



## Full wwPDB EM Validation Report ⓘ

Jun 8, 2026 – 04:24 PM EDT

PDB ID : 9OKL / pdb\_00009okl  
EMDB ID : EMD-70568  
Title : Structure of the Bombyx mori apo-bmCCAN  
Authors : Yatskevich, S.; Ciferri, C.  
Deposited on : 2025-05-10  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

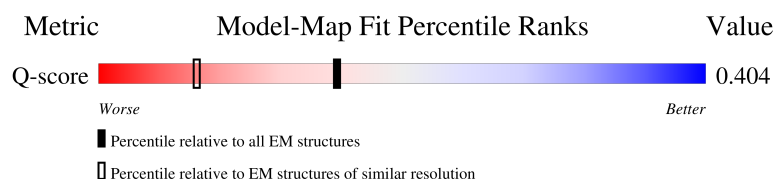
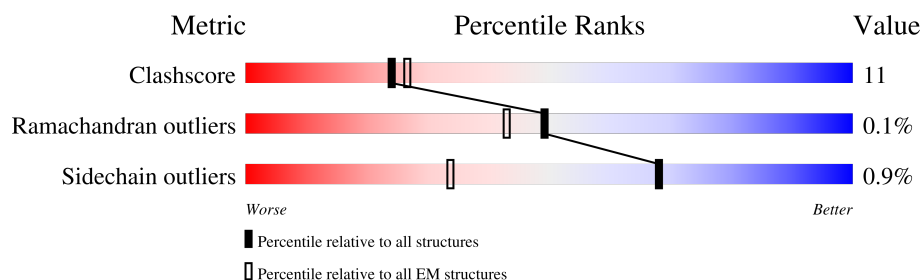
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

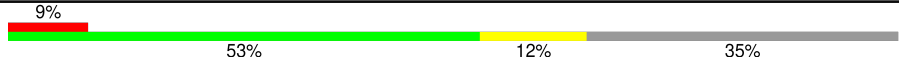
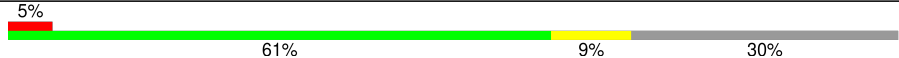


The reported resolution of this entry is 3.00 Å.

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





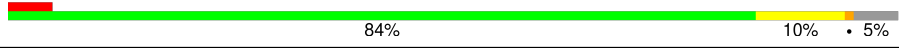



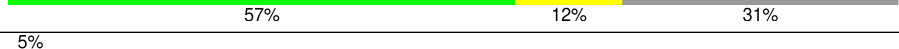
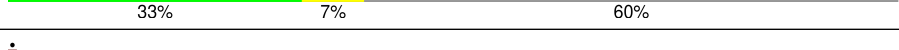
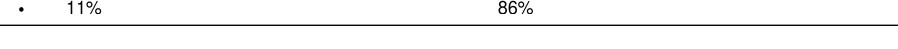
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

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  $\geq 3$ , 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	108	
2	B	82	
3	C	71	
4	D	81	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	H	239	
6	I	661	
7	K	219	
8	L	302	
9	M	180	
10	N	328	
11	O	325	
12	P	638	
13	T	1016	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 39509 atoms, of which 18862 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 CS-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	70	Total	C	H	N	O	0	0
			1108	342	558	99	109		

- Molecule 2 is a protein called CS-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	57	Total	C	H	N	O S	0	0
			907	282	459	74	91 1		

- Molecule 3 is a protein called SFRICE\_007223.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	55	Total	C	H	N	O S	0	0
			880	270	441	78	87 4		

- Molecule 4 is a protein called CS-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	71	Total	C	H	N	O S	0	0
			1050	357	481	103	108 1		

- Molecule 5 is a protein called bm-CENPH.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	228	Total	C	H	N	O S	0	0
			3517	1170	1666	326	345 10		

- Molecule 6 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	534	Total	C	H	N	O S	0	0
			8726	2815	4397	721	774 19		

- Molecule 7 is a protein called bmCENP-K.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	208	Total	C	H	N	O	S	0	0
			3282	1025	1639	272	337	9		

- Molecule 8 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	L	239	Total	C	H	N	O	S	0	0
			3880	1237	1974	309	353	7		

- Molecule 9 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	M	163	Total	C	H	N	O	S	0	0
			2626	818	1340	225	240	3		

- Molecule 10 is a protein called bmCENP-N.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	N	319	Total	C	H	N	O	S	0	0
			5105	1604	2583	440	465	13		

- Molecule 11 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	O	224	Total	C	H	N	O	S	0	0
			3317	1163	1487	320	335	12		

- Molecule 12 is a protein called bmCENP-P.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	P	255	Total	C	H	N	O	S	0	0
			3868	1290	1837	343	387	11		

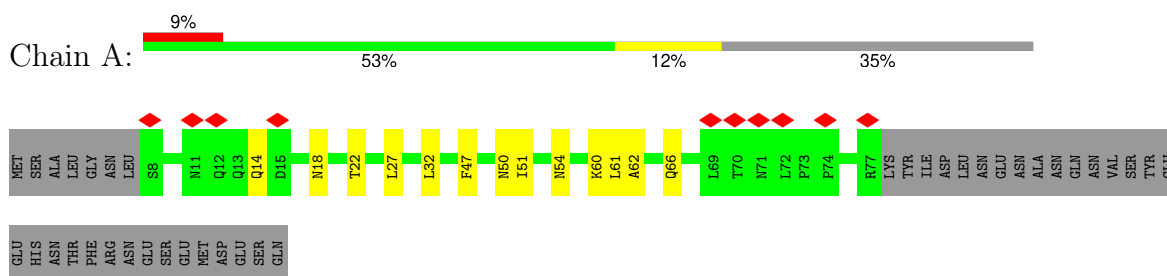
- Molecule 13 is a protein called bmCENP-T.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	146	Total	C	N	O	S	0	0
			1243	803	220	216	4		

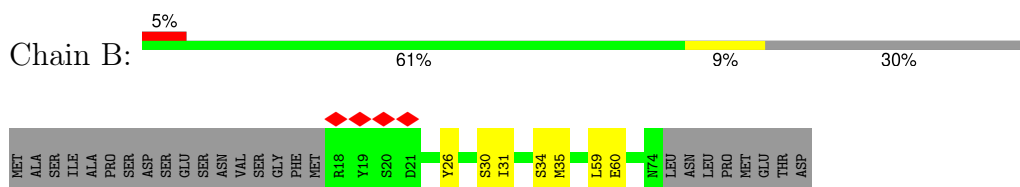
### 3 Residue-property plots [i](#)

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.

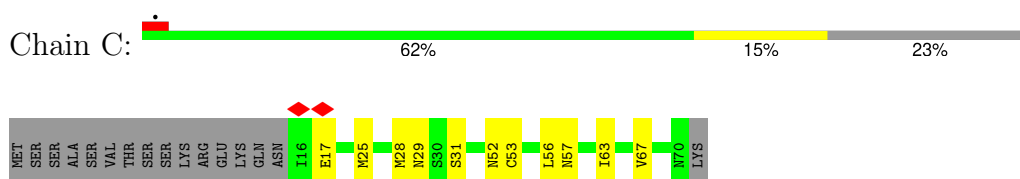
- Molecule 1: CS-1



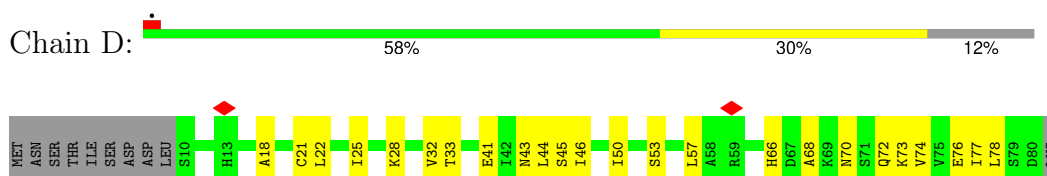
- Molecule 2: CS-2



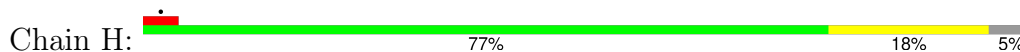
- Molecule 3: SFRICE\_007223

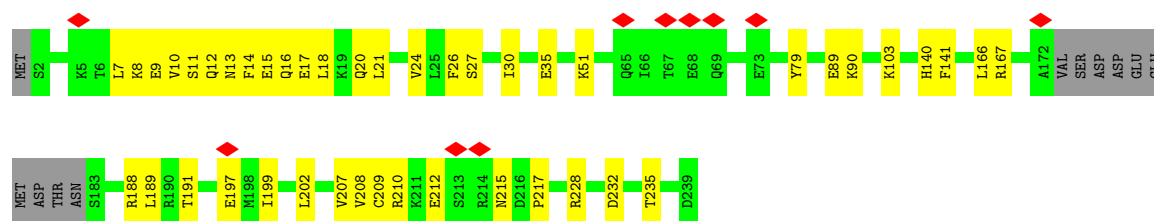


- Molecule 4: CS-4

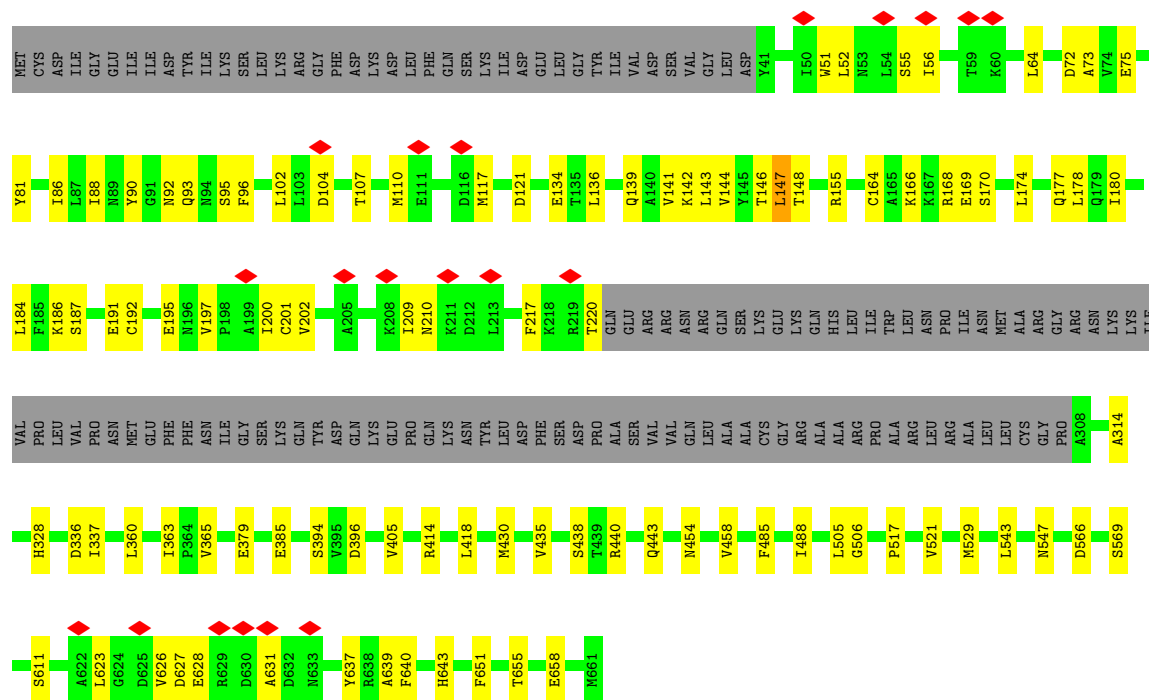


- Molecule 5: bm-CENPH

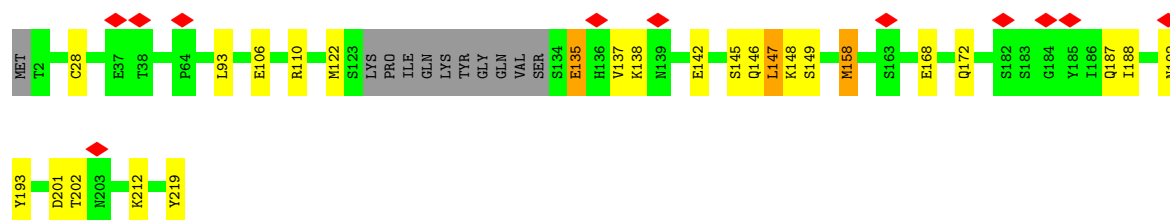
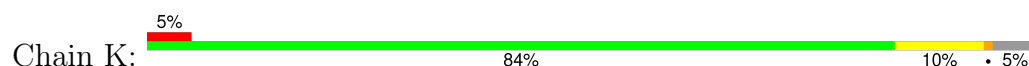




• Molecule 6: Centromere protein I

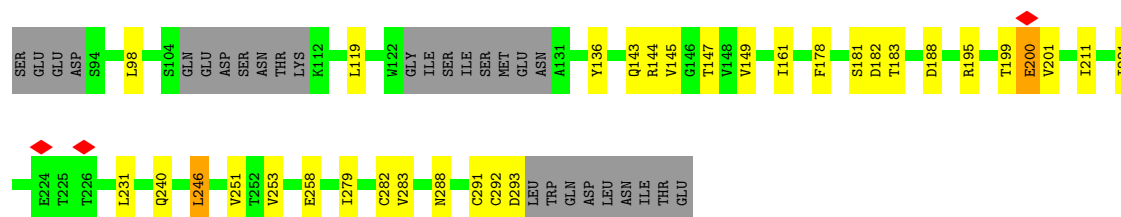


• Molecule 7: bmCENP-K

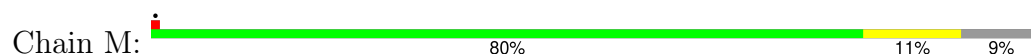


• Molecule 8: Centromere protein L

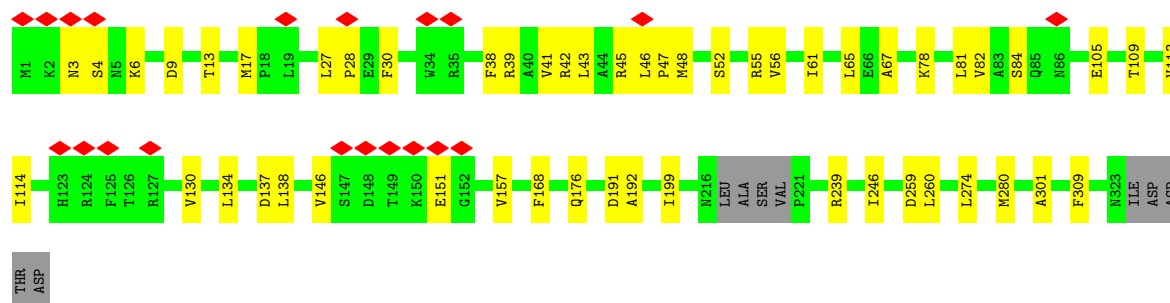
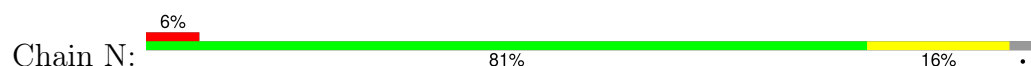




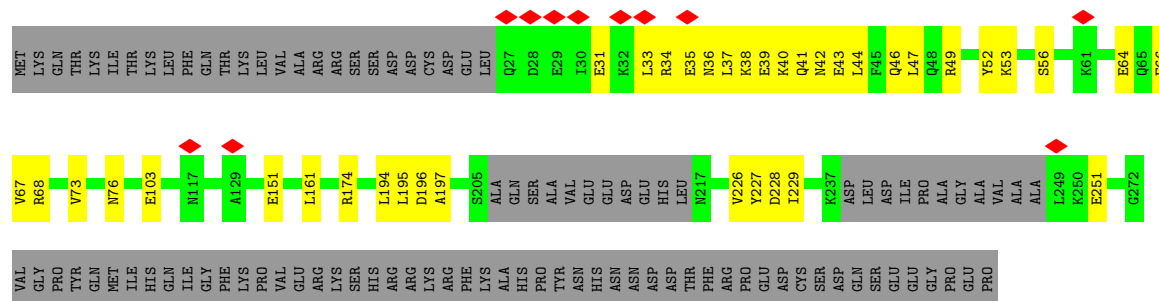
• Molecule 9: Centromere protein M



• Molecule 10: bmCENP-N



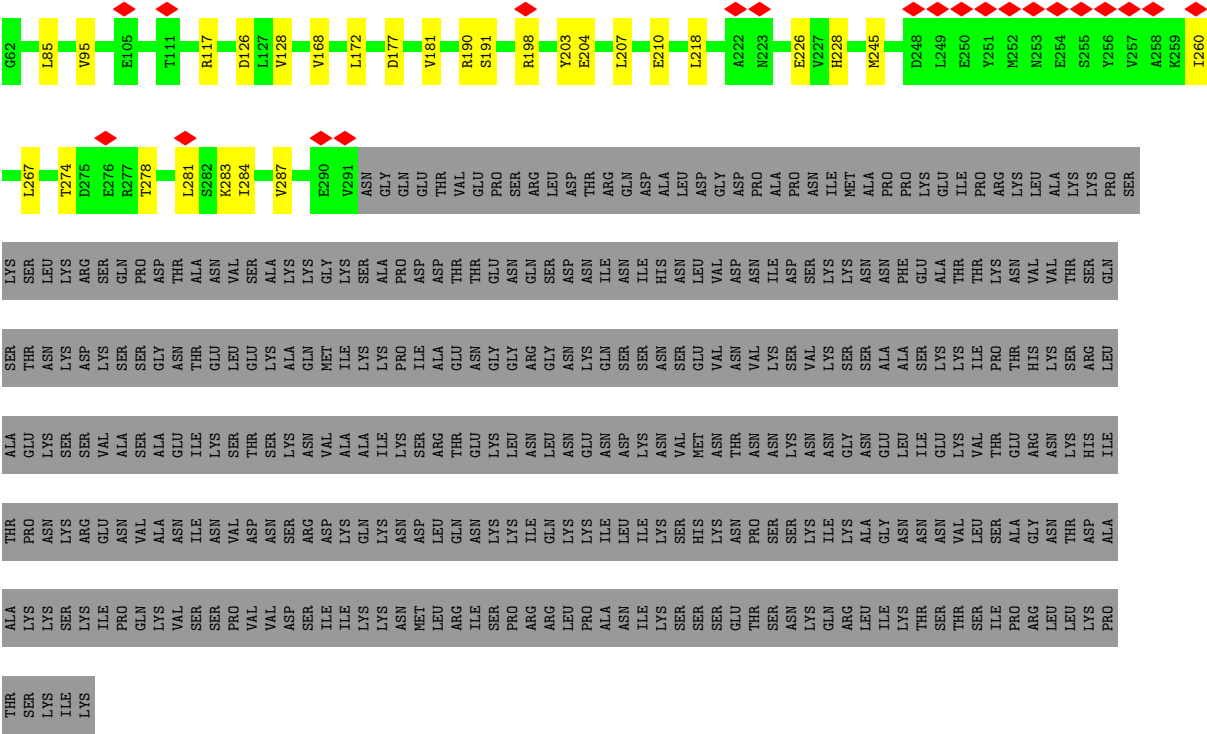
• Molecule 11: Centromere protein O



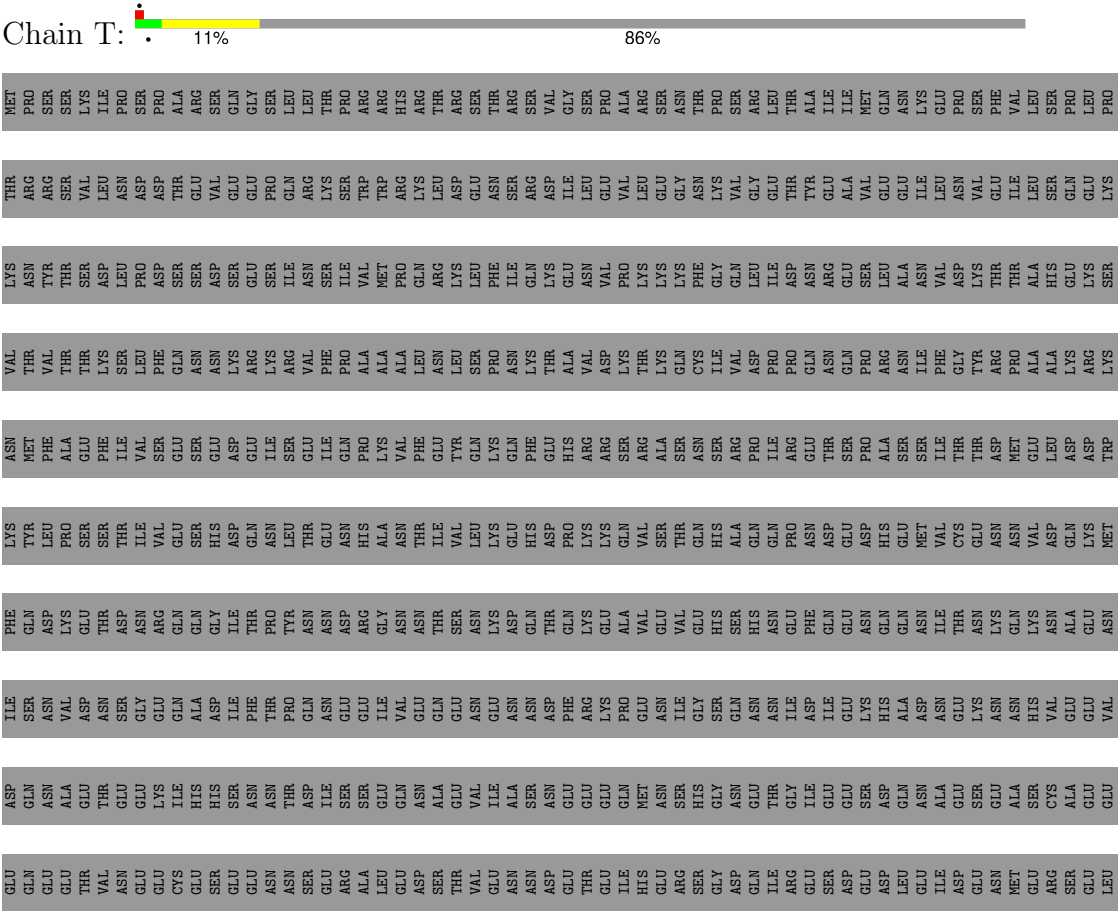
• Molecule 12: bmCENP-P







● Molecule 13: bmCENP-T



D965	T905	PHE	GLY	PRO	GLY
I966	T906	ASN	TRP	GLU	ASN
K967	K907	PHE	ASP	ALA	GLU
K968	R908	LYS	SER	ILE	SER
T969	L909	VAL	HIS	LEU	ASN
H970	Y910	PRO	ARG	HIS	ALA
F971	K911	ALA	THR	ASP	SER
D972	Y912	LYS	THR	LYS	ASN
F973	L913	PRO	ARG	ASN	ASP
Y974	E914	LEU	LYS	GLU	ASP
Q975	D915	PHE	THR	THR	GLU
F976	K916	ALA	LEU	SER	HIS
F977	L917	ARG	ARG	ASP	LEU
H978	E918	HIS	GLN	LEU	TYR
	P919	SER	THR	PHE	LEU
	K920	THR	ASN	THR	SER
	Y921	LYS	HIS	MET	ASP
	D922	PRO	GLY	MET	ASP
	Y923	VAL	ILE	GLY	ASN
	K924	GLN	PHE	ASN	ASP
A925	A925	ASN	THR	ASN	ASP
R926	R926	LYS	THR	THR	GLU
V927	V927	ASN	ARG	ASP	PRO
R928	R928	LYS	LYS	LEU	GLU
A929	A929	VAL	GLN	ARG	ASN
E930	E930	ARG	LEU	LYS	SER
K931	K931	GLU	THR	THR	ALA
L932	L932	MET	ARG	ALA	LYS
V933	V933	LYS	LEU	GLY	ALA
E934	E934	SER	ILE	LEU	ALA
T935	T935	SER	ILE	VAL	ASP
I936	I936	MET	TYR	MET	ILE
Y937	Y937	PRO	L812	GLU	ASN
H938	H938	LEU	Q813	LYS	VAL
F939	F939	ASP	K816	ILE	ASP
T940	T940	LEU	K817	LYS	ASN
K941	K941	PRO	M820	ARG	ASN
E942	E942	PRO	E821	GLN	PRO
V943	V943	GLU	K822	THR	ASN
K944	K944	LEU	N823	ALA	THR
K945	K945	LEU	M824	LEU	PRO
H946	H946	GLU	R825	VAL	ASN
E947	E947	ASP	I826	ASP	LEU
V948	V948	MET	E827	ALA	ASP
A949	A949	MET	E828	LYS	ASN
P950	P950	Y891	Q829	THR	ASN
N951	N951	K892	E829	GLU	GLU
D952	D952	P893	V830	ILE	SER
A953	A953	P894	R831	THR	ILE
V954	V954	K895	N832	LYS	THR
D955	D955	R896	A836	MET	ASP
V956	V956	Q898	LYS	GLN	ARG
L957	L957	Y897	MET	ASN	THR
K958	K958	P899	LYS	THR	VAL
H959	H959	K900	GLN	SER	GLU
E960	E960	N901	CYS	THR	LYS
M961	M961	A902	LYS	GLU	ALA
A962	A962	S903	GLN	ILE	GLU
R963	R963	W904	VAL	PRO	VAL
L964	L964			GLU	SER

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	265941	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.027	Depositor
Minimum map value	-0.822	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0514	Depositor
Map size (Å)	341.066, 346.932, 343.58	wwPDB
Map dimensions	407, 414, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.838, 0.838, 0.83799994	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	0.09	0/554	0.20	0/750
2	B	0.10	0/453	0.25	0/613
3	C	0.10	0/440	0.18	0/591
4	D	0.11	0/573	0.22	0/768
5	H	0.12	0/1872	0.24	0/2508
6	I	0.10	0/4433	0.22	0/6015
7	K	0.11	0/1662	0.22	0/2243
8	L	0.10	0/1935	0.26	0/2614
9	M	0.12	0/1302	0.24	0/1764
10	N	0.12	0/2571	0.25	0/3483
11	O	0.10	0/1858	0.23	0/2490
12	P	0.09	0/2067	0.22	0/2803
13	T	0.09	0/1271	0.22	0/1705
All	All	0.11	0/20991	0.23	0/28347

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	550	558	566	8	0
2	B	448	459	458	9	0
3	C	439	441	449	12	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	569	481	605	24	0
5	H	1851	1666	1938	48	0
6	I	4329	4397	4395	69	0
7	K	1643	1639	1646	20	0
8	L	1906	1974	1969	29	0
9	M	1286	1340	1348	15	0
10	N	2522	2583	2592	48	0
11	O	1830	1487	1866	52	0
12	P	2031	1837	2067	52	0
13	T	1243	0	1284	157	0
All	All	20647	18862	21183	452	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 11.

All (452) 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)
13:T:917:LEU:HD13	13:T:928:ARG:HB3	1.33	1.10
13:T:978:HIS:HA	13:T:986:ARG:HD3	1.43	0.98
13:T:947:GLU:HG2	13:T:948:VAL:HG23	1.42	0.97
13:T:916:LYS:HD3	13:T:966:ILE:HA	1.44	0.96
13:T:900:LYS:H	13:T:900:LYS:HD2	1.32	0.93
13:T:928:ARG:HH21	13:T:964:LEU:HD11	1.33	0.92
10:N:42:ARG:NH2	13:T:890:LYS:O	2.06	0.88
13:T:892:LYS:HD3	13:T:893:PRO:HD2	1.55	0.87
13:T:1007:GLU:HB2	13:T:1010:SER:HB3	1.60	0.83
6:I:566:ASP:O	6:I:569:SER:OG	1.95	0.83
13:T:944:LYS:HE2	13:T:985:ILE:HD11	1.63	0.81
13:T:967:VAL:HG11	13:T:973:PHE:HA	1.63	0.80
5:H:79:TYR:OH	9:M:176:PRO:O	2.00	0.79
6:I:631:ALA:O	6:I:637:TYR:OH	2.00	0.79
7:K:135:GLU:OE1	7:K:135:GLU:N	2.16	0.79
6:I:155:ARG:NH1	6:I:192:CYS:SG	2.55	0.79
5:H:9:GLU:O	5:H:13:ASN:ND2	2.18	0.78
8:L:181:SER:HG	8:L:282:CYS:HG	1.34	0.76
6:I:139:GLN:N	6:I:139:GLN:OE1	2.19	0.76
13:T:828:GLN:O	13:T:832:ASN:ND2	2.18	0.76
8:L:181:SER:OG	8:L:282:CYS:SG	2.44	0.76
6:I:75:GLU:N	6:I:75:GLU:OE1	2.19	0.75
4:D:45:SER:OG	11:O:49:ARG:NH1	2.20	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:217:PHE:O	6:I:220:THR:OG1	2.06	0.73
6:I:394:SER:OG	6:I:396:ASP:OD1	2.05	0.73
13:T:937:TYR:O	13:T:941:LYS:HG3	1.89	0.73
11:O:161:LEU:HD12	12:P:85:LEU:HD11	1.71	0.72
13:T:916:LYS:CD	13:T:966:ILE:HA	2.18	0.72
11:O:151:GLU:N	11:O:151:GLU:OE1	2.21	0.72
13:T:939:PHE:HA	13:T:942:GLU:HG2	1.71	0.72
13:T:969:THR:HG22	13:T:1007:GLU:HA	1.71	0.71
13:T:984:GLU:N	13:T:984:GLU:OE1	2.20	0.71
13:T:999:ILE:HG13	13:T:1000:PRO:HD2	1.72	0.71
7:K:187:GLN:NE2	7:K:188:ILE:O	2.23	0.71
10:N:42:ARG:NH2	13:T:891:TYR:HB2	2.04	0.71
7:K:201:ASP:OD1	13:T:983:ARG:NH1	2.24	0.71
13:T:999:ILE:CD1	13:T:1000:PRO:HD2	2.20	0.71
5:H:167:ARG:NH1	6:I:314:ALA:O	2.23	0.71
4:D:70:ASN:OD1	4:D:73:LYS:N	2.20	0.70
1:A:14:GLN:O	1:A:18:ASN:ND2	2.24	0.70
11:O:37:LEU:HB2	12:P:30:ILE:HG22	1.73	0.70
13:T:897:TYR:OH	13:T:900:LYS:NZ	2.17	0.70
5:H:209:CYS:SG	7:K:158:MET:HE2	2.31	0.70
6:I:360:LEU:O	6:I:440:ARG:NH1	2.25	0.70
5:H:13:ASN:O	5:H:17:GLU:HG2	1.92	0.70
13:T:978:HIS:CA	13:T:986:ARG:HD3	2.22	0.70
4:D:44:LEU:CD2	11:O:49:ARG:HG2	2.21	0.69
10:N:6:LYS:NZ	10:N:67:ALA:O	2.26	0.69
5:H:207:VAL:HG13	5:H:208:VAL:HG13	1.75	0.68
6:I:658:GLU:OE1	6:I:658:GLU:N	2.24	0.68
13:T:999:ILE:CG1	13:T:1000:PRO:HD2	2.24	0.68
13:T:917:LEU:HD13	13:T:928:ARG:CB	2.19	0.68
11:O:33:LEU:HB3	12:P:26:LEU:HD22	1.74	0.68
10:N:55:ARG:NH2	13:T:923:TYR:HB3	2.09	0.67
5:H:103:LYS:NZ	6:I:611:SER:OG	2.26	0.67
13:T:993:ILE:HD12	13:T:993:ILE:H	1.59	0.67
10:N:47:PRO:HA	13:T:893:PRO:HG3	1.76	0.67
13:T:981:MET:HE3	13:T:982:PRO:HD2	1.76	0.67
5:H:27:SER:HB2	11:O:56:SER:HA	1.76	0.67
13:T:958:LYS:HG2	13:T:973:PHE:CE1	2.30	0.67
10:N:13:THR:O	10:N:17:MET:N	2.28	0.66
9:M:36:GLU:OE1	9:M:59:ARG:NH1	2.29	0.66
10:N:45:ARG:NH1	13:T:926:ARG:HG2	2.10	0.66
10:N:48:MET:HE2	13:T:890:LYS:HA	1.78	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:981:MET:HE3	13:T:982:PRO:CD	2.26	0.66
13:T:990:VAL:O	13:T:995:ASN:ND2	2.29	0.66
1:A:50:ASN:O	1:A:54:ASN:ND2	2.28	0.66
6:I:336:ASP:OD1	6:I:337:ILE:N	2.28	0.66
13:T:934:GLU:OE2	13:T:938:HIS:NE2	2.28	0.66
6:I:184:LEU:O	6:I:187:SER:OG	2.12	0.65
6:I:379:GLU:OE1	9:M:160:LYS:NZ	2.17	0.65
3:C:25:MET:O	3:C:29:ASN:ND2	2.29	0.65
6:I:195:GLU:OE1	6:I:195:GLU:N	2.30	0.65
6:I:328:HIS:NE2	8:L:293:ASP:OD1	2.29	0.65
3:C:17:GLU:OE1	3:C:17:GLU:N	2.29	0.64
6:I:166:LYS:HE2	13:T:908:ARG:HG3	1.77	0.64
6:I:170:SER:OG	13:T:903:SER:HA	1.96	0.64
12:P:204:GLU:OE1	12:P:204:GLU:N	2.30	0.64
5:H:51:LYS:NZ	9:M:22:SER:O	2.22	0.64
13:T:999:ILE:HD12	13:T:1000:PRO:HD2	1.79	0.64
8:L:41:VAL:HG22	8:L:161:ILE:CD1	2.27	0.64
11:O:31:GLU:O	11:O:35:GLU:HG2	1.98	0.64
11:O:42:ASN:O	11:O:46:GLN:HG2	1.98	0.63
13:T:890:LYS:HE2	13:T:891:TYR:H	1.63	0.63
6:I:104:ASP:O	6:I:107:THR:OG1	2.14	0.63
4:D:45:SER:OG	11:O:49:ARG:HD2	1.98	0.63
13:T:959:HIS:O	13:T:963:ARG:HG3	1.99	0.63
8:L:41:VAL:HG22	8:L:161:ILE:HD12	1.79	0.62
4:D:33:THR:HG21	5:H:21:LEU:HB3	1.79	0.62
4:D:44:LEU:HD23	11:O:49:ARG:HG2	1.79	0.62
5:H:197:GLU:OE1	7:K:219:TYR:OH	2.17	0.62
11:O:47:LEU:HD12	12:P:37:ILE:HG23	1.81	0.62
13:T:917:LEU:HB2	13:T:925:ALA:HB1	1.81	0.62
13:T:921:TYR:CE2	13:T:928:ARG:HG2	2.35	0.62
2:B:30:SER:HB2	11:O:73:VAL:HG13	1.81	0.62
8:L:84:LEU:HD13	8:L:87:LEU:HD22	1.82	0.62
10:N:30:PHE:CE1	10:N:65:LEU:HD11	2.34	0.62
12:P:27:LEU:O	12:P:30:ILE:HG12	1.99	0.61
13:T:928:ARG:HE	13:T:964:LEU:HD21	1.64	0.61
8:L:279:ILE:O	8:L:283:VAL:HG23	2.00	0.61
7:K:168:GLU:OE1	7:K:172:GLN:NE2	2.33	0.61
11:O:47:LEU:CD1	12:P:37:ILE:HG23	2.31	0.61
12:P:39:GLU:O	12:P:43:LYS:HG3	2.00	0.61
8:L:48:GLN:NE2	8:L:57:TYR:OH	2.34	0.60
12:P:210:GLU:OE1	12:P:210:GLU:N	2.34	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:8:LYS:O	5:H:12:GLN:HG3	2.02	0.60
10:N:41:VAL:HG13	10:N:46:LEU:HD12	1.84	0.60
10:N:45:ARG:NH2	13:T:927:VAL:HA	2.17	0.60
11:O:103:GLU:N	11:O:103:GLU:OE1	2.35	0.60
2:B:26:TYR:CZ	11:O:73:VAL:HG11	2.36	0.60
11:O:64:GLU:N	11:O:64:GLU:OE1	2.27	0.60
13:T:977:PHE:CD1	13:T:981:MET:HG3	2.36	0.60
9:M:36:GLU:OE2	10:N:239:ARG:NH1	2.36	0.59
12:P:20:LEU:HD12	12:P:21:LEU:N	2.18	0.59
5:H:141:PHE:CZ	13:T:830:VAL:HG23	2.38	0.59
13:T:982:PRO:HB2	13:T:984:GLU:OE2	2.03	0.59
8:L:253:VAL:HG21	10:N:301:ALA:HB2	1.85	0.59
13:T:952:ASP:O	13:T:956:VAL:HG23	2.02	0.59
3:C:31:SER:HA	5:H:15:GLU:HG2	1.85	0.59
6:I:639:ALA:HB1	13:T:816:LYS:HE2	1.84	0.59
12:P:245:MET:SD	12:P:267:LEU:HD21	2.42	0.59
4:D:44:LEU:HD11	11:O:53:LYS:HB2	1.85	0.58
5:H:14:PHE:CZ	5:H:18:LEU:HD11	2.38	0.58
13:T:947:GLU:OE1	13:T:947:GLU:N	2.30	0.58
5:H:12:GLN:O	5:H:16:GLN:HG2	2.03	0.58
5:H:35:GLU:OE1	5:H:35:GLU:N	2.31	0.58
10:N:42:ARG:HH22	13:T:891:TYR:HB2	1.66	0.58
11:O:67:VAL:HG22	11:O:68:ARG:H	1.67	0.58
13:T:933:VAL:HA	13:T:936:ILE:HG12	1.86	0.58
6:I:405:VAL:HG22	6:I:430:MET:HE1	1.84	0.58
9:M:33:GLU:OE1	9:M:33:GLU:N	2.33	0.58
10:N:61:ILE:HD12	10:N:65:LEU:HD12	1.85	0.58
13:T:984:GLU:OE2	13:T:985:ILE:HG12	2.04	0.58
13:T:1003:GLY:O	13:T:1006:SER:OG	2.11	0.58
9:M:110:ARG:NE	9:M:180:VAL:O	2.37	0.58
2:B:34:SER:OG	11:O:76:ASN:ND2	2.37	0.57
13:T:954:VAL:O	13:T:958:LYS:HG3	2.04	0.57
6:I:191:GLU:OE1	6:I:191:GLU:N	2.32	0.57
7:K:147:LEU:HD23	7:K:148:LYS:N	2.18	0.57
4:D:78:LEU:HB2	6:I:418:LEU:CD1	2.35	0.57
5:H:7:LEU:O	5:H:10:VAL:HG12	2.05	0.57
6:I:443:GLN:N	6:I:443:GLN:OE1	2.38	0.57
12:P:218:LEU:HD13	12:P:228:HIS:CE1	2.39	0.57
13:T:968:LYS:O	13:T:1008:ILE:HG13	2.05	0.57
13:T:982:PRO:HB2	13:T:984:GLU:CD	2.29	0.57
13:T:901:ASN:OD1	13:T:937:TYR:OH	2.19	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:892:LYS:CD	13:T:893:PRO:HD2	2.31	0.56
3:C:53:CYS:O	3:C:57:ASN:ND2	2.38	0.56
13:T:982:PRO:HB2	13:T:984:GLU:OE1	2.05	0.56
6:I:521:VAL:HG22	6:I:521:VAL:O	2.05	0.56
11:O:36:ASN:O	11:O:39:GLU:HG3	2.06	0.56
11:O:43:GLU:O	11:O:47:LEU:HG	2.06	0.56
5:H:30:ILE:HD13	11:O:52:TYR:HD1	1.70	0.56
8:L:246:LEU:HD13	10:N:280:MET:HE3	1.88	0.56
12:P:28:ASP:O	12:P:31:VAL:HG22	2.06	0.55
13:T:827:GLU:O	13:T:830:VAL:HG12	2.05	0.55
13:T:967:VAL:HG23	13:T:1008:ILE:CD1	2.37	0.55
11:O:33:LEU:HD13	12:P:27:LEU:HD21	1.89	0.55
13:T:952:ASP:OD1	13:T:953:ALA:N	2.38	0.55
4:D:44:LEU:HD21	11:O:49:ARG:O	2.07	0.55
10:N:30:PHE:HE1	10:N:65:LEU:HD11	1.72	0.55
1:A:27:LEU:HD13	2:B:34:SER:HB2	1.89	0.55
5:H:212:GLU:N	5:H:212:GLU:OE1	2.35	0.55
13:T:935:THR:O	13:T:938:HIS:HB2	2.07	0.54
6:I:651:PHE:O	6:I:655:THR:HG22	2.07	0.54
9:M:83:ILE:HB	9:M:114:LEU:HD23	1.89	0.54
13:T:933:VAL:HA	13:T:936:ILE:CD1	2.38	0.54
13:T:937:TYR:CE2	13:T:941:LYS:HD2	2.42	0.54
12:P:35:THR:O	12:P:39:GLU:HG3	2.08	0.54
13:T:902:ALA:HB1	13:T:904:TRP:CE2	2.43	0.54
12:P:203:TYR:HB2	12:P:207:LEU:HD22	1.90	0.54
6:I:134:GLU:OE1	6:I:134:GLU:N	2.38	0.53
12:P:27:LEU:O	12:P:31:VAL:HG13	2.09	0.53
12:P:31:VAL:O	12:P:35:THR:HG23	2.08	0.53
13:T:939:PHE:HA	13:T:942:GLU:CG	2.38	0.53
10:N:176:GLN:OE1	10:N:176:GLN:N	2.38	0.53
13:T:960:GLU:O	13:T:964:LEU:HD13	2.08	0.53
13:T:954:VAL:HG22	13:T:958:LYS:NZ	2.22	0.53
13:T:970:HIS:HD2	13:T:1008:ILE:HG12	1.73	0.53
10:N:138:LEU:HD13	10:N:199:ILE:HD13	1.90	0.53
5:H:11:SER:O	5:H:15:GLU:HG3	2.09	0.53
12:P:260:ILE:HG23	12:P:284:ILE:HD11	1.89	0.53
5:H:26:PHE:O	11:O:56:SER:OG	2.25	0.53
10:N:48:MET:CE	13:T:890:LYS:HA	2.38	0.53
6:I:110:MET:CG	6:I:146:THR:HG21	2.39	0.53
8:L:178:PHE:O	8:L:182:ASP:N	2.41	0.53
10:N:3:ASN:OD1	10:N:4:SER:N	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:26:LEU:O	12:P:30:ILE:HG23	2.09	0.52
10:N:81:LEU:HD12	10:N:84:SER:HB2	1.91	0.52
13:T:939:PHE:CD1	13:T:953:ALA:HB1	2.44	0.52
13:T:944:LYS:CE	13:T:985:ILE:HD11	2.37	0.52
6:I:627:ASP:OD1	6:I:628:GLU:N	2.42	0.52
8:L:145:VAL:O	8:L:149:VAL:HG23	2.09	0.52
13:T:957:LEU:O	13:T:957:LEU:HD23	2.10	0.52
6:I:72:ASP:OD1	6:I:73:ALA:N	2.41	0.52
9:M:167:VAL:HG22	9:M:172:ARG:HH22	1.74	0.52
6:I:169:GLU:H	13:T:906:THR:HG22	1.75	0.52
12:P:283:LYS:O	12:P:287:VAL:HG23	2.10	0.52
13:T:921:TYR:HB3	13:T:924:LYS:HB2	1.92	0.52
4:D:44:LEU:HD23	4:D:44:LEU:C	2.35	0.51
13:T:892:LYS:HD3	13:T:893:PRO:CD	2.34	0.51
13:T:942:GLU:HA	13:T:945:LYS:NZ	2.24	0.51
6:I:64:LEU:C	6:I:64:LEU:HD23	2.36	0.51
6:I:485:PHE:CB	7:K:93:LEU:HD21	2.41	0.51
7:K:106:GLU:OE2	7:K:110:ARG:NH2	2.44	0.51
6:I:505:LEU:HD23	6:I:506:GLY:O	2.09	0.51
13:T:991:PRO:HB3	13:T:997:ILE:HB	1.93	0.51
13:T:1001:ARG:NH2	13:T:1002:ASN:HB2	2.26	0.51
6:I:174:LEU:O	6:I:178:LEU:HD23	2.11	0.51
11:O:47:LEU:HB2	12:P:40:LEU:HD23	1.91	0.51
13:T:992:ASP:OD1	13:T:995:ASN:ND2	2.44	0.51
6:I:86:ILE:O	6:I:90:TYR:N	2.44	0.51
4:D:68:ALA:HB3	4:D:74:VAL:CG2	2.41	0.51
6:I:485:PHE:HB3	7:K:93:LEU:HD21	1.93	0.51
6:I:385:GLU:N	6:I:385:GLU:OE1	2.41	0.51
6:I:643:HIS:NE2	13:T:816:LYS:HD3	2.26	0.50
13:T:977:PHE:O	13:T:981:MET:HB2	2.10	0.50
6:I:488:ILE:HD12	6:I:529:MET:HE1	1.92	0.50
8:L:143:GLN:O	8:L:147:THR:HG23	2.11	0.50
13:T:928:ARG:NE	13:T:964:LEU:HD21	2.26	0.50
4:D:28:LYS:O	4:D:32:VAL:HG23	2.11	0.50
12:P:128:VAL:O	12:P:128:VAL:HG13	2.11	0.50
7:K:142:GLU:O	7:K:145:SER:OG	2.24	0.50
12:P:23:LYS:O	12:P:27:LEU:HG	2.10	0.50
11:O:67:VAL:HG22	11:O:68:ARG:N	2.27	0.50
6:I:93:GLN:HE22	13:T:984:GLU:HB2	1.77	0.50
6:I:363:ILE:HG22	6:I:365:VAL:HG22	1.92	0.50
13:T:905:THR:HG23	13:T:910:TYR:CZ	2.47	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:991:PRO:HA	13:T:997:ILE:HB	1.93	0.50
5:H:140:HIS:CE1	13:T:827:GLU:HB2	2.46	0.50
6:I:517:PRO:HG2	6:I:529:MET:HE3	1.94	0.50
8:L:136:TYR:OH	8:L:288:ASN:OD1	2.22	0.50
9:M:103:VAL:HG11	9:M:112:VAL:HG21	1.93	0.50
13:T:813:GLN:OE1	13:T:817:LYS:HE2	2.11	0.50
6:I:144:VAL:O	6:I:148:THR:OG1	2.27	0.50
11:O:36:ASN:O	11:O:40:LYS:HG3	2.12	0.50
5:H:26:PHE:CZ	11:O:53:LYS:HE3	2.47	0.49
6:I:166:LYS:O	13:T:906:THR:HG21	2.12	0.49
6:I:435:VAL:O	6:I:438:SER:OG	2.28	0.49
13:T:890:LYS:HD3	13:T:891:TYR:CD1	2.47	0.49
6:I:180:ILE:HG23	6:I:202:VAL:HG12	1.94	0.49
1:A:18:ASN:O	1:A:22:THR:HG23	2.12	0.49
5:H:141:PHE:CE2	13:T:830:VAL:HG23	2.47	0.49
8:L:195:ARG:NH2	8:L:258:GLU:OE2	2.45	0.49
13:T:909:LEU:O	13:T:913:LEU:HG	2.13	0.49
13:T:969:THR:HG22	13:T:1007:GLU:CA	2.42	0.49
13:T:999:ILE:HG13	13:T:1000:PRO:CD	2.41	0.49
13:T:993:ILE:HD12	13:T:993:ILE:N	2.26	0.49
10:N:157:VAL:HG22	10:N:168:PHE:CD1	2.47	0.49
13:T:827:GLU:OE2	13:T:831:ARG:NH2	2.45	0.49
10:N:46:LEU:O	13:T:893:PRO:HB3	2.13	0.49
5:H:17:GLU:O	5:H:21:LEU:HG	2.13	0.49
11:O:37:LEU:HB2	12:P:30:ILE:CG2	2.43	0.49
5:H:199:ILE:HB	7:K:147:LEU:HD21	1.93	0.49
1:A:27:LEU:HD11	2:B:31:ILE:HG23	1.94	0.48
6:I:93:GLN:NE2	13:T:984:GLU:HB2	2.28	0.48
7:K:28:CYS:SG	9:M:18:SER:OG	2.67	0.48
2:B:26:TYR:CE2	11:O:73:VAL:HG11	2.47	0.48
10:N:78:LYS:O	10:N:82:VAL:HG23	2.14	0.48
6:I:52:LEU:HD12	6:I:81:TYR:CE2	2.48	0.48
6:I:102:LEU:HD23	6:I:102:LEU:C	2.38	0.48
10:N:45:ARG:HD2	13:T:926:ARG:HD3	1.95	0.48
13:T:938:HIS:O	13:T:942:GLU:HG2	2.12	0.48
13:T:1001:ARG:O	13:T:1001:ARG:HD2	2.14	0.48
13:T:929:ALA:O	13:T:933:VAL:HG23	2.13	0.48
5:H:228:ARG:NE	6:I:121:ASP:OD1	2.41	0.48
12:P:198:ARG:HD2	12:P:278:THR:HG21	1.96	0.48
3:C:63:ILE:HD11	4:D:53:SER:OG	2.14	0.48
5:H:217:PRO:HD3	6:I:88:ILE:HD11	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:41:VAL:O	10:N:45:ARG:N	2.47	0.47
5:H:26:PHE:CE1	11:O:53:LYS:HE3	2.48	0.47
11:O:40:LYS:O	12:P:37:ILE:HD11	2.15	0.47
2:B:31:ILE:HG22	2:B:35:MET:HE2	1.96	0.47
6:I:379:GLU:OE2	6:I:414:ARG:NH2	2.45	0.47
11:O:44:LEU:O	11:O:44:LEU:HD23	2.14	0.47
12:P:274:THR:O	12:P:278:THR:HG23	2.15	0.47
6:I:200:ILE:HG22	6:I:201:CYS:N	2.30	0.47
10:N:134:LEU:N	10:N:134:LEU:HD12	2.29	0.47
4:D:68:ALA:HB3	4:D:74:VAL:HG22	1.97	0.47
3:C:31:SER:N	5:H:15:GLU:OE2	2.48	0.47
13:T:928:ARG:NH2	13:T:964:LEU:HD11	2.16	0.47
13:T:939:PHE:CA	13:T:942:GLU:HG2	2.42	0.47
13:T:949:ALA:HB2	13:T:989:VAL:HG22	1.96	0.47
6:I:623:LEU:O	6:I:626:VAL:HG23	2.14	0.47
8:L:291:CYS:SG	8:L:292:CYS:N	2.85	0.47
11:O:174:ARG:NE	11:O:197:ALA:O	2.47	0.46
12:P:168:VAL:HG22	12:P:168:VAL:O	2.16	0.46
12:P:26:LEU:O	12:P:26:LEU:HD23	2.15	0.46
13:T:981:MET:HE3	13:T:982:PRO:HD3	1.95	0.46
13:T:932:LEU:HD11	13:T:961:MET:SD	2.55	0.46
13:T:954:VAL:C	13:T:958:LYS:HZ3	2.23	0.46
6:I:96:PHE:CD2	6:I:136:LEU:HD11	2.51	0.46
8:L:199:THR:O	8:L:200:GLU:HB2	2.16	0.46
13:T:917:LEU:HD21	13:T:966:ILE:HD11	1.97	0.46
3:C:63:ILE:HG13	4:D:57:LEU:HD11	1.98	0.46
10:N:41:VAL:HG22	10:N:46:LEU:HA	1.97	0.46
3:C:56:LEU:HB2	4:D:50:ILE:HD11	1.98	0.46
5:H:14:PHE:CE2	5:H:18:LEU:HD11	2.50	0.46
12:P:38:ALA:O	12:P:42:THR:HG23	2.16	0.46
13:T:825:ARG:O	13:T:829:GLU:HG3	2.16	0.46
13:T:895:LYS:HG2	13:T:896:ARG:N	2.30	0.46
5:H:21:LEU:O	5:H:24:VAL:HG22	2.16	0.46
11:O:36:ASN:HA	11:O:39:GLU:CG	2.46	0.46
13:T:900:LYS:HD2	13:T:900:LYS:N	2.15	0.46
12:P:207:LEU:HD23	12:P:207:LEU:H	1.81	0.45
11:O:36:ASN:HA	11:O:39:GLU:HG3	1.98	0.45
5:H:20:GLN:OE1	5:H:20:GLN:HA	2.17	0.45
5:H:209:CYS:HB2	7:K:202:THR:HG22	1.99	0.45
13:T:915:ASP:OD1	13:T:916:LYS:N	2.50	0.45
13:T:942:GLU:HA	13:T:945:LYS:HZ3	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:LYS:O	4:D:77:ILE:HG13	2.16	0.45
12:P:260:ILE:HG23	12:P:284:ILE:CD1	2.47	0.45
13:T:933:VAL:HA	13:T:936:ILE:CG1	2.45	0.45
13:T:936:ILE:HG13	13:T:937:TYR:N	2.31	0.45
1:A:47:PHE:O	1:A:51:ILE:HG13	2.17	0.45
8:L:98:LEU:C	8:L:98:LEU:HD23	2.41	0.45
10:N:146:VAL:HG13	10:N:151:GLU:HG2	1.98	0.45
13:T:954:VAL:HG22	13:T:958:LYS:HZ2	1.80	0.45
4:D:72:GLN:O	4:D:76:GLU:HG3	2.17	0.45
10:N:246:ILE:HD12	10:N:309:PHE:CZ	2.51	0.45
9:M:107:LEU:O	9:M:112:VAL:HG23	2.16	0.45
12:P:218:LEU:HD11	12:P:226:GLU:HG3	1.99	0.45
10:N:109:THR:O	10:N:113:VAL:HG23	2.16	0.45
11:O:64:GLU:H	11:O:64:GLU:CD	2.20	0.45
13:T:991:PRO:HA	13:T:995:ASN:OD1	2.17	0.45
10:N:9:ASP:O	10:N:13:THR:OG1	2.29	0.45
8:L:44:LEU:HD11	8:L:119:LEU:HD21	1.99	0.44
13:T:972:ASP:O	13:T:975:GLN:HG3	2.16	0.44
3:C:63:ILE:O	3:C:67:VAL:HG23	2.17	0.44
8:L:240:GLN:HG2	8:L:251:VAL:HG22	1.99	0.44
10:N:114:ILE:HG23	10:N:130:VAL:HG11	1.98	0.44
11:O:228:ASP:OD1	11:O:229:ILE:N	2.50	0.44
13:T:993:ILE:HG22	13:T:993:ILE:O	2.17	0.44
13:T:984:GLU:O	13:T:987:VAL:HG12	2.17	0.44
7:K:146:GLN:O	7:K:149:SER:OG	2.23	0.44
10:N:45:ARG:HH22	13:T:930:GLU:HB2	1.81	0.44
11:O:194:LEU:HD23	11:O:195:LEU:O	2.18	0.44
11:O:39:GLU:OE2	11:O:40:LYS:HG3	2.18	0.44
13:T:951:ASN:O	13:T:954:VAL:HG12	2.18	0.44
8:L:246:LEU:HD13	10:N:280:MET:CE	2.47	0.44
10:N:39:ARG:O	10:N:43:LEU:HD13	2.17	0.44
10:N:45:ARG:HH11	13:T:926:ARG:HG2	1.81	0.44
10:N:259:ASP:OD1	10:N:260:LEU:N	2.50	0.44
13:T:1007:GLU:O	13:T:1010:SER:OG	2.22	0.44
5:H:199:ILE:CB	7:K:147:LEU:HD21	2.47	0.44
8:L:41:VAL:HG21	8:L:119:LEU:CD1	2.48	0.44
13:T:933:VAL:HA	13:T:936:ILE:HD11	1.98	0.44
13:T:935:THR:HG21	13:T:960:GLU:OE2	2.18	0.44
6:I:55:SER:O	6:I:56:ILE:HG23	2.18	0.44
6:I:92:ASN:O	6:I:95:SER:OG	2.31	0.44
10:N:27:LEU:HB2	10:N:28:PRO:HD3	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:46:LEU:O	10:N:46:LEU:HD23	2.17	0.44
8:L:199:THR:O	8:L:200:GLU:CB	2.66	0.44
11:O:33:LEU:HB3	12:P:26:LEU:CD2	2.47	0.44
13:T:912:TYR:HA	13:T:915:ASP:OD2	2.18	0.44
12:P:177:ASP:O	12:P:181:VAL:HG23	2.17	0.43
13:T:921:TYR:O	13:T:924:LYS:HB2	2.18	0.43
12:P:191:SER:OG	12:P:274:THR:HG22	2.19	0.43
13:T:941:LYS:O	13:T:945:LYS:NZ	2.50	0.43
5:H:189:LEU:HD23	7:K:137:VAL:HG22	2.00	0.43
8:L:46:ASN:O	8:L:46:ASN:ND2	2.52	0.43
13:T:918:GLU:N	13:T:919:PRO:HD2	2.34	0.43
4:D:21:CYS:O	4:D:25:ILE:HG13	2.19	0.43
5:H:189:LEU:O	5:H:189:LEU:HD13	2.17	0.43
10:N:52:SER:O	10:N:56:VAL:HG23	2.19	0.43
12:P:40:LEU:HD12	12:P:43:LYS:HD2	2.00	0.43
13:T:812:LEU:C	13:T:812:LEU:HD23	2.43	0.43
11:O:251:GLU:OE1	11:O:251:GLU:N	2.51	0.43
5:H:166:LEU:HA	7:K:122:MET:HE1	2.01	0.43
5:H:202:LEU:C	5:H:202:LEU:HD23	2.44	0.43
10:N:157:VAL:HG22	10:N:168:PHE:HD1	1.84	0.43
11:O:37:LEU:O	11:O:41:GLN:HG3	2.19	0.43
8:L:188:ASP:HB2	8:L:211:ILE:HD12	2.01	0.43
12:P:281:LEU:HA	12:P:284:ILE:HG22	2.00	0.43
6:I:186:LYS:NZ	6:I:197:VAL:O	2.51	0.43
9:M:169:ILE:O	9:M:169:ILE:HG22	2.18	0.43
1:A:61:LEU:HD23	1:A:61:LEU:O	2.19	0.43
6:I:51:TRP:CD1	6:I:64:LEU:HD22	2.54	0.43
13:T:820:MET:O	13:T:824:MET:HG2	2.19	0.43
13:T:822:LYS:O	13:T:826:ILE:HG13	2.18	0.43
13:T:969:THR:HB	13:T:1006:SER:O	2.18	0.43
13:T:991:PRO:HB3	13:T:997:ILE:CG2	2.48	0.43
5:H:7:LEU:HA	5:H:10:VAL:HG12	2.00	0.43
5:H:212:GLU:O	5:H:215:ASN:ND2	2.52	0.43
11:O:196:ASP:O	11:O:197:ALA:C	2.62	0.43
13:T:813:GLN:O	13:T:817:LYS:HG2	2.18	0.43
6:I:117:MET:HE3	6:I:147:LEU:HD23	2.01	0.42
13:T:928:ARG:HE	13:T:964:LEU:CD2	2.30	0.42
3:C:52:ASN:ND2	4:D:43:ASN:OD1	2.52	0.42
13:T:914:GLU:OE1	13:T:914:GLU:HA	2.19	0.42
5:H:188:ARG:O	5:H:191:THR:OG1	2.28	0.42
12:P:20:LEU:HD12	12:P:20:LEU:C	2.44	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:28:ASP:HA	12:P:31:VAL:HG22	2.02	0.42
13:T:947:GLU:O	13:T:988:LYS:HE2	2.19	0.42
12:P:26:LEU:HD23	12:P:26:LEU:C	2.44	0.42
13:T:899:PRO:HB2	13:T:902:ALA:CB	2.49	0.42
7:K:188:ILE:O	7:K:188:ILE:HG23	2.19	0.42
9:M:144:LEU:HD12	9:M:144:LEU:N	2.35	0.42
13:T:947:GLU:O	13:T:988:LYS:HG3	2.19	0.42
5:H:232:ASP:O	5:H:235:THR:HG22	2.20	0.42
8:L:182:ASP:OD1	8:L:183:THR:N	2.52	0.42
13:T:930:GLU:HA	13:T:930:GLU:OE1	2.19	0.42
13:T:969:THR:HG21	13:T:1005:PHE:O	2.20	0.42
1:A:62:ALA:O	1:A:66:GLN:N	2.53	0.42
12:P:172:LEU:HD11	12:P:181:VAL:HG21	2.01	0.42
13:T:921:TYR:HE2	13:T:928:ARG:HG2	1.82	0.42
13:T:977:PHE:HD1	13:T:977:PHE:HA	1.69	0.42
8:L:62:LEU:O	8:L:66:VAL:HG23	2.20	0.41
10:N:38:PHE:CE1	10:N:46:LEU:HD11	2.55	0.41
11:O:64:GLU:HG2	11:O:66:PHE:CE1	2.55	0.41
13:T:948:VAL:HA	13:T:988:LYS:HG3	2.02	0.41
13:T:957:LEU:HD23	13:T:957:LEU:C	2.45	0.41
6:I:141:VAL:HG21	6:I:177:GLN:HB3	2.01	0.41
6:I:143:LEU:C	6:I:143:LEU:HD23	2.45	0.41
6:I:543:LEU:O	6:I:547:ASN:N	2.53	0.41
8:L:221:ILE:O	8:L:231:LEU:HD22	2.20	0.41
12:P:126:ASP:OD1	12:P:190:ARG:NH2	2.53	0.41
13:T:961:MET:CE	13:T:966:ILE:HG21	2.50	0.41
3:C:28:MET:HG3	4:D:22:LEU:HD11	2.02	0.41
11:O:226:VAL:HG13	11:O:227:TYR:N	2.36	0.41
11:O:37:LEU:CB	12:P:30:ILE:HG22	2.45	0.41
12:P:33:CYS:O	12:P:37:ILE:HG13	2.20	0.41
13:T:978:HIS:CB	13:T:986:ARG:HD3	2.50	0.41
5:H:209:CYS:SG	5:H:210:ARG:N	2.93	0.41
6:I:454:ASN:O	6:I:458:VAL:HG23	2.21	0.41
10:N:41:VAL:CG1	10:N:46:LEU:HD12	2.49	0.41
12:P:95:VAL:HG11	12:P:117:ARG:HH21	1.85	0.41
11:O:33:LEU:HD13	12:P:27:LEU:CD2	2.50	0.41
3:C:63:ILE:HG12	4:D:57:LEU:HG	2.02	0.41
4:D:68:ALA:HB1	4:D:73:LYS:HB3	2.03	0.41
5:H:89:GLU:O	5:H:90:LYS:C	2.64	0.41
6:I:169:GLU:HB2	13:T:906:THR:HB	2.03	0.41
12:P:26:LEU:HD23	12:P:30:ILE:HG23	2.03	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:32:TYR:CE1	12:P:36:ARG:HD3	2.56	0.41
2:B:35:MET:HE1	4:D:18:ALA:HA	2.01	0.41
10:N:191:ASP:OD1	10:N:192:ALA:N	2.53	0.41
11:O:34:ARG:O	11:O:38:LYS:HG2	2.21	0.41
11:O:47:LEU:CB	12:P:40:LEU:HD23	2.51	0.41
2:B:59:LEU:O	2:B:60:GLU:C	2.63	0.40
12:P:203:TYR:CB	12:P:207:LEU:HD22	2.51	0.40
5:H:9:GLU:OE1	5:H:9:GLU:HA	2.21	0.40
13:T:899:PRO:HB2	13:T:902:ALA:HB2	2.03	0.40
6:I:209:ILE:HG22	6:I:210:ASN:N	2.36	0.40
8:L:41:VAL:HG12	8:L:42:SER:O	2.21	0.40
13:T:1000:PRO:HG2	13:T:1003:GLY:C	2.46	0.40
7:K:193:TYR:CZ	13:T:1004:VAL:HG11	2.57	0.40
9:M:113:VAL:CG2	9:M:144:LEU:HD13	2.51	0.40
10:N:105:GLU:O	10:N:109:THR:HG22	2.22	0.40
5:H:140:HIS:HB3	13:T:830:VAL:HG11	2.03	0.40
6:I:141:VAL:HG13	6:I:142:LYS:N	2.35	0.40
6:I:164:CYS:O	6:I:168:ARG:NE	2.53	0.40
10:N:138:LEU:CD1	10:N:199:ILE:HD13	2.52	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	68/108 (63%)	67 (98%)	1 (2%)	0	100	100
2	B	55/82 (67%)	55 (100%)	0	0	100	100
3	C	53/71 (75%)	53 (100%)	0	0	100	100
4	D	69/81 (85%)	68 (99%)	1 (1%)	0	100	100
5	H	224/239 (94%)	220 (98%)	4 (2%)	0	100	100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	I	530/661 (80%)	520 (98%)	10 (2%)	0	100	100
7	K	204/219 (93%)	203 (100%)	1 (0%)	0	100	100
8	L	229/302 (76%)	220 (96%)	7 (3%)	2 (1%)	14	48
9	M	161/180 (89%)	160 (99%)	1 (1%)	0	100	100
10	N	315/328 (96%)	302 (96%)	13 (4%)	0	100	100
11	O	218/325 (67%)	209 (96%)	9 (4%)	0	100	100
12	P	251/638 (39%)	247 (98%)	4 (2%)	0	100	100
13	T	142/1016 (14%)	137 (96%)	5 (4%)	0	100	100
All	All	2519/4250 (59%)	2461 (98%)	56 (2%)	2 (0%)	49	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L	200	GLU
8	L	201	VAL

### 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	62/97 (64%)	60 (97%)	2 (3%)	34	67
2	B	53/75 (71%)	53 (100%)	0	100	100
3	C	51/66 (77%)	51 (100%)	0	100	100
4	D	66/76 (87%)	63 (96%)	3 (4%)	24	59
5	H	206/217 (95%)	206 (100%)	0	100	100
6	I	473/584 (81%)	471 (100%)	2 (0%)	84	90
7	K	188/198 (95%)	182 (97%)	6 (3%)	34	67
8	L	218/277 (79%)	215 (99%)	3 (1%)	59	80
9	M	147/161 (91%)	147 (100%)	0	100	100
10	N	282/290 (97%)	280 (99%)	2 (1%)	76	86

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	O	206/295 (70%)	206 (100%)	0	100	100
12	P	231/579 (40%)	231 (100%)	0	100	100
13	T	138/942 (15%)	135 (98%)	3 (2%)	45	74
All	All	2321/3857 (60%)	2300 (99%)	21 (1%)	68	85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	60	LYS
4	D	41	GLU
4	D	46	ILE
4	D	66	HIS
6	I	147	LEU
6	I	640	PHE
7	K	135	GLU
7	K	138	LYS
7	K	147	LEU
7	K	158	MET
7	K	192	ASN
7	K	212	LYS
8	L	31	TYR
8	L	144	ARG
8	L	246	LEU
10	N	137	ASP
10	N	274	LEU
13	T	890	LYS
13	T	923	TYR
13	T	977	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	20	GLN
3	C	52	ASN
3	C	57	ASN
4	D	43	ASN
5	H	69	GLN
5	H	215	ASN
6	I	93	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	I	589	HIS
7	K	172	GLN
8	L	39	ASN
8	L	237	GLN
10	N	5	ASN
10	N	60	HIS
10	N	123	HIS
11	O	76	ASN
11	O	113	HIS
11	O	176	GLN
11	O	217	ASN
11	O	252	GLN
12	P	228	HIS
12	P	243	HIS
13	T	813	GLN
13	T	828	GLN
13	T	970	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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 ⓘ

There are no chain breaks in this entry.

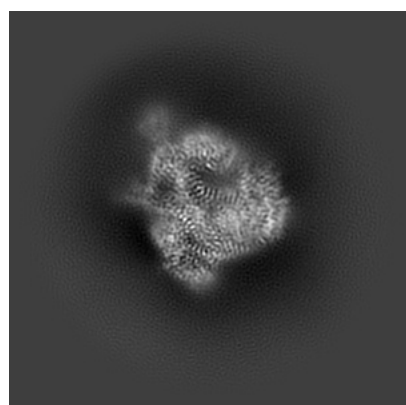
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70568. These allow visual inspection of the internal detail of the map and identification of artifacts.

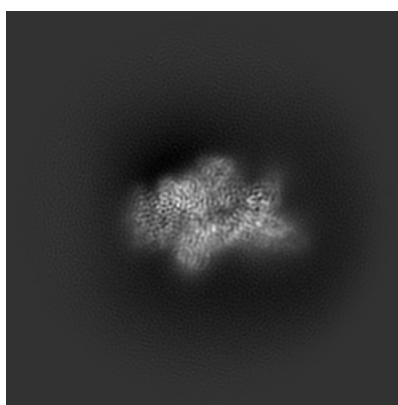
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

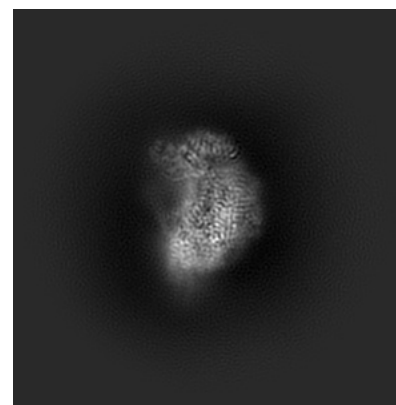
#### 6.1.1 Primary map



X



Y

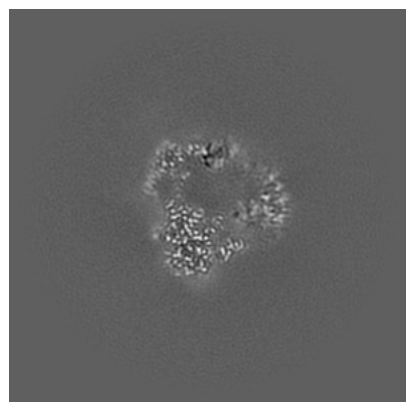


Z

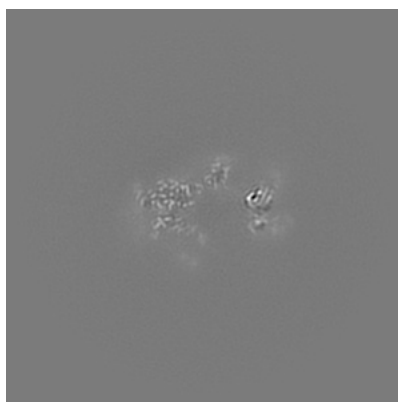
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

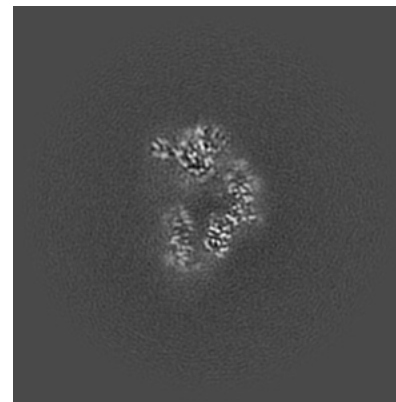
#### 6.2.1 Primary map



X Index: 203



Y Index: 207

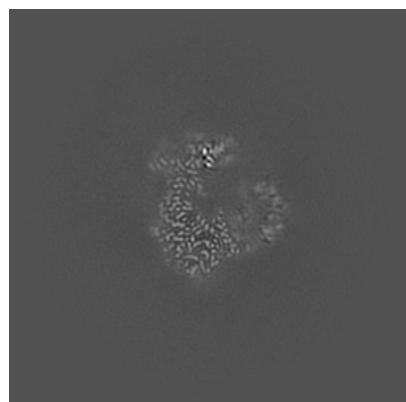


Z Index: 205

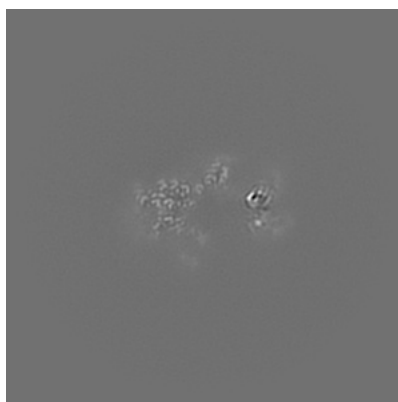
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

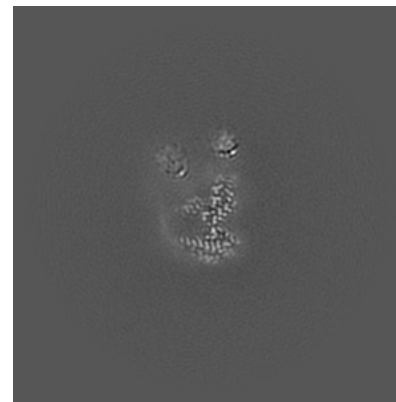
### 6.3.1 Primary map



X Index: 211



Y Index: 206

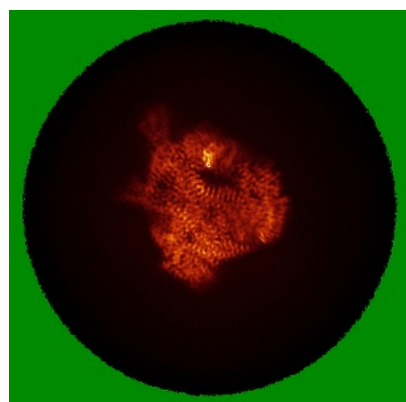


Z Index: 176

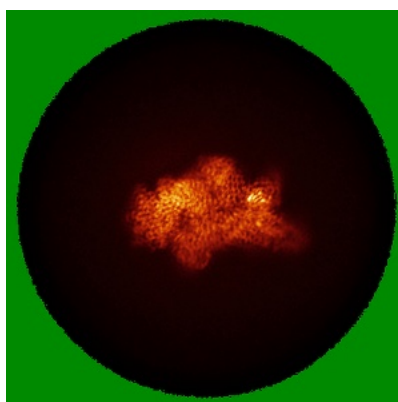
The images above show the largest variance slices of the map in three orthogonal directions.

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

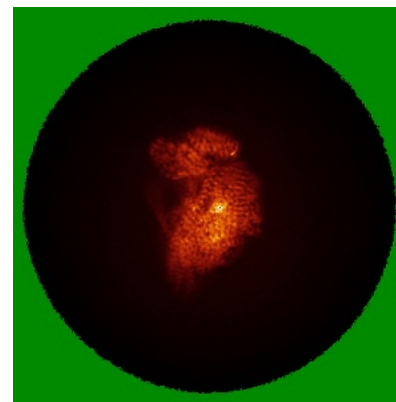
### 6.4.1 Primary map



X



Y

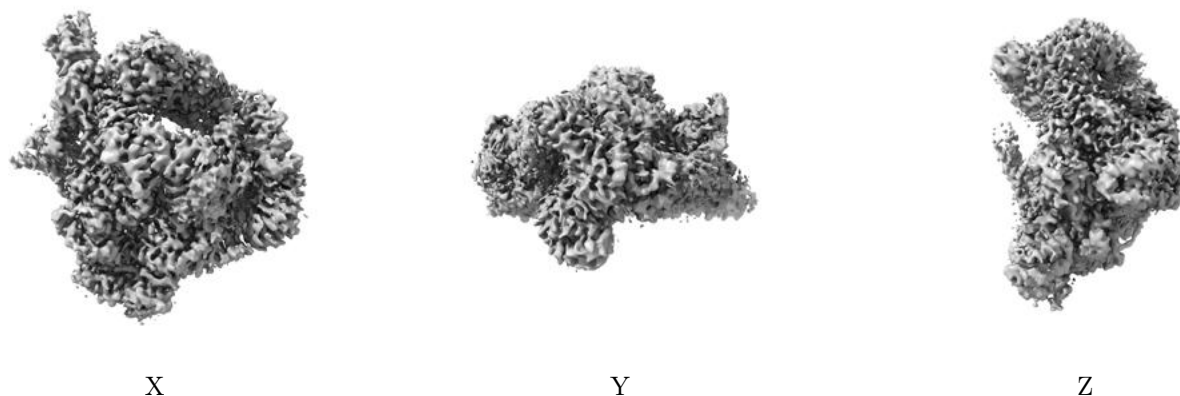


Z

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 0.0514. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

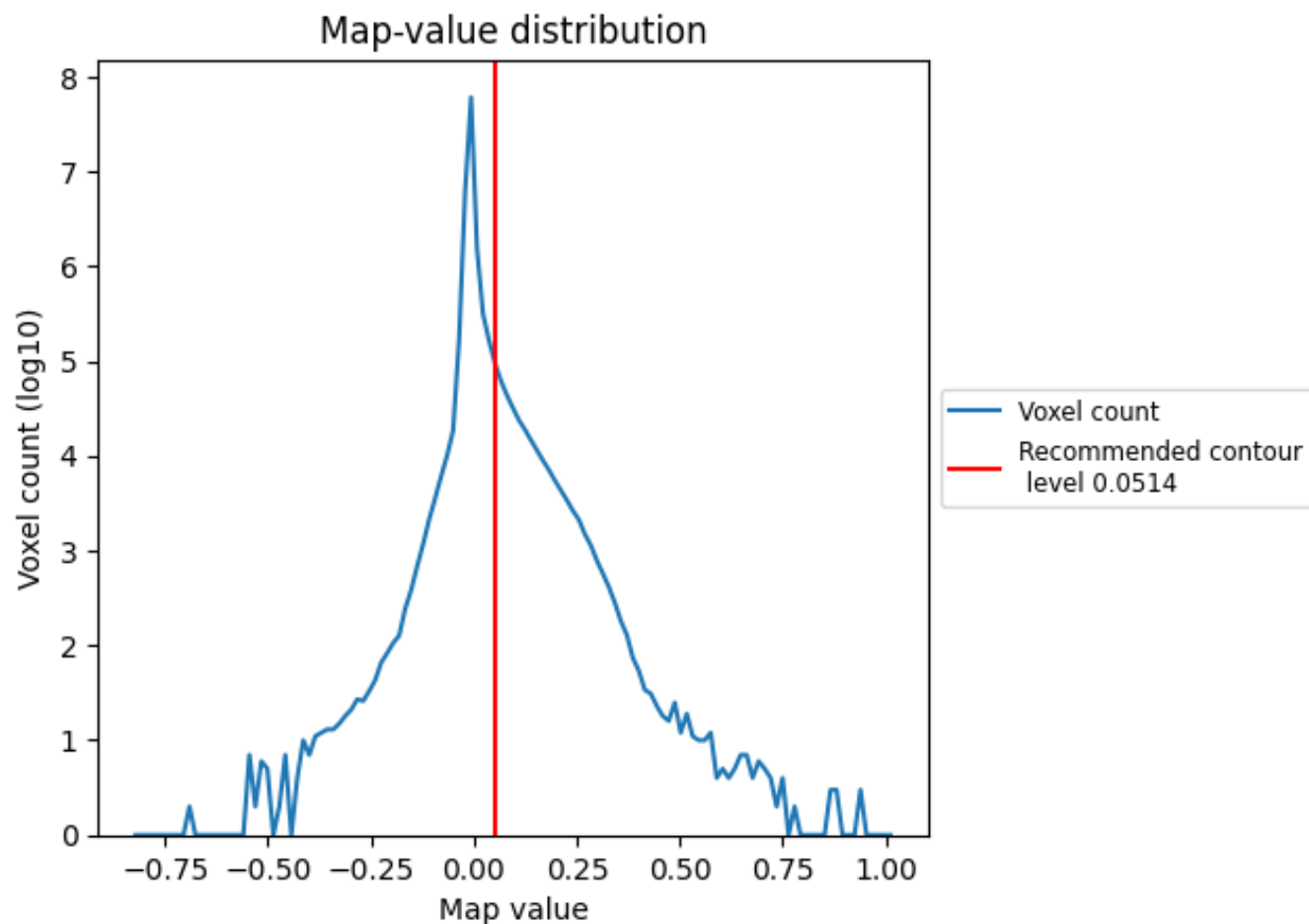
## 6.6 Mask visualisation [i](#)

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.

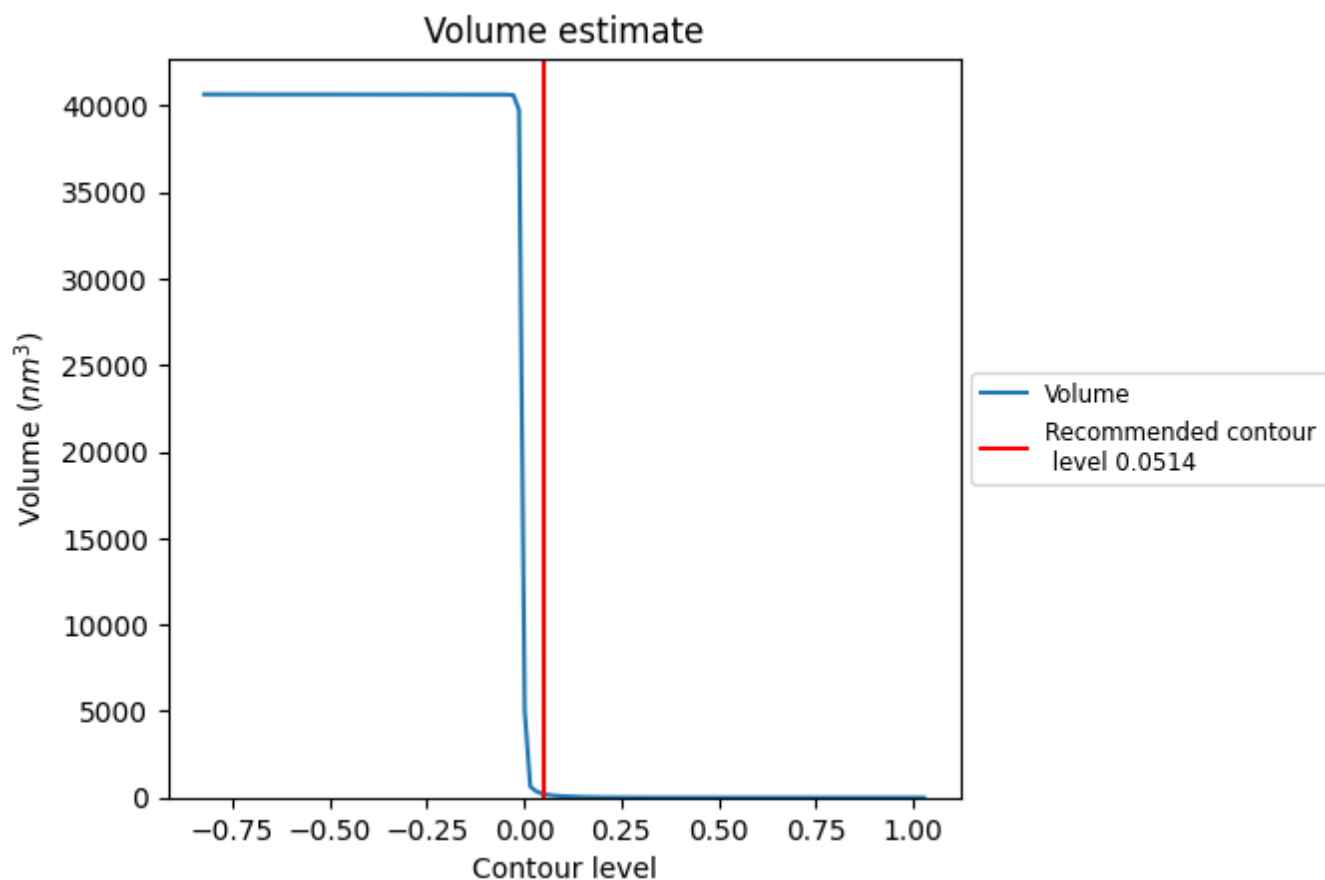
### 7.1 Map-value distribution [i](#)



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 206 nm<sup>3</sup>; this corresponds to an approximate mass of 186 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.

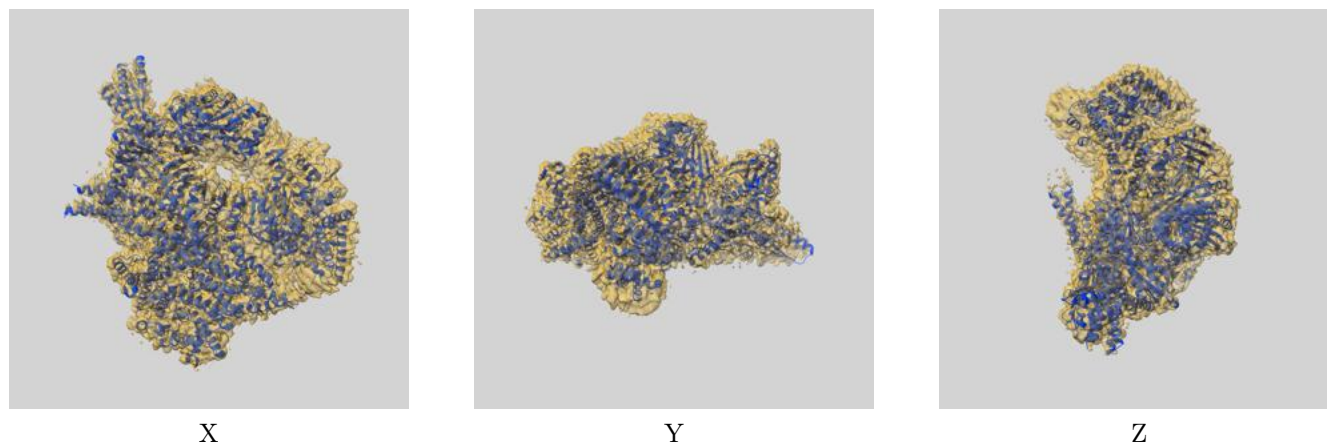
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

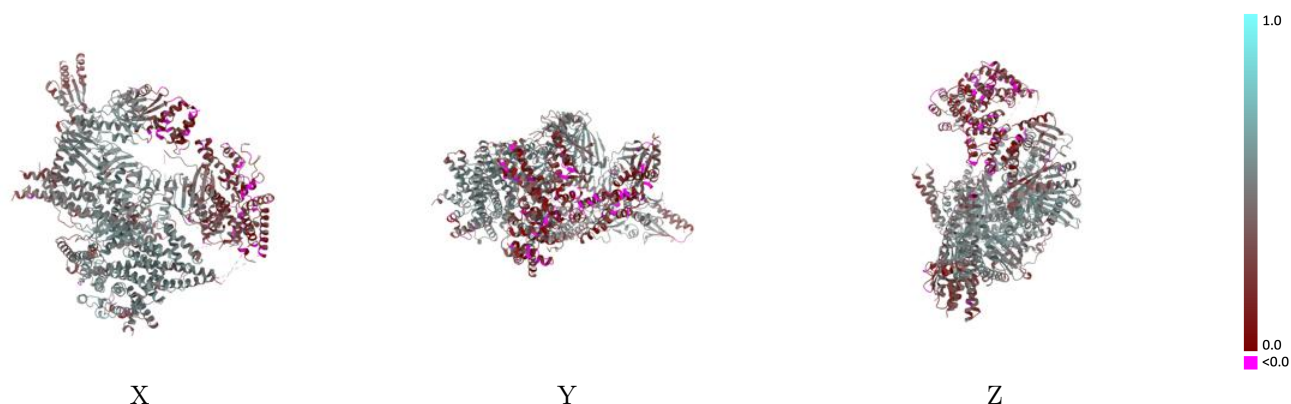
This section contains information regarding the fit between EMDB map EMD-70568 and PDB model 9OKL. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



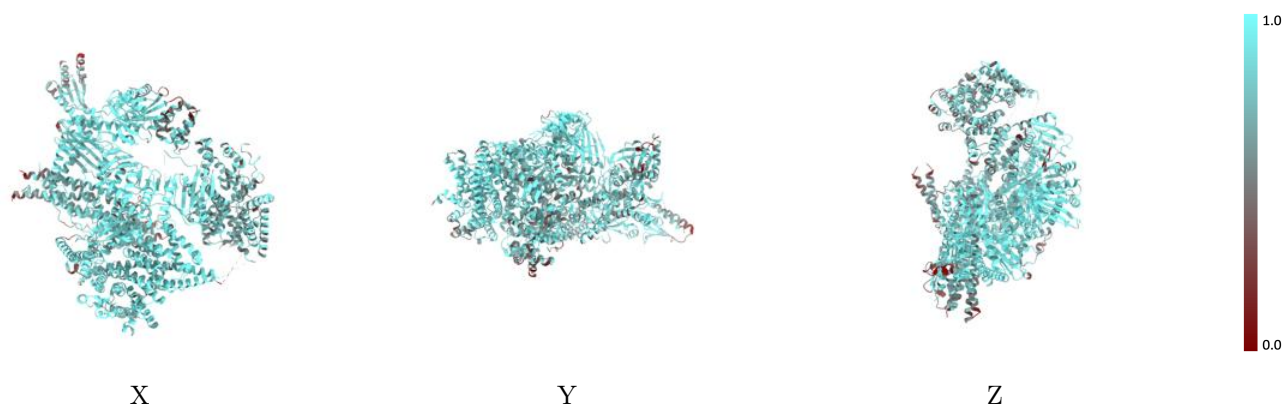
The images above show the 3D surface view of the map at the recommended contour level 0.0514 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



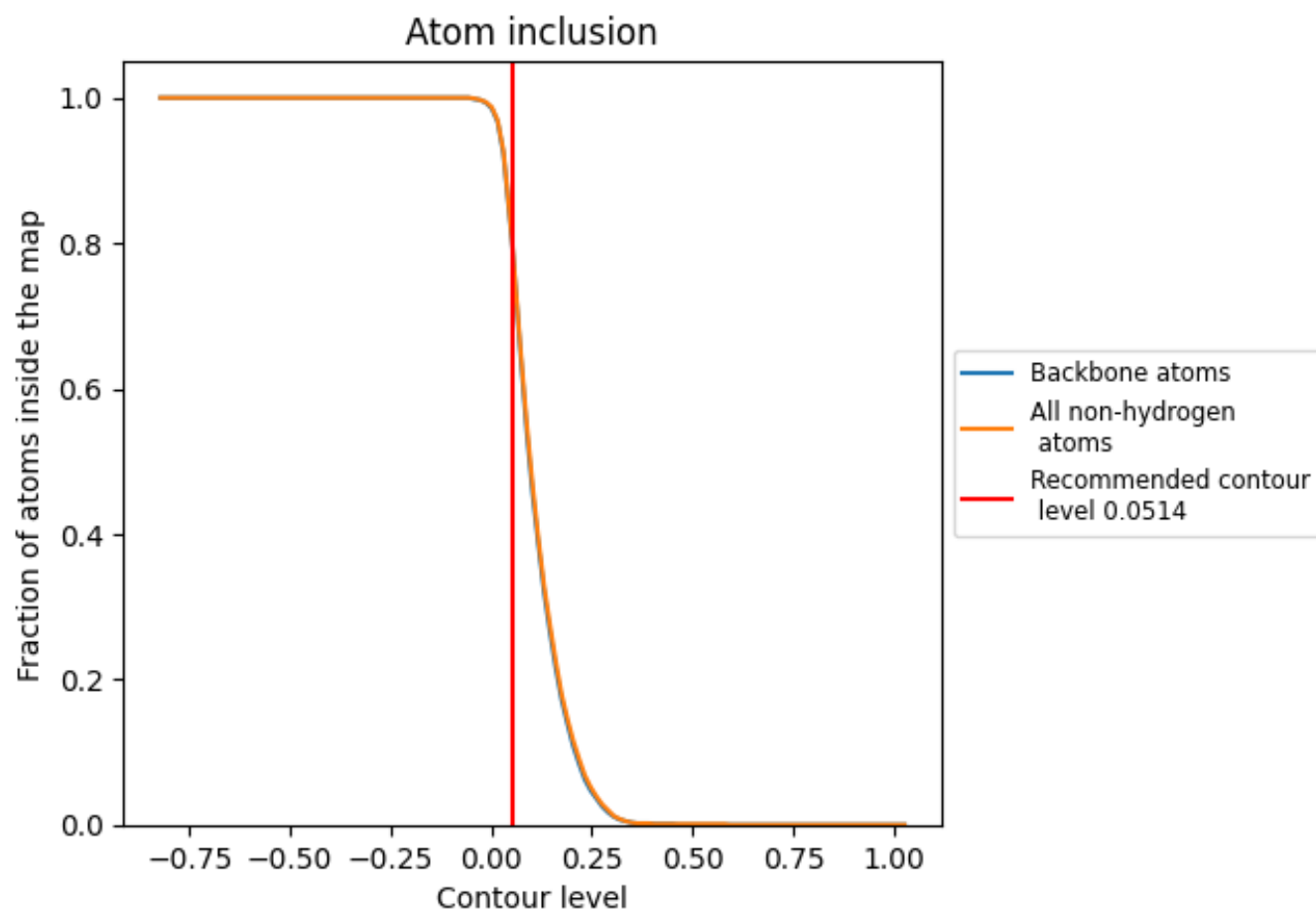
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0514).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 81% 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 (0.0514) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.4040
A	 0.6790	 0.4010
B	 0.7760	 0.4560
C	 0.8060	 0.4600
D	 0.7960	 0.4450
H	 0.8100	 0.4020
I	 0.8390	 0.4050
K	 0.8000	 0.3310
L	 0.8800	 0.4490
M	 0.9130	 0.5320
N	 0.8010	 0.3720
O	 0.8450	 0.4520
P	 0.7500	 0.4140
T	 0.7190	 0.2230

