



Full wwPDB EM Validation Report ⓘ

Nov 18, 2025 – 12:03 PM EST

PDB ID : 9MT4 / pdb_00009mt4
EMDB ID : EMD-48599
Title : Connector structure of phage JohannRWettstein (Bas63)
Authors : Hodgkinson-Bean, J.
Deposited on : 2025-01-10
Resolution : 3.10 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:

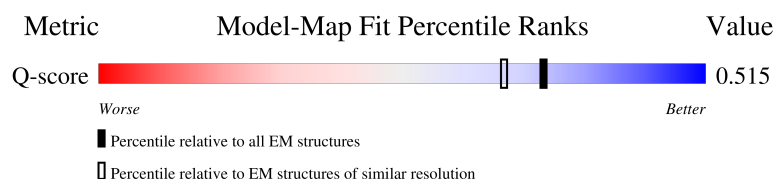
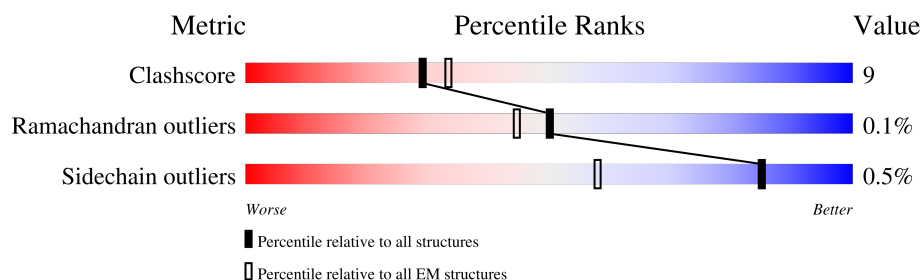
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.10 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	14724 (2.60 - 3.60)

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	488	
1	B	488	
2	E	133	
3	F	199	

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Mol	Chain	Length	Quality of chain
4	O	148	
4	P	148	
5	I	110	
5	J	110	
5	K	110	
5	L	110	
5	M	110	
5	N	110	
6	Q	450	
6	R	450	
7	C	149	
7	D	149	
8	G	166	
8	H	166	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 27234 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	434	Total	C	N	O	S	0	0
			3507	2242	591	654	20		
1	A	434	Total	C	N	O	S	0	0
			3507	2242	591	654	20		

- Molecule 2 is a protein called Head-closure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	132	Total	C	N	O	S	0	0
			1085	677	192	210	6		

- Molecule 3 is a protein called Tail terminator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	196	Total	C	N	O	S	0	0
			1539	970	257	307	5		

- Molecule 4 is a protein called Tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	143	Total	C	N	O	S	0	0
			1102	693	181	222	6		
4	O	140	Total	C	N	O	S	0	0
			1077	676	178	218	5		

- Molecule 5 is a protein called Phage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	96	Total	C	N	O	S	0	0
			729	467	115	146	1		
5	J	85	Total	C	N	O	S	0	0
			596	377	100	118	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	107	Total	C	N	O	S	0	0
			798	506	126	165	1		
5	K	107	Total	C	N	O	S	0	0
			799	507	126	165	1		
5	M	102	Total	C	N	O	S	0	0
			764	488	120	155	1		
5	N	95	Total	C	N	O	S	0	0
			714	453	114	146	1		

- Molecule 6 is a protein called Structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	441	Total	C	N	O	S	0	0
			3374	2126	574	666	8		
6	R	435	Total	C	N	O	S	0	0
			3343	2109	567	660	7		

- Molecule 7 is a protein called Phage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	132	Total	C	N	O	S	0	0
			1045	656	180	203	6		
7	D	132	Total	C	N	O	S	0	0
			1045	656	180	203	6		

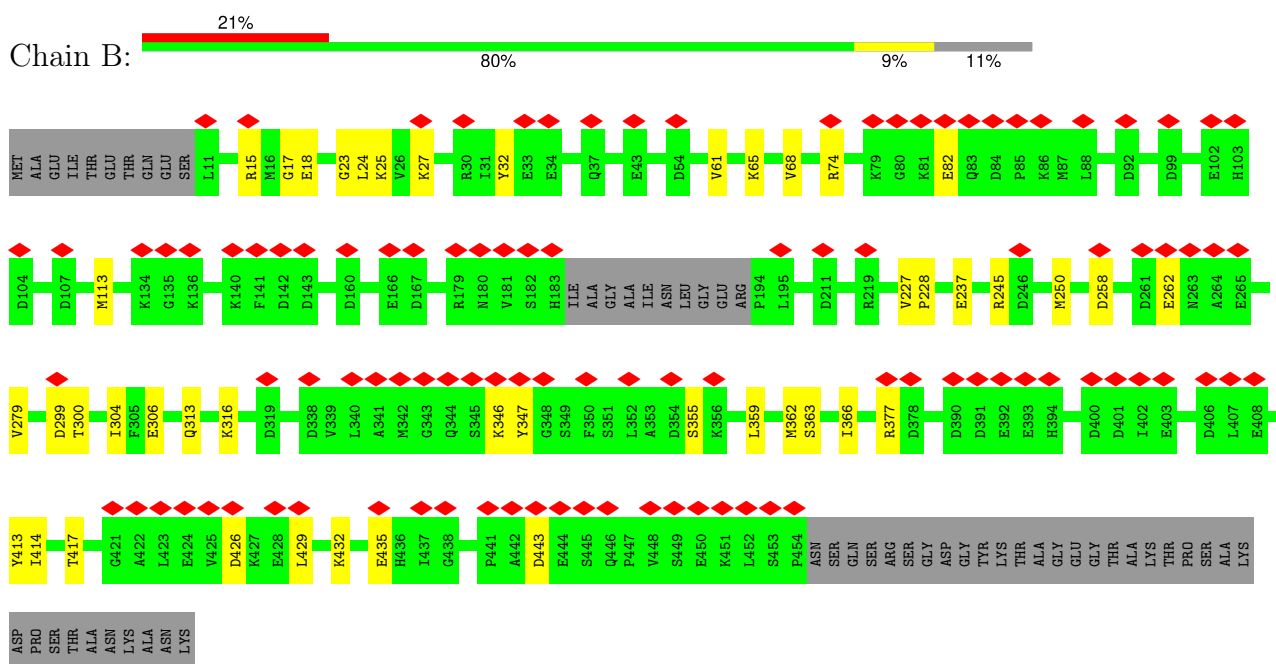
- Molecule 8 is a protein called Collar protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	155	Total	C	N	O	S	0	0
			1203	758	205	233	7		
8	H	129	Total	C	N	O	S	0	0
			1007	636	169	195	7		

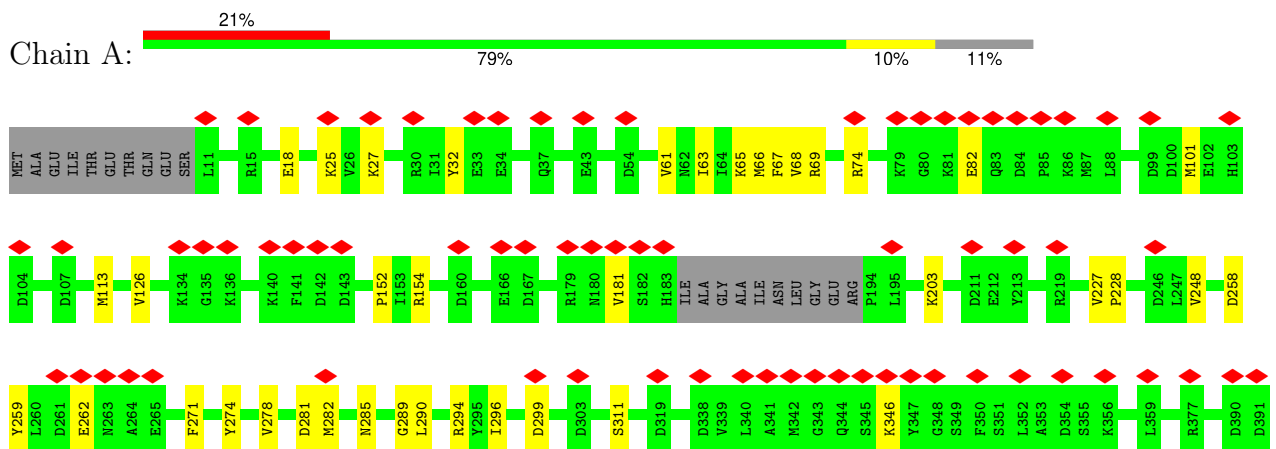
3 Residue-property plots

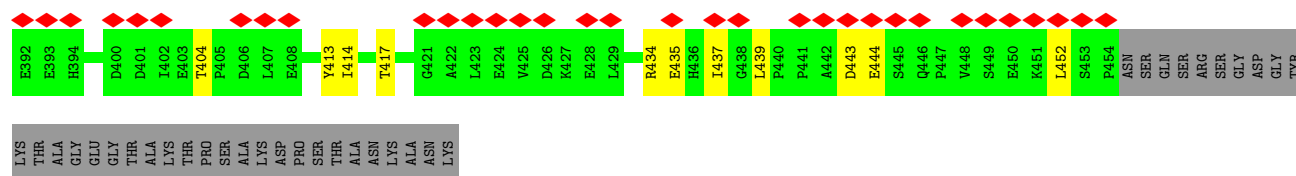
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Portal protein

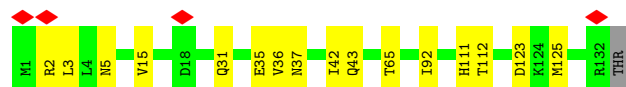
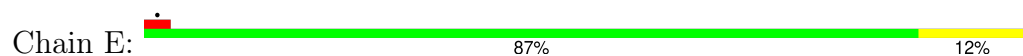


• Molecule 1: Portal protein





- Molecule 2: Head-closure protein



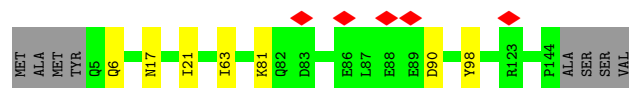
- Molecule 3: Tail terminator protein



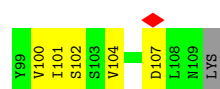
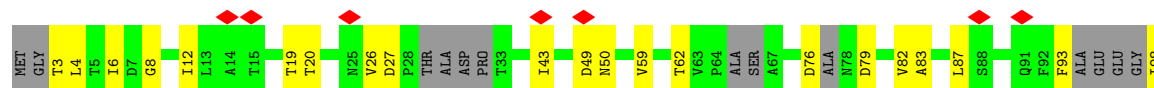
- Molecule 4: Tube protein



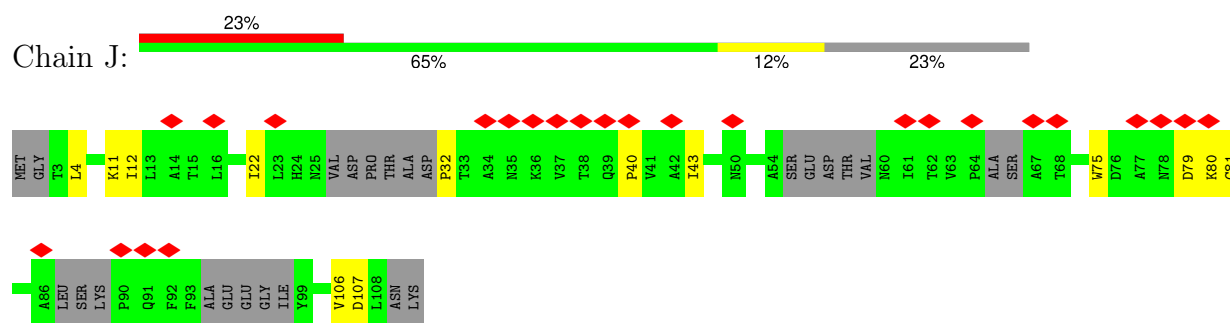
- Molecule 4: Tube protein



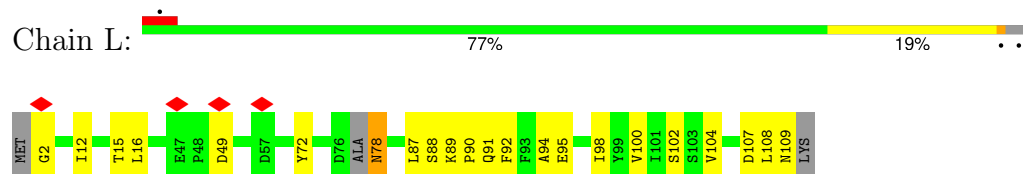
- Molecule 5: Phage protein



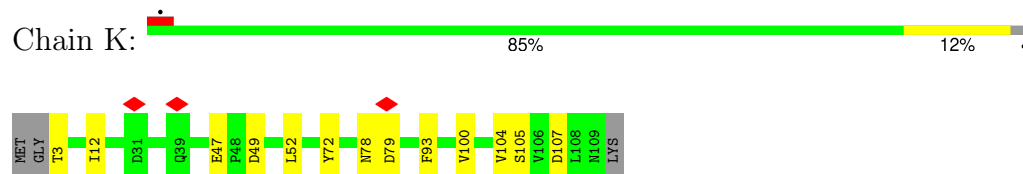
- Molecule 5: Phage protein



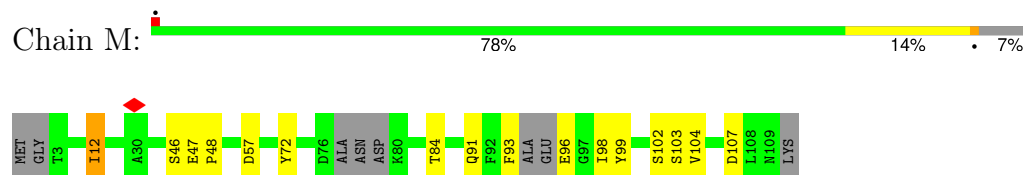
- Molecule 5: Phage protein



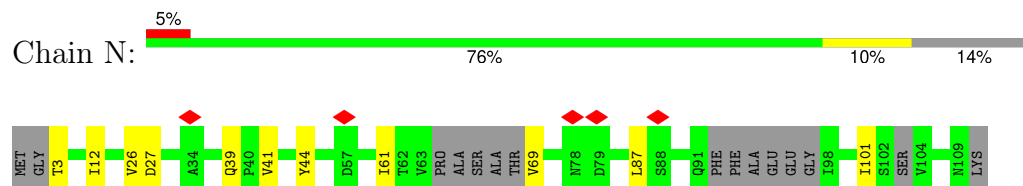
- Molecule 5: Phage protein



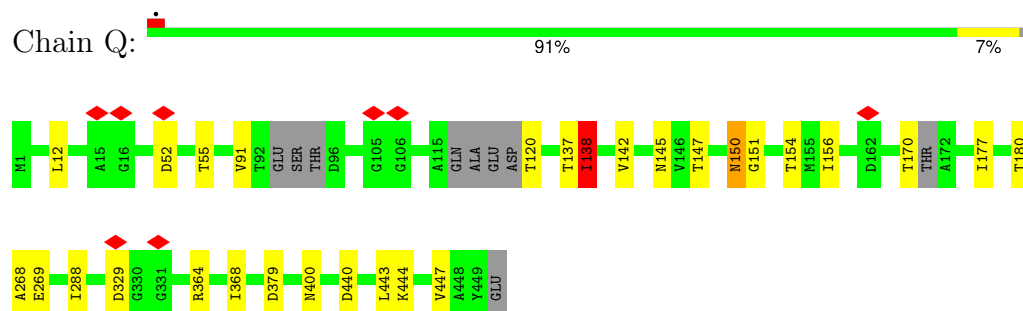
- Molecule 5: Phage protein



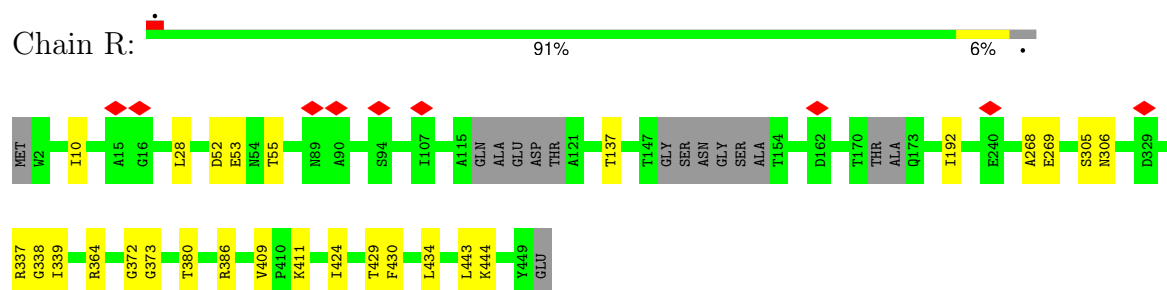
- Molecule 5: Phage protein



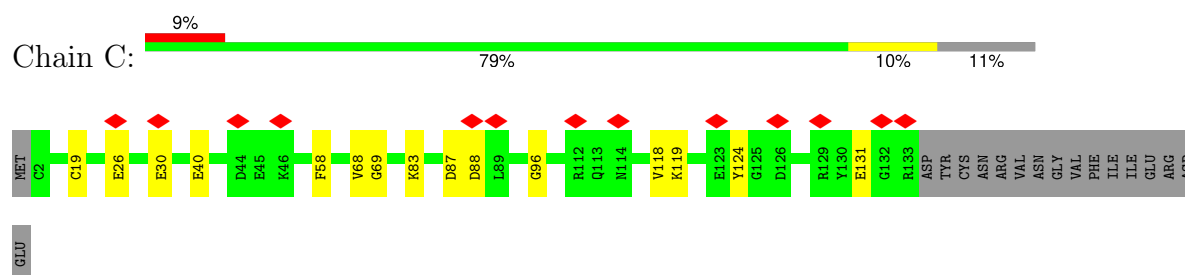
- Molecule 6: Structural protein



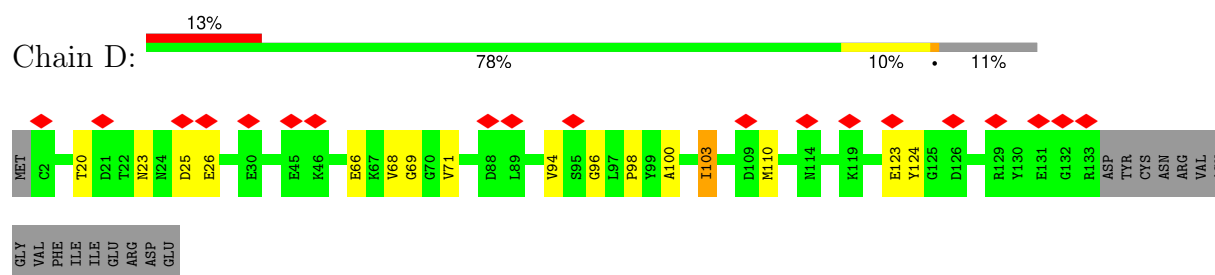
- Molecule 6: Structural protein



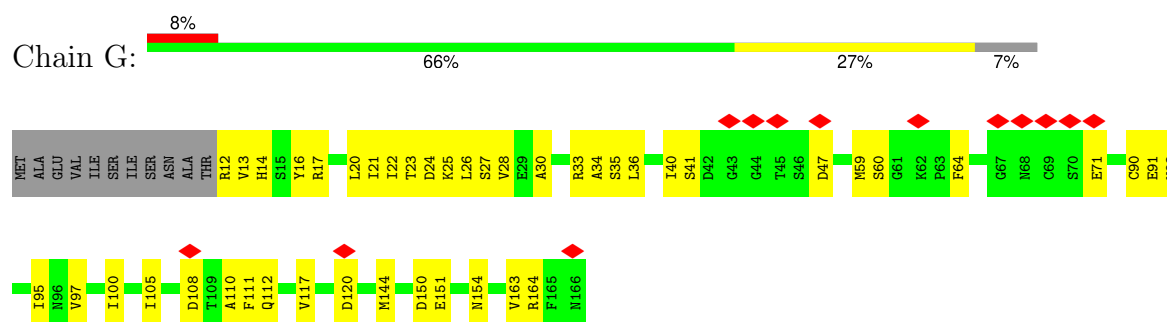
- Molecule 7: Phage protein



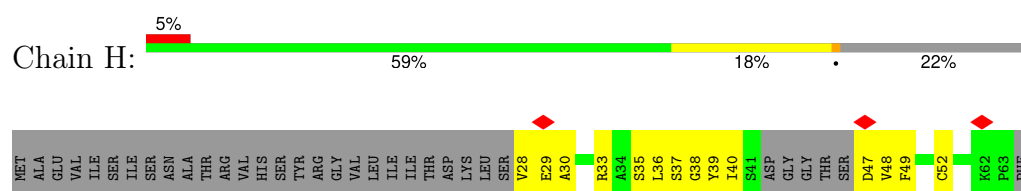
- Molecule 7: Phage protein

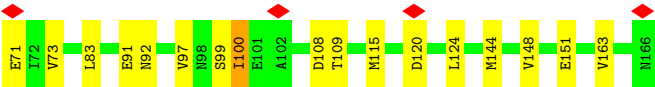


- Molecule 8: Collar protein



- Molecule 8: Collar protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20388	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	3.506	Depositor
Minimum map value	-0.906	Depositor
Average map value	0.036	Depositor
Map value standard deviation	0.152	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	446.61398, 446.61398, 585.31396	wwPDB
Map dimensions	322, 322, 422	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.15	0/3587	0.37	0/4840
1	B	0.14	0/3587	0.37	0/4840
2	E	0.15	0/1106	0.43	0/1496
3	F	0.16	0/1565	0.41	0/2132
4	O	0.14	0/1096	0.35	0/1491
4	P	0.15	0/1122	0.37	0/1526
5	I	0.14	0/740	0.36	0/1012
5	J	0.15	0/601	0.41	0/819
5	K	0.14	0/815	0.34	0/1122
5	L	0.12	0/813	0.33	0/1117
5	M	0.12	0/778	0.31	0/1068
5	N	0.12	0/724	0.32	0/993
6	Q	0.14	0/3431	0.35	0/4672
6	R	0.15	0/3400	0.41	0/4631
7	C	0.19	0/1062	0.40	0/1429
7	D	0.19	0/1062	0.39	0/1429
8	G	0.19	0/1221	0.42	0/1647
8	H	0.18	0/1020	0.39	0/1373
All	All	0.15	0/27730	0.38	0/37637

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3507	0	3491	87	0
1	B	3507	0	3492	73	0
2	E	1085	0	1046	36	0
3	F	1539	0	1522	18	0
4	O	1077	0	1057	17	0
4	P	1102	0	1080	5	0
5	I	729	0	728	41	0
5	J	596	0	570	20	0
5	K	799	0	790	34	0
5	L	798	0	787	64	0
5	M	764	0	762	60	0
5	N	714	0	715	18	0
6	Q	3374	0	3344	57	0
6	R	3343	0	3311	42	0
7	C	1045	0	1035	20	0
7	D	1045	0	1034	42	0
8	G	1203	0	1207	149	0
8	H	1007	0	1012	55	0
All	All	27234	0	26983	491	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 9.

All (491) 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)
5:K:3:THR:N	8:G:28:VAL:CG1	1.72	1.50
5:K:72:TYR:CD2	8:G:36:LEU:HD23	1.53	1.42
8:G:150:ASP:OD2	8:H:49:PHE:N	1.59	1.32
5:L:72:TYR:CD1	8:G:26:LEU:HD13	1.65	1.31
5:L:104:VAL:CG2	8:G:26:LEU:O	1.79	1.30
5:K:72:TYR:CD2	8:G:36:LEU:CD2	2.16	1.27
2:E:43:GLN:OE1	7:C:69:GLY:O	1.53	1.26
5:K:104:VAL:HG23	8:G:35:SER:O	1.32	1.25
1:B:18:GLU:OE2	1:A:126:VAL:HG21	1.12	1.25
5:L:92:PHE:CD2	5:M:96:GLU:O	1.90	1.24
5:K:3:THR:N	8:G:28:VAL:HG13	0.92	1.24
5:N:44:TYR:CE2	6:R:137:THR:CG2	2.20	1.24
5:M:107:ASP:OD1	8:G:12:ARG:N	1.71	1.23
5:M:107:ASP:CG	8:G:12:ARG:HB2	1.61	1.23
1:B:18:GLU:OE2	1:A:126:VAL:CG2	1.88	1.22
5:K:100:VAL:CG2	8:G:41:SER:HB2	1.67	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:72:TYR:CE1	8:G:26:LEU:HD13	1.76	1.20
5:K:72:TYR:CE2	8:G:36:LEU:HD23	1.76	1.20
8:G:90:CYS:SG	8:H:52:CYS:SG	1.20	1.20
1:B:24:LEU:O	1:A:181:VAL:HG13	1.37	1.18
1:A:259:TYR:OH	7:D:94:VAL:HG12	1.43	1.18
5:M:107:ASP:OD1	8:G:12:ARG:CA	1.91	1.18
6:Q:288:ILE:HD11	6:R:372:GLY:C	1.69	1.18
5:M:107:ASP:OD2	8:G:12:ARG:HB2	1.43	1.17
1:A:259:TYR:OH	7:D:94:VAL:CG1	1.90	1.17
5:L:104:VAL:HG23	8:G:26:LEU:C	1.70	1.16
1:B:347:TYR:CE1	1:A:346:LYS:HB2	1.81	1.14
5:N:3:THR:N	8:G:13:VAL:HG23	1.62	1.14
5:N:44:TYR:CE2	6:R:137:THR:HG22	1.81	1.13
1:B:24:LEU:O	1:A:181:VAL:CG1	1.95	1.13
5:L:102:SER:OG	8:G:25:LYS:NZ	1.83	1.11
3:F:154:VAL:HG12	4:O:6:GLN:HG3	1.28	1.09
2:E:112:THR:HG23	7:D:71:VAL:CG2	1.82	1.08
5:L:104:VAL:HG23	8:G:26:LEU:O	0.90	1.07
5:L:94:ALA:CB	5:M:93:PHE:CE1	2.38	1.07
5:L:2:GLY:CA	8:G:34:ALA:HB3	1.85	1.06
6:Q:329:ASP:HB3	6:R:364:ARG:HD2	1.30	1.06
2:E:112:THR:HG23	7:D:71:VAL:HG21	1.37	1.06
1:B:15:ARG:O	1:A:203:LYS:HE2	1.53	1.05
5:I:12:ILE:HG23	5:J:12:ILE:HG23	1.38	1.05
5:I:3:THR:N	8:H:28:VAL:HG13	1.69	1.05
5:M:107:ASP:OD1	8:G:12:ARG:CB	2.05	1.05
5:L:94:ALA:HB2	5:M:93:PHE:CD1	1.92	1.05
5:L:72:TYR:CD1	8:G:26:LEU:CD1	2.39	1.04
2:E:112:THR:CG2	7:D:71:VAL:CG2	2.35	1.04
5:L:87:LEU:HD23	8:G:26:LEU:HD11	1.34	1.04
3:F:125:THR:HG23	4:O:6:GLN:NE2	1.74	1.03
5:L:102:SER:CB	8:G:25:LYS:NZ	2.20	1.02
5:M:98:ILE:HB	8:G:20:LEU:CD1	1.89	1.02
2:E:2:ARG:CG	7:D:26:GLU:OE1	2.08	1.02
5:K:100:VAL:HG23	8:G:41:SER:HB2	1.02	1.01
6:Q:288:ILE:HD11	6:R:372:GLY:CA	1.89	1.01
1:B:359:LEU:HD21	1:A:63:ILE:HD11	1.40	1.01
1:B:347:TYR:CD1	1:A:346:LYS:HB2	1.95	1.00
5:M:107:ASP:OD1	8:G:12:ARG:HB2	1.61	0.99
5:L:94:ALA:CB	5:M:93:PHE:CD1	2.46	0.99
6:Q:147:THR:HG22	8:G:16:TYR:HE1	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:107:ASP:OD2	8:H:33:ARG:HB2	1.64	0.97
5:L:102:SER:CB	8:G:25:LYS:HZ2	1.78	0.97
2:E:2:ARG:HD2	7:D:26:GLU:OE1	1.65	0.96
2:E:2:ARG:CD	7:D:26:GLU:OE1	2.14	0.96
6:Q:147:THR:CG2	8:G:16:TYR:CE1	2.48	0.96
5:L:92:PHE:HD2	5:M:96:GLU:O	1.48	0.96
6:Q:147:THR:HG22	8:G:16:TYR:CE1	2.00	0.96
2:E:15:VAL:CG1	8:G:92:ASN:HB3	1.96	0.96
6:Q:288:ILE:CD1	6:R:372:GLY:C	2.38	0.96
5:M:107:ASP:CG	8:G:12:ARG:CB	2.39	0.95
2:E:15:VAL:HG12	8:G:92:ASN:HB3	1.49	0.95
5:M:107:ASP:OD2	8:G:12:ARG:CB	2.14	0.94
6:Q:329:ASP:CB	6:R:364:ARG:HD2	1.97	0.94
3:F:125:THR:CG2	4:O:6:GLN:NE2	2.32	0.93
5:I:4:LEU:HD12	8:H:30:ALA:HB2	1.51	0.92
5:L:102:SER:HB2	8:G:25:LYS:NZ	1.84	0.92
5:K:3:THR:CA	8:G:28:VAL:HG13	2.00	0.91
5:K:72:TYR:CE2	8:G:36:LEU:CD2	2.45	0.91
5:M:46:SER:OG	6:Q:180:THR:CG2	2.19	0.91
6:Q:288:ILE:HD11	6:R:372:GLY:HA2	1.53	0.90
2:E:112:THR:CG2	7:D:71:VAL:HG23	2.02	0.90
5:M:98:ILE:HB	8:G:20:LEU:HD11	1.54	0.89
4:O:98:TYR:CD2	6:Q:379:ASP:OD2	2.25	0.89
1:B:18:GLU:CD	1:A:126:VAL:HG21	1.98	0.89
1:A:285:ASN:OD1	7:D:124:TYR:HB2	1.73	0.88
5:L:94:ALA:HB2	5:M:93:PHE:CE1	2.06	0.88
3:F:125:THR:CG2	4:O:6:GLN:HE21	1.85	0.88
5:I:12:ILE:CG2	5:J:12:ILE:HG23	2.03	0.88
5:K:100:VAL:HG23	8:G:41:SER:CB	1.99	0.88
5:I:104:VAL:HG23	8:H:35:SER:O	1.74	0.87
5:N:44:TYR:CZ	6:R:137:THR:HG22	2.09	0.86
5:L:87:LEU:CD2	8:G:26:LEU:HD11	2.04	0.86
5:L:2:GLY:C	8:G:34:ALA:HB3	2.01	0.86
2:E:2:ARG:HG3	7:D:26:GLU:OE1	1.75	0.85
2:E:123:ASP:OD1	3:F:140:ASN:O	1.93	0.85
5:N:3:THR:N	8:G:13:VAL:CG2	2.39	0.85
5:L:102:SER:CB	8:G:25:LYS:HZ1	1.90	0.85
5:L:94:ALA:HB3	5:M:93:PHE:HE1	1.39	0.84
5:L:94:ALA:CB	5:M:93:PHE:HE1	1.86	0.84
5:N:44:TYR:CZ	6:R:137:THR:CG2	2.59	0.84
8:G:100:ILE:HD11	8:H:49:PHE:CE2	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:44:TYR:CE2	6:R:137:THR:HG21	2.10	0.83
2:E:112:THR:HG22	2:E:112:THR:O	1.77	0.83
5:L:72:TYR:CG	8:G:26:LEU:HD13	2.13	0.83
5:I:93:PHE:HZ	8:H:40:ILE:HG22	1.40	0.83
5:I:8:GLY:O	5:I:12:ILE:HG13	1.78	0.83
5:I:50:ASN:OD1	8:G:111:PHE:N	2.11	0.82
5:K:3:THR:N	8:G:28:VAL:HG11	1.91	0.82
5:M:103:SER:OG	6:Q:156:ILE:CD1	2.27	0.82
5:L:94:ALA:HB2	5:M:93:PHE:HD1	1.42	0.82
2:E:112:THR:CG2	7:D:71:VAL:HG21	2.06	0.81
1:B:250:MET:CE	1:A:290:LEU:HD12	2.10	0.81
6:Q:145:ASN:HB3	6:Q:156:ILE:HG22	1.63	0.81
6:Q:288:ILE:CD1	6:R:372:GLY:CA	2.58	0.81
1:B:15:ARG:O	1:A:203:LYS:CE	2.28	0.81
1:B:426:ASP:HB3	1:A:434:ARG:HH12	1.46	0.80
1:B:426:ASP:HB3	1:A:434:ARG:NH1	1.96	0.80
5:M:107:ASP:OD2	8:G:12:ARG:CG	2.29	0.80
1:A:259:TYR:HH	7:D:94:VAL:HG12	1.45	0.79
8:G:150:ASP:OD2	8:H:48:VAL:HA	1.82	0.79
5:I:101:ILE:HG23	8:H:36:LEU:HD11	1.65	0.79
1:B:429:LEU:HD13	1:A:439:LEU:CD1	2.13	0.79
5:M:46:SER:OG	6:Q:180:THR:HG23	1.83	0.79
6:Q:329:ASP:HB3	6:R:364:ARG:CD	2.11	0.78
2:E:43:GLN:CD	7:C:69:GLY:O	2.26	0.77
6:Q:147:THR:HG21	8:G:16:TYR:CE1	2.19	0.77
3:F:125:THR:HG21	4:O:6:GLN:HE21	1.47	0.77
5:I:93:PHE:CZ	8:H:40:ILE:CG2	2.67	0.77
5:L:94:ALA:HB3	5:M:93:PHE:CE1	2.13	0.77
5:N:44:TYR:HE2	6:R:137:THR:CG2	1.90	0.77
5:L:72:TYR:CE1	8:G:26:LEU:CD1	2.62	0.77
1:B:359:LEU:HD21	1:A:63:ILE:CD1	2.16	0.76
8:G:150:ASP:OD2	8:H:48:VAL:C	2.26	0.76
6:Q:145:ASN:HB3	6:Q:156:ILE:CG2	2.15	0.76
5:M:47:GLU:HG3	5:M:48:PRO:HD2	1.67	0.76
5:L:12:ILE:HG23	5:K:12:ILE:HG23	1.67	0.75
1:B:347:TYR:CE1	1:A:346:LYS:CB	2.65	0.75
5:M:47:GLU:CG	5:M:48:PRO:HD2	2.15	0.75
5:M:103:SER:O	8:G:16:TYR:HD2	1.69	0.75
5:K:3:THR:CA	8:G:28:VAL:CG1	2.62	0.74
1:A:282:MET:HA	7:D:103:ILE:HD11	1.67	0.74
4:P:98:TYR:OH	6:R:411:LYS:NZ	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:43:ILE:HD13	5:I:59:VAL:HG21	1.70	0.73
5:M:107:ASP:OD1	8:G:12:ARG:C	2.31	0.73
5:K:72:TYR:CD2	8:G:36:LEU:HD22	2.19	0.73
5:L:2:GLY:HA3	8:G:34:ALA:HB3	1.70	0.72
1:B:429:LEU:CD1	1:A:439:LEU:HD11	2.19	0.72
4:O:98:TYR:CE2	6:Q:379:ASP:CG	2.67	0.72
5:M:98:ILE:CB	8:G:20:LEU:HD11	2.19	0.72
3:F:154:VAL:HG12	4:O:6:GLN:CG	2.15	0.72
5:K:72:TYR:CG	8:G:36:LEU:CD2	2.72	0.72
5:M:103:SER:OG	6:Q:156:ILE:HD11	1.90	0.72
5:I:93:PHE:HZ	8:H:40:ILE:CG2	2.00	0.72
1:A:281:ASP:C	7:D:103:ILE:HD11	2.14	0.71
1:B:363:SER:HB3	1:A:66:MET:HE2	1.72	0.71
2:E:5:ASN:OD1	7:D:25:ASP:OD1	2.08	0.71
5:I:6:ILE:HD11	8:G:110:ALA:O	1.89	0.71
1:B:237:GLU:CD	7:C:124:TYR:O	2.34	0.71
5:I:12:ILE:CG2	5:J:12:ILE:CG2	2.68	0.71
6:Q:154:THR:HG23	8:G:14:HIS:HE1	1.56	0.70
6:R:337:ARG:O	6:R:339:ILE:HG23	1.91	0.70
5:I:83:ALA:HB2	5:J:4:LEU:HD23	1.72	0.70
8:G:150:ASP:OD2	8:H:48:VAL:CA	2.39	0.70
6:R:268:ALA:HB3	6:R:269:GLU:OE1	1.91	0.70
6:Q:288:ILE:CD1	6:R:372:GLY:HA2	2.20	0.70
1:A:27:LYS:HE3	1:A:32:TYR:CE2	2.27	0.70
1:B:27:LYS:HE3	1:B:32:TYR:CE2	2.27	0.70
5:K:104:VAL:CG2	8:G:35:SER:O	2.26	0.70
5:L:78:ASN:O	5:L:78:ASN:ND2	2.22	0.69
1:A:262:GLU:OE2	7:C:96:GLY:N	2.24	0.69
5:K:100:VAL:CG2	8:G:41:SER:CB	2.59	0.69
5:M:57:ASP:HB2	6:Q:184:THR:HG23	1.74	0.69
5:I:93:PHE:CZ	8:H:40:ILE:HG22	2.24	0.69
5:I:4:LEU:HD12	8:H:30:ALA:CB	2.23	0.69
5:I:50:ASN:OD1	8:G:111:PHE:CA	2.41	0.69
5:K:93:PHE:CE1	8:G:40:ILE:CD1	2.76	0.69
5:L:72:TYR:CE1	8:G:26:LEU:HD22	2.28	0.69
5:M:46:SER:OG	6:Q:180:THR:HG21	1.91	0.68
5:I:93:PHE:CZ	8:H:40:ILE:HG21	2.28	0.68
5:L:92:PHE:CE2	5:M:96:GLU:O	2.45	0.68
6:Q:443:LEU:HD21	6:R:430:PHE:CD1	2.29	0.68
1:B:250:MET:HE2	1:A:290:LEU:HD12	1.76	0.68
4:O:98:TYR:CE2	6:Q:379:ASP:OD2	2.47	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:104:VAL:CB	8:G:26:LEU:O	2.42	0.68
5:N:44:TYR:CZ	6:R:137:THR:HG21	2.28	0.68
5:L:72:TYR:CZ	8:G:26:LEU:HD13	2.29	0.68
2:E:112:THR:HG23	7:D:71:VAL:HG23	1.63	0.67
4:O:98:TYR:CE2	6:Q:379:ASP:OD1	2.48	0.67
1:A:281:ASP:O	7:D:103:ILE:HD11	1.95	0.67
1:B:24:LEU:C	1:A:181:VAL:HG13	2.18	0.67
3:F:141:THR:HG22	3:F:142:ASP:OD1	1.96	0.66
5:M:98:ILE:CB	8:G:20:LEU:CD1	2.69	0.66
4:O:98:TYR:HD2	6:Q:379:ASP:OD2	1.79	0.66
5:L:108:LEU:HD23	8:G:30:ALA:HB3	1.78	0.66
6:Q:329:ASP:CG	6:R:364:ARG:HD2	2.21	0.65
6:Q:154:THR:CG2	8:G:14:HIS:CE1	2.80	0.65
5:I:62:THR:HG22	5:I:98:ILE:HD12	1.79	0.64
5:L:16:LEU:HG	5:K:12:ILE:HD11	1.79	0.64
5:M:99:TYR:OH	8:G:17:ARG:NE	2.23	0.64
1:B:300:THR:HG21	1:A:296:ILE:HG21	1.79	0.63
1:B:24:LEU:O	1:A:181:VAL:HG12	1.94	0.63
5:K:107:ASP:HB2	8:G:33:ARG:HB2	1.79	0.63
5:L:102:SER:OG	8:G:23:THR:CG2	2.46	0.63
5:M:107:ASP:OD2	8:G:12:ARG:HD2	2.00	0.62
1:B:306:GLU:OE1	1:A:294:ARG:NH2	2.33	0.62
5:L:107:ASP:OD1	5:L:108:LEU:N	2.32	0.62
2:E:112:THR:CG2	2:E:112:THR:O	2.47	0.62
5:M:98:ILE:HB	8:G:20:LEU:HD13	1.79	0.62
6:Q:154:THR:CG2	8:G:14:HIS:HE1	2.11	0.62
1:B:23:GLY:C	1:A:181:VAL:HG11	2.24	0.62
2:E:112:THR:HG21	7:D:71:VAL:HG23	1.78	0.61
1:B:25:LYS:HB2	1:B:25:LYS:NZ	2.16	0.61
5:K:72:TYR:CG	8:G:36:LEU:HD22	2.35	0.61
1:A:25:LYS:HB2	1:A:25:LYS:NZ	2.16	0.61
6:Q:443:LEU:HD21	6:R:430:PHE:CE1	2.36	0.61
5:I:19:THR:HG23	5:I:20:THR:HG23	1.83	0.61
1:A:282:MET:HA	7:D:103:ILE:CD1	2.30	0.61
3:F:125:THR:HG23	4:O:6:GLN:HE22	1.61	0.60
1:B:377:ARG:NH1	1:A:101:MET:O	2.34	0.60
8:G:150:ASP:CG	8:H:49:PHE:N	2.53	0.60
1:B:359:LEU:CD2	1:A:63:ILE:HD11	2.25	0.60
1:B:432:LYS:HE3	1:A:437:ILE:O	2.02	0.60
1:B:429:LEU:HD12	1:A:439:LEU:HD11	1.83	0.60
1:A:274:TYR:CE1	7:D:98:PRO:O	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:154:VAL:CG1	4:O:6:GLN:HG3	2.18	0.60
6:Q:255:MET:HE3	6:Q:255:MET:HA	1.82	0.60
1:B:313:GLN:HB3	1:A:311:SER:HB2	1.83	0.60
1:B:304:ILE:O	1:A:294:ARG:HD3	2.02	0.59
1:B:262:GLU:OE2	7:D:96:GLY:N	2.34	0.59
5:M:91:GLN:OE1	8:G:17:ARG:NH1	2.34	0.59
5:M:107:ASP:OD2	8:G:12:ARG:CD	2.49	0.59
1:B:366:ILE:HG21	1:A:69:ARG:NH1	2.17	0.59
1:B:300:THR:HG21	1:A:296:ILE:CG2	2.32	0.59
1:A:262:GLU:OE2	7:C:96:GLY:CA	2.50	0.59
5:L:72:TYR:CD1	8:G:26:LEU:HD11	2.37	0.59
5:L:94:ALA:HB1	5:M:93:PHE:CD1	2.37	0.58
1:B:313:GLN:HB2	1:A:311:SER:HB3	1.85	0.58
1:B:313:GLN:HB2	1:A:311:SER:CB	2.33	0.58
5:L:2:GLY:HA2	8:G:34:ALA:HB3	1.78	0.58
8:G:25:LYS:HE3	8:G:25:LYS:HA	1.85	0.58
6:Q:288:ILE:CD1	6:R:373:GLY:N	2.67	0.58
1:B:18:GLU:CD	1:A:126:VAL:CG2	2.69	0.58
1:B:355:SER:OG	1:A:404:THR:OG1	2.22	0.58
5:N:44:TYR:OH	6:R:137:THR:HG21	2.04	0.57
2:E:15:VAL:HG13	8:G:92:ASN:HD22	1.69	0.57
1:A:282:MET:CA	7:D:103:ILE:HD11	2.33	0.57
5:L:95:GLU:HG3	5:M:91:GLN:HE22	1.70	0.57
5:M:103:SER:O	8:G:16:TYR:CD2	2.56	0.57
1:B:313:GLN:CB	1:A:311:SER:HB2	2.35	0.57
5:I:101:ILE:HG23	8:H:36:LEU:CD1	2.33	0.57
6:Q:154:THR:HG21	8:G:14:HIS:CE1	2.39	0.57
5:I:43:ILE:HD13	5:I:59:VAL:CG2	2.35	0.56
5:L:89:LYS:HD2	5:L:90:PRO:HD2	1.87	0.56
5:J:106:VAL:HG12	5:J:107:ASP:N	2.21	0.56
5:L:102:SER:HB2	8:G:25:LYS:HZ2	1.55	0.56
2:E:2:ARG:HH21	7:D:23:ASN:HD21	1.53	0.56
5:L:87:LEU:HA	8:G:26:LEU:HD21	1.87	0.56
1:B:61:VAL:HG12	1:B:65:LYS:HD3	1.87	0.56
7:C:83:LYS:O	7:C:87:ASP:OD2	2.24	0.56
1:A:259:TYR:OH	7:D:94:VAL:HG11	1.98	0.55
7:C:58:PHE:CB	7:D:20:THR:HG21	2.36	0.55
1:A:61:VAL:HG12	1:A:65:LYS:HD3	1.87	0.55
6:Q:443:LEU:CD2	6:R:430:PHE:CE1	2.90	0.55
5:L:72:TYR:CG	8:G:26:LEU:CD1	2.82	0.55
5:L:72:TYR:HE1	8:G:26:LEU:HD22	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:94:ALA:CB	5:M:93:PHE:HD1	2.04	0.55
1:B:250:MET:CE	1:A:290:LEU:CD1	2.83	0.55
8:H:100:ILE:HG23	8:H:148:VAL:HG13	1.89	0.55
5:J:32:PRO:HB2	5:J:81:CYS:SG	2.47	0.54
5:K:93:PHE:CE1	8:G:40:ILE:HD12	2.42	0.54
7:C:58:PHE:HB3	7:D:20:THR:HG21	1.90	0.54
1:B:262:GLU:OE2	7:D:96:GLY:CA	2.55	0.54
5:L:104:VAL:CG2	8:G:27:SER:HA	2.37	0.54
1:B:279:VAL:HG13	1:A:289:GLY:HA3	1.90	0.54
1:A:413:TYR:O	1:A:417:THR:HG23	2.08	0.54
6:R:10:ILE:O	6:R:10:ILE:HG22	2.08	0.54
2:E:3:LEU:HD23	7:C:68:VAL:HG23	1.89	0.54
5:J:80:LYS:HG2	5:J:80:LYS:O	2.08	0.54
5:M:72:TYR:OH	8:G:13:VAL:HG12	2.08	0.54
5:K:72:TYR:CE2	8:G:36:LEU:HD22	2.39	0.54
8:G:117:VAL:O	8:G:117:VAL:HG13	2.08	0.54
1:B:413:TYR:O	1:B:417:THR:HG23	2.08	0.53
7:C:26:GLU:O	7:C:26:GLU:HG3	2.07	0.53
7:C:40:GLU:HA	7:C:40:GLU:OE1	2.08	0.53
1:A:271:PHE:CE1	7:D:98:PRO:HD3	2.43	0.53
5:M:98:ILE:CG2	8:G:20:LEU:CD1	2.86	0.53
6:Q:440:ASP:HB2	6:R:424:ILE:HG13	1.91	0.53
8:G:95:ILE:HD13	8:H:49:PHE:CZ	2.43	0.53
6:Q:269:GLU:N	6:Q:269:GLU:OE1	2.42	0.53
1:B:250:MET:HE1	1:A:282:MET:HE3	1.91	0.53
6:Q:150:ASN:OD1	6:Q:151:GLY:N	2.41	0.53
5:K:100:VAL:HG21	8:G:41:SER:HB2	1.79	0.53
5:N:44:TYR:CE2	6:R:137:THR:HG23	2.37	0.53
1:B:359:LEU:CD2	1:A:63:ILE:CD1	2.85	0.53
2:E:15:VAL:CG1	8:G:92:ASN:HD22	2.22	0.52
4:P:56:ASP:C	4:P:56:ASP:OD1	2.53	0.52
8:H:99:SER:O	8:H:100:ILE:HB	2.09	0.52
3:F:183:GLU:HB3	3:F:184:PRO:HD3	1.91	0.52
1:A:262:GLU:OE2	7:C:96:GLY:HA2	2.09	0.52
2:E:15:VAL:HG13	8:G:92:ASN:ND2	2.24	0.52
1:B:262:GLU:OE2	7:D:96:GLY:HA2	2.08	0.52
1:B:363:SER:CB	1:A:66:MET:HE2	2.39	0.52
6:R:28:LEU:HD13	6:R:192:ILE:CD1	2.39	0.52
7:D:110:MET:HE2	7:D:110:MET:HA	1.92	0.52
8:G:59:MET:HE1	8:H:49:PHE:CE2	2.44	0.52
1:B:299:ASP:OD1	1:B:299:ASP:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:71:GLU:N	8:G:71:GLU:OE1	2.43	0.52
5:M:12:ILE:HG23	5:N:12:ILE:HG23	1.90	0.52
1:A:299:ASP:C	1:A:299:ASP:OD1	2.53	0.52
7:C:30:GLU:OE2	7:C:30:GLU:HA	2.10	0.51
7:C:131:GLU:OE2	7:C:131:GLU:N	2.43	0.51
6:Q:443:LEU:CD2	6:R:430:PHE:HE1	2.24	0.51
1:B:237:GLU:OE1	7:C:124:TYR:O	2.29	0.51
5:M:47:GLU:HG2	5:M:48:PRO:HD2	1.89	0.51
2:E:31:GLN:N	2:E:31:GLN:OE1	2.44	0.51
6:Q:288:ILE:HD13	6:R:373:GLY:N	2.26	0.51
1:A:82:GLU:N	1:A:82:GLU:OE1	2.44	0.51
5:I:50:ASN:OD1	8:G:111:PHE:C	2.53	0.51
5:K:93:PHE:CE1	8:G:40:ILE:HD11	2.45	0.51
6:Q:444:LYS:O	6:R:429:THR:HA	2.11	0.51
8:G:47:ASP:OD2	8:G:47:ASP:C	2.53	0.51
1:B:18:GLU:OE1	1:A:154:ARG:NH1	2.44	0.51
5:L:100:VAL:O	8:G:23:THR:HA	2.10	0.51
1:B:426:ASP:CG	1:A:443:ASP:HB3	2.36	0.51
2:E:35:GLU:N	2:E:35:GLU:OE1	2.44	0.51
1:B:366:ILE:CG2	1:A:69:ARG:NH1	2.74	0.51
5:L:95:GLU:HG3	5:M:91:GLN:NE2	2.25	0.51
8:G:97:VAL:HG12	8:G:97:VAL:O	2.11	0.51
5:K:47:GLU:OE1	5:K:47:GLU:HA	2.11	0.50
5:M:12:ILE:HG23	5:N:12:ILE:CG2	2.41	0.50
8:G:91:GLU:N	8:G:91:GLU:OE2	2.43	0.50
5:I:50:ASN:HB3	8:G:112:GLN:N	2.26	0.50
6:R:443:LEU:HD23	6:R:444:LYS:N	2.26	0.50
5:M:107:ASP:OD1	8:G:12:ARG:O	2.29	0.50
8:G:120:ASP:OD2	8:G:120:ASP:C	2.54	0.50
5:M:98:ILE:CG2	8:G:20:LEU:HD11	2.41	0.50
5:M:57:ASP:HB2	6:Q:184:THR:CG2	2.41	0.50
6:R:269:GLU:OE1	6:R:269:GLU:N	2.45	0.50
5:M:102:SER:HB3	8:G:16:TYR:HB2	1.94	0.50
1:B:82:GLU:OE1	1:B:82:GLU:N	2.44	0.50
1:B:237:GLU:OE2	7:C:124:TYR:O	2.28	0.50
5:J:106:VAL:HG22	8:H:28:VAL:HB	1.94	0.50
5:I:12:ILE:HG23	5:J:12:ILE:CG2	2.23	0.49
1:B:68:VAL:HG11	1:B:113:MET:SD	2.53	0.49
2:E:65:THR:HG21	3:F:140:ASN:ND2	2.27	0.49
8:G:95:ILE:HD13	8:H:49:PHE:HZ	1.75	0.49
5:L:15:THR:OG1	5:K:12:ILE:HD13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG11	1:A:113:MET:SD	2.53	0.49
2:E:111:HIS:HB2	7:D:66:GLU:OE1	2.11	0.49
6:Q:145:ASN:ND2	8:G:16:TYR:HB3	2.27	0.49
8:H:91:GLU:C	8:H:91:GLU:OE1	2.56	0.49
5:N:61:ILE:HD12	5:N:101:ILE:HD11	1.94	0.49
1:A:271:PHE:CD1	7:D:98:PRO:HD3	2.48	0.49
5:L:49:ASP:OD1	5:L:49:ASP:C	2.55	0.49
8:G:151:GLU:OE2	8:H:47:ASP:HB3	2.14	0.48
5:L:91:GLN:CD	8:G:22:ILE:HD13	2.37	0.48
1:B:347:TYR:HE1	1:A:346:LYS:CB	2.26	0.48
5:J:43:ILE:HG23	5:J:43:ILE:O	2.13	0.48
5:L:104:VAL:HG22	8:G:27:SER:HA	1.95	0.48
5:L:104:VAL:CG2	8:G:26:LEU:C	2.62	0.48
1:B:443:ASP:O	1:A:452:LEU:HD21	2.14	0.48
6:Q:400:ASN:O	6:Q:400:ASN:ND2	2.47	0.48
5:J:22:ILE:HD12	5:J:75:TRP:CZ2	2.50	0.47
1:A:444:GLU:OE2	1:A:444:GLU:O	2.32	0.47
5:K:52:LEU:HD11	5:K:105:SER:HB2	1.95	0.47
4:P:88:GLU:N	4:P:88:GLU:OE1	2.47	0.47
5:I:26:VAL:HG12	5:I:27:ASP:N	2.30	0.47
7:D:123:GLU:N	7:D:123:GLU:OE1	2.48	0.47
8:H:120:ASP:OD1	8:H:120:ASP:C	2.58	0.47
8:H:144:MET:CE	8:H:163:VAL:HG11	2.44	0.47
1:B:366:ILE:CG2	1:A:69:ARG:HH11	2.28	0.47
8:G:59:MET:HE1	8:H:49:PHE:CZ	2.49	0.47
5:I:87:LEU:HD23	8:H:36:LEU:HD23	1.95	0.47
6:Q:137:THR:O	6:Q:138:ILE:HG22	2.15	0.47
6:Q:443:LEU:HD23	6:Q:444:LYS:N	2.30	0.47
8:G:60:SER:HA	8:H:52:CYS:O	2.15	0.47
5:M:103:SER:OG	6:Q:156:ILE:HD12	2.09	0.47
3:F:125:THR:HG21	4:O:6:GLN:NE2	2.15	0.47
1:A:281:ASP:O	7:D:103:ILE:CD1	2.62	0.46
1:B:313:GLN:CB	1:A:311:SER:CB	2.93	0.46
2:E:43:GLN:NE2	7:C:69:GLY:O	2.48	0.46
5:I:79:ASP:OD1	5:I:79:ASP:O	2.33	0.46
5:I:102:SER:N	8:H:37:SER:O	2.48	0.46
5:M:104:VAL:HG13	8:G:14:HIS:O	2.14	0.46
6:Q:52:ASP:OD1	6:Q:55:THR:HG23	2.16	0.46
8:G:95:ILE:HG21	8:H:49:PHE:HZ	1.81	0.46
5:L:72:TYR:CE1	8:G:26:LEU:CD2	2.99	0.46
8:G:100:ILE:HD11	8:H:49:PHE:HE2	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:MET:N	7:D:103:ILE:HD11	2.30	0.46
3:F:106:LYS:HD2	3:F:132:ILE:HD11	1.97	0.46
5:I:100:VAL:O	8:H:38:GLY:HA3	2.16	0.46
5:L:98:ILE:HB	8:G:21:ILE:HG12	1.98	0.46
8:G:154:ASN:ND2	8:H:48:VAL:HG23	2.31	0.46
1:B:245:ARG:NH2	1:A:282:MET:O	2.49	0.46
2:E:15:VAL:HG21	8:G:64:PHE:CD1	2.51	0.45
5:J:107:ASP:OD2	8:H:29:GLU:OE1	2.34	0.45
5:I:98:ILE:O	8:H:40:ILE:HA	2.17	0.45
8:H:91:GLU:O	8:H:92:ASN:HB2	2.16	0.45
5:L:107:ASP:OD1	5:L:109:ASN:ND2	2.50	0.45
8:H:71:GLU:OE1	8:H:71:GLU:HA	2.16	0.45
3:F:113:SER:O	3:F:114:VAL:HB	2.17	0.45
4:O:21:ILE:HG21	4:O:63:ILE:HD11	1.99	0.45
5:J:22:ILE:HD12	5:J:75:TRP:HZ2	1.82	0.45
2:E:125:MET:HE2	3:F:96:LYS:HG3	1.98	0.45
5:I:12:ILE:HG21	5:J:12:ILE:CG2	2.45	0.45
8:H:83:LEU:C	8:H:83:LEU:HD23	2.42	0.45
4:O:90:ASP:OD1	4:O:90:ASP:C	2.60	0.45
6:R:386:ARG:HG3	6:R:409:VAL:HG11	1.98	0.45
6:R:305:SER:O	6:R:306:ASN:HB3	2.18	0.44
1:B:300:THR:CG2	1:A:296:ILE:HG21	2.44	0.44
5:I:8:GLY:O	5:I:12:ILE:CG1	2.56	0.44
5:J:106:VAL:CG1	5:J:107:ASP:N	2.80	0.44
8:H:73:VAL:HB	8:H:163:VAL:HG12	1.99	0.44
5:I:76:ASP:OD2	5:J:11:LYS:NZ	2.51	0.44
8:G:105:ILE:HD11	8:G:144:MET:HE2	2.00	0.44
4:O:81:LYS:HB2	4:O:81:LYS:NZ	2.33	0.44
5:L:12:ILE:HD12	5:K:12:ILE:HG23	1.98	0.44
2:E:111:HIS:HD2	7:D:66:GLU:OE2	2.01	0.44
5:L:88:SER:HB3	8:G:24:ASP:OD1	2.18	0.44
8:G:163:VAL:HG12	8:G:164:ARG:N	2.33	0.44
8:H:91:GLU:OE1	8:H:91:GLU:O	2.34	0.44
6:R:53:GLU:N	6:R:53:GLU:OE1	2.51	0.43
7:D:68:VAL:O	7:D:69:GLY:C	2.59	0.43
5:L:102:SER:OG	8:G:23:THR:HG21	2.17	0.43
5:K:107:ASP:CB	8:G:33:ARG:HB2	2.48	0.43
8:G:25:LYS:O	8:G:26:LEU:C	2.61	0.43
5:L:88:SER:CB	8:G:24:ASP:OD1	2.67	0.43
6:Q:170:THR:HG22	6:Q:177:ILE:HD12	2.00	0.43
5:I:100:VAL:N	8:H:39:TYR:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:84:THR:O	5:N:3:THR:OG1	2.37	0.43
7:C:26:GLU:O	7:C:26:GLU:CG	2.66	0.43
8:H:97:VAL:HG23	8:H:100:ILE:HD12	2.01	0.43
8:H:97:VAL:O	8:H:97:VAL:HG13	2.19	0.43
2:E:36:VAL:HG12	2:E:37:ASN:N	2.34	0.42
6:Q:364:ARG:HG2	6:Q:368:ILE:HD12	2.01	0.42
7:C:88:ASP:OD1	7:C:88:ASP:C	2.62	0.42
8:H:115:MET:HE2	8:H:124:LEU:HB3	2.02	0.42
4:P:13:VAL:HG11	6:R:380:THR:HA	2.01	0.42
2:E:112:THR:HG22	7:D:68:VAL:HB	2.01	0.42
1:B:316:LYS:NZ	1:A:248:VAL:O	2.51	0.42
5:M:107:ASP:O	8:G:12:ARG:N	2.52	0.42
5:N:26:VAL:HG12	5:N:27:ASP:N	2.35	0.42
6:Q:268:ALA:HB3	6:Q:269:GLU:OE1	2.20	0.42
1:B:258:ASP:OD1	1:B:258:ASP:C	2.62	0.42
1:A:27:LYS:HB3	1:A:32:TYR:CD2	2.54	0.42
1:A:227:VAL:HB	1:A:228:PRO:HD3	2.01	0.42
2:E:2:ARG:NH2	7:D:23:ASN:HD21	2.16	0.42
3:F:55:ILE:HG12	3:F:93:VAL:HG22	2.02	0.42
6:R:52:ASP:OD1	6:R:55:THR:HG23	2.20	0.42
1:B:227:VAL:HB	1:B:228:PRO:HD3	2.01	0.42
5:K:79:ASP:OD1	5:K:79:ASP:O	2.38	0.42
1:A:258:ASP:OD1	1:A:258:ASP:C	2.62	0.42
6:Q:154:THR:HG23	8:G:14:HIS:CE1	2.42	0.42
7:D:23:ASN:C	7:D:23:ASN:OD1	2.63	0.42
3:F:113:SER:HA	3:F:116:ASP:OD1	2.19	0.41
5:K:78:ASN:OD1	5:K:78:ASN:N	2.53	0.41
8:H:151:GLU:OE1	8:H:151:GLU:N	2.52	0.41
5:J:75:TRP:HB2	5:J:79:ASP:O	2.20	0.41
5:N:39:GLN:O	5:N:41:VAL:HG23	2.20	0.41
1:B:362:MET:HE1	1:A:67:PHE:CE1	2.54	0.41
5:J:22:ILE:HD11	5:J:40:PRO:HG3	2.02	0.41
1:B:429:LEU:CD1	1:A:439:LEU:CD1	2.81	0.41
5:I:100:VAL:O	8:H:38:GLY:CA	2.69	0.41
6:Q:91:VAL:HG21	6:Q:120:THR:C	2.45	0.41
6:Q:138:ILE:O	6:Q:142:VAL:HG22	2.20	0.41
8:G:108:ASP:O	8:G:108:ASP:OD2	2.39	0.41
1:B:27:LYS:HB3	1:B:32:TYR:CD2	2.54	0.41
4:P:27:ASP:OD1	4:P:27:ASP:N	2.53	0.41
5:K:49:ASP:OD1	5:K:49:ASP:O	2.39	0.41
5:N:69:VAL:HG23	5:N:87:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:337:ARG:O	6:R:338:GLY:C	2.61	0.41
5:I:49:ASP:OD1	5:I:49:ASP:C	2.63	0.41
5:I:49:ASP:OD1	5:I:49:ASP:O	2.39	0.41
5:M:107:ASP:OD2	8:G:12:ARG:HG3	2.16	0.41
6:Q:447:VAL:HG11	6:R:434:LEU:HD21	2.03	0.41
8:H:108:ASP:O	8:H:109:THR:HG22	2.21	0.41
1:B:17:GLY:HA2	1:A:126:VAL:HG13	2.02	0.40
1:B:74:ARG:HB3	1:B:74:ARG:CZ	2.51	0.40
1:A:278:VAL:HG22	7:D:100:ALA:CB	2.51	0.40
5:M:107:ASP:CG	8:G:12:ARG:CG	2.91	0.40
8:H:108:ASP:C	8:H:109:THR:HG22	2.46	0.40
8:H:108:ASP:C	8:H:108:ASP:OD2	2.64	0.40
5:M:98:ILE:CG2	8:G:20:LEU:HD12	2.51	0.40
7:C:19:CYS:O	7:C:19:CYS:SG	2.80	0.40
8:G:97:VAL:O	8:G:97:VAL:CG1	2.69	0.40
8:G:100:ILE:CD1	8:H:49:PHE:CE2	2.97	0.40
2:E:42:ILE:HD13	2:E:92:ILE:HD11	2.03	0.40
5:I:82:VAL:O	5:J:4:LEU:HD22	2.22	0.40
6:Q:288:ILE:HD11	6:R:372:GLY:O	2.11	0.40
1:B:18:GLU:CD	1:A:152:PRO:HG3	2.46	0.40
5:L:104:VAL:HG23	8:G:27:SER:HA	2.04	0.40
1:A:74:ARG:CZ	1:A:74:ARG:HB3	2.51	0.40
5:J:75:TRP:HB3	5:J:81:CYS:HA	2.02	0.40
8:G:100:ILE:HD11	8:H:49:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	430/488 (88%)	416 (97%)	14 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	430/488 (88%)	416 (97%)	14 (3%)	0	100	100
2	E	130/133 (98%)	127 (98%)	3 (2%)	0	100	100
3	F	194/199 (98%)	186 (96%)	8 (4%)	0	100	100
4	O	138/148 (93%)	136 (99%)	2 (1%)	0	100	100
4	P	141/148 (95%)	139 (99%)	2 (1%)	0	100	100
5	I	86/110 (78%)	82 (95%)	4 (5%)	0	100	100
5	J	73/110 (66%)	66 (90%)	7 (10%)	0	100	100
5	K	105/110 (96%)	104 (99%)	1 (1%)	0	100	100
5	L	103/110 (94%)	100 (97%)	3 (3%)	0	100	100
5	M	96/110 (87%)	94 (98%)	2 (2%)	0	100	100
5	N	87/110 (79%)	85 (98%)	2 (2%)	0	100	100
6	Q	433/450 (96%)	424 (98%)	7 (2%)	2 (0%)	25	58
6	R	427/450 (95%)	411 (96%)	16 (4%)	0	100	100
7	C	130/149 (87%)	124 (95%)	6 (5%)	0	100	100
7	D	130/149 (87%)	125 (96%)	5 (4%)	0	100	100
8	G	153/166 (92%)	146 (95%)	7 (5%)	0	100	100
8	H	123/166 (74%)	114 (93%)	8 (6%)	1 (1%)	16	48
All	All	3409/3794 (90%)	3295 (97%)	111 (3%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Q	138	ILE
8	H	100	ILE
6	Q	150	ASN

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	384/424 (91%)	381 (99%)	3 (1%)	79	89
1	B	384/424 (91%)	381 (99%)	3 (1%)	79	89
2	E	120/122 (98%)	120 (100%)	0	100	100
3	F	173/177 (98%)	172 (99%)	1 (1%)	84	91
4	O	121/127 (95%)	120 (99%)	1 (1%)	79	89
4	P	123/127 (97%)	123 (100%)	0	100	100
5	I	86/94 (92%)	86 (100%)	0	100	100
5	J	62/94 (66%)	62 (100%)	0	100	100
5	K	92/94 (98%)	92 (100%)	0	100	100
5	L	92/94 (98%)	91 (99%)	1 (1%)	70	84
5	M	89/94 (95%)	88 (99%)	1 (1%)	70	84
5	N	84/94 (89%)	84 (100%)	0	100	100
6	Q	357/365 (98%)	354 (99%)	3 (1%)	79	89
6	R	355/365 (97%)	355 (100%)	0	100	100
7	C	113/129 (88%)	111 (98%)	2 (2%)	54	76
7	D	113/129 (88%)	112 (99%)	1 (1%)	75	88
8	G	139/148 (94%)	139 (100%)	0	100	100
8	H	117/148 (79%)	117 (100%)	0	100	100
All	All	3004/3249 (92%)	2988 (100%)	16 (0%)	85	92

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

Mol	Chain	Res	Type
1	B	346	LYS
1	B	414	ILE
1	B	435	GLU
1	A	18	GLU
1	A	414	ILE
1	A	435	GLU
3	F	121	GLU
4	O	17	ASN
5	L	78	ASN
5	M	12	ILE
6	Q	12	LEU
6	Q	138	ILE
6	Q	223	LYS
7	C	118	VAL

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Mol	Chain	Res	Type
7	C	119	LYS
7	D	103	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
2	E	5	ASN
2	E	41	ASN
2	E	43	GLN
2	E	108	GLN
2	E	111	HIS
4	P	17	ASN
4	P	114	GLN
4	O	6	GLN
4	O	73	GLN
5	L	50	ASN
5	M	35	ASN
6	Q	82	GLN
6	Q	131	GLN
6	R	220	GLN
7	C	59	GLN
8	G	14	HIS
8	G	92	ASN
8	G	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

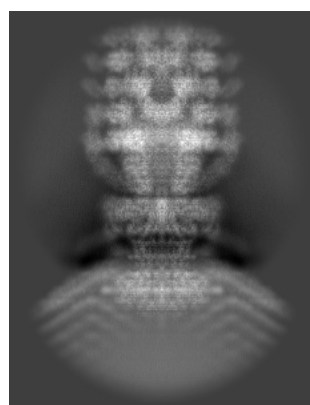
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48599. These allow visual inspection of the internal detail of the map and identification of artifacts.

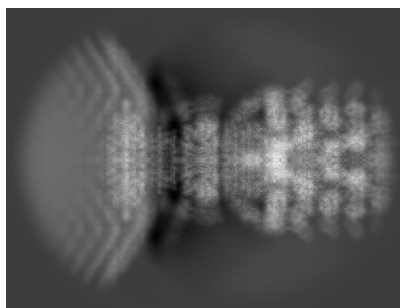
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

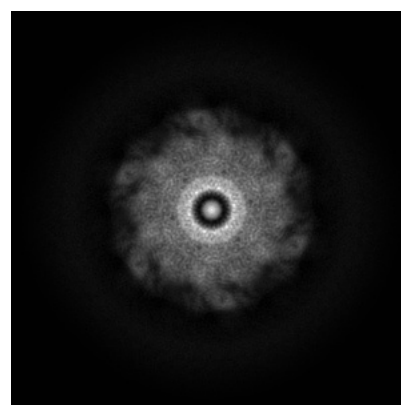
6.1.1 Primary map



X



Y

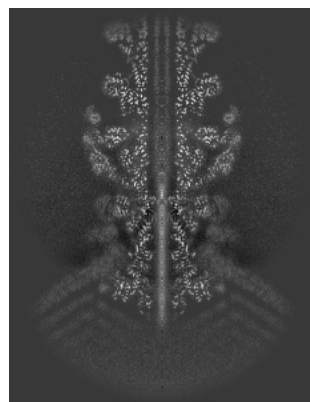


Z

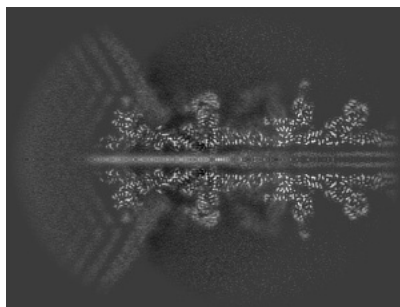
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

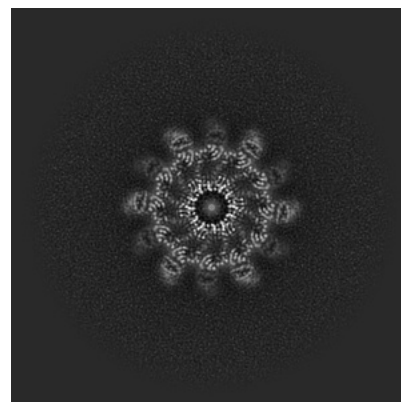
6.2.1 Primary map



X Index: 161



Y Index: 161

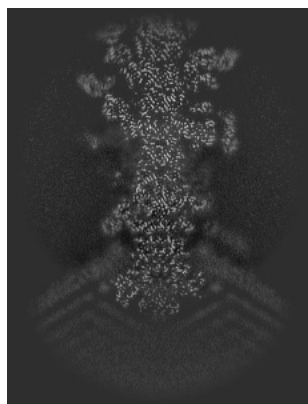


Z Index: 211

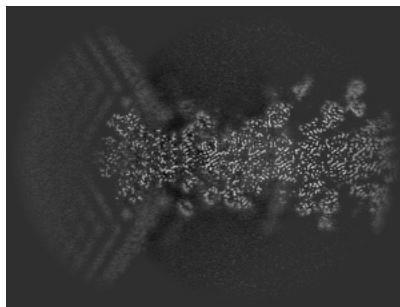
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

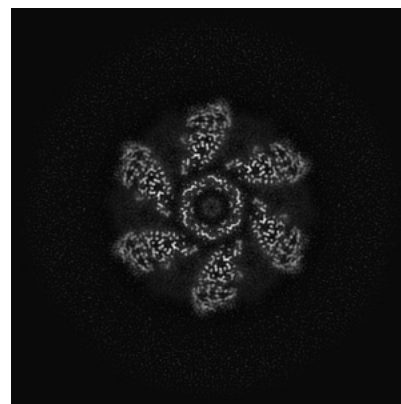
6.3.1 Primary map



X Index: 145



Y Index: 145

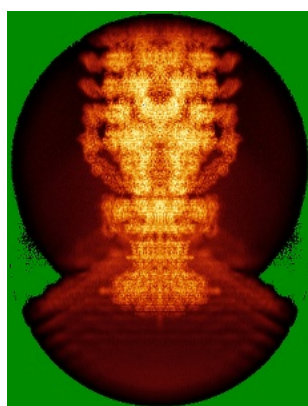


Z Index: 283

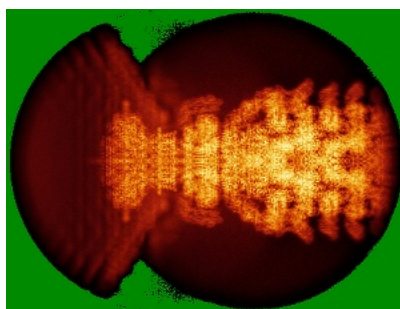
The images above show the largest variance slices of the map in three orthogonal directions.

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

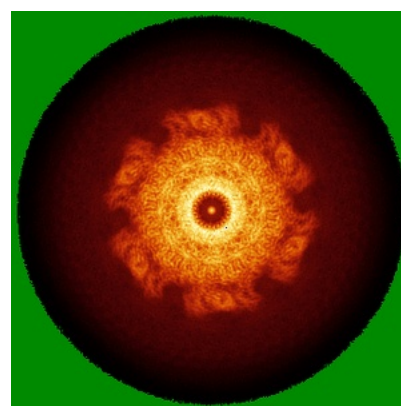
6.4.1 Primary map



X



Y

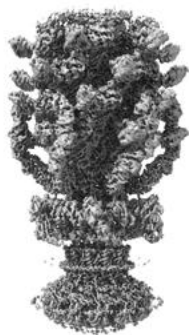


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

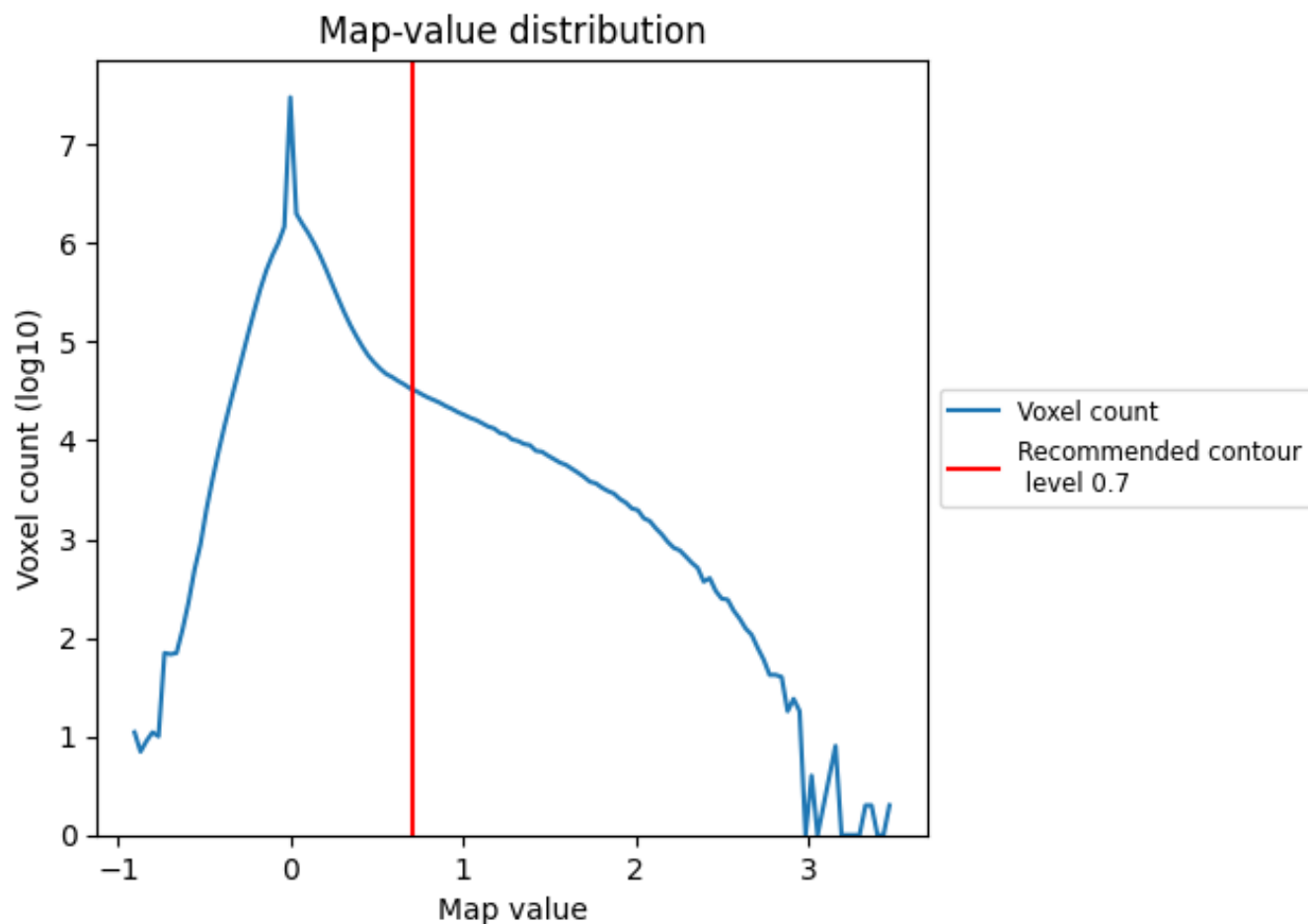
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

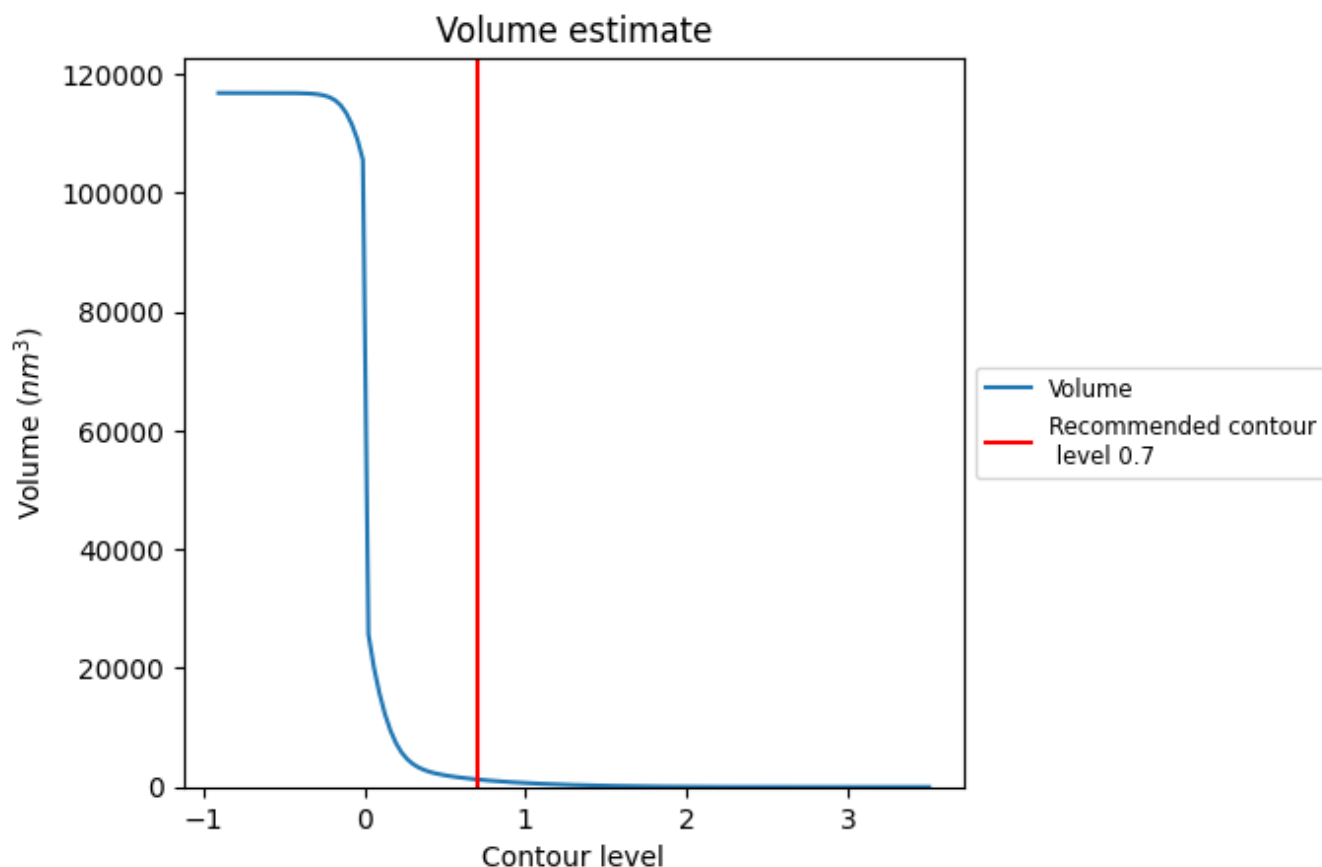
This section contains the results of statistical analysis of the map.

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 1263 nm³; this corresponds to an approximate mass of 1141 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation ⓘ

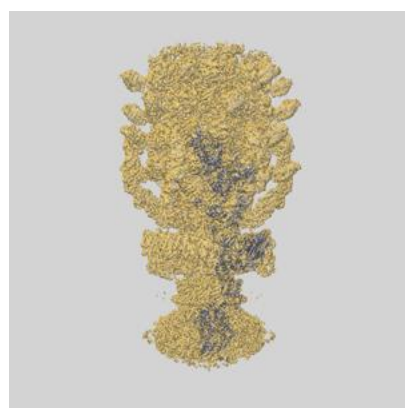
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

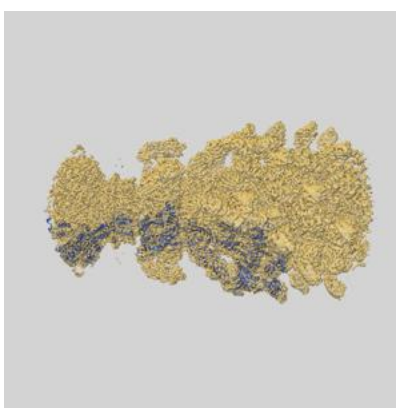
This section contains information regarding the fit between EMDB map EMD-48599 and PDB model 9MT4. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

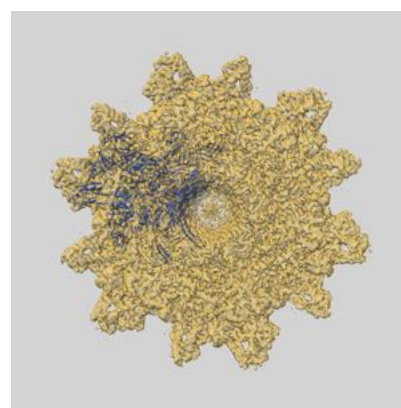
9.1.1 Map-model overlay [i](#)



X

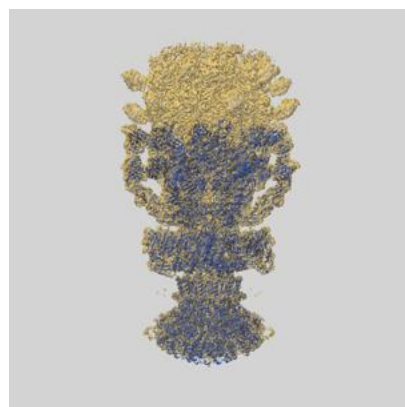


Y

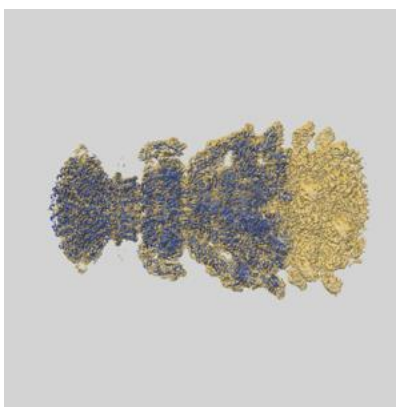


Z

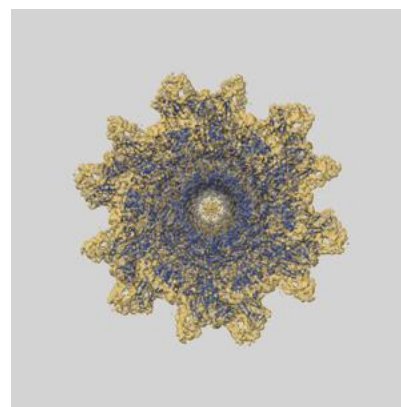
9.1.2 Map-model assembly overlay [i](#)



X



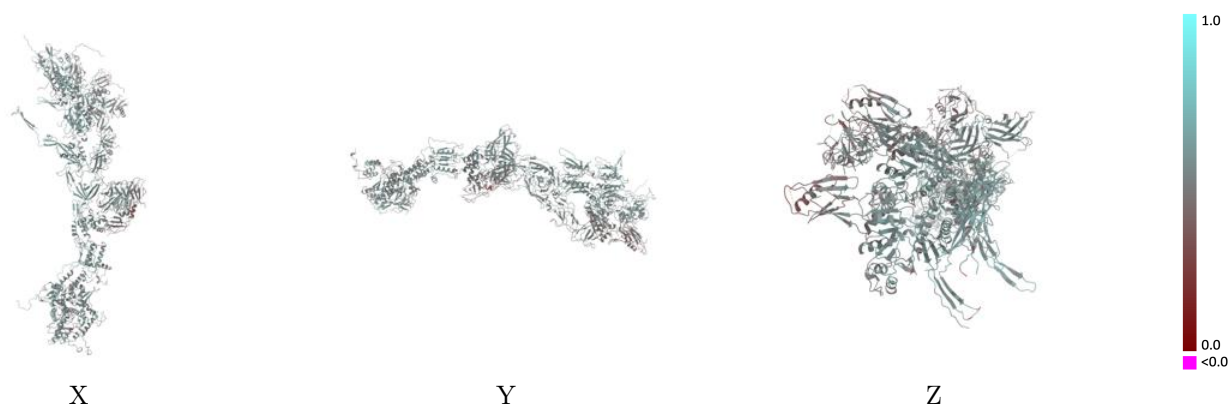
Y



Z

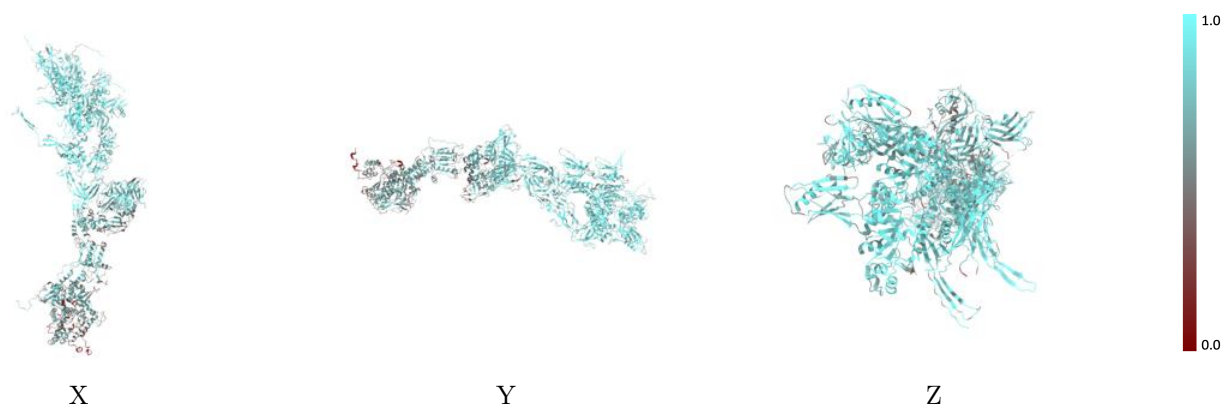
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



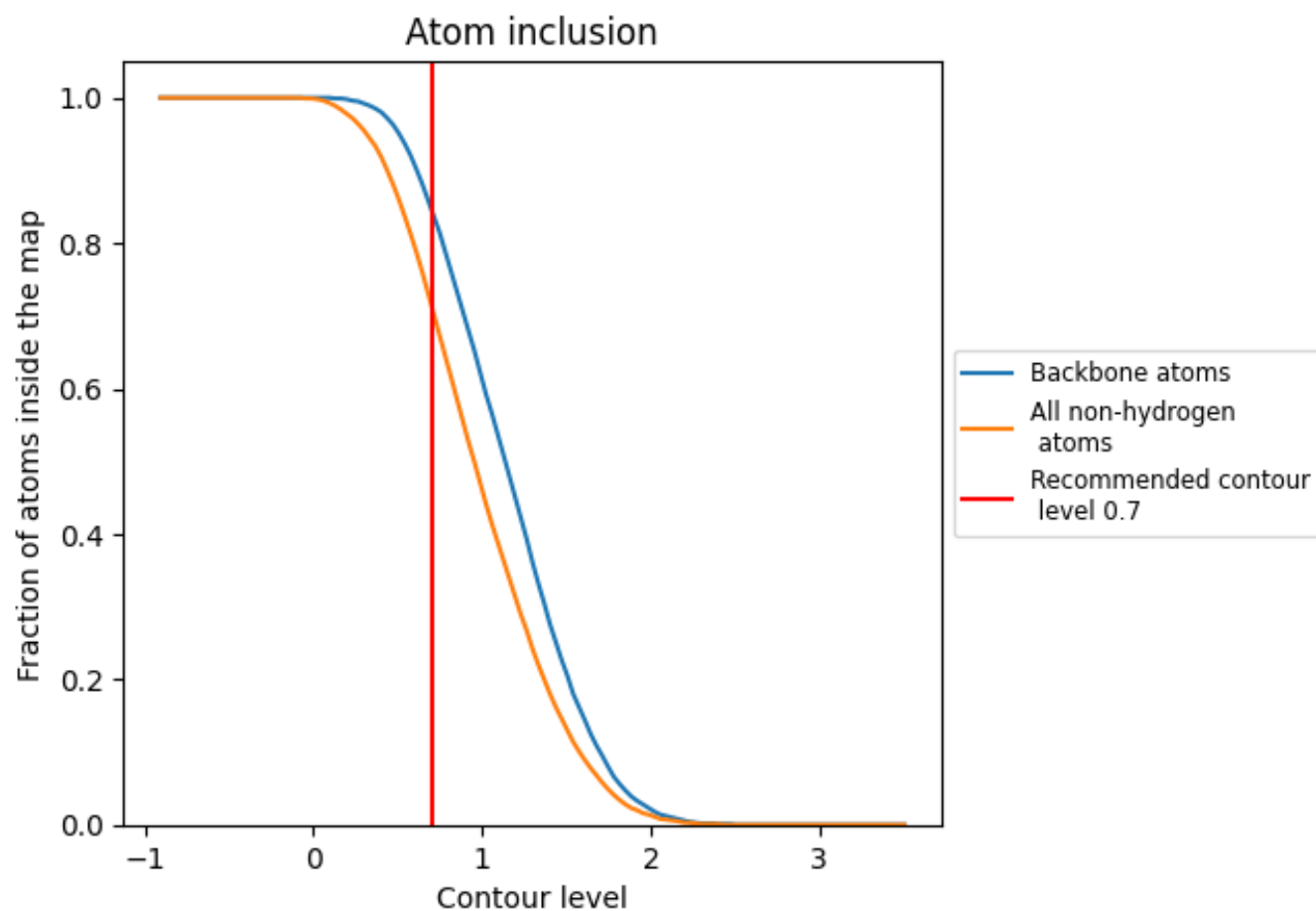
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 72% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.5150
A	 0.5700	 0.5270
B	 0.5560	 0.5130
C	 0.6510	 0.5280
D	 0.6400	 0.5170
E	 0.8060	 0.5490
F	 0.8070	 0.5370
G	 0.7280	 0.5100
H	 0.7280	 0.5160
I	 0.6500	 0.4380
J	 0.5240	 0.4160
K	 0.7650	 0.5160
L	 0.7640	 0.4960
M	 0.8090	 0.4800
N	 0.7370	 0.4420
O	 0.8080	 0.5470
P	 0.8000	 0.5470
Q	 0.8300	 0.5250
R	 0.8170	 0.5140

