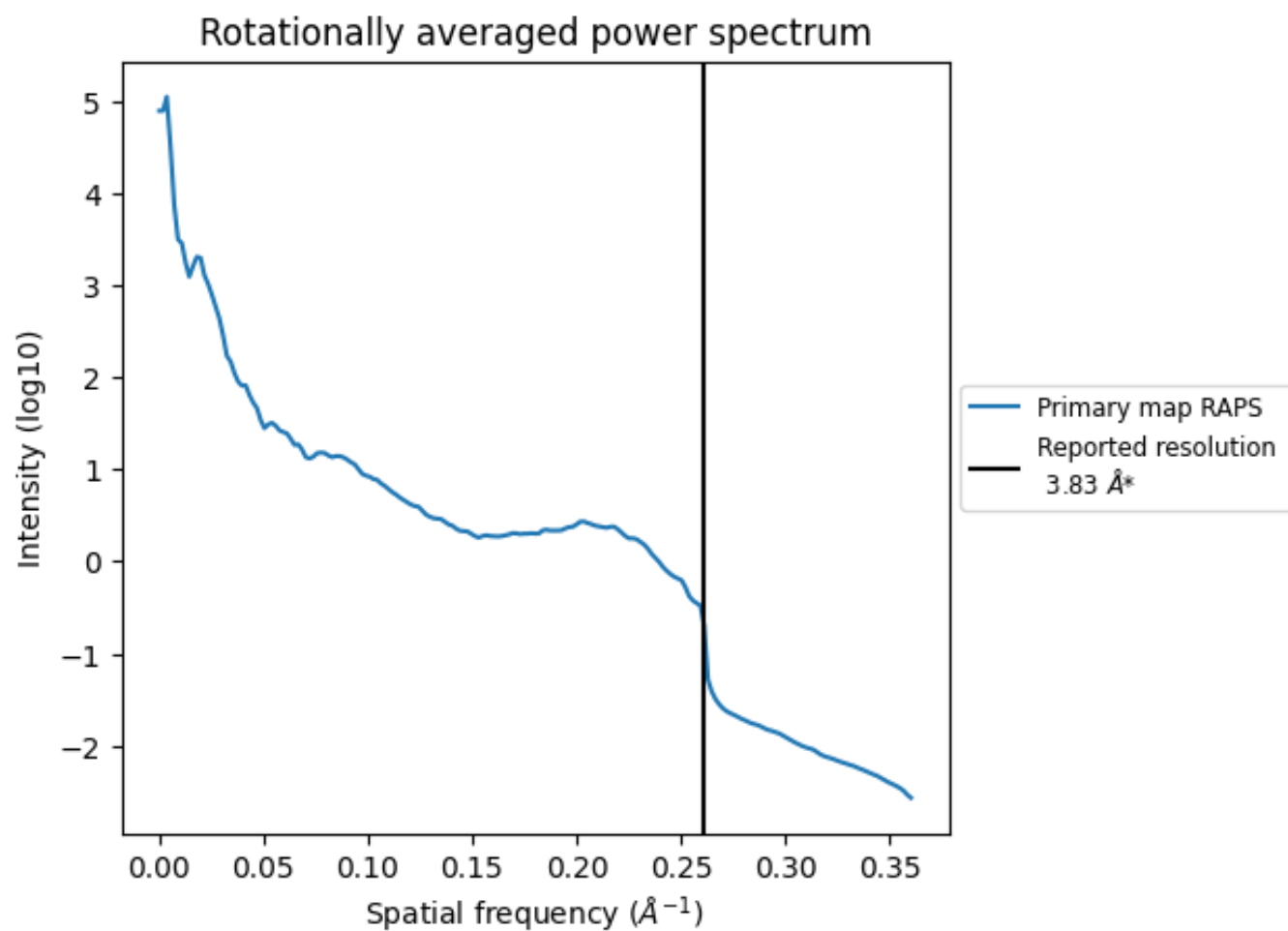
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1704 nm³; this corresponds to an approximate mass of 1539 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.261 Å⁻¹

8 Fourier-Shell correlation ⓘ

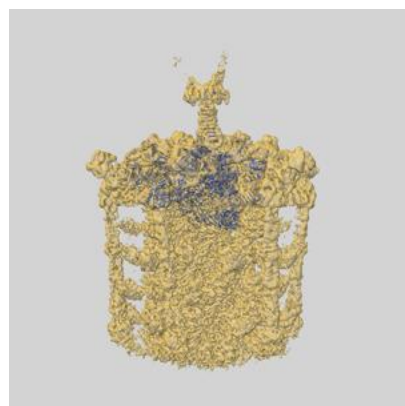
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

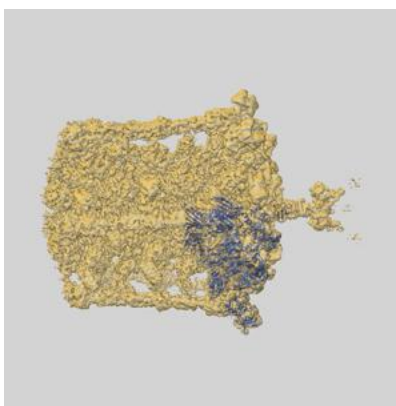
This section contains information regarding the fit between EMDB map EMD-49281 and PDB model 9NDY. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlays

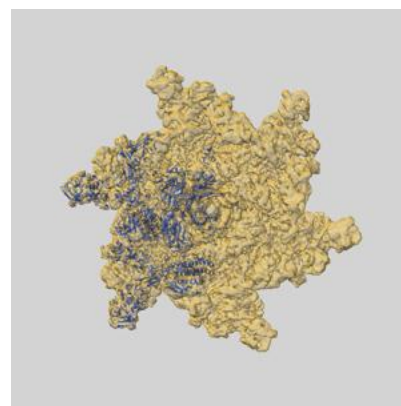
9.1.1 Map-model overlay [i](#)



X

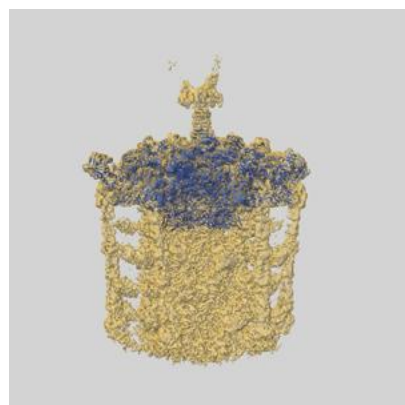


Y

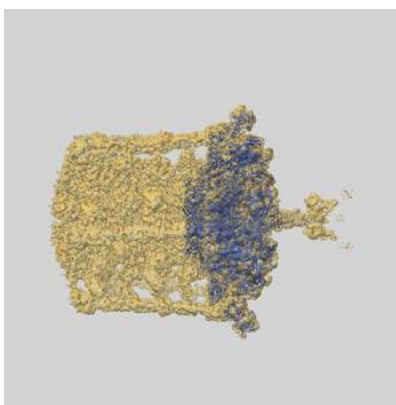


Z

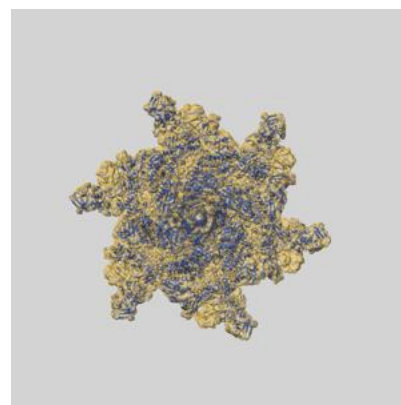
9.1.2 Map-model assembly overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.78 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](#)



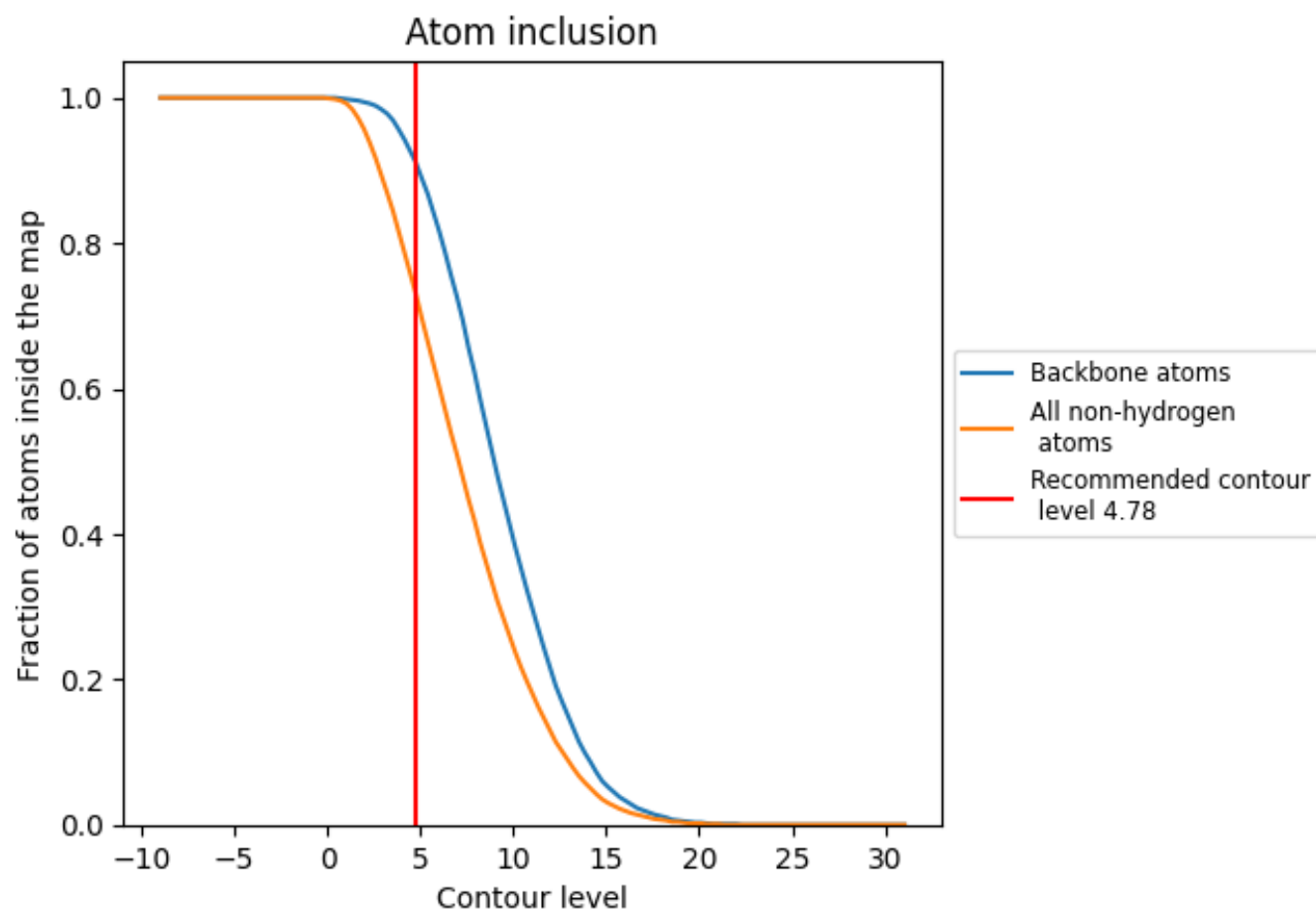
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.78).













































9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 73% 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 (4.78) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7280	 0.3750
A	 0.5960	 0.4410
B	 0.5700	 0.4400
C	 0.6380	 0.4510
D	 0.6490	 0.4550
E	 0.7400	 0.4690
F	 0.6200	 0.3940
G	 0.8310	 0.4350
H	 0.7520	 0.3280
I	 0.7340	 0.3380
J	 0.6810	 0.3400
K	 0.7420	 0.3290
L	 0.7370	 0.3430
M	 0.6980	 0.3770
N	 0.7460	 0.4440
O	 0.7560	 0.4450
P	 0.8680	 0.2610
Q	 0.8400	 0.2560
R	 0.9000	 0.2760
S	 0.8000	 0.3190
T	 0.9000	 0.3380
U	 0.8480	 0.3000

