Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 12:33 PM EST

PDB ID	:	6N06
EMDB ID	:	EMD-9311
Title	:	Cryo-EM structure of the HO BMC shell: BMC-T1 in the assembled shell
Authors	:	Greber, B.J.; Sutter, M.; Kerfeld, C.A.
Deposited on	:	2018-11-06
Resolution	:	3.40 Å(reported)
Based on initial models	:	5V74, 5DIH

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

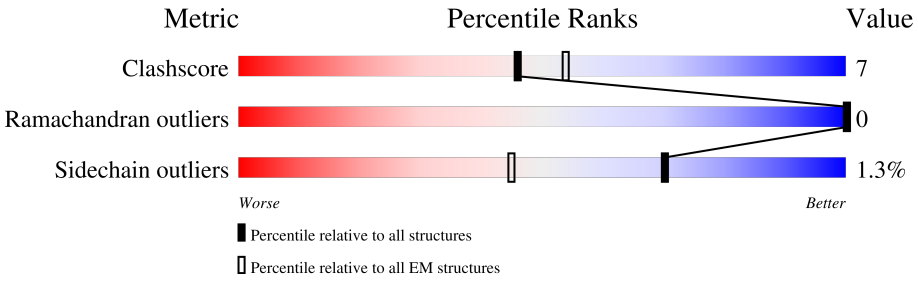
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	205	81% 17%
1	B	205	87% 11%
1	C	205	80% 18%
2	GA	99	74% 19% 7%
2	GB	99	77% 16% 7%
2	GC	99	74% 19% 7%
2	GD	99	77% 16% 7%
2	GE	99	78% 15% 7%

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Mol	Chain	Length	Quality of chain
2	GF	99	80% 13% 7%
2	HA	99	73% 20% 7%
2	HB	99	80% 13% 7%
2	HC	99	74% 19% 7%
2	HD	99	76% 16% 7%
2	HE	99	74% 19% 7%
2	HF	99	78% 15% 7%
2	IA	99	75% 18% 7%
2	IB	99	75% 18% 7%
2	IC	99	77% 16% 7%
2	ID	99	79% 14% 7%
2	IE	99	79% 14% 7%
2	IF	99	78% 15% 7%
2	JA	99	77% 16% 7%
2	JB	99	80% 13% 7%
2	JC	99	74% 19% 7%
2	JD	99	79% 14% 7%
2	JE	99	74% 19% 7%
2	JF	99	78% 15% 7%
2	KA	99	77% 16% 7%
2	KB	99	74% 19% 7%
2	KC	99	74% 19% 7%
2	KD	99	80% 13% 7%
2	KE	99	77% 16% 7%
2	KF	99	77% 16% 7%

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Mol	Chain	Length	Quality of chain
2	LA	99	77% 16% 7%
2	LB	99	80% 13% 7%
2	LC	99	76% 17% 7%
2	LD	99	80% 13% 7%
2	LE	99	73% 20% 7%
2	LF	99	78% 15% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28197 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 Microcompartments protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	201	Total	C	N	O	S	0	0
			1503	948	261	286	8		
1	B	201	Total	C	N	O	S	0	0
			1503	948	261	286	8		
1	C	201	Total	C	N	O	S	0	0
			1503	948	261	286	8		

- Molecule 2 is a protein called Microcompartments protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	GA	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	GB	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	GC	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	GD	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	GE	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	GF	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	HA	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	HB	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	HC	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	HD	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	HE	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	HF	92	Total	C	N	O	S	0	0
			658	413	120	122	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	IA	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	IB	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	IC	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	ID	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	IE	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	IF	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	JA	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	JB	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	JC	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	JD	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	JE	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	JF	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	KA	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	KB	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	KC	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	KD	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	KE	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	KF	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	LA	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	LB	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	LC	92	Total	C	N	O	S	0	0
			658	413	120	122	3		

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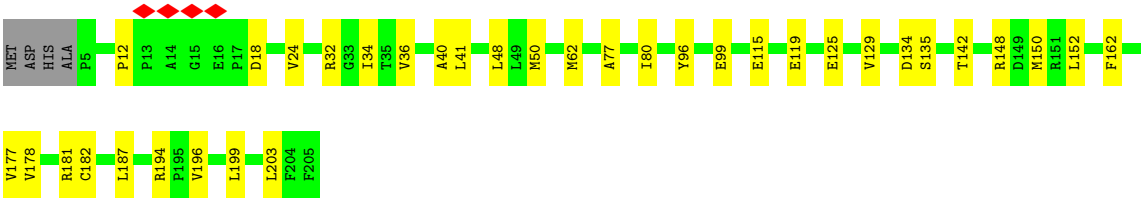
Mol	Chain	Residues	Atoms					AltConf	Trace
2	LD	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	LE	92	Total	C	N	O	S	0	0
			658	413	120	122	3		
2	LF	92	Total	C	N	O	S	0	0
			658	413	120	122	3		

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.

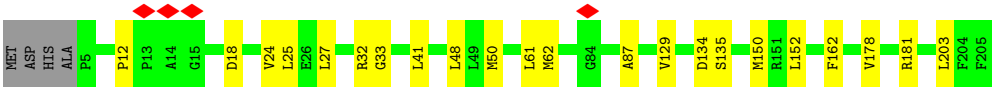
• Molecule 1: Microcompartments protein

Chain A:



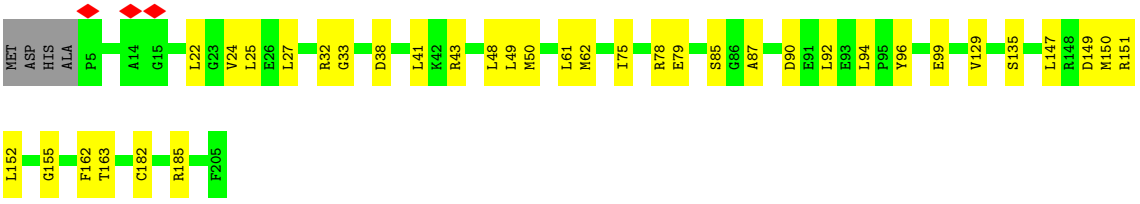
• Molecule 1: Microcompartments protein

Chain B:



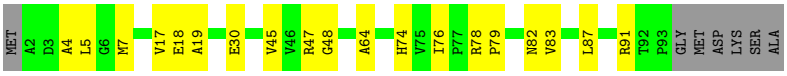
• Molecule 1: Microcompartments protein

Chain C:



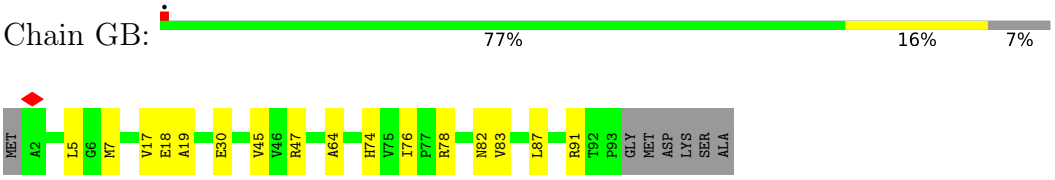
• Molecule 2: Microcompartments protein

Chain GA:



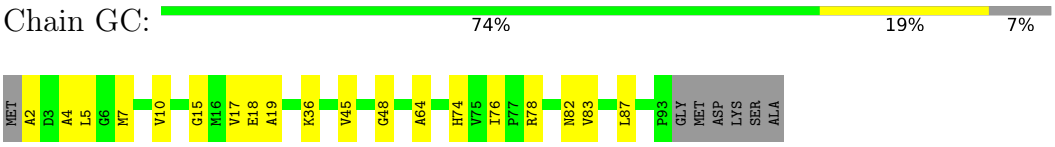
• Molecule 2: Microcompartments protein

Chain GB:



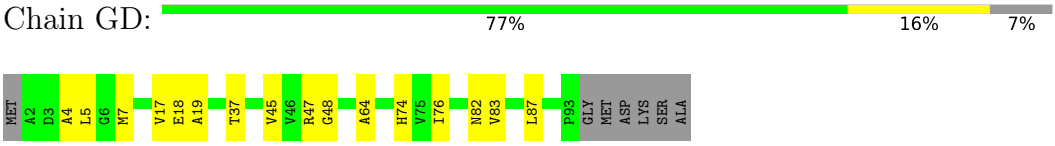
• Molecule 2: Microcompartments protein

Chain GC:



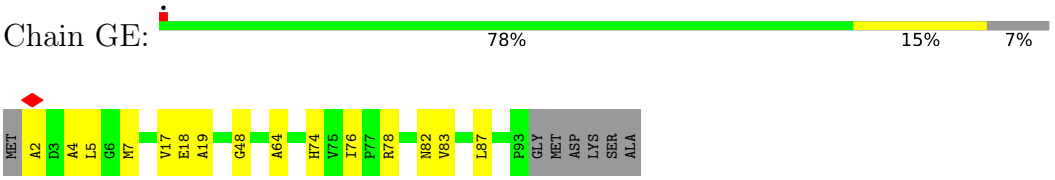
• Molecule 2: Microcompartments protein

Chain GD:



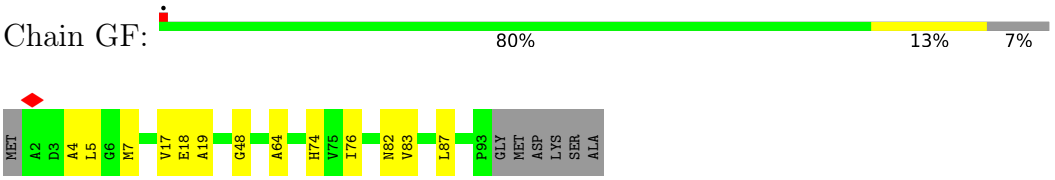
• Molecule 2: Microcompartments protein

Chain GE:



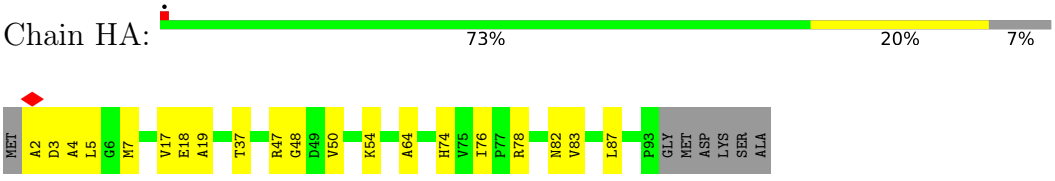
• Molecule 2: Microcompartments protein

Chain GF:



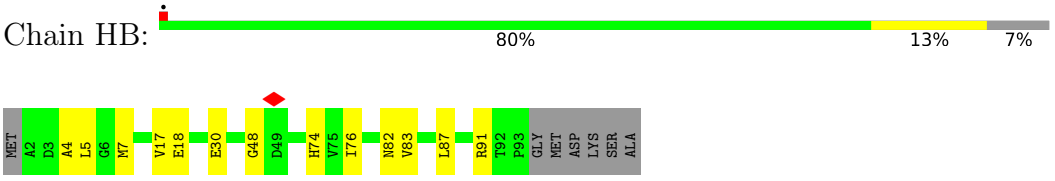
• Molecule 2: Microcompartments protein

Chain HA:



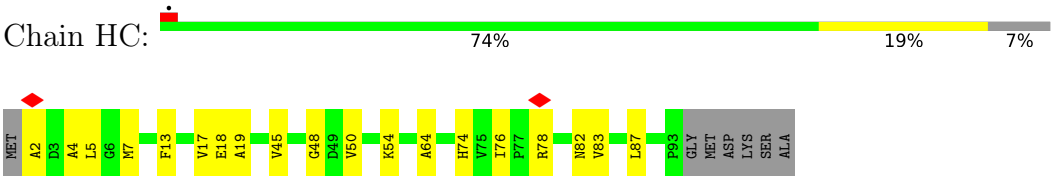
• Molecule 2: Microcompartments protein

Chain HB:



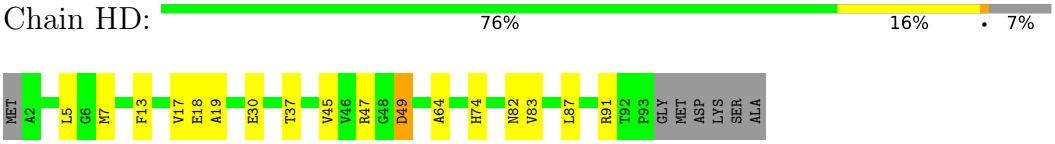
• Molecule 2: Microcompartments protein

Chain HC:



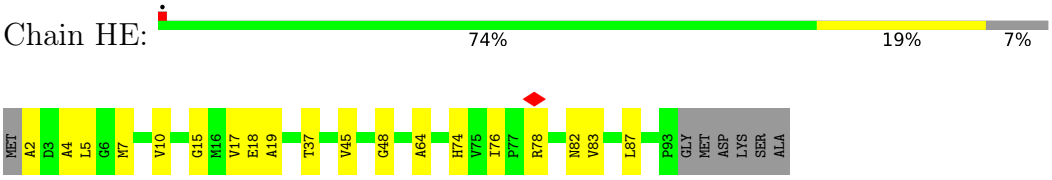
• Molecule 2: Microcompartments protein

Chain HD:



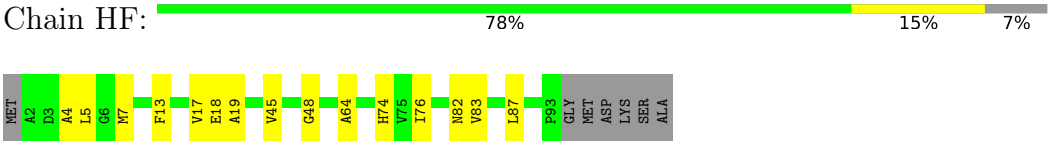
• Molecule 2: Microcompartments protein

Chain HE:



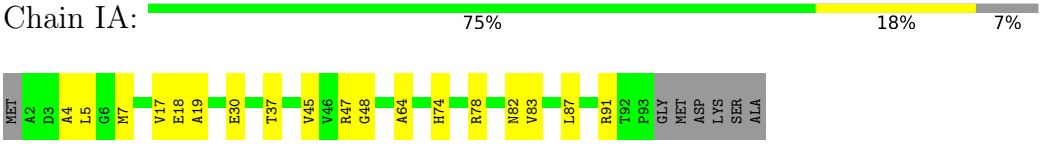
• Molecule 2: Microcompartments protein

Chain HF:



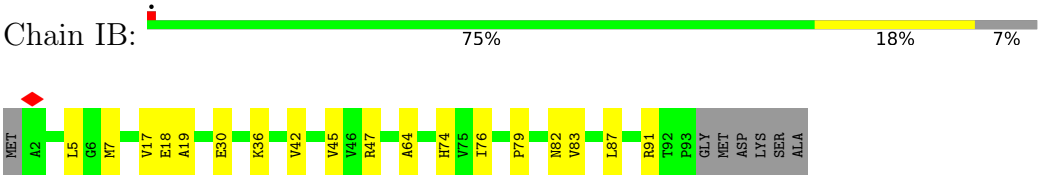
• Molecule 2: Microcompartments protein

Chain IA:



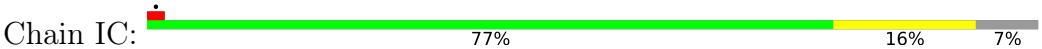
• Molecule 2: Microcompartments protein

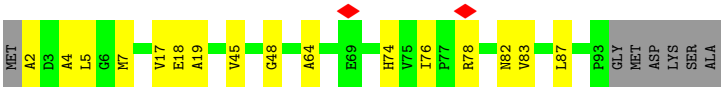
Chain IB:



• Molecule 2: Microcompartments protein

Chain IC:



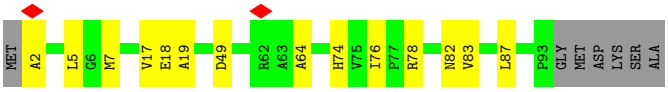


• Molecule 2: Microcompartments protein

Chain ID:

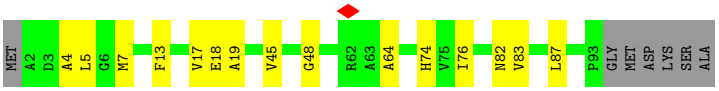
• Molecule 2: Microcompartments protein

Chain IE:



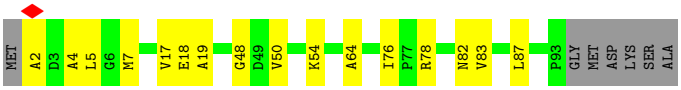
• Molecule 2: Microcompartments protein

Chain IF:



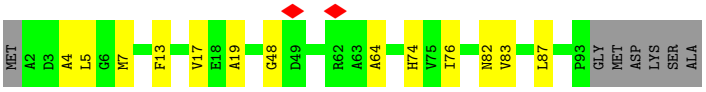
• Molecule 2: Microcompartments protein

Chain JA:



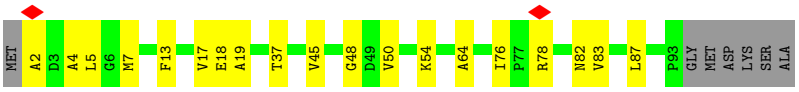
• Molecule 2: Microcompartments protein

Chain JB:



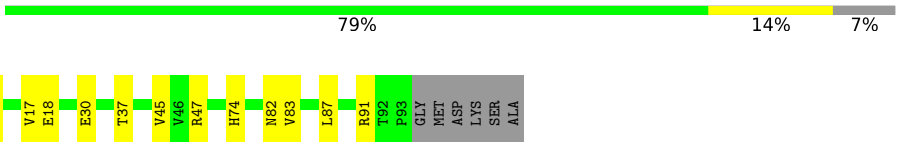
• Molecule 2: Microcompartments protein

Chain JC:



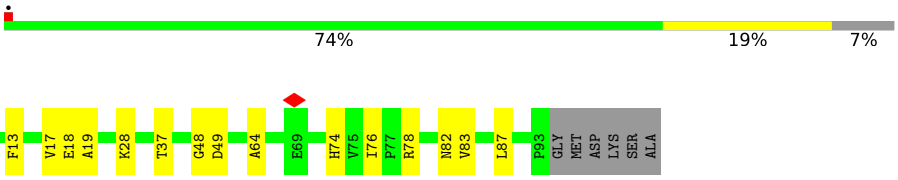
• Molecule 2: Microcompartments protein

Chain JD:



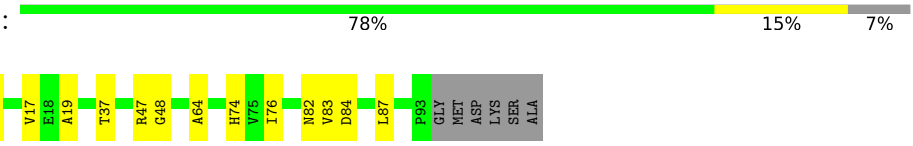
• Molecule 2: Microcompartments protein

Chain JE:



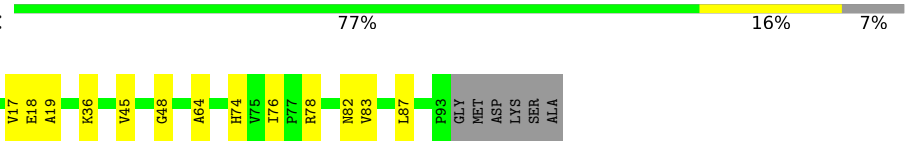
• Molecule 2: Microcompartments protein

Chain JF:



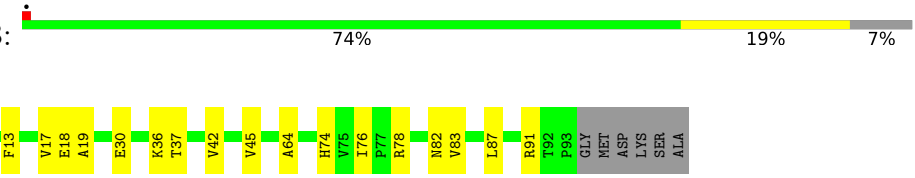
• Molecule 2: Microcompartments protein

Chain KA:



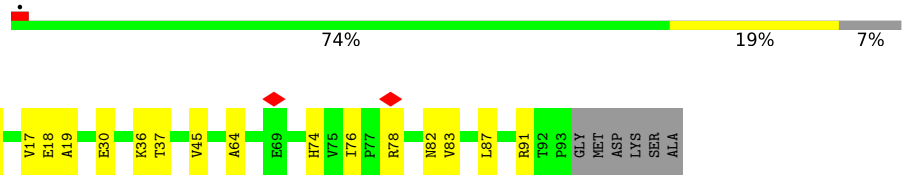
• Molecule 2: Microcompartments protein

Chain KB:



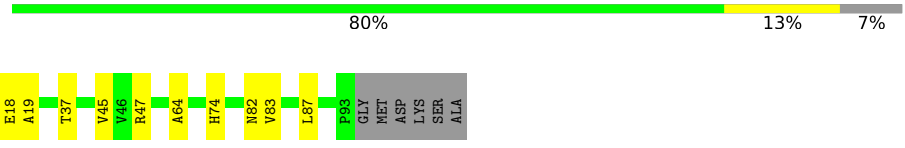
• Molecule 2: Microcompartments protein

Chain KC:



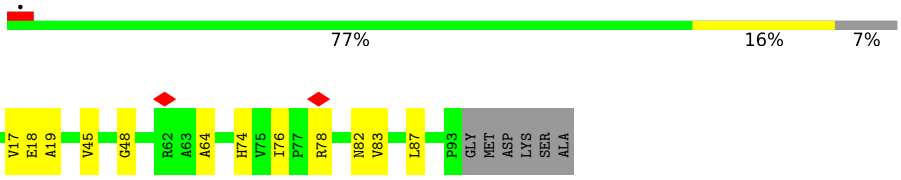
• Molecule 2: Microcompartments protein

Chain KD:



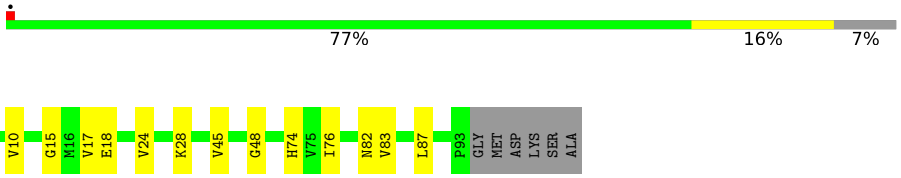
• Molecule 2: Microcompartments protein

Chain KE:



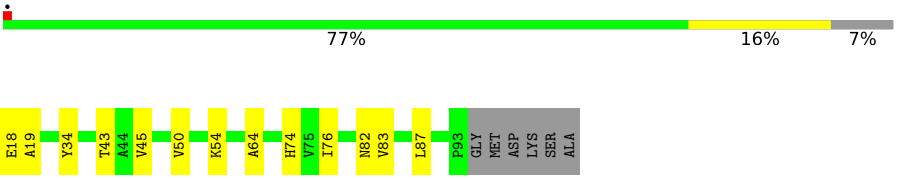
• Molecule 2: Microcompartments protein

Chain KF:



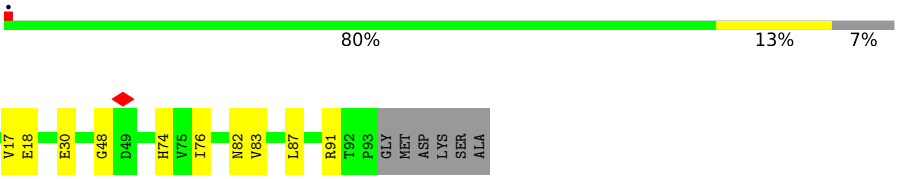
• Molecule 2: Microcompartments protein

Chain LA:



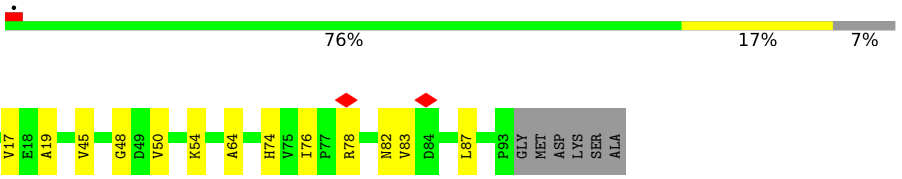
• Molecule 2: Microcompartments protein

Chain LB:



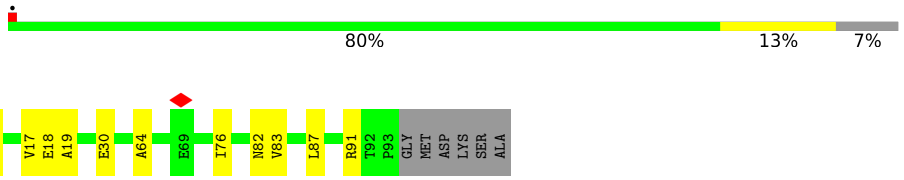
• Molecule 2: Microcompartments protein

Chain LC:



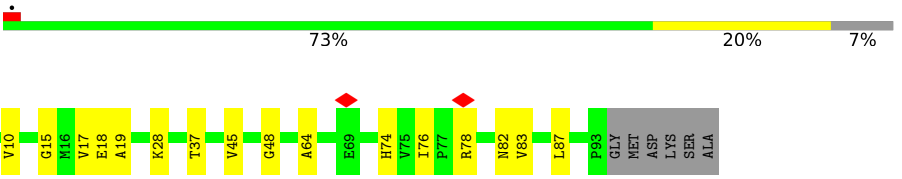
• Molecule 2: Microcompartments protein

Chain LD:



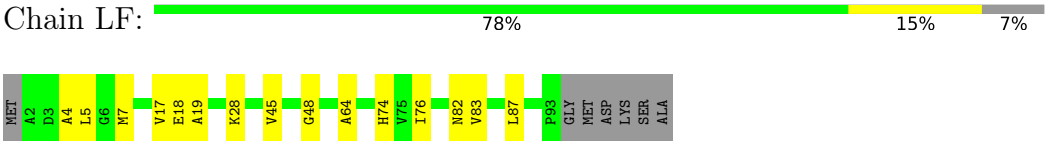
• Molecule 2: Microcompartments protein

Chain LE:



• Molecule 2: Microcompartments protein

Chain LF:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	177642	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Initial CTF fitting using CTFFIND4, CTF correction applied within RELION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	48543	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	527.36, 527.36, 527.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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	0.30	0/1526	0.55	0/2073
1	B	0.30	0/1526	0.56	0/2073
1	C	0.31	0/1526	0.57	0/2073
2	GA	0.33	0/666	0.51	0/904
2	GB	0.33	0/666	0.50	0/904
2	GC	0.32	0/666	0.52	0/904
2	GD	0.31	0/666	0.51	0/904
2	GE	0.32	0/666	0.51	0/904
2	GF	0.33	0/666	0.52	0/904
2	HA	0.33	0/666	0.52	0/904
2	HB	0.31	0/666	0.51	0/904
2	HC	0.31	0/666	0.50	0/904
2	HD	0.33	0/666	0.50	0/904
2	HE	0.33	0/666	0.51	0/904
2	HF	0.33	0/666	0.51	0/904
2	IA	0.34	0/666	0.51	0/904
2	IB	0.33	0/666	0.51	0/904
2	IC	0.31	0/666	0.52	0/904
2	ID	0.31	0/666	0.51	0/904
2	IE	0.32	0/666	0.51	0/904
2	IF	0.32	0/666	0.51	0/904
2	JA	0.34	0/666	0.52	0/904
2	JB	0.32	0/666	0.51	0/904
2	JC	0.31	0/666	0.51	0/904
2	JD	0.32	0/666	0.49	0/904
2	JE	0.33	0/666	0.51	0/904
2	JF	0.33	0/666	0.52	0/904
2	KA	0.33	0/666	0.52	0/904
2	KB	0.33	0/666	0.52	0/904
2	KC	0.31	0/666	0.51	0/904
2	KD	0.31	0/666	0.51	0/904
2	KE	0.32	0/666	0.51	0/904
2	KF	0.33	0/666	0.53	0/904
2	LA	0.34	0/666	0.52	0/904

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	LB	0.31	0/666	0.51	0/904
2	LC	0.31	0/666	0.51	0/904
2	LD	0.32	0/666	0.51	0/904
2	LE	0.33	0/666	0.52	0/904
2	LF	0.33	0/666	0.50	0/904
All	All	0.32	0/28554	0.52	0/38763

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	HD	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	HD	49	ASP	Peptide

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	1503	0	1529	24	0
1	B	1503	0	1529	13	0
1	C	1503	0	1529	21	0
2	GA	658	0	678	14	0
2	GB	658	0	678	13	0
2	GC	658	0	678	14	0
2	GD	658	0	678	13	0
2	GE	658	0	678	11	0
2	GF	658	0	678	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	HA	658	0	678	14	0
2	HB	658	0	678	10	0
2	HC	658	0	678	14	0
2	HD	658	0	678	14	0
2	HE	658	0	678	14	0
2	HF	658	0	678	12	0
2	IA	658	0	678	14	0
2	IB	658	0	678	14	0
2	IC	658	0	678	12	0
2	ID	658	0	678	11	0
2	IE	658	0	678	11	0
2	IF	658	0	678	12	0
2	JA	658	0	678	11	0
2	JB	658	0	678	10	0
2	JC	658	0	678	14	0
2	JD	658	0	678	12	0
2	JE	658	0	678	15	0
2	JF	658	0	678	11	0
2	KA	658	0	678	13	0
2	KB	658	0	678	15	0
2	KC	658	0	678	15	0
2	KD	658	0	678	12	0
2	KE	658	0	678	12	0
2	KF	658	0	678	13	0
2	LA	658	0	678	12	0
2	LB	658	0	678	10	0
2	LC	658	0	678	12	0
2	LD	658	0	678	10	0
2	LE	658	0	678	15	0
2	LF	658	0	678	12	0
All	All	28197	0	28995	380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (380) 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)
2:LB:4:ALA:HB3	2:LB:48:GLY:O	1.83	0.77
2:HB:4:ALA:HB3	2:HB:48:GLY:O	1.86	0.75
2:JC:4:ALA:HB3	2:JC:48:GLY:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LC:4:ALA:HB3	2:LC:48:GLY:O	1.91	0.71
2:IC:4:ALA:HB3	2:IC:48:GLY:O	1.93	0.68
2:JB:4:ALA:HB3	2:JB:48:GLY:O	1.94	0.67
2:HC:4:ALA:HB3	2:HC:48:GLY:O	1.97	0.64
2:IF:4:ALA:HB3	2:IF:48:GLY:O	1.98	0.63
2:GC:83:VAL:HG13	2:GC:87:LEU:HD12	1.81	0.62
2:HD:17:VAL:HG22	2:HE:87:LEU:HD13	1.82	0.62
2:KD:17:VAL:HG22	2:KE:87:LEU:HD13	1.82	0.62
2:IB:17:VAL:HG22	2:IC:87:LEU:HD13	1.80	0.62
2:KF:4:ALA:HB3	2:KF:48:GLY:O	2.00	0.62
2:LD:17:VAL:HG22	2:LE:87:LEU:HD13	1.82	0.61
1:A:40:ALA:HB2	1:A:77:ALA:HB2	1.81	0.61
1:C:135:SER:OG	1:C:182:CYS:SG	2.57	0.61
2:GB:17:VAL:HG22	2:GC:87:LEU:HD13	1.81	0.61
2:HA:4:ALA:HB3	2:HA:48:GLY:O	2.00	0.61
2:LC:83:VAL:HG13	2:LC:87:LEU:HD12	1.83	0.61
1:B:24:VAL:HG22	1:B:62:MET:HG2	1.82	0.61
2:KE:4:ALA:HB3	2:KE:48:GLY:O	2.00	0.61
2:KC:83:VAL:HG13	2:KC:87:LEU:HD12	1.83	0.60
1:A:24:VAL:HG22	1:A:62:MET:HG2	1.83	0.60
2:HE:83:VAL:HG13	2:HE:87:LEU:HD12	1.82	0.60
2:JA:87:LEU:HD13	2:JF:17:VAL:HG22	1.84	0.60
2:ID:17:VAL:HG22	2:IE:87:LEU:HD13	1.83	0.59
2:LA:83:VAL:HG13	2:LA:87:LEU:HD12	1.85	0.59
2:JF:83:VAL:HG13	2:JF:87:LEU:HD12	1.85	0.59
2:IC:83:VAL:HG13	2:IC:87:LEU:HD12	1.83	0.59
2:KB:17:VAL:HG22	2:KC:87:LEU:HD13	1.84	0.58
2:LA:17:VAL:HG11	2:LB:7:MET:HE3	1.84	0.58
2:JF:5:LEU:HD23	2:JF:76:ILE:HD12	1.85	0.58
1:B:129:VAL:HG13	1:B:152:LEU:HD22	1.85	0.58
2:JA:2:ALA:O	2:JA:78:ARG:NH1	2.36	0.58
2:KC:7:MET:HG2	2:KC:45:VAL:HG22	1.85	0.58
2:IA:74:HIS:NE2	2:IF:18:GLU:OE1	2.36	0.58
2:IF:5:LEU:HD23	2:IF:76:ILE:HD12	1.86	0.58
2:JE:28:LYS:HD3	2:KB:78:ARG:HH22	1.67	0.58
1:B:12:PRO:HG3	1:B:18:ASP:HA	1.84	0.58
2:JB:17:VAL:HG22	2:JC:87:LEU:HD13	1.86	0.58
2:HA:87:LEU:HD13	2:HF:17:VAL:HG22	1.84	0.58
2:GF:83:VAL:HG13	2:GF:87:LEU:HD12	1.85	0.58
2:HA:83:VAL:HG13	2:HA:87:LEU:HD12	1.85	0.58
2:KE:17:VAL:HG22	2:KF:87:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LE:4:ALA:HB3	2:LE:48:GLY:O	2.04	0.57
2:GC:7:MET:HG2	2:GC:45:VAL:HG22	1.86	0.57
2:GE:17:VAL:HG22	2:GF:87:LEU:HD13	1.85	0.57
2:JD:17:VAL:HG22	2:JE:87:LEU:HD13	1.85	0.57
2:GD:5:LEU:HD23	2:GD:76:ILE:HD12	1.86	0.57
2:GF:5:LEU:HD23	2:GF:76:ILE:HD12	1.85	0.57
2:JC:5:LEU:HD23	2:JC:76:ILE:HD12	1.87	0.57
2:JE:17:VAL:HG22	2:JF:87:LEU:HD13	1.86	0.57
2:HA:2:ALA:O	2:HA:78:ARG:NH1	2.37	0.57
2:HC:83:VAL:HG13	2:HC:87:LEU:HD12	1.86	0.57
2:JC:83:VAL:HG13	2:JC:87:LEU:HD12	1.85	0.57
2:KB:5:LEU:HD23	2:KB:76:ILE:HD12	1.87	0.57
2:ID:5:LEU:HD23	2:ID:76:ILE:HD12	1.86	0.56
2:KE:5:LEU:HD23	2:KE:76:ILE:HD12	1.86	0.56
2:IC:7:MET:HG2	2:IC:45:VAL:HG22	1.86	0.56
2:LA:87:LEU:HD13	2:LF:17:VAL:HG22	1.86	0.56
2:HB:5:LEU:HD23	2:HB:76:ILE:HD12	1.86	0.56
2:HF:5:LEU:HD23	2:HF:76:ILE:HD12	1.87	0.56
2:GD:17:VAL:HG22	2:GE:87:LEU:HD13	1.88	0.56
2:IA:87:LEU:HD13	2:IF:17:VAL:HG22	1.88	0.56
2:IC:18:GLU:OE1	2:ID:74:HIS:NE2	2.39	0.56
2:KC:2:ALA:O	2:KC:78:ARG:NH1	2.38	0.56
2:JA:83:VAL:HG13	2:JA:87:LEU:HD12	1.87	0.56
2:JB:17:VAL:HG11	2:JC:7:MET:HE1	1.88	0.56
2:GA:87:LEU:HD13	2:GF:17:VAL:HG22	1.88	0.56
2:KA:7:MET:HE1	2:KF:17:VAL:HG11	1.88	0.56
2:GE:4:ALA:HB3	2:GE:48:GLY:O	2.06	0.56
2:JA:5:LEU:HD23	2:JA:76:ILE:HD12	1.88	0.56
2:HE:17:VAL:HG22	2:HF:87:LEU:HD13	1.87	0.55
2:HF:7:MET:HG2	2:HF:45:VAL:HG22	1.86	0.55
2:IE:19:ALA:HB2	2:IE:64:ALA:HB2	1.88	0.55
1:A:34:ILE:HD13	1:B:203:LEU:HD23	1.88	0.55
2:JE:83:VAL:HG13	2:JE:87:LEU:HD12	1.87	0.55
1:A:32:ARG:NH2	1:A:80:ILE:O	2.40	0.55
2:JD:17:VAL:HG11	2:JE:7:MET:HE1	1.88	0.55
2:KF:5:LEU:HD23	2:KF:76:ILE:HD12	1.88	0.55
2:LB:5:LEU:HD23	2:LB:76:ILE:HD12	1.87	0.55
2:LE:83:VAL:HG13	2:LE:87:LEU:HD12	1.89	0.55
2:HF:4:ALA:HB3	2:HF:48:GLY:O	2.07	0.55
2:KB:18:GLU:OE1	2:KC:74:HIS:NE2	2.39	0.55
2:LE:18:GLU:OE1	2:LF:74:HIS:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HD:18:GLU:OE1	2:HE:74:HIS:NE2	2.39	0.55
2:IE:17:VAL:HG22	2:IF:87:LEU:HD13	1.88	0.55
2:KD:17:VAL:HG11	2:KE:7:MET:HE3	1.89	0.55
2:GA:7:MET:HE3	2:GF:17:VAL:HG11	1.87	0.55
2:IC:2:ALA:O	2:IC:78:ARG:NH1	2.39	0.55
2:GA:18:GLU:OE1	2:GB:74:HIS:NE2	2.40	0.55
2:KA:87:LEU:HD13	2:KF:17:VAL:HG22	1.89	0.55
2:HA:3:ASP:O	2:HA:47:ARG:NH2	2.40	0.54
2:IA:17:VAL:HG22	2:IB:87:LEU:HD13	1.89	0.54
2:IF:83:VAL:HG13	2:IF:87:LEU:HD12	1.88	0.54
2:LA:17:VAL:HG22	2:LB:87:LEU:HD13	1.89	0.54
1:A:18:ASP:OD2	2:LF:28:LYS:NZ	2.39	0.54
1:A:135:SER:OG	1:A:182:CYS:SG	2.60	0.54
2:LE:17:VAL:HG22	2:LF:87:LEU:HD13	1.90	0.54
1:B:32:ARG:HD2	1:B:87:ALA:HB3	1.89	0.54
2:GA:74:HIS:NE2	2:GF:18:GLU:OE1	2.40	0.54
2:JC:17:VAL:HG22	2:JD:87:LEU:HD13	1.89	0.54
1:C:41:LEU:HD11	1:C:48:LEU:HB2	1.90	0.54
2:HB:83:VAL:HG13	2:HB:87:LEU:HD12	1.89	0.54
2:LF:5:LEU:HD23	2:LF:76:ILE:HD12	1.89	0.54
2:LC:17:VAL:HG22	2:LD:87:LEU:HD13	1.89	0.54
2:JA:17:VAL:HG11	2:JB:7:MET:HE3	1.90	0.54
2:JD:18:GLU:OE1	2:JE:74:HIS:NE2	2.41	0.54
2:KF:83:VAL:HG13	2:KF:87:LEU:HD12	1.90	0.54
2:HC:17:VAL:HG22	2:HD:87:LEU:HD13	1.90	0.53
2:JB:5:LEU:HD23	2:JB:76:ILE:HD12	1.90	0.53
2:IA:17:VAL:HG11	2:IB:7:MET:HE1	1.90	0.53
2:KB:83:VAL:HG13	2:KB:87:LEU:HD12	1.90	0.53
2:LC:5:LEU:HD23	2:LC:76:ILE:HD12	1.88	0.53
2:HA:17:VAL:HG11	2:HB:7:MET:HE1	1.89	0.53
2:HC:17:VAL:HG11	2:HD:7:MET:HE3	1.91	0.53
2:IA:83:VAL:HG13	2:IA:87:LEU:HD12	1.90	0.53
2:JE:2:ALA:O	2:JE:78:ARG:NH1	2.41	0.53
2:HD:17:VAL:HG11	2:HE:7:MET:HE1	1.91	0.53
2:JB:83:VAL:HG13	2:JB:87:LEU:HD12	1.91	0.53
2:LB:83:VAL:HG13	2:LB:87:LEU:HD12	1.89	0.53
2:GC:18:GLU:OE1	2:GD:74:HIS:NE2	2.41	0.53
2:IA:18:GLU:OE1	2:IB:74:HIS:NE2	2.42	0.53
2:ID:7:MET:HG2	2:ID:45:VAL:HG22	1.91	0.53
2:IB:30:GLU:OE1	2:IB:91:ARG:NH2	2.41	0.53
1:C:129:VAL:HG13	1:C:152:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GC:2:ALA:O	2:GC:78:ARG:NH1	2.42	0.53
2:HD:5:LEU:HD13	2:HD:47:ARG:HH11	1.73	0.53
2:HF:83:VAL:HG13	2:HF:87:LEU:HD12	1.91	0.53
2:IE:17:VAL:HG11	2:IF:7:MET:HE1	1.91	0.53
2:JA:17:VAL:HG22	2:JB:87:LEU:HD13	1.91	0.53
2:HB:17:VAL:HG11	2:HC:7:MET:HE3	1.91	0.53
1:C:32:ARG:HD2	1:C:87:ALA:HB3	1.90	0.52
2:IF:19:ALA:HB2	2:IF:64:ALA:HB2	1.91	0.52
2:GD:17:VAL:HG11	2:GE:7:MET:HE1	1.91	0.52
2:LD:17:VAL:HG11	2:LE:7:MET:HE1	1.90	0.52
1:C:150:MET:HG3	1:C:162:PHE:HB3	1.92	0.52
2:GA:83:VAL:HG13	2:GA:87:LEU:HD12	1.91	0.52
2:GD:7:MET:HG2	2:GD:45:VAL:HG22	1.91	0.52
2:JC:17:VAL:HG11	2:JD:7:MET:HE1	1.92	0.52
2:JD:83:VAL:HG13	2:JD:87:LEU:HD12	1.92	0.52
2:LA:5:LEU:HD23	2:LA:76:ILE:HD12	1.91	0.52
2:GB:17:VAL:HG11	2:GC:7:MET:HE1	1.92	0.52
2:GE:83:VAL:HG13	2:GE:87:LEU:HD12	1.91	0.52
2:GF:4:ALA:HB3	2:GF:48:GLY:O	2.09	0.52
2:HE:2:ALA:O	2:HE:78:ARG:NH1	2.42	0.52
2:IA:19:ALA:HB2	2:IA:64:ALA:HB2	1.91	0.52
2:KD:7:MET:HG2	2:KD:45:VAL:HG22	1.91	0.52
2:GA:17:VAL:HG11	2:GB:7:MET:HE1	1.91	0.52
2:HA:7:MET:HE3	2:HF:17:VAL:HG11	1.89	0.52
2:HB:17:VAL:HG22	2:HC:87:LEU:HD13	1.90	0.52
2:LE:2:ALA:O	2:LE:78:ARG:NH1	2.42	0.52
2:KE:83:VAL:HG13	2:KE:87:LEU:HD12	1.91	0.52
2:HA:17:VAL:HG22	2:HB:87:LEU:HD13	1.91	0.52
2:IB:17:VAL:HG11	2:IC:7:MET:HE1	1.92	0.52
2:IE:83:VAL:HG13	2:IE:87:LEU:HD12	1.91	0.52
2:KA:83:VAL:HG13	2:KA:87:LEU:HD12	1.92	0.52
2:KE:2:ALA:O	2:KE:78:ARG:NH1	2.43	0.52
2:GE:2:ALA:O	2:GE:78:ARG:NH1	2.42	0.52
2:HA:5:LEU:HD23	2:HA:76:ILE:HD12	1.91	0.52
2:HC:5:LEU:HD23	2:HC:76:ILE:HD12	1.91	0.52
2:JE:18:GLU:OE1	2:JF:74:HIS:NE2	2.42	0.52
2:KB:17:VAL:HG11	2:KC:7:MET:HE1	1.91	0.52
1:B:25:LEU:HB2	1:B:61:LEU:HB2	1.91	0.52
2:LC:17:VAL:HG11	2:LD:7:MET:HE3	1.92	0.52
2:GB:18:GLU:OE1	2:GC:74:HIS:NE2	2.42	0.51
2:IA:4:ALA:HB3	2:IA:48:GLY:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LD:13:PHE:HB2	2:LE:37:THR:HG21	1.92	0.51
2:HA:18:GLU:OE1	2:HB:74:HIS:NE2	2.42	0.51
1:A:125:GLU:HG3	1:A:187:LEU:HB2	1.93	0.51
2:GA:7:MET:HG2	2:GA:45:VAL:HG22	1.92	0.51
2:GA:17:VAL:HG22	2:GB:87:LEU:HD13	1.92	0.51
2:HE:17:VAL:HG11	2:HF:7:MET:HE1	1.92	0.51
2:IC:17:VAL:HG11	2:ID:7:MET:HE1	1.91	0.51
2:IC:17:VAL:HG22	2:ID:87:LEU:HD13	1.92	0.51
2:KC:5:LEU:HD23	2:KC:76:ILE:HD12	1.92	0.51
2:KC:17:VAL:HG22	2:KD:87:LEU:HD13	1.92	0.51
2:LA:18:GLU:OE1	2:LB:74:HIS:NE2	2.44	0.51
2:LD:30:GLU:OE1	2:LD:91:ARG:NH2	2.40	0.51
2:GE:5:LEU:HD23	2:GE:76:ILE:HD12	1.93	0.51
2:KC:18:GLU:OE1	2:KD:74:HIS:NE2	2.44	0.51
1:B:41:LEU:HD11	1:B:48:LEU:HB2	1.92	0.51
2:JE:17:VAL:HG11	2:JF:7:MET:HE1	1.92	0.51
2:LB:17:VAL:HG22	2:LC:87:LEU:HD13	1.92	0.51
1:A:41:LEU:O	2:GA:78:ARG:NH1	2.43	0.51
2:LD:18:GLU:OE1	2:LE:74:HIS:NE2	2.44	0.51
2:LF:4:ALA:HB3	2:LF:48:GLY:O	2.10	0.51
2:GC:17:VAL:HG11	2:GD:7:MET:HE1	1.93	0.51
2:HC:2:ALA:O	2:HC:78:ARG:NH1	2.44	0.51
2:LE:5:LEU:HD23	2:LE:76:ILE:HD12	1.93	0.50
2:IB:18:GLU:OE1	2:IC:74:HIS:NE2	2.44	0.50
1:A:134:ASP:OD1	1:A:181:ARG:NH2	2.45	0.50
2:GC:17:VAL:HG22	2:GD:87:LEU:HD13	1.93	0.50
2:LC:2:ALA:O	2:LC:78:ARG:NH1	2.45	0.50
1:B:41:LEU:O	2:IA:78:ARG:NH1	2.44	0.50
2:LF:19:ALA:HB2	2:LF:64:ALA:HB2	1.94	0.50
2:GF:19:ALA:HB2	2:GF:64:ALA:HB2	1.93	0.50
2:LE:7:MET:HG2	2:LE:45:VAL:HG22	1.94	0.50
2:GE:17:VAL:HG11	2:GF:7:MET:HE1	1.94	0.50
2:KE:17:VAL:HG11	2:KF:7:MET:HE1	1.93	0.50
1:B:135:SER:HB3	1:B:178:VAL:HG22	1.94	0.50
2:GE:19:ALA:HB2	2:GE:64:ALA:HB2	1.94	0.50
2:HA:50:VAL:O	2:HA:54:LYS:HB2	2.11	0.50
2:HE:7:MET:HG2	2:HE:45:VAL:HG22	1.94	0.49
2:IB:5:LEU:HD13	2:IB:47:ARG:HH11	1.76	0.49
2:ID:17:VAL:HG11	2:IE:7:MET:HE3	1.94	0.49
2:IB:83:VAL:HG13	2:IB:87:LEU:HD12	1.93	0.49
2:JA:4:ALA:HB3	2:JA:48:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KA:17:VAL:HG22	2:KB:87:LEU:HD13	1.94	0.49
2:LD:83:VAL:HG13	2:LD:87:LEU:HD12	1.93	0.49
2:LF:83:VAL:HG13	2:LF:87:LEU:HD12	1.94	0.49
2:JC:19:ALA:HB2	2:JC:64:ALA:HB2	1.94	0.49
2:KE:18:GLU:OE1	2:KF:74:HIS:NE2	2.45	0.49
2:HF:19:ALA:HB2	2:HF:64:ALA:HB2	1.93	0.49
2:LE:17:VAL:HG11	2:LF:7:MET:HE1	1.95	0.49
2:HE:4:ALA:HB3	2:HE:48:GLY:O	2.13	0.49
2:IA:7:MET:HE1	2:IF:17:VAL:HG11	1.95	0.49
2:ID:83:VAL:HG13	2:ID:87:LEU:HD12	1.94	0.49
1:C:25:LEU:HB2	1:C:61:LEU:HB2	1.95	0.48
1:C:149:ASP:OD1	1:C:163:THR:OG1	2.24	0.48
2:HC:18:GLU:OE1	2:HD:74:HIS:NE2	2.46	0.48
2:JD:13:PHE:HB2	2:JE:37:THR:HG21	1.96	0.48
2:ID:4:ALA:HB3	2:ID:48:GLY:O	2.13	0.48
2:KA:74:HIS:NE2	2:KF:18:GLU:OE1	2.46	0.48
2:KE:7:MET:HG2	2:KE:45:VAL:HG22	1.96	0.48
2:HB:18:GLU:OE1	2:HC:74:HIS:NE2	2.47	0.48
2:KA:19:ALA:HB2	2:KA:64:ALA:HB2	1.94	0.48
2:KA:5:LEU:HD23	2:KA:76:ILE:HD12	1.95	0.48
2:KD:83:VAL:HG13	2:KD:87:LEU:HD12	1.95	0.48
2:LD:5:LEU:HD23	2:LD:76:ILE:HD12	1.95	0.48
2:JE:5:LEU:HD23	2:JE:76:ILE:HD12	1.95	0.48
1:B:50:MET:HG2	1:B:62:MET:HB2	1.96	0.47
2:HE:18:GLU:OE1	2:HF:74:HIS:NE2	2.46	0.47
2:IB:19:ALA:HB2	2:IB:64:ALA:HB2	1.96	0.47
2:JC:2:ALA:O	2:JC:78:ARG:NH1	2.47	0.47
2:JF:4:ALA:HB3	2:JF:48:GLY:O	2.13	0.47
2:LB:17:VAL:HG11	2:LC:7:MET:HE1	1.96	0.47
2:JA:7:MET:HE1	2:JF:17:VAL:HG11	1.96	0.47
1:A:115:GLU:OE1	1:A:148:ARG:NH1	2.40	0.47
2:LA:7:MET:HE1	2:LF:17:VAL:HG11	1.96	0.47
2:HD:30:GLU:OE1	2:HD:91:ARG:NH2	2.40	0.47
2:IB:47:ARG:HH12	2:IB:79:PRO:HG3	1.80	0.47
2:GA:4:ALA:HB3	2:GA:48:GLY:O	2.14	0.47
2:GA:5:LEU:HD23	2:GA:76:ILE:HD12	1.97	0.47
2:GC:4:ALA:HB3	2:GC:48:GLY:O	2.14	0.47
2:HE:5:LEU:HD23	2:HE:76:ILE:HD12	1.96	0.47
2:HC:7:MET:HG2	2:HC:45:VAL:HG22	1.97	0.47
2:IC:5:LEU:HD23	2:IC:76:ILE:HD12	1.96	0.47
2:IC:19:ALA:HB2	2:IC:64:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ID:18:GLU:OE1	2:IE:74:HIS:NE2	2.47	0.47
2:KA:17:VAL:HG11	2:KB:7:MET:HE1	1.97	0.47
1:A:36:VAL:HG13	1:A:77:ALA:HB1	1.97	0.47
2:HC:19:ALA:HB2	2:HC:64:ALA:HB2	1.97	0.47
1:C:151:ARG:HH21	1:C:155:GLY:HA3	1.79	0.46
2:HA:37:THR:HG21	2:HF:13:PHE:HB2	1.97	0.46
2:JE:19:ALA:HB2	2:JE:64:ALA:HB2	1.97	0.46
2:KD:18:GLU:OE1	2:KE:74:HIS:NE2	2.48	0.46
1:C:32:ARG:NH1	1:C:85:SER:O	2.48	0.46
2:IE:5:LEU:HD23	2:IE:76:ILE:HD12	1.98	0.46
2:KA:18:GLU:OE1	2:KB:74:HIS:NE2	2.48	0.46
1:A:41:LEU:HD11	1:A:48:LEU:HB2	1.98	0.46
2:KF:10:VAL:HG11	2:KF:15:GLY:HA3	1.98	0.46
1:A:194:ARG:NH1	2:KF:24:VAL:O	2.48	0.46
2:JE:4:ALA:HB3	2:JE:48:GLY:O	2.16	0.46
1:C:90:ASP:OD2	1:C:185:ARG:NH1	2.42	0.46
2:GD:83:VAL:HG13	2:GD:87:LEU:HD12	1.96	0.46
2:JD:30:GLU:OE1	2:JD:91:ARG:NH2	2.40	0.46
1:A:96:TYR:OH	1:A:99:GLU:OE2	2.33	0.46
2:GD:19:ALA:HB2	2:GD:64:ALA:HB2	1.97	0.46
2:JC:50:VAL:O	2:JC:54:LYS:HB2	2.16	0.46
2:KF:7:MET:HG2	2:KF:45:VAL:HG22	1.97	0.46
2:KD:5:LEU:HD13	2:KD:47:ARG:HH11	1.81	0.46
2:GE:18:GLU:OE1	2:GF:74:HIS:NE2	2.48	0.46
2:LA:50:VAL:O	2:LA:54:LYS:HB2	2.16	0.46
2:JC:18:GLU:OE1	2:JD:74:HIS:NE2	2.49	0.45
2:LA:34:TYR:HA	2:LA:43:THR:O	2.16	0.45
2:LC:7:MET:HG2	2:LC:45:VAL:HG22	1.97	0.45
2:LD:19:ALA:HB2	2:LD:64:ALA:HB2	1.98	0.45
1:A:150:MET:HG3	1:A:162:PHE:HB3	1.98	0.45
2:GA:47:ARG:HH12	2:GA:79:PRO:HG3	1.81	0.45
2:JB:19:ALA:HB2	2:JB:64:ALA:HB2	1.98	0.45
2:IB:5:LEU:HD23	2:IB:76:ILE:HD12	1.97	0.45
2:JD:7:MET:HG2	2:JD:45:VAL:HG22	1.98	0.45
2:GA:19:ALA:HB2	2:GA:64:ALA:HB2	1.98	0.45
2:KA:36:LYS:HE3	2:KB:37:THR:HA	1.98	0.45
1:B:27:LEU:HD22	1:B:33:GLY:HA2	1.98	0.45
2:LB:30:GLU:OE1	2:LB:91:ARG:NH2	2.44	0.45
2:ID:19:ALA:HB2	2:ID:64:ALA:HB2	1.99	0.45
1:A:129:VAL:HG13	1:A:152:LEU:HD22	1.98	0.45
2:GD:18:GLU:OE1	2:GE:74:HIS:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:N	1:C:62:MET:O	2.48	0.45
2:KC:30:GLU:OE1	2:KC:91:ARG:NH2	2.49	0.45
1:C:50:MET:HG2	1:C:62:MET:HB2	1.98	0.45
2:JF:19:ALA:HB2	2:JF:64:ALA:HB2	1.99	0.45
2:GB:30:GLU:OE1	2:GB:91:ARG:NH2	2.40	0.44
2:KB:30:GLU:OE1	2:KB:91:ARG:NH2	2.45	0.44
2:GD:4:ALA:HB3	2:GD:48:GLY:O	2.16	0.44
2:HD:19:ALA:HB2	2:HD:64:ALA:HB2	1.99	0.44
2:KD:19:ALA:HB2	2:KD:64:ALA:HB2	1.99	0.44
2:GA:30:GLU:OE1	2:GA:91:ARG:NH2	2.44	0.44
2:GB:83:VAL:HG13	2:GB:87:LEU:HD12	2.00	0.44
1:A:50:MET:HG2	1:A:62:MET:HB2	2.00	0.44
1:B:150:MET:HG3	1:B:162:PHE:HB3	1.99	0.44
1:C:96:TYR:OH	1:C:99:GLU:OE2	2.35	0.44
2:HA:19:ALA:HB2	2:HA:64:ALA:HB2	1.99	0.44
2:KC:17:VAL:HG11	2:KD:7:MET:HE1	1.99	0.44
2:JA:19:ALA:HB2	2:JA:64:ALA:HB2	2.00	0.44
2:GB:5:LEU:HD13	2:GB:47:ARG:HH11	1.83	0.44
2:HE:19:ALA:HB2	2:HE:64:ALA:HB2	2.00	0.44
2:IF:7:MET:HG2	2:IF:45:VAL:HG22	2.00	0.44
1:A:12:PRO:HG3	1:A:18:ASP:HA	1.99	0.43
1:C:43:ARG:NH2	1:C:79:GLU:OE2	2.51	0.43
2:GC:10:VAL:HG11	2:GC:15:GLY:HA3	1.99	0.43
2:HC:50:VAL:O	2:HC:54:LYS:HB2	2.19	0.43
2:JA:18:GLU:OE1	2:JB:74:HIS:NE2	2.51	0.43
2:GC:19:ALA:HB2	2:GC:64:ALA:HB2	2.01	0.43
1:A:135:SER:HB3	1:A:178:VAL:HG22	2.00	0.43
2:GB:19:ALA:HB2	2:GB:64:ALA:HB2	1.99	0.43
2:IE:2:ALA:O	2:IE:78:ARG:NH1	2.51	0.43
1:C:41:LEU:O	2:KA:78:ARG:NH1	2.51	0.43
2:GB:5:LEU:HD23	2:GB:76:ILE:HD12	2.00	0.43
2:IA:30:GLU:OE1	2:IA:91:ARG:NH2	2.45	0.43
2:LC:19:ALA:HB2	2:LC:64:ALA:HB2	2.00	0.43
1:A:135:SER:HG	1:A:182:CYS:HG	1.49	0.43
2:GC:5:LEU:HD23	2:GC:76:ILE:HD12	2.00	0.43
2:JA:50:VAL:O	2:JA:54:LYS:HB2	2.18	0.43
2:JB:13:PHE:HB2	2:JC:37:THR:HG21	2.00	0.43
1:C:27:LEU:HD22	1:C:33:GLY:HA2	2.01	0.43
2:JC:7:MET:HG2	2:JC:45:VAL:HG22	2.01	0.43
2:KB:19:ALA:HB2	2:KB:64:ALA:HB2	2.00	0.43
2:LE:10:VAL:HG11	2:LE:15:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GC:36:LYS:HE3	2:GD:37:THR:HA	2.01	0.43
2:KA:4:ALA:HB3	2:KA:48:GLY:O	2.18	0.43
1:A:142:THR:HG21	1:A:177:VAL:HG11	2.00	0.42
1:A:196:VAL:HG23	1:C:38:ASP:HB2	2.01	0.42
2:KC:13:PHE:HB2	2:KD:37:THR:HG21	2.00	0.42
2:KE:19:ALA:HB2	2:KE:64:ALA:HB2	2.01	0.42
2:LF:7:MET:HG2	2:LF:45:VAL:HG22	2.01	0.42
2:HD:13:PHE:HB2	2:HE:37:THR:HG21	2.01	0.42
1:C:24:VAL:HB	1:C:92:LEU:HB3	2.01	0.42
1:C:147:LEU:HD11	1:C:162:PHE:HB2	2.00	0.42
2:IB:36:LYS:HG2	2:IB:42:VAL:HG12	2.01	0.42
2:HA:74:HIS:NE2	2:HF:18:GLU:OE1	2.52	0.42
2:IE:49:ASP:OD1	2:IE:49:ASP:N	2.52	0.42
2:JE:49:ASP:N	2:JE:49:ASP:OD1	2.53	0.42
1:A:199:LEU:HG	1:A:203:LEU:HD23	2.02	0.42
2:HD:7:MET:HG2	2:HD:45:VAL:HG22	2.02	0.42
2:IB:7:MET:HG2	2:IB:45:VAL:HG22	2.02	0.42
2:GD:5:LEU:HD13	2:GD:47:ARG:HH11	1.85	0.42
2:JE:13:PHE:HB2	2:JF:37:THR:HG21	2.01	0.42
2:LA:19:ALA:HB2	2:LA:64:ALA:HB2	2.01	0.42
2:IE:18:GLU:OE1	2:IF:74:HIS:NE2	2.52	0.42
2:KA:7:MET:HG2	2:KA:45:VAL:HG22	2.02	0.42
2:LC:50:VAL:O	2:LC:54:LYS:HB2	2.20	0.42
2:LE:19:ALA:HB2	2:LE:64:ALA:HB2	2.00	0.42
2:IA:37:THR:HG21	2:IF:13:PHE:HB2	2.02	0.42
2:JF:47:ARG:NH2	2:JF:84:ASP:OD2	2.53	0.42
2:KB:36:LYS:HG2	2:KB:42:VAL:HG12	2.01	0.42
2:LA:7:MET:HG2	2:LA:45:VAL:HG22	2.00	0.42
2:GB:7:MET:HG2	2:GB:45:VAL:HG22	2.02	0.41
1:A:119:GLU:HG3	2:KF:28:LYS:HD3	2.02	0.41
2:HD:83:VAL:HG13	2:HD:87:LEU:HD12	2.02	0.41
2:IA:5:LEU:HD13	2:IA:47:ARG:HH11	1.85	0.41
1:C:75:ILE:HD12	1:C:78:ARG:HD2	2.03	0.41
2:IA:7:MET:HG2	2:IA:45:VAL:HG22	2.02	0.41
1:B:134:ASP:OD1	1:B:181:ARG:NH2	2.53	0.41
2:KC:36:LYS:HE3	2:KD:37:THR:HA	2.02	0.41
1:C:22:LEU:HD23	1:C:94:LEU:HD12	2.03	0.41
2:KB:7:MET:HG2	2:KB:45:VAL:HG22	2.03	0.41
2:JC:13:PHE:HB2	2:JD:37:THR:HG21	2.02	0.41
2:KB:13:PHE:HB2	2:KC:37:THR:HG21	2.02	0.41
2:KC:19:ALA:HB2	2:KC:64:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LB:18:GLU:OE1	2:LC:74:HIS:NE2	2.54	0.41
2:HB:30:GLU:OE1	2:HB:91:ARG:NH2	2.44	0.41
2:LA:74:HIS:NE2	2:LF:18:GLU:OE1	2.54	0.40
2:HD:49:ASP:N	2:HD:49:ASP:OD1	2.53	0.40
2:GB:78:ARG:HH11	2:LE:28:LYS:HB2	1.86	0.40
2:HC:13:PHE:HB2	2:HD:37:THR:HG21	2.04	0.40
2:HE:10:VAL:HG11	2:HE:15:GLY:HA3	2.02	0.40
2:JD:5:LEU:HD13	2:JD:47:ARG:HH11	1.87	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	199/205 (97%)	189 (95%)	10 (5%)	0	100	100
1	B	199/205 (97%)	190 (96%)	9 (4%)	0	100	100
1	C	199/205 (97%)	186 (94%)	13 (6%)	0	100	100
2	GA	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	GB	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	GC	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	GD	90/99 (91%)	90 (100%)	0	0	100	100
2	GE	90/99 (91%)	88 (98%)	2 (2%)	0	100	100
2	GF	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	HA	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	HB	90/99 (91%)	88 (98%)	2 (2%)	0	100	100
2	HC	90/99 (91%)	87 (97%)	3 (3%)	0	100	100
2	HD	90/99 (91%)	90 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	HE	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	HF	90/99 (91%)	90 (100%)	0	0	100	100
2	IA	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	IB	90/99 (91%)	90 (100%)	0	0	100	100
2	IC	90/99 (91%)	88 (98%)	2 (2%)	0	100	100
2	ID	90/99 (91%)	90 (100%)	0	0	100	100
2	IE	90/99 (91%)	87 (97%)	3 (3%)	0	100	100
2	IF	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	JA	90/99 (91%)	87 (97%)	3 (3%)	0	100	100
2	JB	90/99 (91%)	90 (100%)	0	0	100	100
2	JC	90/99 (91%)	90 (100%)	0	0	100	100
2	JD	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	JE	90/99 (91%)	90 (100%)	0	0	100	100
2	JF	90/99 (91%)	90 (100%)	0	0	100	100
2	KA	90/99 (91%)	90 (100%)	0	0	100	100
2	KB	90/99 (91%)	88 (98%)	2 (2%)	0	100	100
2	KC	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	KD	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	KE	90/99 (91%)	87 (97%)	3 (3%)	0	100	100
2	KF	90/99 (91%)	88 (98%)	2 (2%)	0	100	100
2	LA	90/99 (91%)	88 (98%)	2 (2%)	0	100	100
2	LB	90/99 (91%)	88 (98%)	2 (2%)	0	100	100
2	LC	90/99 (91%)	88 (98%)	2 (2%)	0	100	100
2	LD	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	LE	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
2	LF	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
All	All	3837/4179 (92%)	3763 (98%)	74 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	153/156 (98%)	153 (100%)	0	100	100
1	B	153/156 (98%)	153 (100%)	0	100	100
1	C	153/156 (98%)	153 (100%)	0	100	100
2	GA	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	GB	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	GC	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	GD	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	GE	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	GF	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	HA	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	HB	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	HC	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	HD	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	HE	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	HF	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	IA	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	IB	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	IC	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	ID	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	IE	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	IF	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	JA	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	JB	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	JC	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	JD	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	JE	63/68 (93%)	62 (98%)	1 (2%)	62	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	JF	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	KA	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	KB	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	KC	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	KD	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	KE	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	KF	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	LA	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	LB	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	LC	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	LD	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	LE	63/68 (93%)	62 (98%)	1 (2%)	62	81
2	LF	63/68 (93%)	62 (98%)	1 (2%)	62	81
All	All	2727/2916 (94%)	2691 (99%)	36 (1%)	70	84

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	GA	82	ASN
2	GB	82	ASN
2	GC	82	ASN
2	GD	82	ASN
2	GE	82	ASN
2	GF	82	ASN
2	HA	82	ASN
2	HB	82	ASN
2	HC	82	ASN
2	HD	82	ASN
2	HE	82	ASN
2	HF	82	ASN
2	IA	82	ASN
2	IB	82	ASN
2	IC	82	ASN
2	ID	82	ASN
2	IE	82	ASN
2	IF	82	ASN
2	JA	82	ASN

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Mol	Chain	Res	Type
2	JB	82	ASN
2	JC	82	ASN
2	JD	82	ASN
2	JE	82	ASN
2	JF	82	ASN
2	KA	82	ASN
2	KB	82	ASN
2	KC	82	ASN
2	KD	82	ASN
2	KE	82	ASN
2	KF	82	ASN
2	LA	82	ASN
2	LB	82	ASN
2	LC	82	ASN
2	LD	82	ASN
2	LE	82	ASN
2	LF	82	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
2	GD	82	ASN
2	GE	82	ASN
2	HB	82	ASN
2	HC	82	ASN
2	HF	82	ASN
2	IA	82	ASN
2	IC	82	ASN
2	IE	82	ASN
2	JC	82	ASN
2	JF	82	ASN
2	KC	82	ASN
2	KE	82	ASN
2	KF	82	ASN
2	LC	82	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

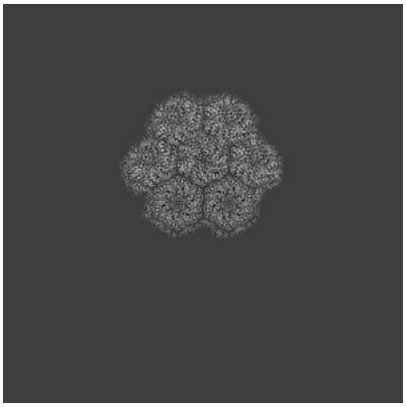
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9311. These allow visual inspection of the internal detail of the map and identification of artifacts.

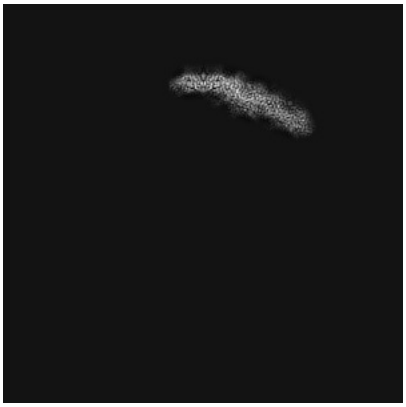
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

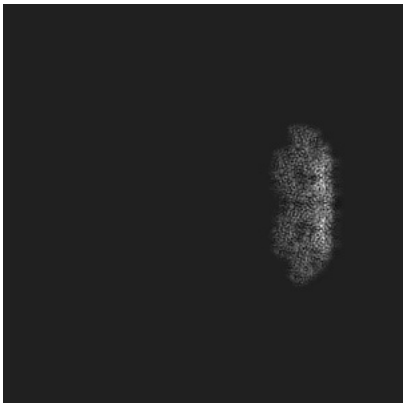
6.1.1 Primary map



X



Y

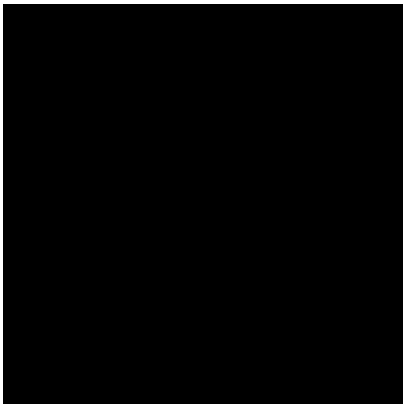


Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 256

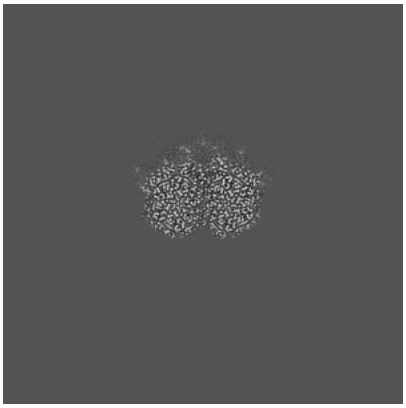
Y Index: 256

Z Index: 256

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: 410

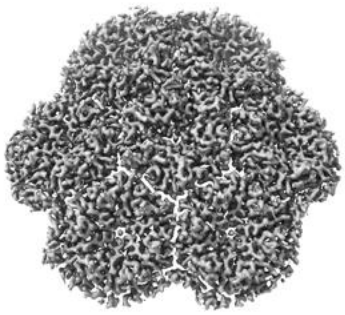
Y Index: 279

Z Index: 298

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

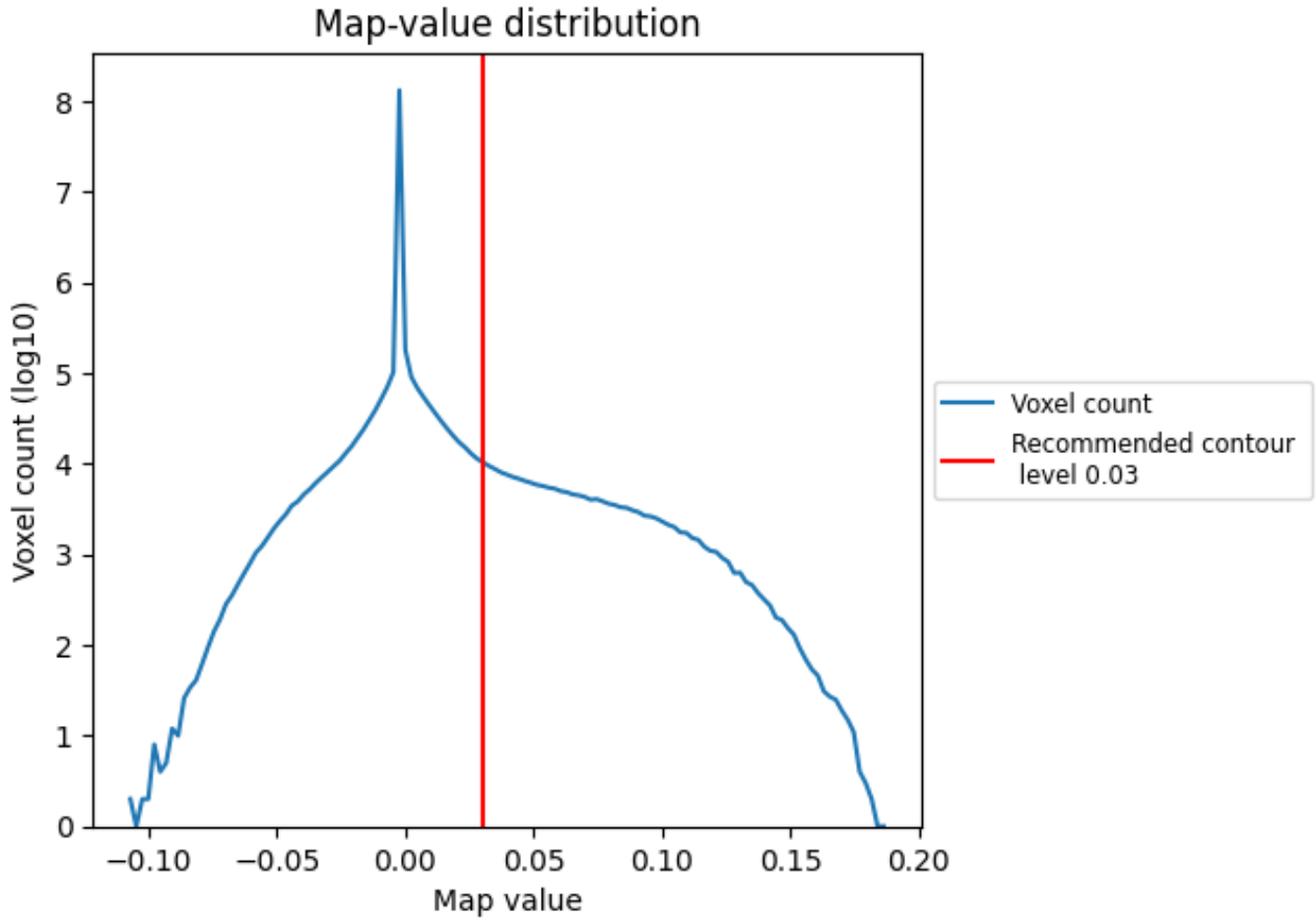
6.5 Mask visualisation (i)

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

7 Map analysis

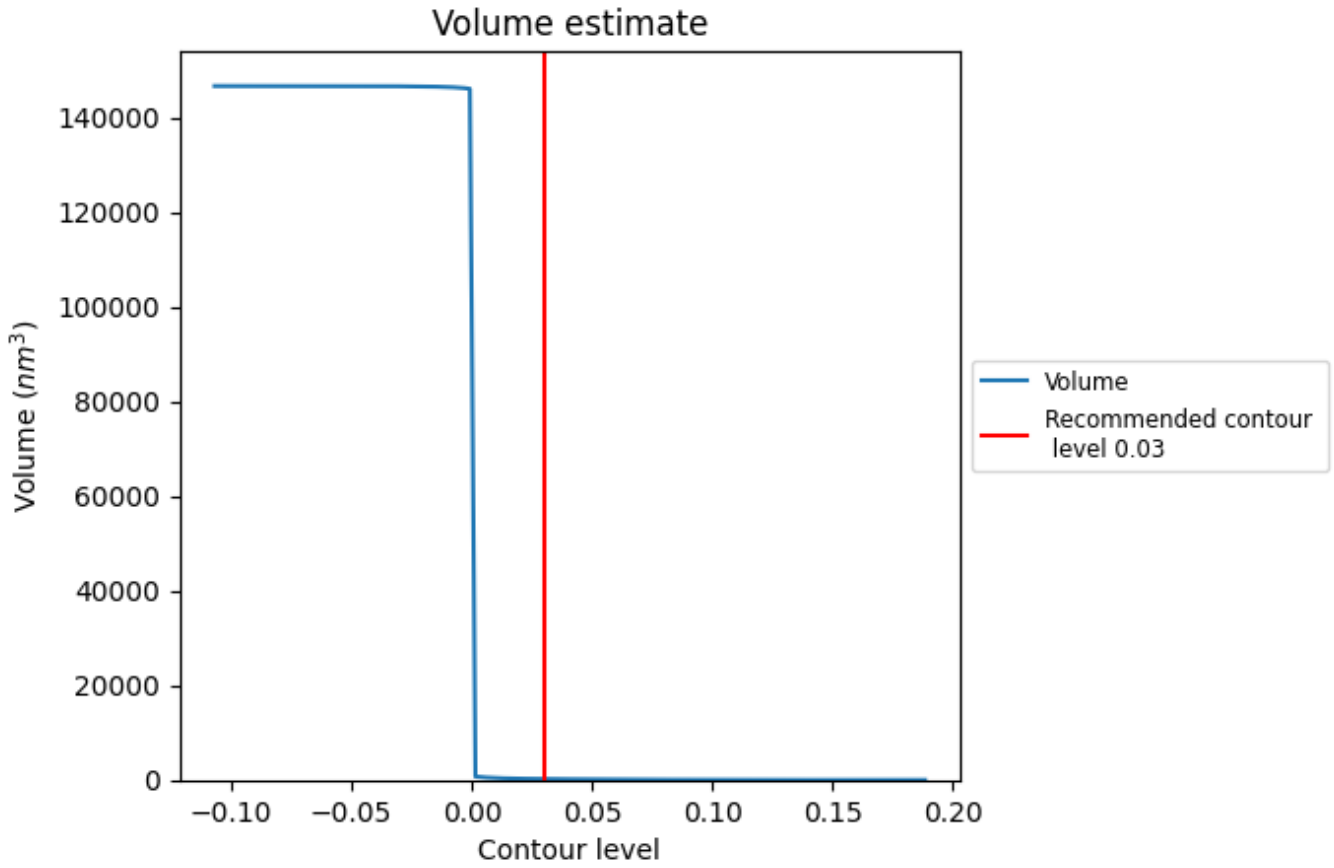
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

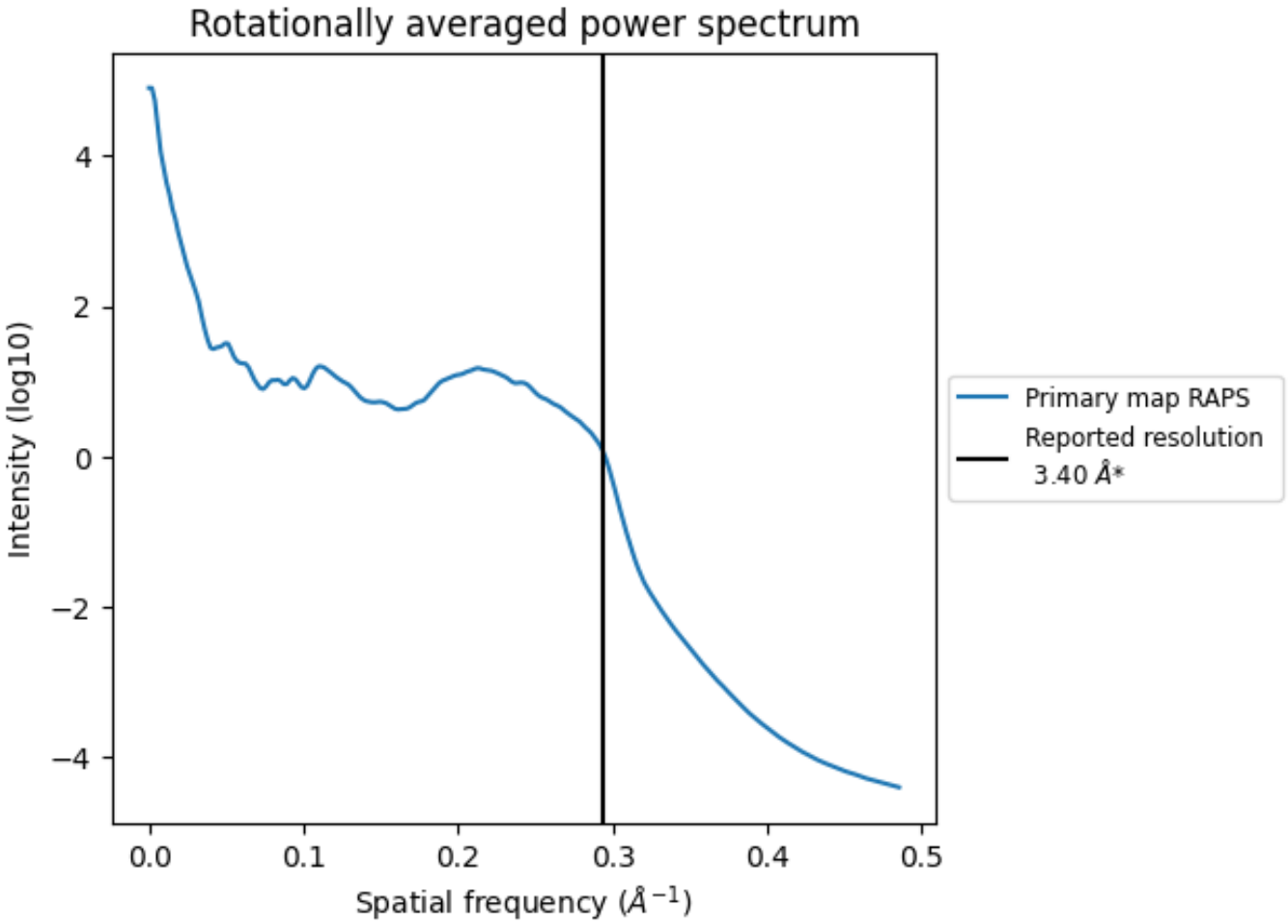
7.2 Volume estimate



The volume at the recommended contour level is 197 nm^3; this corresponds to an approximate mass of 178 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

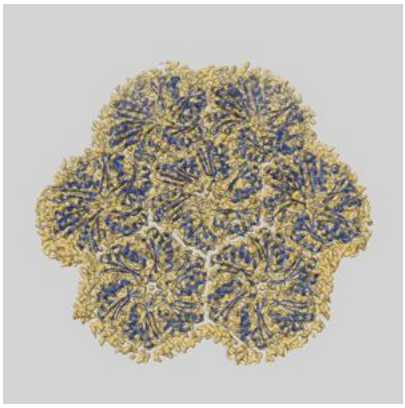
8 Fourier-Shell correlation

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

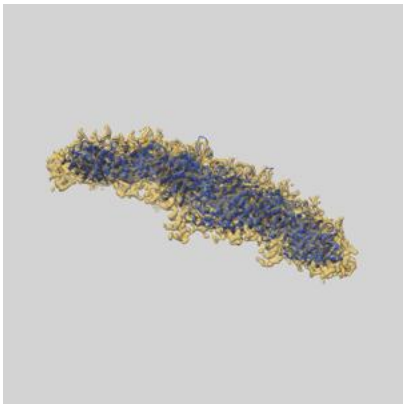
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9311 and PDB model 6N06. Per-residue inclusion information can be found in section 3 on page 8.

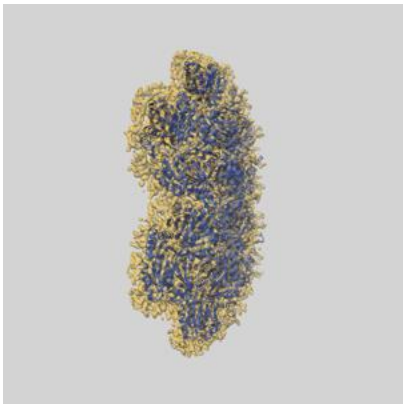
9.1 Map-model overlay



X



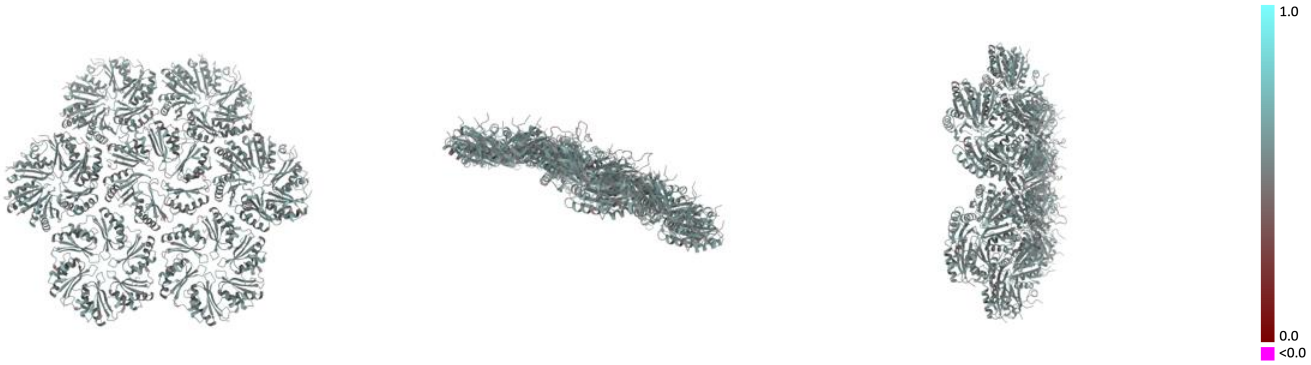
Y



Z

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

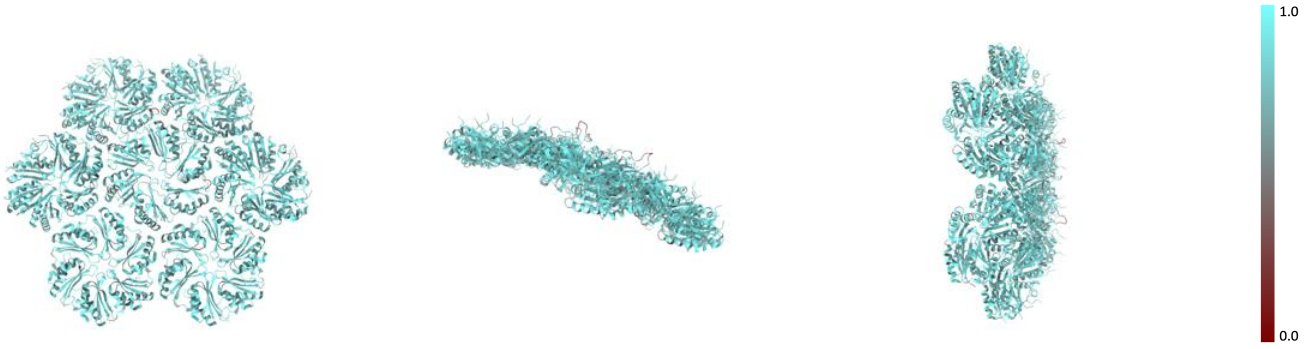
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

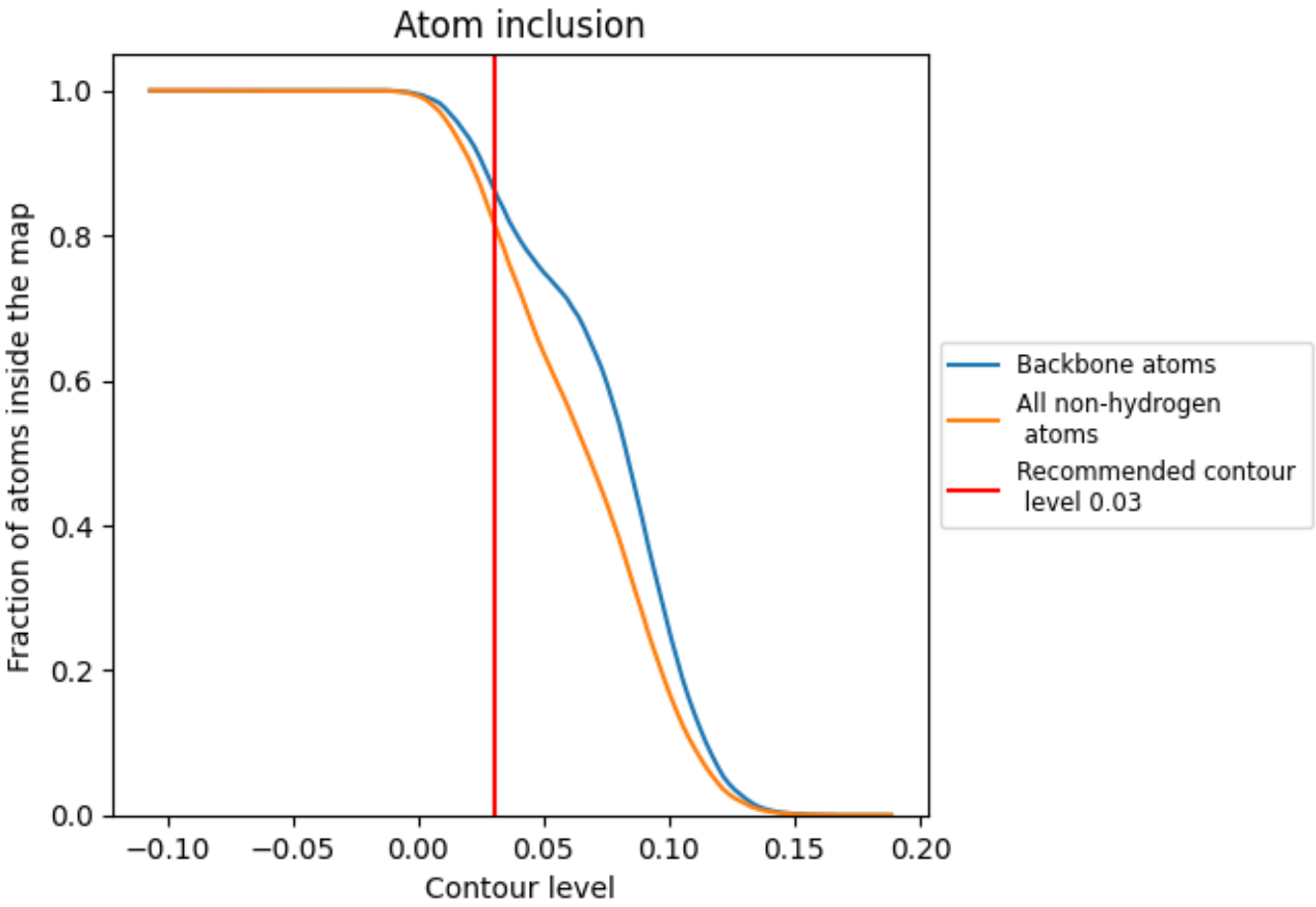
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8184	0.5300
A	0.8086	0.5260
B	0.7997	0.5180
C	0.8079	0.5210
GA	0.8323	0.5360
GB	0.8230	0.5360
GC	0.8199	0.5290
GD	0.8152	0.5290
GE	0.8121	0.5300
GF	0.8183	0.5290
HA	0.8168	0.5370
HB	0.8121	0.5180
HC	0.8137	0.5280
HD	0.8199	0.5350
HE	0.8214	0.5320
HF	0.8447	0.5380
IA	0.8214	0.5320
IB	0.8230	0.5370
IC	0.8121	0.5280
ID	0.8168	0.5280
IE	0.8043	0.5250
IF	0.8292	0.5290
JA	0.8276	0.5420
JB	0.8261	0.5230
JC	0.8075	0.5290
JD	0.8214	0.5280
JE	0.8307	0.5320
JF	0.8354	0.5350
KA	0.8339	0.5310
KB	0.8214	0.5380
KC	0.8043	0.5250
KD	0.8043	0.5240
KE	0.8106	0.5270
KF	0.8261	0.5310
LA	0.8292	0.5380

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Chain	Atom inclusion	Q-score
LB	0.8183	0.5240
LC	0.8090	0.5290
LD	0.8152	0.5360
LE	0.8276	0.5360
LF	0.8478	0.5340