



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:39 AM UTC

PDB ID : 9DYJ / pdb\_00009dyj  
EMDB ID : EMD-47306  
Title : BEST2 + GABA open state  
Authors : Owji, A.P.; Kittredge, A.K.; Zhang, Y.; Yang, T.  
Deposited on : 2024-10-14  
Resolution : 2.31 Å(reported)  
Based on initial model : 8D1E

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>.

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMD 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

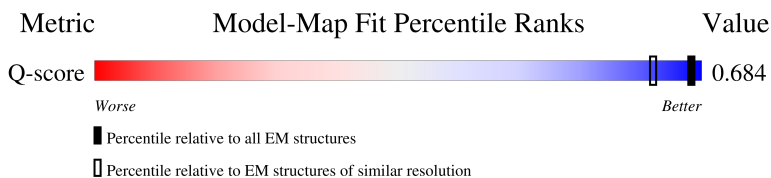
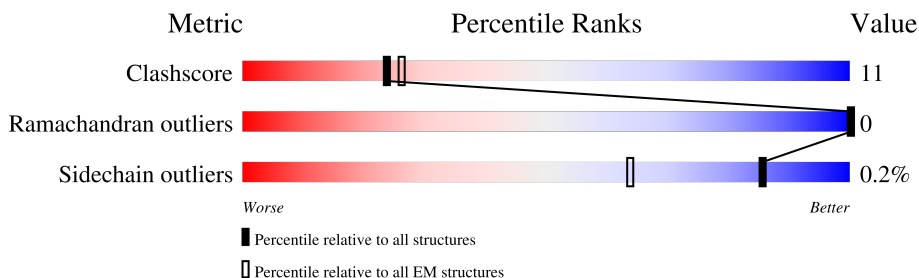
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.31 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	4306 ( 1.81 - 2.81 )

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	509	50% 18% 32%
1	B	509	51% 17% 32%
1	C	509	51% 17% 32%
1	D	509	51% 17% 32%

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Mol	Chain	Length	Quality of chain
1	E	509	 A horizontal bar chart showing the quality of chain E. The bar is divided into three segments: a green segment representing 50%, a yellow segment representing 18%, and a grey segment representing 32%. The percentages are labeled below the corresponding segments.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14431 atoms, of which 40 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.

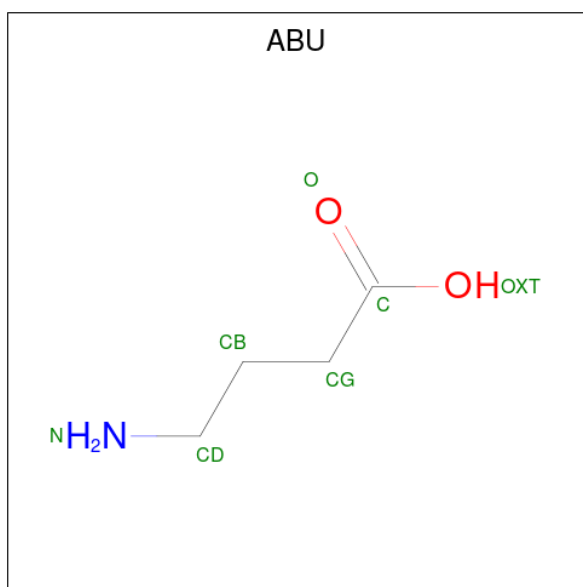
- Molecule 1 is a protein called Bestrophin-2a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	347	Total	C	N	O	S	2	0
			2870	1885	471	498	16		
1	B	347	Total	C	N	O	S	2	0
			2870	1885	471	498	16		
1	C	347	Total	C	N	O	S	2	0
			2870	1885	471	498	16		
1	D	347	Total	C	N	O	S	2	0
			2870	1885	471	498	16		
1	A	347	Total	C	N	O	S	2	0
			2870	1885	471	498	16		

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	E	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	
2	A	1	Total	Ca	0
			1	1	

- Molecule 3 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	H	N	O	0
			15	4	8	1	2	
3	B	1	Total	C	H	N	O	0
			15	4	8	1	2	
3	C	1	Total	C	H	N	O	0
			15	4	8	1	2	
3	D	1	Total	C	H	N	O	0
			15	4	8	1	2	
3	A	1	Total	C	H	N	O	0
			15	4	8	1	2	

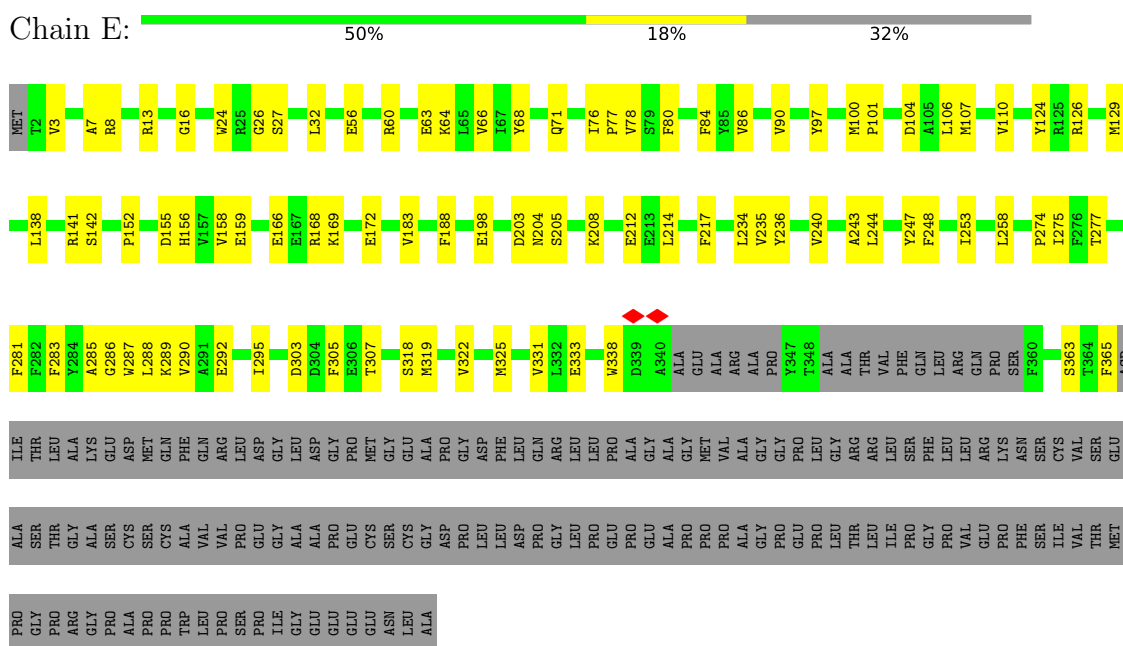
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Cl	0
			1	1	

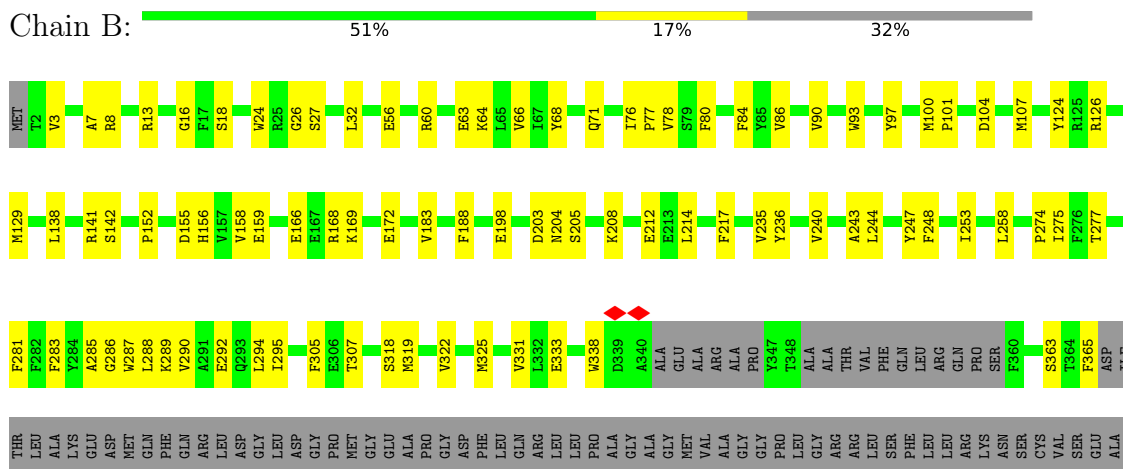
### 3 Residue-property plots

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

#### • Molecule 1: Bestrophin-2a



#### • Molecule 1: Bestrophin-2a



[illegible]

- Molecule 1: Bestrophin-2a

Chain C:  51% 17% 32%

ARG	GLY	ALA	F282	L138	MET
	GLY	ALA	F283		T3
PRO	PRO	GLU	Y284	R141	V2
ALA	ALA	ASP	A285	S142	
PRO	PRO	SER	G286		A7
PRO	PRO	GLN	W287	P152	R8
TRP	ALA	PHE	L288		
LEU	VAL	GLN	K289	D155	R13
PRO	VAL	ARG	V290	H156	
SER	PRO	LEU	A291	V157	G16
PRO	PRO	ASP	E292	V158	
ILE	GLY	GLY	Q293	E159	G26
GLY	ALA	LEU	L294		
GLU	GLU	ASP	L295	E166	L32
GLU	GLU	GLY		E167	
GLU	GLU	PRO	F305	E168	E56
GLU	GLY	MET	E306	K169	
ASN	SER	GLY	T307		R60
LEU	ALA	GLU		E172	
	GLY	ALA	M319		E63
	ASP	PRO		V183	K64
PRO	PRO	GLY	V322		L85
LEU	LEU	ASP		F188	V66
LEU	LEU	PHE	K325		I67
ASP	ASP	LEU		E198	Y68
PRO	PRO	GLN	V331		Q71
GLY	GLY	ARG	L332	D203	
LEU	LEU	LEU	E333	N204	
PRO	PRO	LEU		S205	I76
GLU	GLU	PRO	W338		P77
PRO	ALA	ALA	D339	K208	V78
GLU	GLU	ALA	A340	E212	S79
PRO	PRO	GLY	ALA	E213	F80
PRO	PRO	MET	GLU	L214	F84
PRO	PRO	VAL	ALA	ALA	Y85
ALA	ALA	ALA	ARG	F217	V86
GLY	GLY	GLY	ALA		
PRO	PRO	PRO	PRO	V235	V90
PRO	PRO	GLY	Y347	Y236	
PRO	GLU	LEU	T348		W33
LEU	LEU	GLY	ALA	V240	
THR	THR	ARG	ALA		Y97
LEU	ARG	ARG	THR	A243	
ILE	ILE	LEU	VAL	L244	M100
PRO	PRO	SER	PHE	Y245	P101
GLY	GLY	PHE	GLN	S246	
PRO	PRO	LEU	LEU	Y247	D104
VAL	VAL	LEU	ARG	F248	A105
GLU	GLU	LEU	GLN		L106
PRO	PRO	ARG	PRO		M107
PHE	PHE	ASN	SER	I253	
SER	SER	ASN	F360	L258	V110
ILE	ILE	CYS			
VAL	VAL	VAL	S363	P274	Y124
THR	THR	SER	T364	I275	R125
MET	MET	GLU	F365	F276	R126
PRO	PRO	ALA	ASP	T277	
GLY	GLY	SER	ILE		M129
PRO	PRO	THR	THR	F381	

- Molecule 1: Bestrophin-2a

Chain D:  51% 17% 32%

GLY	THR	F283	L138	MET
PRO	LEU	T284		T2
ARG	ALA	A285	R141	V3
GLY	LYS	G286	S142	
PRO	GLU	W287		A7
ALA	CYS	L288	P152	R8
PRO	MET	K289		
PRO	GLN	V290	D155	R13
PRO	PHE	A291	H156	
TRP	GLN	E292	V157	G16
LEU	ARG	G293	V158	
PRO	VAL	L294	E159	G26
SER	LEU	T296		
PRO	ASP		E166	L32
ILE	GLY		E167	
GLY	LEU	D303	G168	
GLY	ALA	A304	R169	E56
GLU	ASP	F305		
GLU	PRO	E306		R60
GLU	GLY	T307	E172	
GLU	MET			
ASN	GLY			E63
LEU	GLU	S318	V183	K64
ALA	ALA	K319	F188	L65
	ASP			V66
	PRO	V322	E198	I67
	LEU			Y68
	ASP	K325		
	PHE			Q71
	LEU		D203	
	ASP		N204	I76
	PRO	V331	S205	P77
	GLN	L332		
	ARG	E333		V78
	LEU		K208	S79
	LEU			
	PRO	W338	E212	F80
	GLU	A339	E213	
	ALA	A340	L214	
	ALA			F84
	GLY			Y85
	PRO		F217	V86
	PRO		ALA	
	VAL	ARG		
	ALA	ALA	V235	V90
	GLY	PRO	Y236	
	GLY			
	GLY	T347		W93
	PRO	T348	V240	
	LEU	ALA		Y97
	GLY	ALA	A243	
	ARG	THR	L244	M100
	ARG	VAL		P101
	LEU	PHE	Y247	
	PRO	GLN	F248	D104
	PHE	LEU	I253	A105
	LEU	LEU		L106
	VAL	GLN	L258	M107
	GLU	PRO		
	LYS	SER		V110
	ASN		P274	
	SER	F360	I275	Y124
	CYS		F276	R125
	VAL	S363	T277	R126
	THR	T364		
	SER	F365		
	GLU	ASP	F281	M129
	ALA		E293	

- Molecule 1: Bestrophin-2a

Chain A:  50% 18% 32%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	103839	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 ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.203	Depositor
Minimum map value	-2.456	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ABU, CL

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	0.16	0/2953	0.29	0/4005
1	B	0.17	0/2953	0.29	0/4005
1	C	0.16	0/2953	0.29	0/4005
1	D	0.17	0/2953	0.29	0/4005
1	E	0.16	0/2953	0.29	0/4005
All	All	0.16	0/14765	0.29	0/20025

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	2870	0	2838	75	0
1	B	2870	0	2838	75	0
1	C	2870	0	2838	74	0
1	D	2870	0	2838	74	0
1	E	2870	0	2838	76	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	7	8	0	0	0
3	B	7	8	0	0	0
3	C	7	8	0	0	0
3	D	7	8	0	0	0
3	E	7	8	0	0	0
4	A	1	0	0	0	0
All	All	14391	40	14190	311	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 (311) 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)
1:D:286:GLY:O	1:D:290:VAL:HG23	1.74	0.88
1:A:286:GLY:O	1:A:290:VAL:HG23	1.74	0.88
1:A:155:ASP:OD1	1:A:168:ARG:NH1	2.08	0.87
1:C:155:ASP:OD1	1:C:168:ARG:NH1	2.08	0.87
1:B:286:GLY:O	1:B:290:VAL:HG23	1.74	0.87
1:E:286:GLY:O	1:E:290:VAL:HG23	1.74	0.86
1:B:155:ASP:OD1	1:B:168:ARG:NH1	2.08	0.86
1:D:155:ASP:OD1	1:D:168:ARG:NH1	2.08	0.86
1:C:286:GLY:O	1:C:290:VAL:HG23	1.74	0.86
1:E:155:ASP:OD1	1:E:168:ARG:NH1	2.08	0.83
1:E:235:VAL:HG21	1:D:290:VAL:HG13	1.67	0.77
1:B:235:VAL:HG21	1:A:290:VAL:HG13	1.67	0.77
1:E:290:VAL:HG13	1:A:235:VAL:HG21	1.67	0.77
1:C:63:GLU:HG2	1:C:258:LEU:HD22	1.67	0.76
1:E:63:GLU:HG2	1:E:258:LEU:HD22	1.67	0.76
1:B:63:GLU:HG2	1:B:258:LEU:HD22	1.67	0.75
1:C:290:VAL:HG13	1:D:235:VAL:HG21	1.68	0.75
1:D:63:GLU:HG2	1:D:258:LEU:HD22	1.68	0.75
1:B:290:VAL:HG13	1:C:235:VAL:HG21	1.68	0.75
1:A:63:GLU:HG2	1:A:258:LEU:HD22	1.67	0.75
1:B:285:ALA:O	1:B:289:LYS:HG2	1.91	0.71
1:C:285:ALA:O	1:C:289:LYS:HG2	1.91	0.70
1:E:285:ALA:O	1:E:289:LYS:HG2	1.91	0.70
1:D:285:ALA:O	1:D:289:LYS:HG2	1.91	0.70
1:A:285:ALA:O	1:A:289:LYS:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:HD13	1:C:289:LYS:HG3	1.74	0.70
1:D:32:LEU:HD13	1:D:289:LYS:HG3	1.74	0.69
1:B:32:LEU:HD13	1:B:289:LYS:HG3	1.74	0.69
1:E:32:LEU:HD13	1:E:289:LYS:HG3	1.74	0.69
1:A:32:LEU:HD13	1:A:289:LYS:HG3	1.74	0.69
1:E:86:VAL:HG21	1:E:287:TRP:CD1	2.31	0.66
1:C:86:VAL:HG21	1:C:287:TRP:CD1	2.31	0.66
1:A:86:VAL:HG21	1:A:287:TRP:CD1	2.31	0.65
1:B:86:VAL:HG21	1:B:287:TRP:CD1	2.31	0.65
1:D:86:VAL:HG21	1:D:287:TRP:CD1	2.31	0.65
1:E:325:MET:HE1	1:A:183:VAL:HG13	1.80	0.63
1:B:325:MET:HE1	1:C:183:VAL:HG13	1.80	0.63
1:B:183:VAL:HG13	1:A:325:MET:HE1	1.80	0.62
1:C:325:MET:HE1	1:D:183:VAL:HG13	1.80	0.62
1:E:183:VAL:HG13	1:D:325:MET:HE1	1.80	0.62
1:B:124:TYR:OH	1:B:198:GLU:OE1	2.13	0.62
1:C:124:TYR:OH	1:C:198:GLU:OE1	2.13	0.59
1:E:243:ALA:HA	1:D:283:PHE:CZ	2.38	0.58
1:C:283:PHE:CZ	1:D:243:ALA:HA	2.39	0.58
1:B:243:ALA:HA	1:A:283:PHE:CZ	2.38	0.58
1:E:283:PHE:CZ	1:A:243:ALA:HA	2.38	0.58
1:D:97:TYR:HB2	1:D:305:PHE:CZ	2.39	0.58
1:B:283:PHE:CZ	1:C:243:ALA:HA	2.39	0.57
1:C:283:PHE:CE2	1:D:76:ILE:HG23	2.40	0.57
1:C:104:ASP:O	1:C:107:MET:HG2	2.05	0.57
1:E:104:ASP:O	1:E:107:MET:HG2	2.05	0.57
1:B:129:MET:HB2	1:B:319:MET:HE1	1.86	0.57
1:C:97:TYR:HB2	1:C:305:PHE:CZ	2.39	0.57
1:D:129:MET:HB2	1:D:319:MET:HE1	1.87	0.57
1:E:97:TYR:HB2	1:E:305:PHE:CZ	2.39	0.57
1:B:283:PHE:CE2	1:C:76:ILE:HG23	2.40	0.57
1:A:97:TYR:HB2	1:A:305:PHE:CZ	2.39	0.57
1:B:76:ILE:HG23	1:A:283:PHE:CE2	2.40	0.57
1:A:60:ARG:O	1:A:64:LYS:HG3	2.05	0.57
1:B:104:ASP:O	1:B:107:MET:HG2	2.05	0.56
1:B:290:VAL:HG13	1:C:235:VAL:CG2	2.35	0.56
1:E:76:ILE:HG23	1:D:283:PHE:CE2	2.41	0.56
1:E:235:VAL:CG2	1:D:290:VAL:HG13	2.34	0.56
1:E:283:PHE:CE2	1:A:76:ILE:HG23	2.40	0.56
1:B:97:TYR:HB2	1:B:305:PHE:CZ	2.39	0.56
1:A:104:ASP:O	1:A:107:MET:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ARG:O	1:E:64:LYS:HG3	2.05	0.56
1:B:60:ARG:O	1:B:64:LYS:HG3	2.05	0.56
1:D:60:ARG:O	1:D:64:LYS:HG3	2.05	0.56
1:B:235:VAL:CG2	1:A:290:VAL:HG13	2.34	0.56
1:D:104:ASP:O	1:D:107:MET:HG2	2.05	0.56
1:B:325:MET:CE	1:C:183:VAL:HG13	2.36	0.56
1:B:183:VAL:HG13	1:A:325:MET:CE	2.36	0.56
1:E:274:PRO:HB2	1:E:277:THR:HB	1.88	0.56
1:E:325:MET:CE	1:A:183:VAL:HG13	2.36	0.56
1:C:129:MET:HB2	1:C:319:MET:HE1	1.86	0.56
1:A:129:MET:HB2	1:A:319:MET:HE1	1.87	0.56
1:C:325:MET:CE	1:D:183:VAL:HG13	2.36	0.55
1:E:129:MET:HB2	1:E:319:MET:HE1	1.87	0.55
1:C:60:ARG:O	1:C:64:LYS:HG3	2.05	0.55
1:C:290:VAL:HG13	1:D:235:VAL:CG2	2.35	0.55
1:E:290:VAL:HG13	1:A:235:VAL:CG2	2.34	0.55
1:D:274:PRO:HB2	1:D:277:THR:HB	1.88	0.55
1:A:274:PRO:HB2	1:A:277:THR:HB	1.88	0.55
1:D:208:LYS:O	1:D:212:GLU:HG3	2.07	0.55
1:A:208:LYS:O	1:A:212:GLU:HG3	2.07	0.55
1:C:208:LYS:O	1:C:212:GLU:HG3	2.07	0.54
1:E:208:LYS:O	1:E:212:GLU:HG3	2.07	0.54
1:E:183:VAL:HG13	1:D:325:MET:CE	2.36	0.54
1:B:274:PRO:HB2	1:B:277:THR:HB	1.88	0.54
1:C:274:PRO:HB2	1:C:277:THR:HB	1.88	0.54
1:B:208:LYS:O	1:B:212:GLU:HG3	2.07	0.54
1:B:18:SER:HG	1:C:245:TYR:HH	1.52	0.53
1:D:292:GLU:O	1:D:295:ILE:HG22	2.09	0.53
1:E:292:GLU:O	1:E:295:ILE:HG22	2.09	0.52
1:A:208:LYS:NZ	1:A:212:GLU:OE2	2.40	0.52
1:D:56:GLU:O	1:D:60:ARG:HG2	2.09	0.52
1:E:56:GLU:O	1:E:60:ARG:HG2	2.09	0.52
1:C:292:GLU:O	1:C:295:ILE:HG22	2.09	0.52
1:A:129:MET:CG	1:A:322:VAL:HG11	2.39	0.52
1:A:292:GLU:O	1:A:295:ILE:HG22	2.09	0.52
1:E:129:MET:CG	1:E:322:VAL:HG11	2.39	0.52
1:C:129:MET:CG	1:C:322:VAL:HG11	2.39	0.52
1:B:56:GLU:O	1:B:60:ARG:HG2	2.09	0.52
1:B:292:GLU:O	1:B:295:ILE:HG22	2.09	0.52
1:A:56:GLU:O	1:A:60:ARG:HG2	2.09	0.52
1:B:129:MET:CG	1:B:322:VAL:HG11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG21	1:B:168:ARG:HG3	1.92	0.52
1:E:158:VAL:HG21	1:E:168:ARG:HG3	1.92	0.51
1:D:129:MET:CG	1:D:322:VAL:HG11	2.39	0.51
1:D:158:VAL:HG21	1:D:168:ARG:HG3	1.92	0.51
1:A:124:TYR:OH	1:A:198:GLU:OE1	2.13	0.51
1:C:56:GLU:O	1:C:60:ARG:HG2	2.09	0.51
1:C:158:VAL:HG21	1:C:168:ARG:HG3	1.91	0.51
1:A:158:VAL:HG21	1:A:168:ARG:HG3	1.92	0.51
1:B:208:LYS:NZ	1:B:212:GLU:OE2	2.40	0.50
1:E:208:LYS:NZ	1:E:212:GLU:OE2	2.40	0.48
1:A:244:LEU:HD22	1:A:288:LEU:HD23	1.96	0.48
1:B:244:LEU:HD22	1:B:288:LEU:HD23	1.96	0.48
1:E:244:LEU:HD22	1:E:288:LEU:HD23	1.96	0.47
1:C:244:LEU:HD22	1:C:288:LEU:HD23	1.96	0.47
1:C:338:TRP:CZ3	1:D:126:ARG:HD3	2.50	0.47
1:D:331:VAL:O	1:D:333:GLU:OE2	2.33	0.47
1:E:126:ARG:HD3	1:D:338:TRP:CZ3	2.50	0.47
1:E:331:VAL:O	1:E:333:GLU:OE2	2.33	0.47
1:D:244:LEU:HD22	1:D:288:LEU:HD23	1.96	0.47
1:A:77:PRO:HB2	1:A:80:PHE:HB3	1.97	0.46
1:A:331:VAL:O	1:A:333:GLU:OE2	2.33	0.46
1:E:13:ARG:HG3	1:E:16:GLY:HA2	1.97	0.46
1:B:13:ARG:HG3	1:B:16:GLY:HA2	1.97	0.46
1:B:77:PRO:HB2	1:B:80:PHE:HB3	1.97	0.46
1:B:126:ARG:HD3	1:A:338:TRP:CZ3	2.51	0.46
1:E:124:TYR:OH	1:E:198:GLU:OE1	2.13	0.46
1:B:13:ARG:CG	1:B:16:GLY:HA2	2.45	0.46
1:C:13:ARG:CG	1:C:16:GLY:HA2	2.45	0.46
1:D:13:ARG:HG3	1:D:16:GLY:HA2	1.97	0.46
1:D:77:PRO:HB2	1:D:80:PHE:HB3	1.97	0.46
1:D:100:MET:CE	1:D:307:THR:HG22	2.46	0.46
1:A:13:ARG:CG	1:A:16:GLY:HA2	2.45	0.46
1:A:100:MET:CE	1:A:307:THR:HG22	2.45	0.46
1:C:331:VAL:O	1:C:333:GLU:OE2	2.33	0.46
1:A:13:ARG:HG3	1:A:16:GLY:HA2	1.97	0.46
1:D:129:MET:HG3	1:D:322:VAL:HG11	1.97	0.46
1:A:24:TRP:O	1:A:27:SER:OG	2.30	0.46
1:B:100:MET:CE	1:B:307:THR:HG22	2.45	0.46
1:C:100:MET:CE	1:C:307:THR:HG22	2.45	0.46
1:C:208:LYS:NZ	1:C:212:GLU:OE2	2.40	0.46
1:A:129:MET:HG3	1:A:322:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:HD22	1:B:288:LEU:CD2	2.46	0.46
1:B:331:VAL:O	1:B:333:GLU:OE2	2.33	0.46
1:D:275:ILE:HD12	1:D:275:ILE:H	1.81	0.46
1:E:13:ARG:CG	1:E:16:GLY:HA2	2.45	0.46
1:B:275:ILE:HD12	1:B:275:ILE:H	1.81	0.46
1:C:13:ARG:HG3	1:C:16:GLY:HA2	1.97	0.45
1:C:77:PRO:HB2	1:C:80:PHE:HB3	1.97	0.45
1:C:129:MET:HG3	1:C:322:VAL:HG11	1.97	0.45
1:E:100:MET:CE	1:E:307:THR:HG22	2.45	0.45
1:D:13:ARG:CG	1:D:16:GLY:HA2	2.45	0.45
1:D:248:PHE:CZ	1:D:281:PHE:HA	2.52	0.45
1:A:66:VAL:HG22	1:A:253:ILE:O	2.16	0.45
1:E:66:VAL:HG22	1:E:253:ILE:O	2.16	0.45
1:E:338:TRP:CZ3	1:A:126:ARG:HD3	2.51	0.45
1:B:3:VAL:HG21	1:B:26:GLY:HA3	1.98	0.45
1:B:129:MET:HG3	1:B:322:VAL:HG11	1.97	0.45
1:B:338:TRP:CZ3	1:C:126:ARG:HD3	2.51	0.45
1:C:8:ARG:O	1:C:13:ARG:NH1	2.50	0.45
1:D:8:ARG:O	1:D:13:ARG:NH1	2.50	0.45
1:E:244:LEU:HD22	1:E:288:LEU:CD2	2.46	0.45
1:C:3:VAL:HG21	1:C:26:GLY:HA3	1.98	0.45
1:C:248:PHE:CZ	1:C:281:PHE:HA	2.52	0.45
1:C:275:ILE:HD12	1:C:275:ILE:H	1.81	0.45
1:D:244:LEU:HD22	1:D:288:LEU:CD2	2.46	0.45
1:A:3:VAL:HG21	1:A:26:GLY:HA3	1.98	0.45
1:B:248:PHE:CZ	1:B:281:PHE:HA	2.52	0.45
1:C:66:VAL:HG22	1:C:253:ILE:O	2.16	0.45
1:A:168:ARG:O	1:A:172:GLU:HG2	2.17	0.45
1:E:77:PRO:HB2	1:E:80:PHE:HB3	1.97	0.45
1:B:66:VAL:HG22	1:B:253:ILE:O	2.16	0.45
1:C:236:TYR:O	1:C:240[B]:VAL:HG23	2.17	0.45
1:D:78:VAL:HG21	1:D:247:TYR:CG	2.52	0.45
1:D:168:ARG:O	1:D:172:GLU:HG2	2.17	0.45
1:E:129:MET:HG3	1:E:322:VAL:HG11	1.97	0.45
1:E:236:TYR:O	1:E:240[B]:VAL:HG23	2.17	0.45
1:E:248:PHE:CZ	1:E:281:PHE:HA	2.52	0.45
1:B:8:ARG:O	1:B:13:ARG:NH1	2.50	0.45
1:A:8:ARG:O	1:A:13:ARG:NH1	2.50	0.45
1:E:142:SER:HA	1:C:365:PHE:CE2	2.52	0.45
1:E:275:ILE:HD12	1:E:275:ILE:H	1.81	0.45
1:B:236:TYR:O	1:B:240[B]:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:VAL:HG21	1:C:247:TYR:CG	2.52	0.45
1:D:236:TYR:O	1:D:240[B]:VAL:HG23	2.17	0.45
1:A:236:TYR:O	1:A:240[B]:VAL:HG23	2.17	0.45
1:A:244:LEU:HD22	1:A:288:LEU:CD2	2.46	0.45
1:A:275:ILE:H	1:A:275:ILE:HD12	1.81	0.45
1:B:107:MET:HB3	1:B:129:MET:HE2	1.99	0.45
1:A:107:MET:HB3	1:A:129:MET:HE2	1.99	0.45
1:E:287:TRP:CZ2	1:A:84:PHE:CD1	3.06	0.44
1:B:203:ASP:OD2	1:B:205[A]:SER:OG	2.32	0.44
1:E:8:ARG:O	1:E:13:ARG:NH1	2.50	0.44
1:B:68:TYR:HA	1:B:71:GLN:HE21	1.83	0.44
1:B:168:ARG:O	1:B:172:GLU:HG2	2.17	0.44
1:C:68:TYR:HA	1:C:71:GLN:HE21	1.83	0.44
1:C:101:PRO:HB2	1:C:217:PHE:CE2	2.53	0.44
1:D:66:VAL:HG22	1:D:253:ILE:O	2.16	0.44
1:D:68:TYR:HA	1:D:71:GLN:HE21	1.83	0.44
1:C:86:VAL:O	1:C:90:VAL:HG23	2.18	0.44
1:C:244:LEU:HD22	1:C:288:LEU:CD2	2.46	0.44
1:D:203:ASP:OD2	1:D:205[A]:SER:OG	2.32	0.44
1:A:248:PHE:CZ	1:A:281:PHE:HA	2.52	0.44
1:E:24:TRP:O	1:E:27:SER:OG	2.30	0.44
1:E:101:PRO:HB2	1:E:217:PHE:CE2	2.53	0.44
1:E:203:ASP:OD2	1:E:205[A]:SER:OG	2.32	0.44
1:C:107:MET:HB3	1:C:129:MET:HE2	1.99	0.44
1:B:287:TRP:CZ2	1:C:84:PHE:CD1	3.06	0.44
1:D:208:LYS:NZ	1:D:212:GLU:OE2	2.40	0.44
1:D:365:PHE:CE2	1:A:142:SER:HA	2.52	0.44
1:A:86:VAL:O	1:A:90:VAL:HG23	2.18	0.44
1:A:152:PRO:HG2	1:A:156:HIS:CE1	2.53	0.44
1:E:3:VAL:HG21	1:E:26:GLY:HA3	1.98	0.44
1:E:287:TRP:HZ2	1:A:84:PHE:CD1	2.36	0.44
1:B:86:VAL:O	1:B:90:VAL:HG23	2.18	0.44
1:B:101:PRO:HB2	1:B:217:PHE:CE2	2.53	0.44
1:D:3:VAL:HG21	1:D:26:GLY:HA3	1.98	0.44
1:A:78:VAL:HG21	1:A:247:TYR:CG	2.52	0.44
1:E:107:MET:HB3	1:E:129:MET:HE2	1.99	0.44
1:E:152:PRO:HG2	1:E:156:HIS:CE1	2.53	0.44
1:E:168:ARG:O	1:E:172:GLU:HG2	2.17	0.44
1:E:188:PHE:CG	1:E:214:LEU:HD13	2.53	0.44
1:B:188:PHE:CG	1:B:214:LEU:HD13	2.53	0.44
1:C:100:MET:HE3	1:C:307:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:SER:HA	1:A:365:PHE:CE2	2.53	0.44
1:A:68:TYR:HA	1:A:71:GLN:HE21	1.83	0.44
1:A:101:PRO:HB2	1:A:217:PHE:CE2	2.53	0.44
1:E:7:ALA:HB2	1:D:363:SER:O	2.18	0.44
1:E:78:VAL:HG21	1:E:247:TYR:CG	2.52	0.44
1:B:84:PHE:CD1	1:A:287:TRP:CZ2	3.06	0.44
1:C:168:ARG:O	1:C:172:GLU:HG2	2.17	0.44
1:D:86:VAL:O	1:D:90:VAL:HG23	2.18	0.44
1:B:84:PHE:CD1	1:A:287:TRP:HZ2	2.36	0.43
1:D:101:PRO:HB2	1:D:217:PHE:CE2	2.53	0.43
1:D:152:PRO:HG2	1:D:156:HIS:CE1	2.53	0.43
1:B:363:SER:O	1:C:7:ALA:HB2	2.18	0.43
1:C:152:PRO:HG2	1:C:156:HIS:CE1	2.53	0.43
1:D:107:MET:HB3	1:D:129:MET:HE2	1.99	0.43
1:E:68:TYR:HA	1:E:71:GLN:HE21	1.83	0.43
1:E:86:VAL:O	1:E:90:VAL:HG23	2.18	0.43
1:B:152:PRO:HG2	1:B:156:HIS:CE1	2.53	0.43
1:D:124:TYR:OH	1:D:198:GLU:OE1	2.13	0.43
1:E:84:PHE:CD1	1:D:287:TRP:CZ2	3.06	0.43
1:B:78:VAL:HG21	1:B:247:TYR:CG	2.52	0.43
1:C:287:TRP:CZ2	1:D:84:PHE:CD1	3.06	0.43
1:C:363:SER:O	1:D:7:ALA:HB2	2.18	0.43
1:D:166:GLU:HA	1:D:169:LYS:HE2	2.01	0.43
1:A:100:MET:HE3	1:A:307:THR:HG22	2.00	0.43
1:A:188:PHE:CG	1:A:214:LEU:HD13	2.53	0.43
1:E:205[A]:SER:OG	1:A:204:ASN:HB3	2.19	0.43
1:B:287:TRP:HZ2	1:C:84:PHE:CD1	2.36	0.43
1:C:166:GLU:HA	1:C:169:LYS:HE2	2.01	0.43
1:E:100:MET:HE3	1:E:307:THR:HG22	2.00	0.43
1:B:100:MET:HE3	1:B:307:THR:HG22	2.00	0.43
1:C:86:VAL:HG21	1:C:287:TRP:HD1	1.83	0.43
1:C:287:TRP:HZ2	1:D:84:PHE:CD1	2.37	0.43
1:E:166:GLU:HA	1:E:169:LYS:HE2	2.01	0.43
1:B:205[A]:SER:OG	1:C:204:ASN:HB3	2.19	0.43
1:C:188:PHE:CG	1:C:214:LEU:HD13	2.53	0.43
1:D:100:MET:HE3	1:D:307:THR:HG22	2.00	0.43
1:E:84:PHE:CD1	1:D:287:TRP:HZ2	2.36	0.43
1:D:188:PHE:CG	1:D:214:LEU:HD13	2.53	0.43
1:B:7:ALA:HB2	1:A:363:SER:O	2.18	0.42
1:B:155:ASP:O	1:B:159:GLU:OE2	2.38	0.42
1:B:365:PHE:CE2	1:D:142:SER:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ASN:HB3	1:A:205[A]:SER:OG	2.19	0.42
1:C:155:ASP:O	1:C:159:GLU:OE2	2.38	0.42
1:D:155:ASP:O	1:D:159:GLU:OE2	2.38	0.42
1:A:166:GLU:HA	1:A:169:LYS:HE2	2.01	0.42
1:B:166:GLU:HA	1:B:169:LYS:HE2	2.01	0.42
1:C:205[A]:SER:OG	1:D:204:ASN:HB3	2.20	0.42
1:E:155:ASP:O	1:E:159:GLU:OE2	2.38	0.42
1:E:204:ASN:HB3	1:D:205[A]:SER:OG	2.20	0.42
1:E:363:SER:O	1:A:7:ALA:HB2	2.19	0.42
1:B:86:VAL:HG21	1:B:287:TRP:HD1	1.83	0.42
1:A:155:ASP:O	1:A:159:GLU:OE2	2.38	0.42
1:E:365:PHE:CE2	1:B:142:SER:HA	2.54	0.41
1:C:203:ASP:OD2	1:C:205[A]:SER:OG	2.32	0.41
1:E:248:PHE:CE1	1:E:281:PHE:HA	2.55	0.41
1:E:318:SER:O	1:E:322:VAL:HG22	2.21	0.41
1:B:24:TRP:O	1:B:27:SER:OG	2.30	0.41
1:B:318:SER:O	1:B:322:VAL:HG22	2.21	0.41
1:C:248:PHE:CE1	1:C:281:PHE:HA	2.55	0.41
1:A:106:LEU:O	1:A:110:VAL:HG23	2.21	0.41
1:A:138:LEU:O	1:A:141:ARG:HG2	2.21	0.41
1:B:138:LEU:O	1:B:141:ARG:HG2	2.21	0.41
1:B:248:PHE:CE1	1:B:281:PHE:HA	2.55	0.41
1:E:138:LEU:O	1:E:141:ARG:HG2	2.21	0.41
1:B:93:TRP:CD1	1:B:294:LEU:HD22	2.56	0.41
1:D:106:LEU:O	1:D:110:VAL:HG23	2.21	0.41
1:D:318:SER:O	1:D:322:VAL:HG22	2.21	0.41
1:C:106:LEU:O	1:C:110:VAL:HG23	2.21	0.41
1:C:138:LEU:O	1:C:141:ARG:HG2	2.21	0.41
1:A:93:TRP:CD1	1:A:294:LEU:HD22	2.56	0.41
1:A:203:ASP:OD2	1:A:205[A]:SER:OG	2.32	0.41
1:A:318:SER:O	1:A:322:VAL:HG22	2.21	0.41
1:A:248:PHE:CE1	1:A:281:PHE:HA	2.55	0.40
1:C:93:TRP:CD1	1:C:294:LEU:HD22	2.56	0.40
1:D:138:LEU:O	1:D:141:ARG:HG2	2.21	0.40
1:D:248:PHE:CE1	1:D:281:PHE:HA	2.56	0.40
1:D:93:TRP:CD1	1:D:294:LEU:HD22	2.56	0.40
1:E:26:GLY:O	1:A:234:LEU:HD23	2.22	0.40
1:E:86:VAL:HG21	1:E:287:TRP:HD1	1.83	0.40
1:E:106:LEU:O	1:E:110:VAL:HG23	2.21	0.40
1:E:234:LEU:HD23	1:D:26:GLY:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	343/509 (67%)	336 (98%)	7 (2%)	0	100	100
1	B	343/509 (67%)	336 (98%)	7 (2%)	0	100	100
1	C	343/509 (67%)	336 (98%)	7 (2%)	0	100	100
1	D	343/509 (67%)	336 (98%)	7 (2%)	0	100	100
1	E	343/509 (67%)	336 (98%)	7 (2%)	0	100	100
All	All	1715/2545 (67%)	1680 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/428 (71%)	304 (100%)	1 (0%)	86	92
1	B	305/428 (71%)	305 (100%)	0	100	100
1	C	305/428 (71%)	305 (100%)	0	100	100
1	D	305/428 (71%)	304 (100%)	1 (0%)	86	92
1	E	305/428 (71%)	304 (100%)	1 (0%)	86	92
All	All	1525/2140 (71%)	1522 (100%)	3 (0%)	85	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	303	ASP
1	D	303	ASP
1	A	303	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	71	GLN
1	B	71	GLN
1	C	71	GLN
1	D	71	GLN
1	A	71	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ABU	A	602	-	6,6,6	0.88	0	6,6,6	1.23	0
3	ABU	E	602	-	6,6,6	0.87	0	6,6,6	1.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ABU	D	602	-	6,6,6	0.87	0	6,6,6	1.23	0
3	ABU	C	602	-	6,6,6	0.87	0	6,6,6	1.23	0
3	ABU	B	602	-	6,6,6	0.87	0	6,6,6	1.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ABU	A	602	-	-	0/4/4/4	-
3	ABU	E	602	-	-	0/4/4/4	-
3	ABU	D	602	-	-	0/4/4/4	-
3	ABU	C	602	-	-	0/4/4/4	-
3	ABU	B	602	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

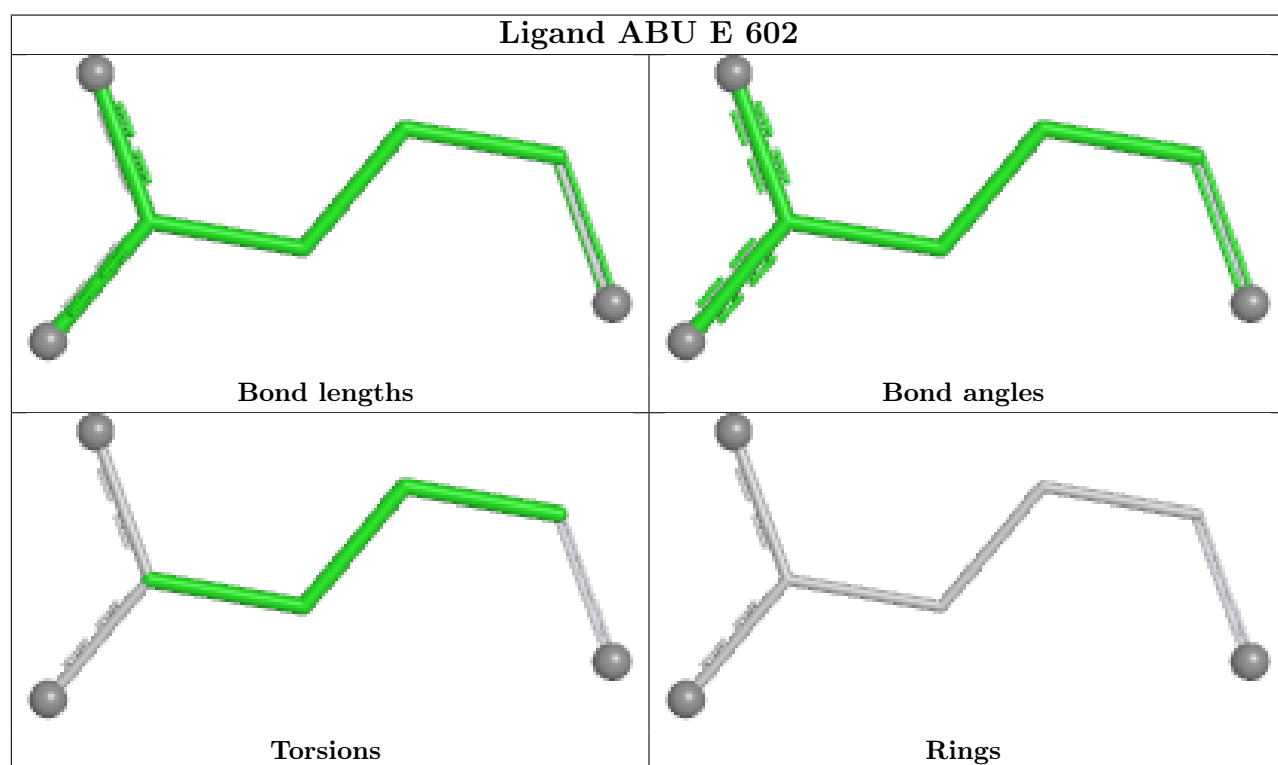
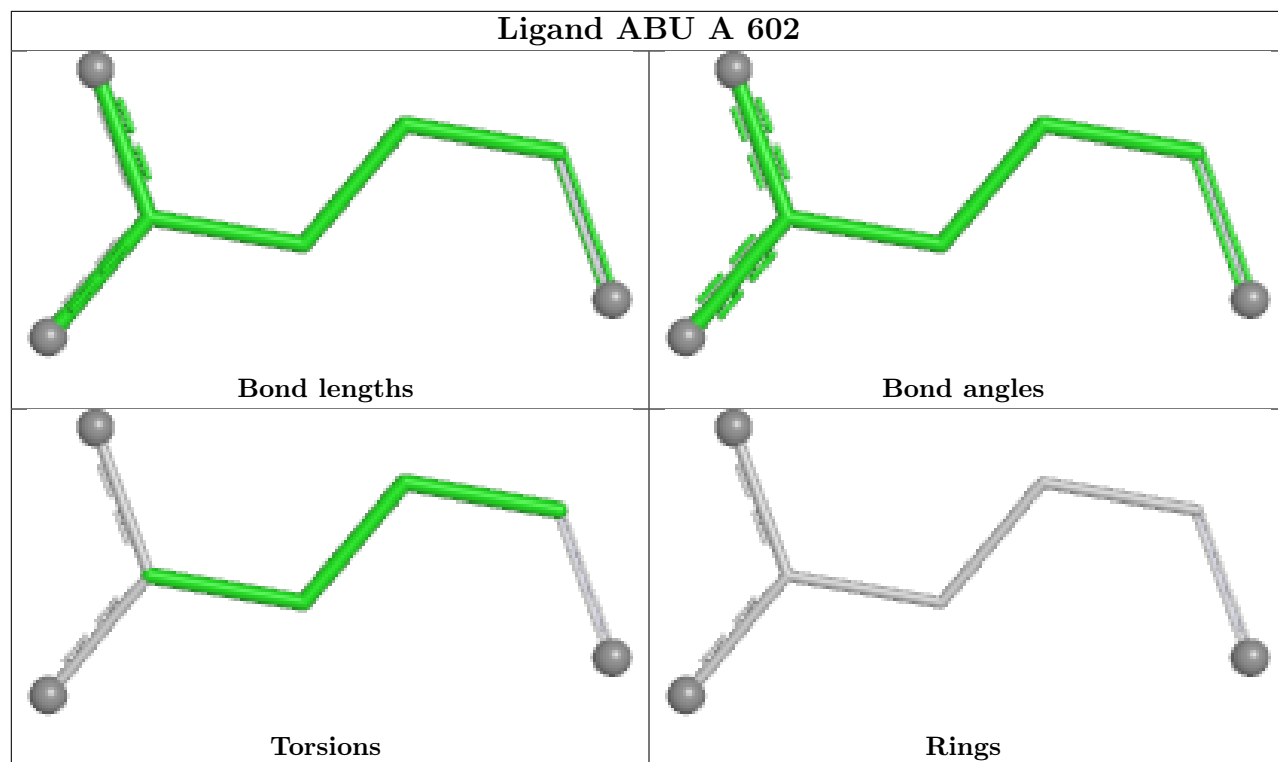
There are no chirality outliers.

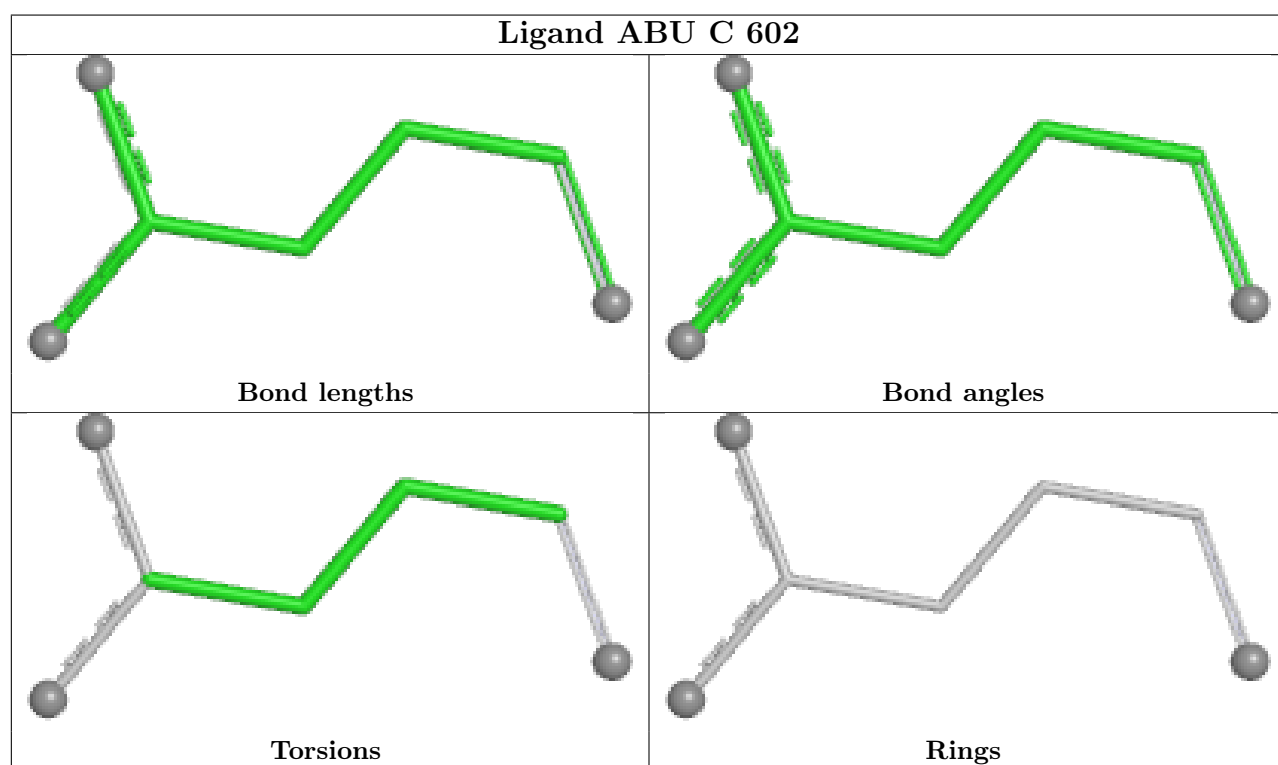
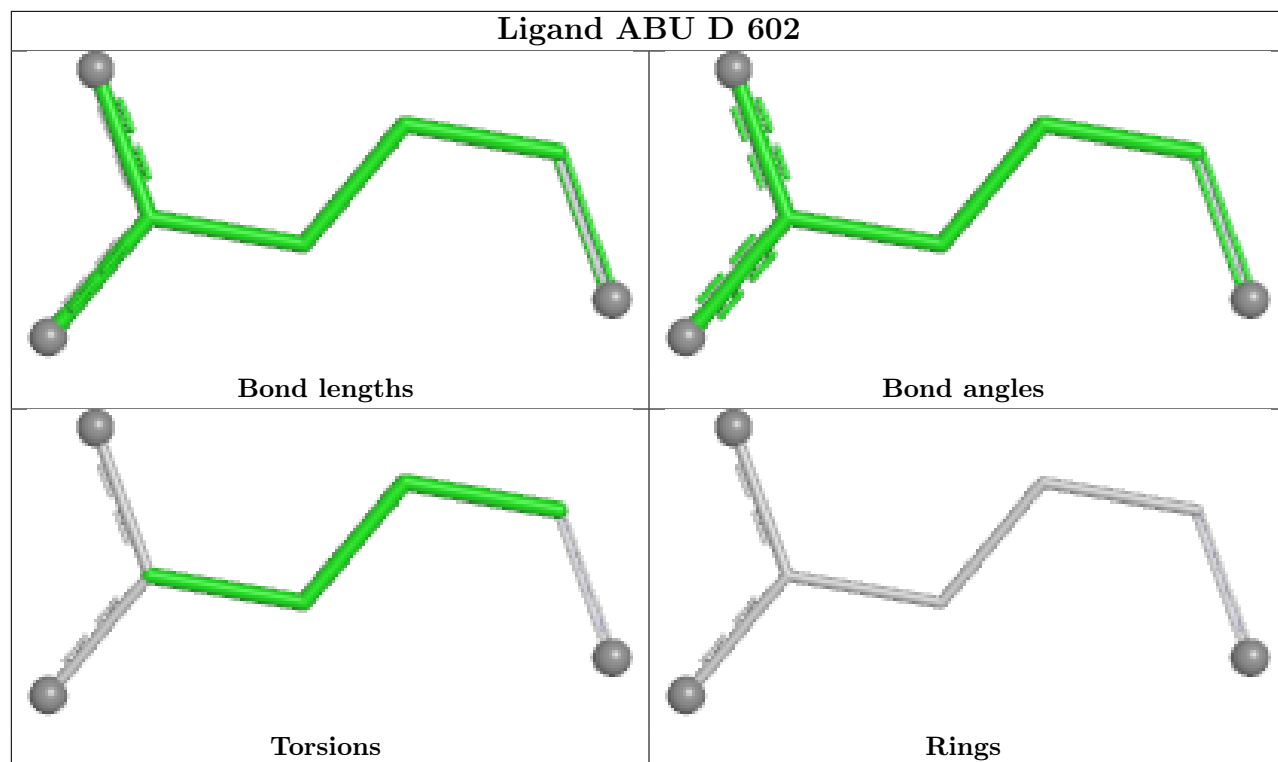
There are no torsion outliers.

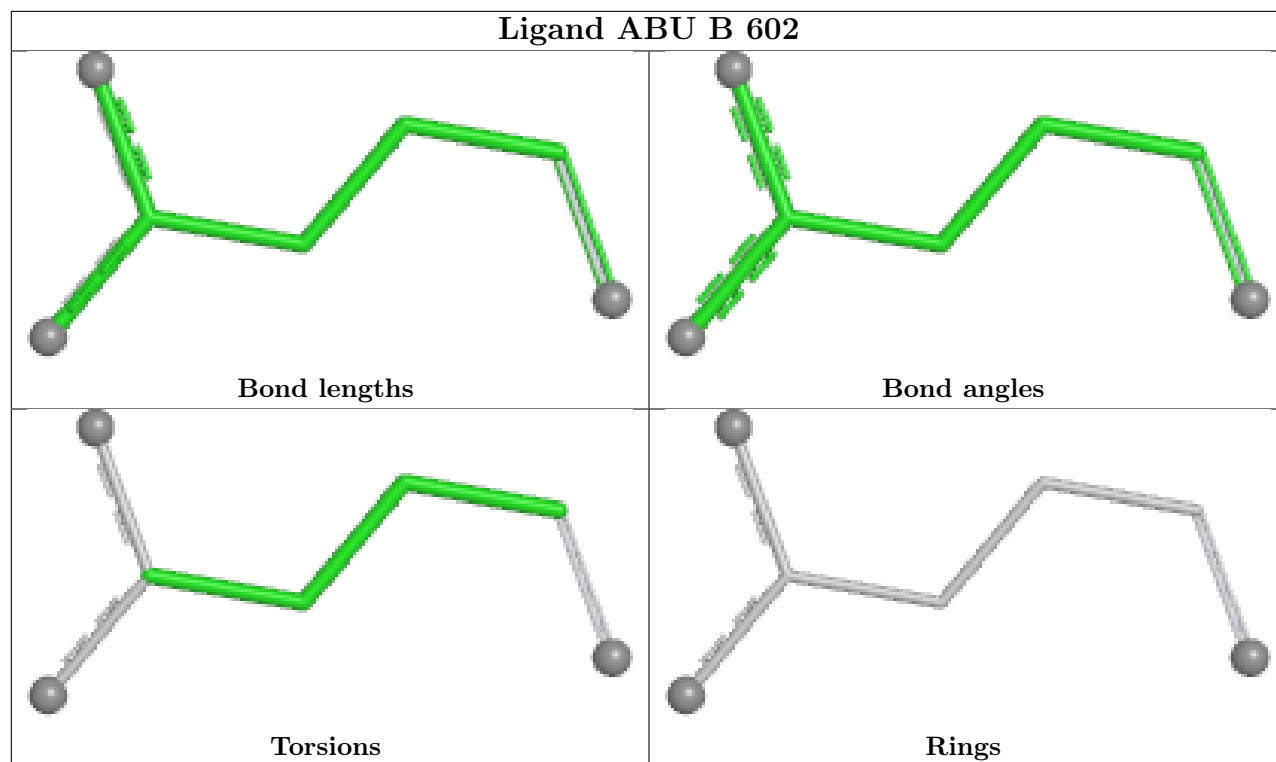
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



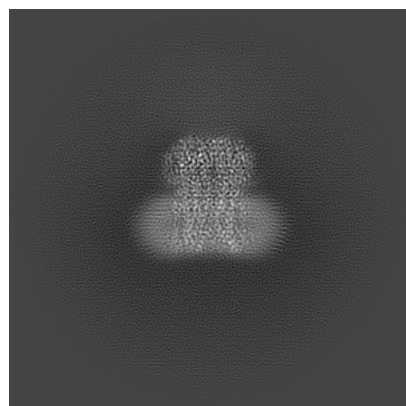
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47306. These allow visual inspection of the internal detail of the map and identification of artifacts.

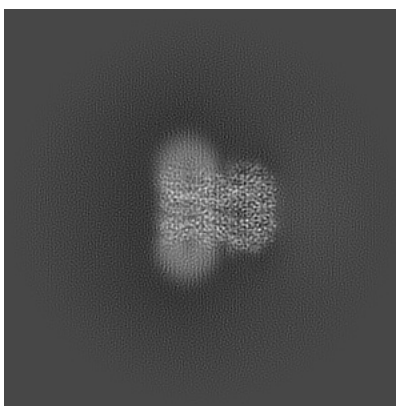
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

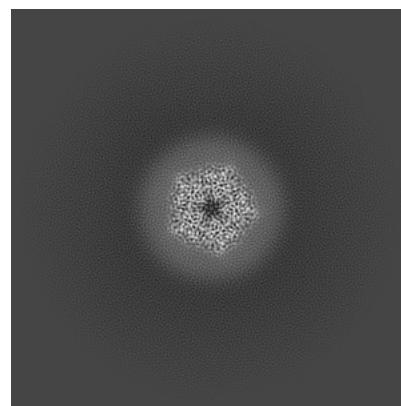
#### 6.1.1 Primary map



X

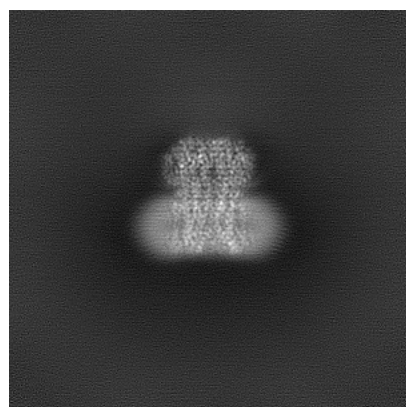


Y

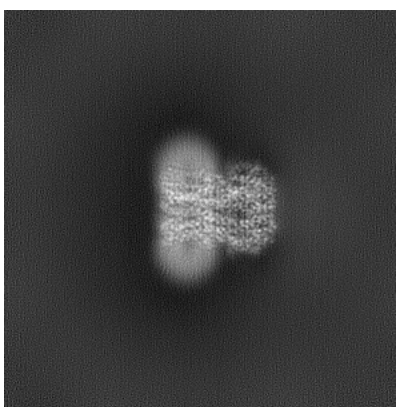


Z

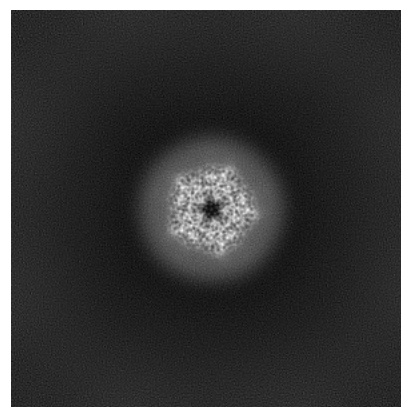
#### 6.1.2 Raw map



X



Y

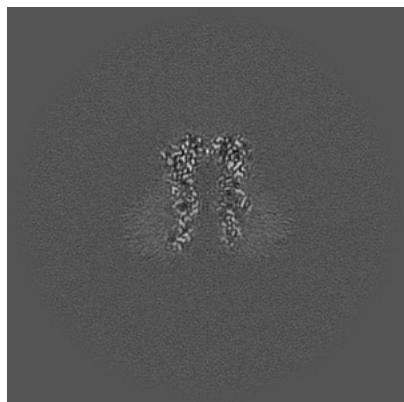


Z

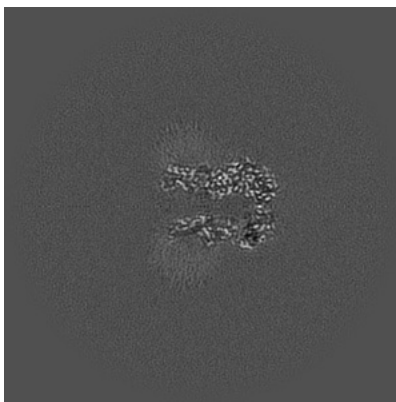
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

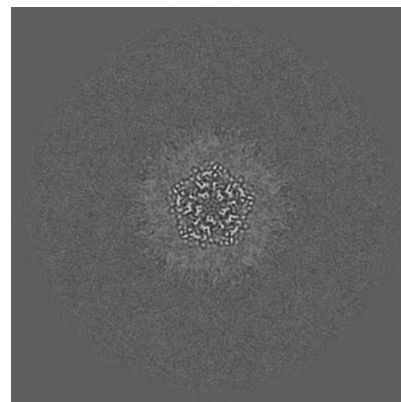
### 6.2.1 Primary map



X Index: 200

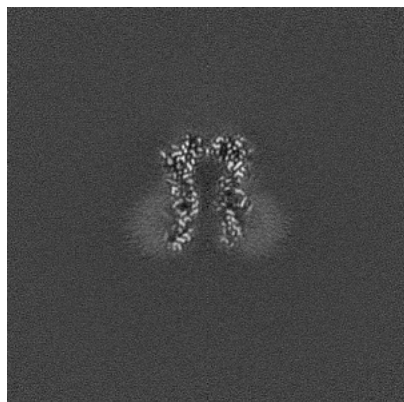


Y Index: 200

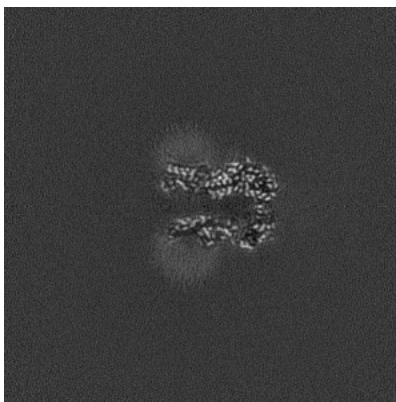


Z Index: 200

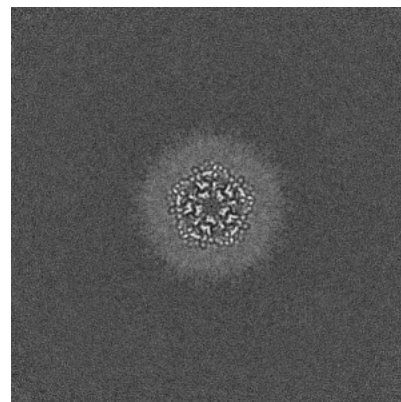
### 6.2.2 Raw map



X Index: 200



Y Index: 200

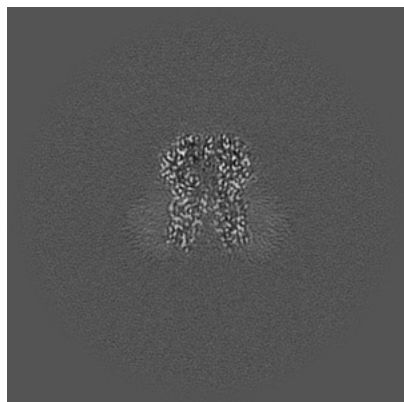


Z Index: 200

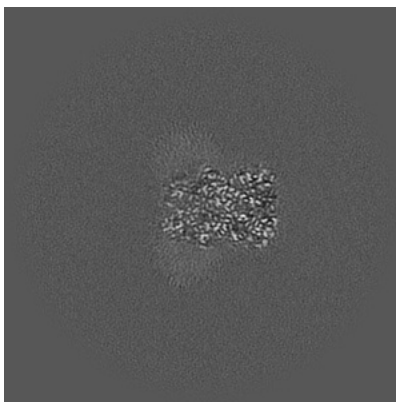
The images above show central slices of the map in three orthogonal directions.

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

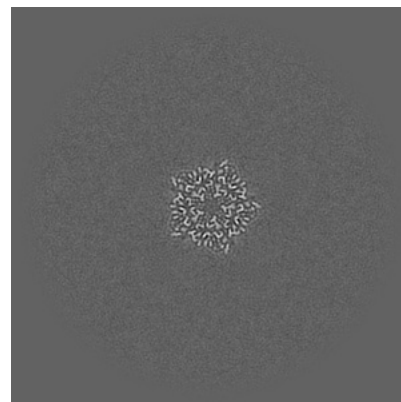
### 6.3.1 Primary map



X Index: 210

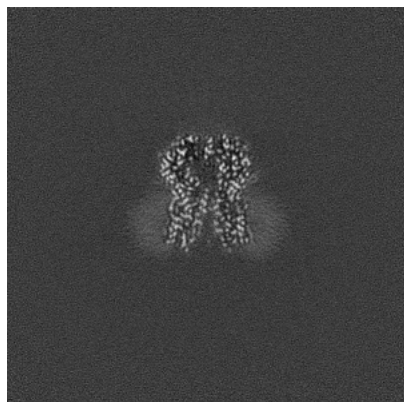


Y Index: 214

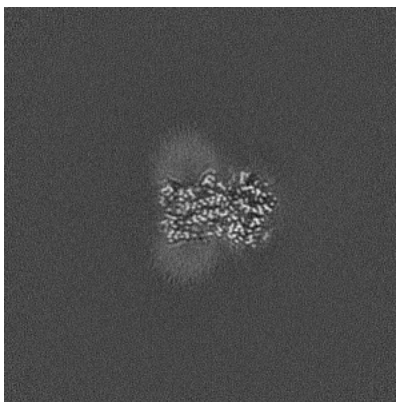


Z Index: 243

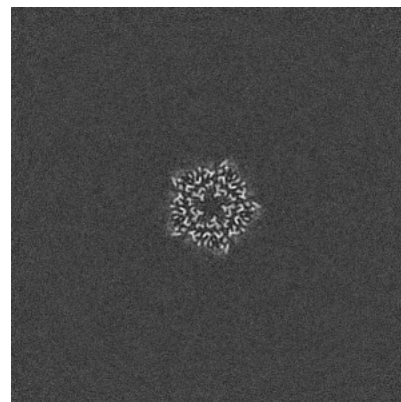
### 6.3.2 Raw map



X Index: 210



Y Index: 222



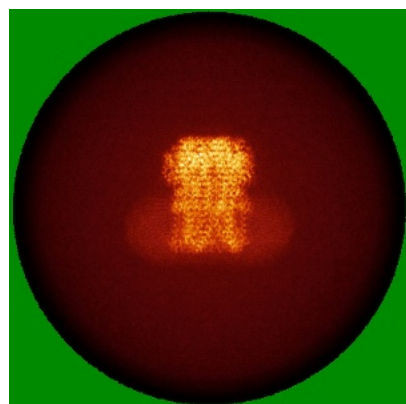
Z Index: 243

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

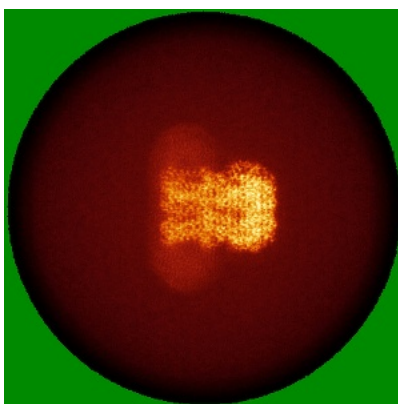


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

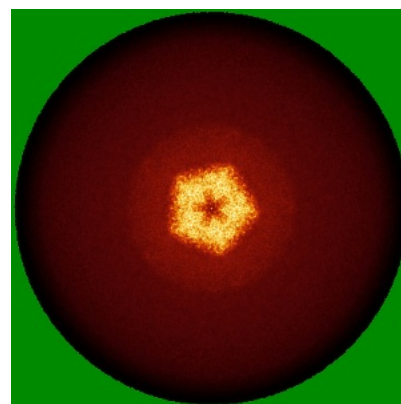
### 6.4.1 Primary map



X

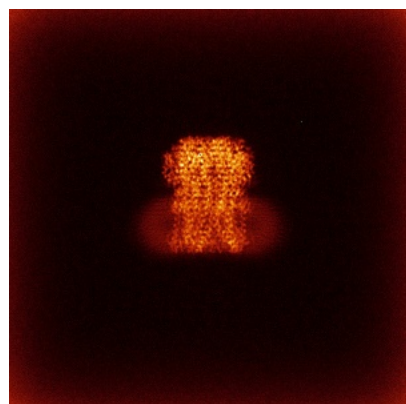


Y

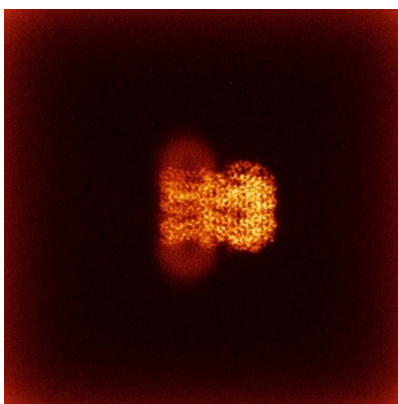


Z

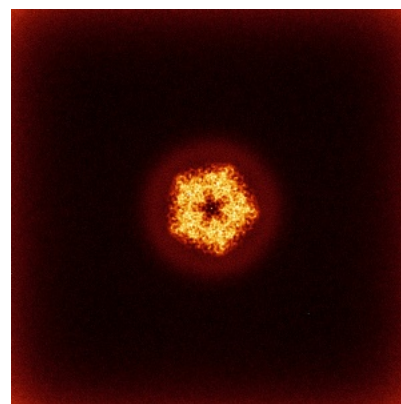
### 6.4.2 Raw map



X



Y

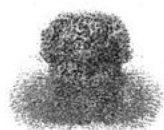


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



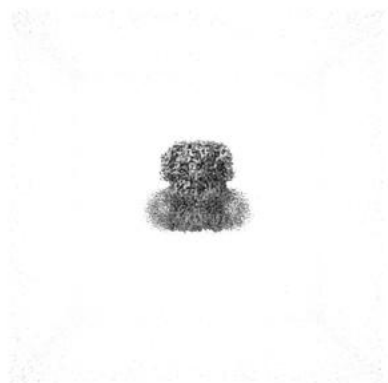
Y



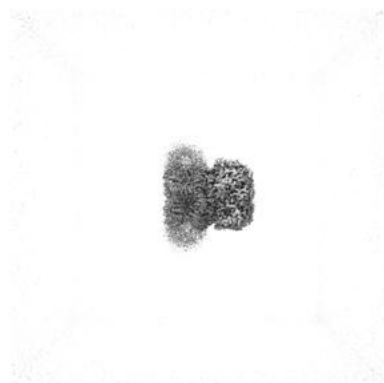
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

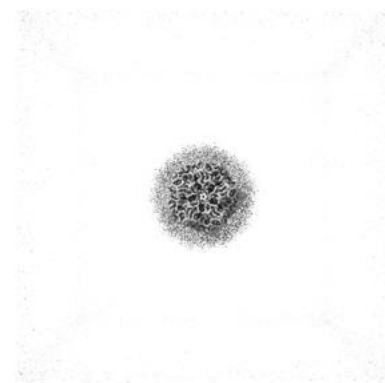
### 6.5.2 Raw map



X



Y



Z

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

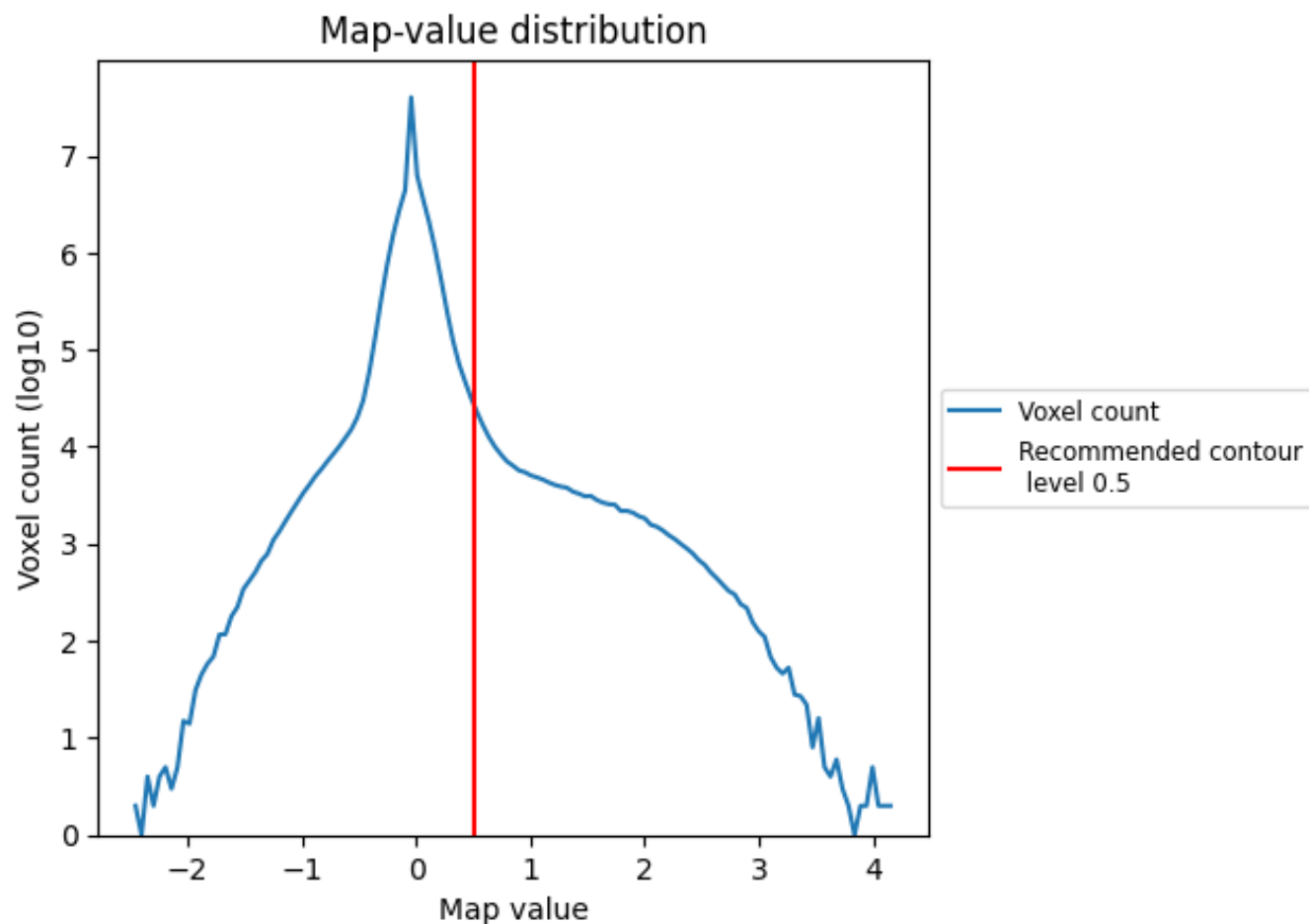
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

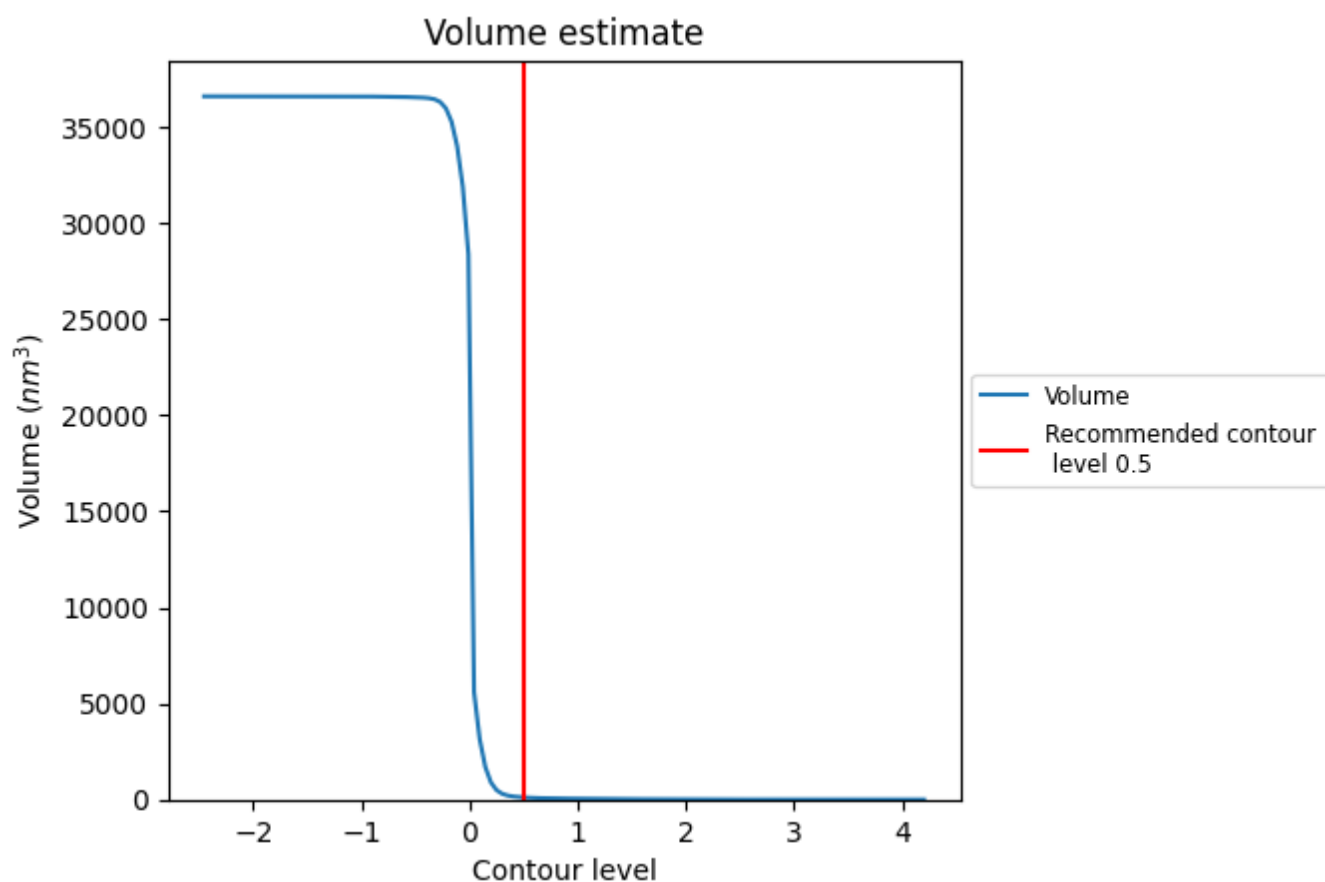
This section contains the results of statistical analysis of the map.

### 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.

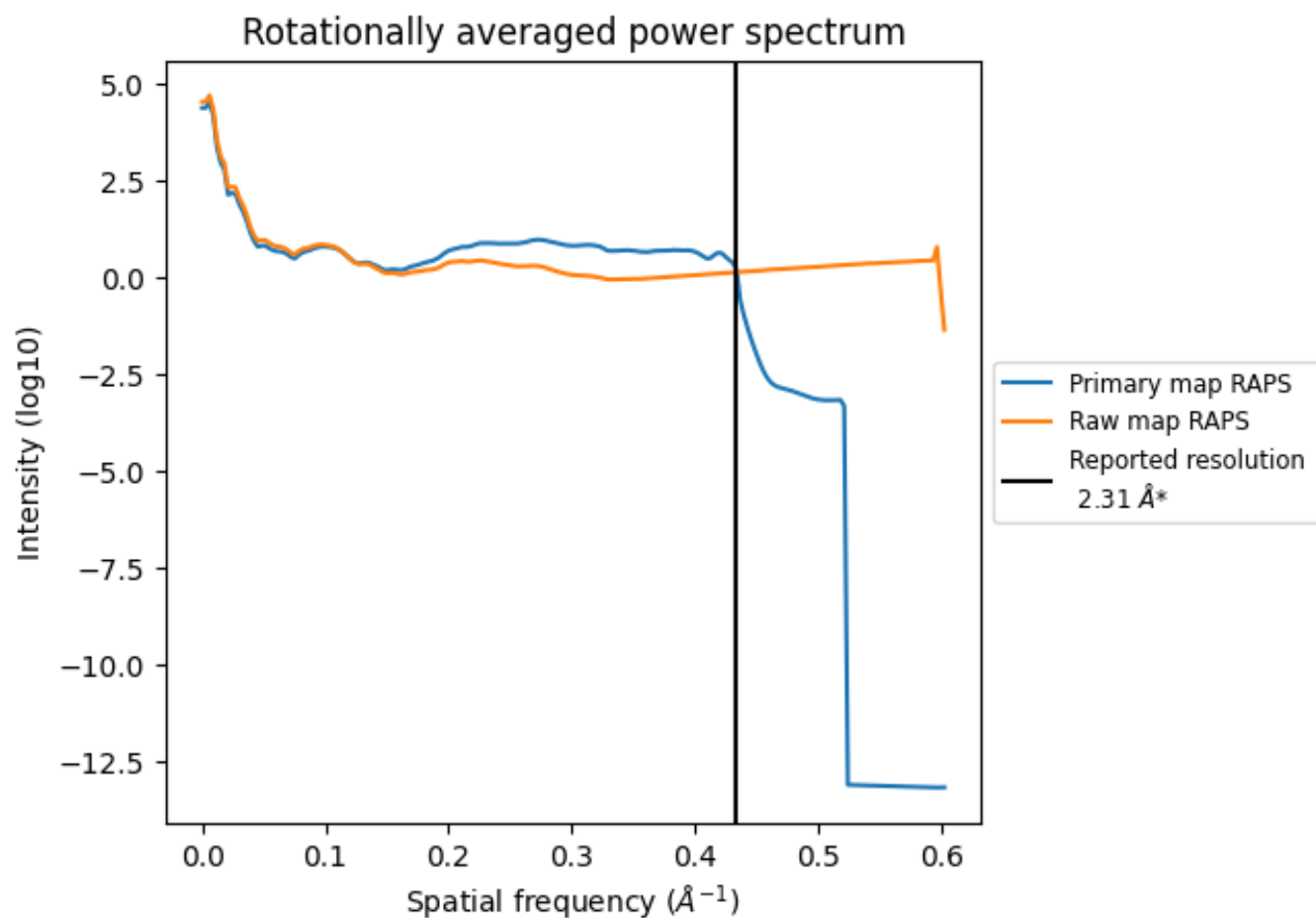
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm<sup>3</sup>; this corresponds to an approximate mass of 99 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



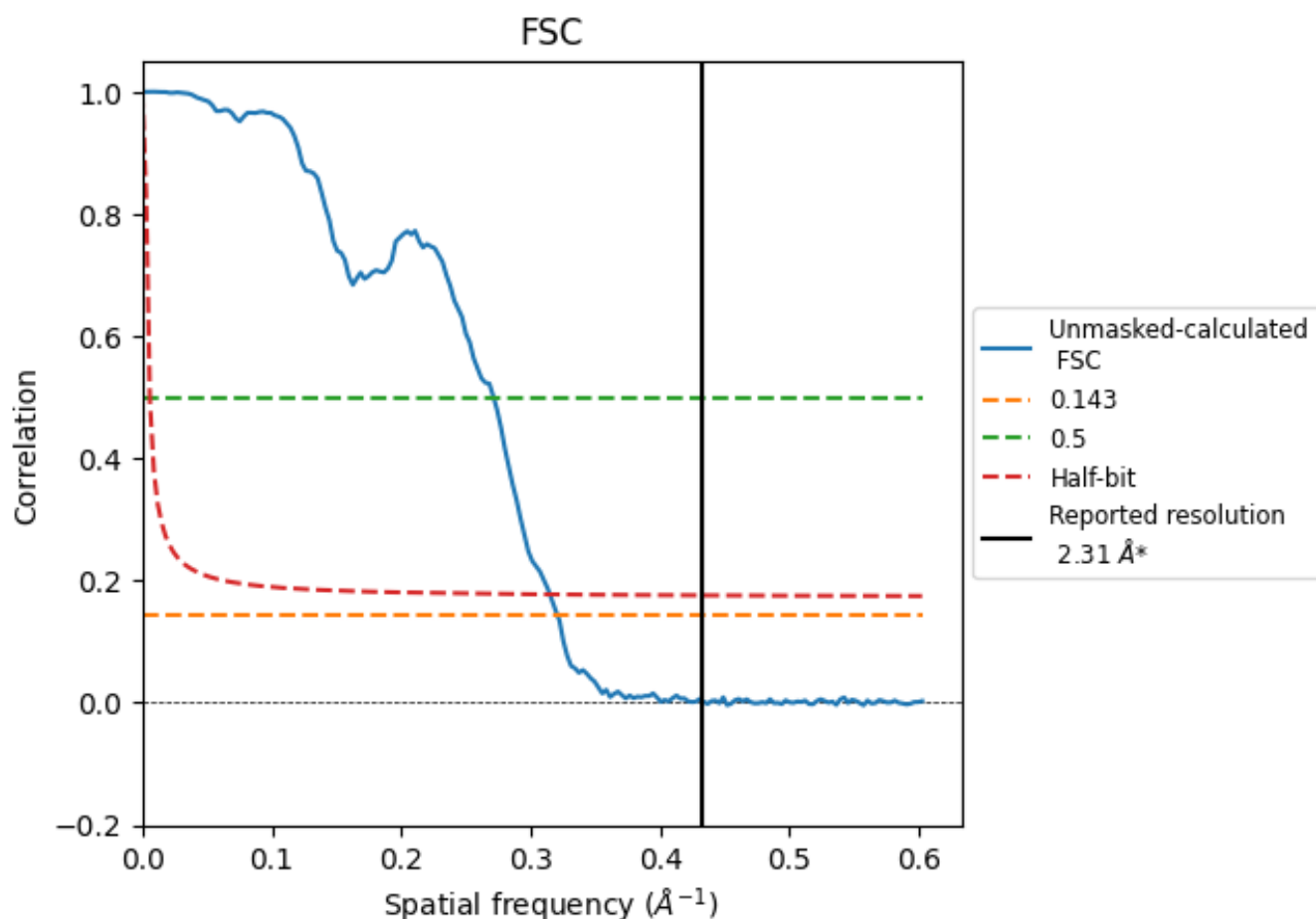
\*Reported resolution corresponds to spatial frequency of 0.433  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.433 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

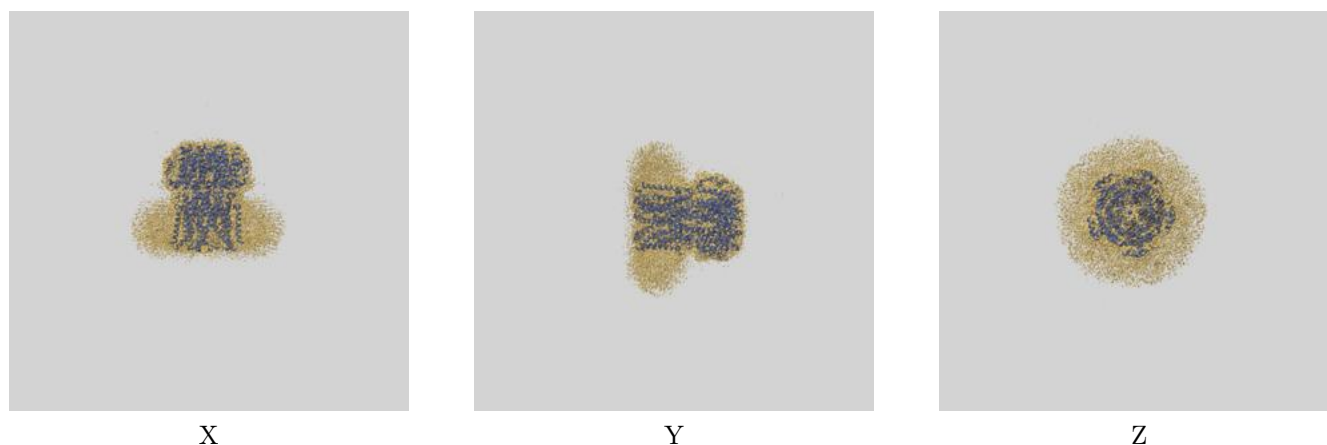
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	3.69	3.18

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.31 by more than 10 %

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

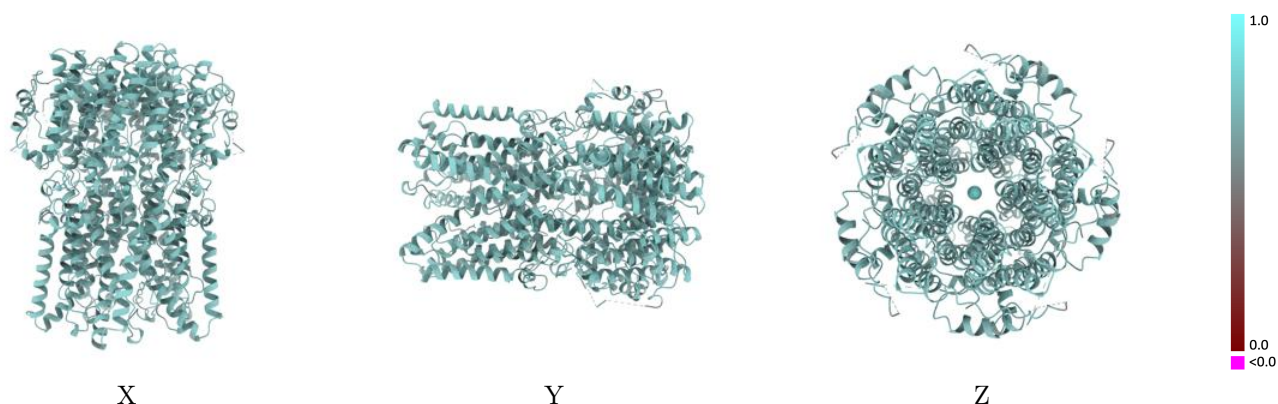
This section contains information regarding the fit between EMDB map EMD-47306 and PDB model 9DYJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



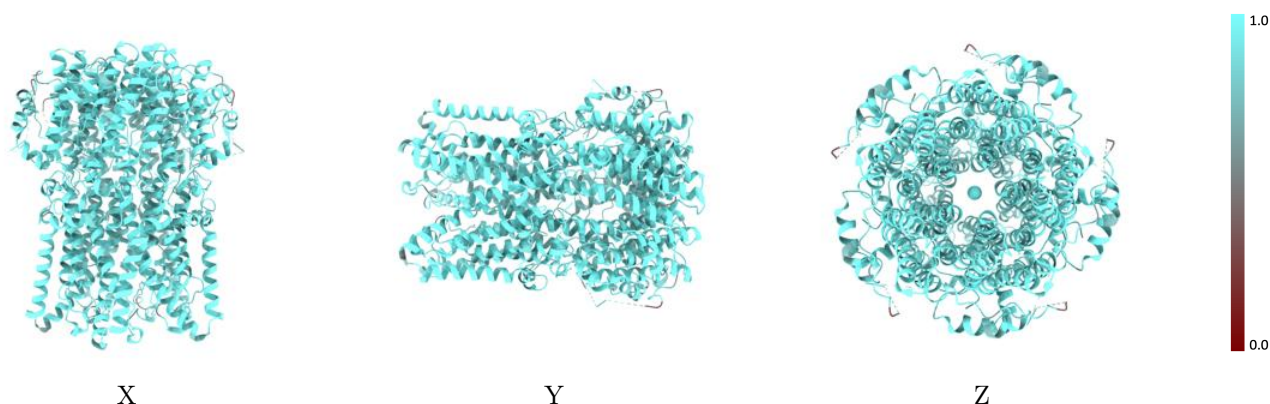
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



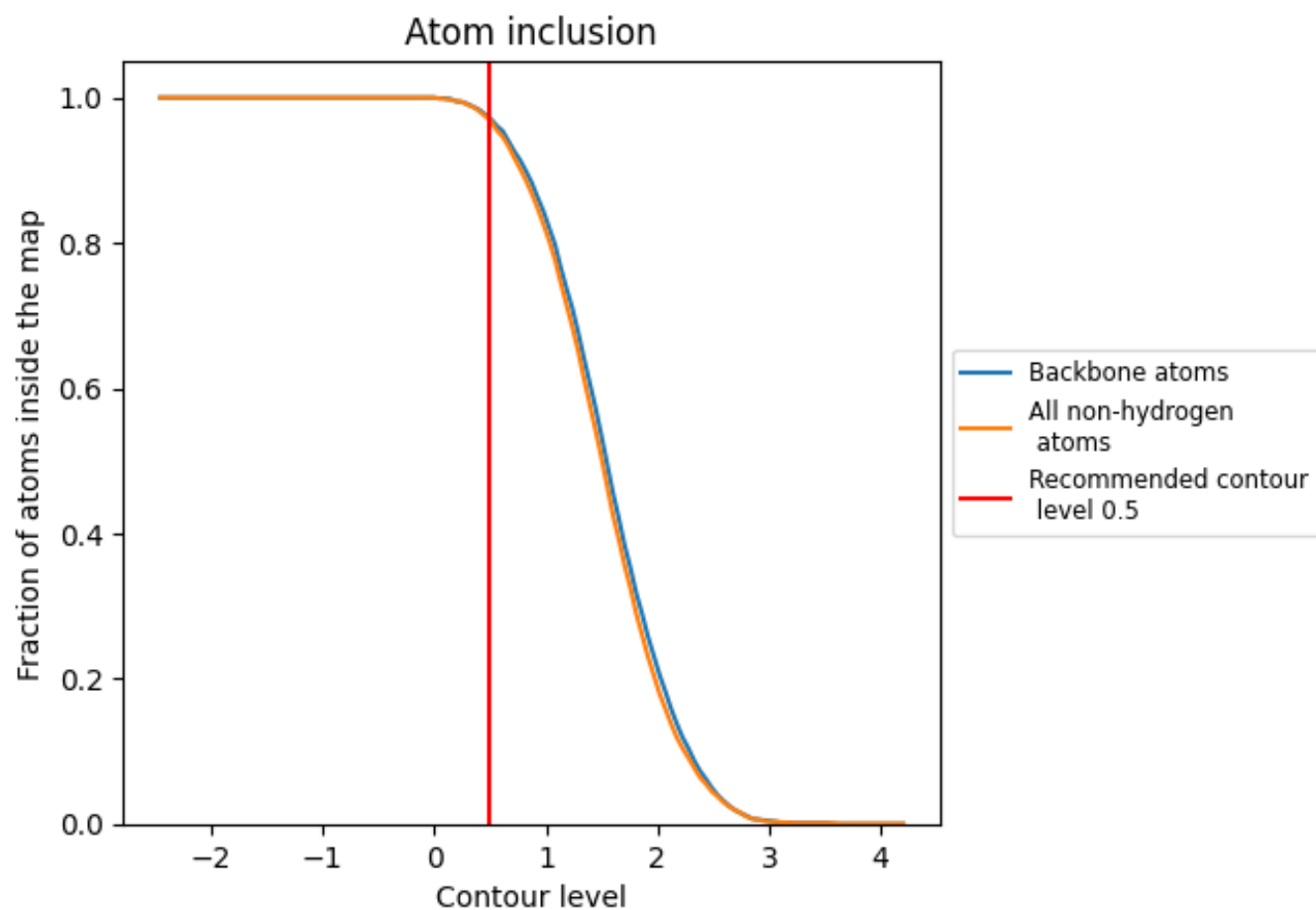
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9690	<div><div></div></div> 0.6840
A	<div><div></div></div> 0.9700	<div><div></div></div> 0.6840
B	<div><div></div></div> 0.9710	<div><div></div></div> 0.6840
C	<div><div></div></div> 0.9690	<div><div></div></div> 0.6840
D	<div><div></div></div> 0.9700	<div><div></div></div> 0.6830
E	<div><div></div></div> 0.9700	<div><div></div></div> 0.6850

