



Full wwPDB EM Validation Report ⓘ

May 13, 2024 – 12:47 PM EDT

PDB ID : 8SGK
EMDB ID : EMD-40458
Title : CryoEM structure of Deinococcus radiodurans BphP photosensory module in Pr state
Authors : Li, H.; Li, H.
Deposited on : 2023-04-12
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

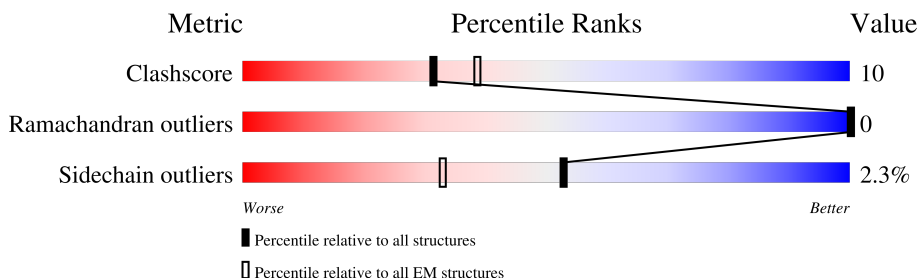
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 $\leq 5\%$. 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	777	<div> <div>49%</div> <div>14%</div> <div>37%</div> </div>
1	B	777	<div> <div>49%</div> <div>14%</div> <div>37%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7622 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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	493	Total	C	N	O	S	0	0
			3768	2395	671	691	11		
1	B	493	Total	C	N	O	S	0	0
			3768	2395	671	691	11		

There are 44 discrepancies between the modelled and reference sequences:

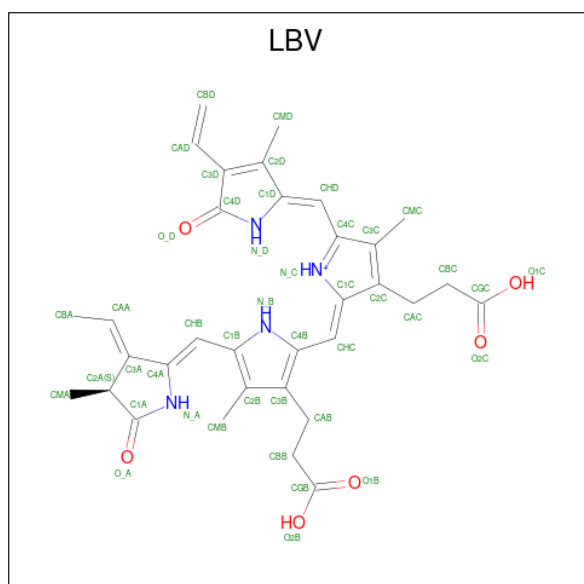
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q9RZA4
A	-12	ALA	-	expression tag	UNP Q9RZA4
A	-11	SER	-	expression tag	UNP Q9RZA4
A	-10	MET	-	expression tag	UNP Q9RZA4
A	-9	THR	-	expression tag	UNP Q9RZA4
A	-8	GLY	-	expression tag	UNP Q9RZA4
A	-7	GLY	-	expression tag	UNP Q9RZA4
A	-6	GLN	-	expression tag	UNP Q9RZA4
A	-5	GLN	-	expression tag	UNP Q9RZA4
A	-4	MET	-	expression tag	UNP Q9RZA4
A	-3	GLY	-	expression tag	UNP Q9RZA4
A	-2	ARG	-	expression tag	UNP Q9RZA4
A	-1	GLY	-	expression tag	UNP Q9RZA4
A	0	SER	-	expression tag	UNP Q9RZA4
A	756	LEU	-	expression tag	UNP Q9RZA4
A	757	GLU	-	expression tag	UNP Q9RZA4
A	758	HIS	-	expression tag	UNP Q9RZA4
A	759	HIS	-	expression tag	UNP Q9RZA4
A	760	HIS	-	expression tag	UNP Q9RZA4
A	761	HIS	-	expression tag	UNP Q9RZA4
A	762	HIS	-	expression tag	UNP Q9RZA4
A	763	HIS	-	expression tag	UNP Q9RZA4
B	-13	MET	-	initiating methionine	UNP Q9RZA4
B	-12	ALA	-	expression tag	UNP Q9RZA4
B	-11	SER	-	expression tag	UNP Q9RZA4
B	-10	MET	-	expression tag	UNP Q9RZA4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	THR	-	expression tag	UNP Q9RZA4
B	-8	GLY	-	expression tag	UNP Q9RZA4
B	-7	GLY	-	expression tag	UNP Q9RZA4
B	-6	GLN	-	expression tag	UNP Q9RZA4
B	-5	GLN	-	expression tag	UNP Q9RZA4
B	-4	MET	-	expression tag	UNP Q9RZA4
B	-3	GLY	-	expression tag	UNP Q9RZA4
B	-2	ARG	-	expression tag	UNP Q9RZA4
B	-1	GLY	-	expression tag	UNP Q9RZA4
B	0	SER	-	expression tag	UNP Q9RZA4
B	756	LEU	-	expression tag	UNP Q9RZA4
B	757	GLU	-	expression tag	UNP Q9RZA4
B	758	HIS	-	expression tag	UNP Q9RZA4
B	759	HIS	-	expression tag	UNP Q9RZA4
B	760	HIS	-	expression tag	UNP Q9RZA4
B	761	HIS	-	expression tag	UNP Q9RZA4
B	762	HIS	-	expression tag	UNP Q9RZA4
B	763	HIS	-	expression tag	UNP Q9RZA4

- Molecule 2 is 3-[2-[(Z)-[3-(2-carboxyethyl)-5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-4-methyl-pyrrol-1-ium -2-ylidene]methyl]-5-[(Z)-[(3E)-3-ethylidene-4-methyl-5-oxidanylidene-pyrrolidin-2-ylidene]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (three-letter code: LBV) (formula: C₃₃H₃₇N₄O₆) (labeled as "Ligand of Interest" by depositor).

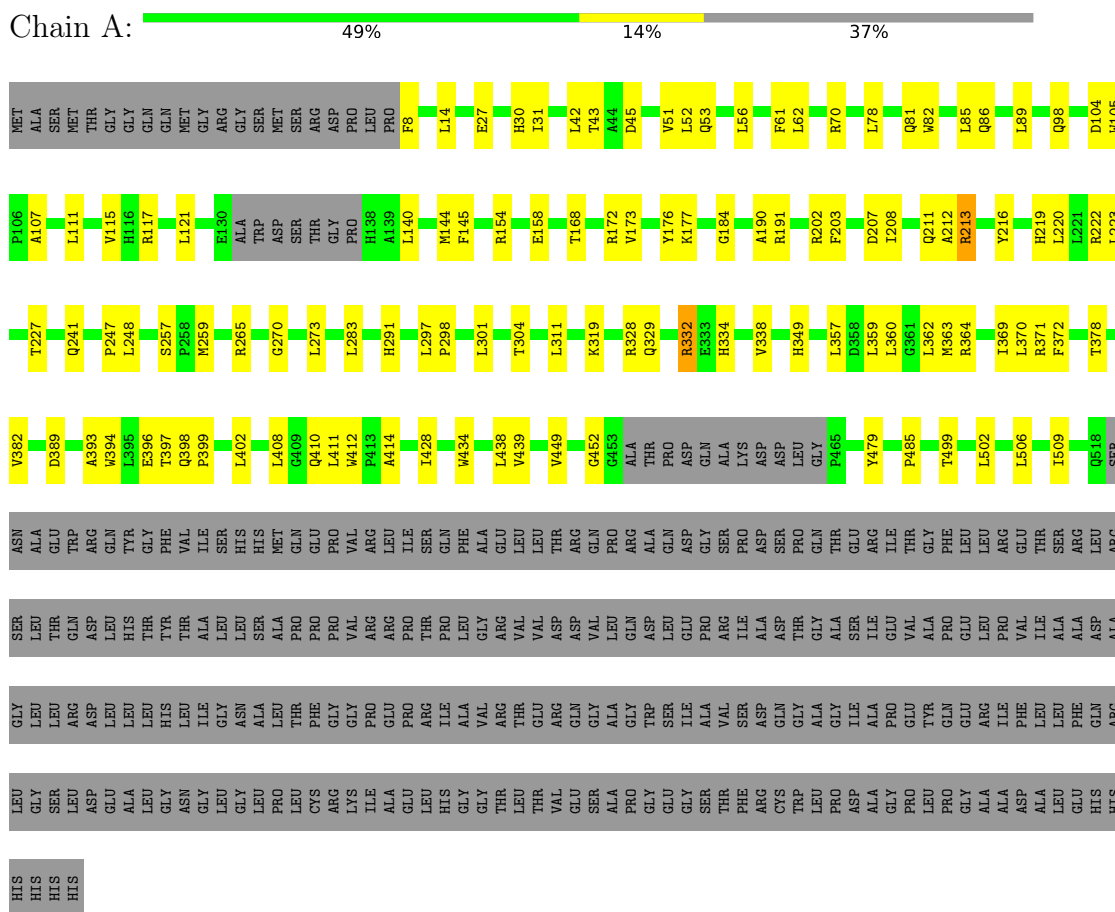


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			43	33	4	6	
2	B	1	Total	C	N	O	0
			43	33	4	6	

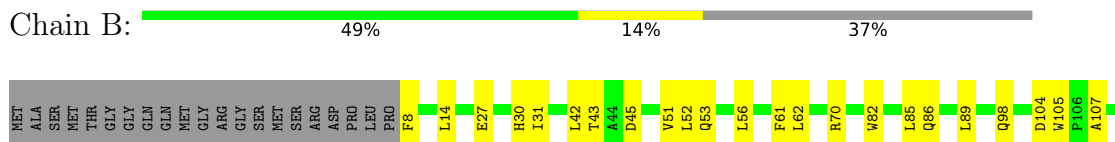
3 Residue-property plots

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: Bacteriophytochrome



• Molecule 1: Bacteriophytochrome



HIS	GLN	ASP	LEU	Q518	P384	Q247	L111
	ARG	ALA	ARG	SER	V388	P247	V115
	ARG	GLY	SER	ASN	D389	S257	H116
	GLY	LEU	LEU	ALA	SER	P258	R117
	SER	LEU	THR	GLU	TRP	M259	L121
	LEU	ARG	GLN	TRP	ARG	A393	L121
	ASP	ASP	ASP	ARG	W394	R265	E130
	GLU	LEU	LEU	GLN	L395	G270	ALA
	ALA	LEU	HIS	TYR	E396	T397	ASP
	HIS	LEU	THR	THR	PHE	L402	TRP
HIS	ASN	LEU	THR	VAL	L402	L273	ASP
	GLY	ILE	ALA	ILE	L408	V279	THR
	LEU	GLY	LEU	SER	G409	Q282	GLY
	GLY	ASN	LEU	HIS	L410	L283	PRO
	LEU	ALA	SER	HIS	Q410	H138	H138
	LEU	LEU	ALA	MET	L411	A139	A139
	THR	THR	PRO	GLN	W412	H291	L140
	LEU	PHE	PRO	GLU	P413	L297	M144
	CYS	ARG	GLY	PRO	A414	P298	F145
	ARG	GLY	VAL	VAL	L428	L301	F145
HIS	ILE	PRO	ARG	ARG	L428	L301	R154
	ALA	GLU	ARG	LEU	W434	L301	R154
	GLU	PRO	PRO	ILE	L438	T304	E158
	LEU	ARG	THR	SER	L438	L311	T168
	ARG	ILE	PRO	GLN	V439	L312	R172
	GLY	ALA	LEU	PHE	L447	K319	V173
	GLY	VAL	GLY	ALA	L447	Q328	Y176
	THR	ARG	VAL	GLU	E448	R329	L177
	LEU	THR	VAL	LEU	V449	G453	G184
	THR	GLU	ASP	THR	ALA	PRO	A190
HIS	VAL	ARG	ASP	ARG	THR	R332	R191
	GLN	GLY	VAL	GLN	PRO	E333	R191
	ALA	ALA	LEU	ARG	GLN	H334	R191
	GLY	TRP	ASP	ALA	GLN	V338	R202
	ILE	SER	ALA	GLY	LYS	H349	R202
	VAL	VAL	ARG	SER	ASP	L357	D207
	ASP	SER	ILE	PRO	ASP	D358	L208
	ARG	ASN	ALA	ASP	LEU	L359	Q211
	GLN	GLY	THR	SER	P465	A212	A212
	GLY	GLY	ALA	GLN	K476	R213	R213
HIS	ILE	ILE	SER	GLU	Y479	Y216	Y216
	ALA	ALA	ILE	ARG	P485	H219	H219
	PRO	GLU	VAL	THR	T499	L370	L220
	PRO	GLU	VAL	THR	L502	R371	L221
	GLN	PRO	ALA	PHE	F372	R222	R222
	LEU	GLU	LEU	LEU	T378	L223	L223
	ARG	ARG	LEU	LEU	L506	T227	T227
	ILE	VAL	VAL	GLU	V382	Q241	Q241
	LEU	LEU	ILE	THR	L509	L283	L283
	THR	PHE	ALA	SER	A393		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209952	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.881	Depositor
Minimum map value	-1.485	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.063	Depositor
Map size (\AA)	298.08002, 298.08002, 298.08002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82800007, 0.82800007, 0.82800007	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LBV

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	0.24	0/3863	0.49	0/5282
1	B	0.24	0/3863	0.49	0/5282
All	All	0.24	0/7726	0.49	0/10564

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

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	3768	0	3746	77	0
1	B	3768	0	3746	75	0
2	A	43	0	34	2	0
2	B	43	0	34	2	0
All	All	7622	0	7560	145	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 10.

All (145) 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:B:297:LEU:HD11	1:B:301:LEU:HD22	1.67	0.76
1:A:207:ASP:HB3	2:A:801:LBV:HHD1	1.68	0.75
1:B:207:ASP:HB3	2:B:801:LBV:HHD1	1.68	0.75
1:A:297:LEU:HD11	1:A:301:LEU:HD22	1.67	0.74
1:A:328:ARG:O	1:A:332:ARG:NH1	2.27	0.67
1:B:140:LEU:HD22	1:B:304:THR:HG23	1.76	0.67
1:B:328:ARG:O	1:B:332:ARG:NH1	2.27	0.67
1:A:140:LEU:HD22	1:A:304:THR:HG23	1.77	0.67
1:A:329:GLN:O	1:A:329:GLN:NE2	2.30	0.65
1:B:329:GLN:O	1:B:329:GLN:NE2	2.30	0.65
1:A:362:LEU:HD23	1:A:363:MET:HG2	1.81	0.62
1:B:362:LEU:HD23	1:B:363:MET:HG2	1.81	0.62
1:A:89:LEU:O	1:A:117:ARG:NH2	2.33	0.62
1:B:220:LEU:O	1:B:222:ARG:NH2	2.32	0.61
1:B:227:THR:O	1:B:265:ARG:NH1	2.33	0.61
1:A:227:THR:O	1:A:265:ARG:NH1	2.33	0.61
1:B:297:LEU:HD12	1:B:298:PRO:HD2	1.83	0.61
1:B:89:LEU:O	1:B:117:ARG:NH2	2.33	0.61
1:A:172:ARG:HG2	1:A:191:ARG:HG3	1.84	0.60
1:B:172:ARG:HG2	1:B:191:ARG:HG3	1.84	0.60
1:A:220:LEU:O	1:A:222:ARG:NH2	2.32	0.60
1:A:27:GLU:O	1:A:211:GLN:NE2	2.31	0.59
1:B:334:HIS:HB3	1:B:362:LEU:HD12	1.84	0.59
1:A:334:HIS:HB3	1:A:362:LEU:HD12	1.84	0.59
1:A:297:LEU:HD12	1:A:298:PRO:HD2	1.83	0.59
1:A:499:THR:HG22	1:B:499:THR:HG22	1.84	0.59
1:A:154:ARG:NH1	1:A:158:GLU:OE1	2.37	0.58
1:B:27:GLU:O	1:B:211:GLN:NE2	2.31	0.58
1:B:223:LEU:HD13	1:B:273:LEU:HD12	1.85	0.58
1:A:223:LEU:HD13	1:A:273:LEU:HD12	1.85	0.57
1:A:42:LEU:HD11	1:A:62:LEU:HD11	1.87	0.57
1:A:371:ARG:NH2	1:A:396:GLU:OE2	2.38	0.57
1:B:154:ARG:NH1	1:B:158:GLU:OE1	2.37	0.57
1:B:52:LEU:HD12	1:B:121:LEU:HD21	1.86	0.56
1:B:202:ARG:HH11	1:B:449:VAL:HG11	1.70	0.56
1:B:371:ARG:NH2	1:B:396:GLU:OE2	2.38	0.56
1:A:52:LEU:HD12	1:A:121:LEU:HD21	1.86	0.56
1:A:202:ARG:HH11	1:A:449:VAL:HG11	1.70	0.55
1:B:42:LEU:HD11	1:B:62:LEU:HD11	1.87	0.55
1:A:51:VAL:O	1:A:70:ARG:NH2	2.40	0.55
1:B:51:VAL:O	1:B:70:ARG:NH2	2.40	0.54
1:A:105:TRP:HD1	1:A:107:ALA:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:MET:HG2	1:A:311:LEU:HD11	1.91	0.53
1:B:144:MET:HG2	1:B:311:LEU:HD11	1.91	0.53
1:B:329:GLN:HA	1:B:332:ARG:HD3	1.90	0.53
1:A:212:ALA:O	1:A:216:TYR:N	2.41	0.53
1:B:338:VAL:HG12	1:B:357:LEU:HD22	1.91	0.52
1:A:329:GLN:HA	1:A:332:ARG:HD3	1.90	0.52
1:A:43:THR:HG22	1:A:121:LEU:HD22	1.92	0.52
1:A:410:GLN:NE2	1:A:479:TYR:OH	2.43	0.52
1:B:212:ALA:O	1:B:216:TYR:N	2.41	0.52
1:B:43:THR:HG22	1:B:121:LEU:HD22	1.92	0.52
1:B:410:GLN:NE2	1:B:479:TYR:OH	2.43	0.52
1:A:378:THR:HB	1:A:382:VAL:HG11	1.93	0.51
1:B:105:TRP:HD1	1:B:107:ALA:H	1.57	0.51
1:B:45:ASP:OD1	1:B:241:GLN:NE2	2.44	0.51
1:A:208:ILE:O	1:A:213:ARG:NH2	2.44	0.51
1:A:338:VAL:HG12	1:A:357:LEU:HD22	1.92	0.50
1:A:349:HIS:CD2	1:A:372:PHE:HB2	2.46	0.50
1:B:104:ASP:OD1	1:B:104:ASP:N	2.39	0.50
1:B:378:THR:HB	1:B:382:VAL:HG11	1.93	0.50
1:B:208:ILE:O	1:B:213:ARG:NH2	2.44	0.50
1:A:370:LEU:HD23	1:A:438:LEU:HD21	1.92	0.50
1:A:412:TRP:HE3	1:A:414:ALA:H	1.57	0.50
1:B:349:HIS:CD2	1:B:372:PHE:HB2	2.46	0.50
1:B:370:LEU:HD23	1:B:438:LEU:HD21	1.92	0.50
1:A:173:VAL:HB	1:A:190:ALA:HB3	1.93	0.50
1:B:173:VAL:HB	1:B:190:ALA:HB3	1.93	0.49
1:A:45:ASP:OD1	1:A:241:GLN:NE2	2.44	0.49
1:A:369:ILE:HB	1:A:439:VAL:HB	1.94	0.49
1:B:412:TRP:HE3	1:B:414:ALA:H	1.57	0.49
1:A:502:LEU:HD12	1:B:506:LEU:HD13	1.94	0.49
1:B:369:ILE:HB	1:B:439:VAL:HB	1.94	0.48
1:A:402:LEU:HD12	1:A:428:ILE:HG22	1.95	0.48
1:B:402:LEU:HD12	1:B:428:ILE:HG22	1.94	0.48
1:B:43:THR:HB	1:B:53:GLN:HB2	1.96	0.48
1:A:176:TYR:HE1	1:A:184:GLY:HA3	1.79	0.47
1:B:82:TRP:O	1:B:86:GLN:HG2	2.14	0.47
1:A:506:LEU:HB2	1:B:506:LEU:HB2	1.96	0.47
1:A:369:ILE:HG12	1:A:378:THR:HG22	1.97	0.47
1:A:82:TRP:O	1:A:86:GLN:HG2	2.14	0.47
1:B:369:ILE:HG12	1:B:378:THR:HG22	1.97	0.47
1:B:332:ARG:N	1:B:332:ARG:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:LEU:HA	1:A:509:ILE:HG22	1.97	0.46
1:B:506:LEU:HA	1:B:509:ILE:HG22	1.96	0.46
1:A:332:ARG:N	1:A:332:ARG:HD2	2.30	0.46
1:A:43:THR:HB	1:A:53:GLN:HB2	1.96	0.46
1:B:176:TYR:HE1	1:B:184:GLY:HA3	1.79	0.46
1:B:213:ARG:HG3	1:B:283:LEU:HD23	1.98	0.46
1:B:312:LEU:HD23	1:B:312:LEU:HA	1.82	0.46
1:A:213:ARG:HG3	1:A:283:LEU:HD23	1.98	0.45
1:A:104:ASP:N	1:A:104:ASP:OD1	2.39	0.45
1:B:85:LEU:HD11	1:B:115:VAL:HG21	1.98	0.45
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.84	0.45
1:A:85:LEU:HD11	1:A:115:VAL:HG21	1.98	0.45
1:A:502:LEU:CD1	1:B:506:LEU:HD13	2.47	0.44
1:B:144:MET:HG2	1:B:311:LEU:CD1	2.47	0.44
1:A:31:ILE:HG22	1:A:247:PRO:HA	1.98	0.44
1:A:144:MET:HG2	1:A:311:LEU:CD1	2.47	0.44
1:B:31:ILE:HG22	1:B:247:PRO:HA	1.98	0.44
1:A:270:GLY:N	1:A:291:HIS:O	2.43	0.44
1:A:371:ARG:NH1	1:A:434:TRP:O	2.48	0.44
1:B:219:HIS:O	1:B:222:ARG:NH1	2.51	0.44
1:B:297:LEU:HD12	1:B:298:PRO:CD	2.47	0.44
1:B:408:LEU:HD12	1:B:408:LEU:HA	1.79	0.44
1:A:98:GLN:HB2	1:B:145:PHE:CE1	2.53	0.43
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.79	0.43
1:A:219:HIS:O	1:A:222:ARG:NH1	2.51	0.43
1:B:270:GLY:N	1:B:291:HIS:O	2.43	0.43
1:A:393:ALA:O	1:A:397:THR:HG23	2.19	0.43
1:A:61:PHE:HE1	1:A:111:LEU:HD11	1.84	0.43
1:B:61:PHE:HE1	1:B:111:LEU:HD11	1.84	0.43
1:B:216:TYR:OH	2:B:801:LBV:HAC1	2.19	0.43
1:A:297:LEU:HD12	1:A:298:PRO:CD	2.47	0.43
1:B:371:ARG:NH1	1:B:434:TRP:O	2.48	0.43
1:B:438:LEU:HD23	1:B:438:LEU:HA	1.84	0.43
1:A:216:TYR:OH	2:A:801:LBV:HAC1	2.19	0.42
1:A:332:ARG:HD2	1:A:332:ARG:H	1.84	0.42
1:A:389:ASP:N	1:A:389:ASP:OD1	2.52	0.42
1:B:393:ALA:O	1:B:397:THR:HG23	2.19	0.42
1:A:257:SER:OG	1:A:259:MET:HG3	2.19	0.42
1:A:394:TRP:HZ2	1:A:411:LEU:HG	1.84	0.42
1:B:168:THR:HG22	1:B:301:LEU:HD21	2.01	0.42
1:B:332:ARG:HD2	1:B:332:ARG:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:SER:OG	1:B:259:MET:HG3	2.20	0.42
1:A:168:THR:HG22	1:A:301:LEU:HD21	2.01	0.42
1:B:389:ASP:N	1:B:389:ASP:OD1	2.52	0.42
1:B:394:TRP:HZ2	1:B:411:LEU:HG	1.84	0.42
1:A:145:PHE:CE1	1:B:98:GLN:HB2	2.55	0.41
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.86	0.41
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.92	0.41
1:A:398:GLN:HA	1:A:399:PRO:HD3	1.96	0.41
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.84	0.41
1:A:506:LEU:HD13	1:B:502:LEU:HD12	2.01	0.41
1:B:279:VAL:O	1:B:282:GLN:NE2	2.54	0.41
1:B:394:TRP:CZ2	1:B:411:LEU:HG	2.56	0.41
1:B:384:PRO:O	1:B:388:VAL:HG23	2.22	0.40
1:A:203:PHE:CE1	1:A:452:GLY:HA3	2.56	0.40
1:A:394:TRP:CZ2	1:A:411:LEU:HG	2.57	0.40
1:B:447:LEU:O	1:B:476:LYS:HB3	2.22	0.40
1:A:176:TYR:CE1	1:A:184:GLY:HA3	2.57	0.40
1:B:56:LEU:HA	1:B:56:LEU:HD23	1.84	0.40
1:A:78:LEU:HD13	1:A:81:GLN:HB2	2.04	0.40
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.96	0.40
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.86	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	487/777 (63%)	485 (100%)	2 (0%)	0	100	100
1	B	487/777 (63%)	485 (100%)	2 (0%)	0	100	100
All	All	974/1554 (63%)	970 (100%)	4 (0%)	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	388/615 (63%)	379 (98%)	9 (2%)	50	71
1	B	388/615 (63%)	379 (98%)	9 (2%)	50	71
All	All	776/1230 (63%)	758 (98%)	18 (2%)	53	71

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	30	HIS
1	A	177	LYS
1	A	213	ARG
1	A	319	LYS
1	A	332	ARG
1	A	359	LEU
1	A	364	ARG
1	A	485	PRO
1	B	8	PHE
1	B	30	HIS
1	B	177	LYS
1	B	213	ARG
1	B	319	LYS
1	B	332	ARG
1	B	359	LEU
1	B	364	ARG
1	B	485	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	GLN

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Mol	Chain	Res	Type
1	B	410	GLN
1	B	513	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	LBV	A	801	1	42,46,46	1.50	3 (7%)	47,67,67	1.10	4 (8%)
2	LBV	B	801	1	42,46,46	1.49	3 (7%)	47,67,67	1.10	4 (8%)

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
2	LBV	A	801	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LBV	B	801	1	-	10/26/74/74	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	LBV	CHC-C1C	6.57	1.40	1.35
2	B	801	LBV	CHC-C1C	6.54	1.40	1.35
2	A	801	LBV	C1C-C2C	-3.33	1.40	1.45
2	B	801	LBV	C1C-C2C	-3.32	1.40	1.45
2	A	801	LBV	C4C-C3C	-2.55	1.40	1.45
2	B	801	LBV	C4C-C3C	-2.51	1.40	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	LBV	CHC-C1C-N-C	-2.49	125.37	128.83
2	B	801	LBV	CHC-C1C-N-C	-2.49	125.38	128.83
2	A	801	LBV	CAA-C3A-C4A	-2.39	123.47	126.36
2	B	801	LBV	CAA-C3A-C4A	-2.38	123.49	126.36
2	A	801	LBV	CMC-C3C-C4C	2.17	128.40	125.06
2	B	801	LBV	CMC-C3C-C4C	2.16	128.39	125.06
2	B	801	LBV	O-A-C1A-C2A	2.06	128.26	126.28
2	A	801	LBV	O-A-C1A-C2A	2.05	128.26	126.28

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	LBV	C3A-C4A-CHB-C1B
2	A	801	LBV	A-N-C4A-CHB-C1B
2	A	801	LBV	C3C-C4C-CHD-C1D
2	A	801	LBV	C-N-C4C-CHD-C1D
2	B	801	LBV	C3A-C4A-CHB-C1B
2	B	801	LBV	A-N-C4A-CHB-C1B
2	B	801	LBV	C3C-C4C-CHD-C1D
2	B	801	LBV	C-N-C4C-CHD-C1D
2	A	801	LBV	D-N-C1D-CHD-C4C
2	B	801	LBV	D-N-C1D-CHD-C4C
2	A	801	LBV	C2C-CAC-CBC-CGC
2	B	801	LBV	C2C-CAC-CBC-CGC
2	A	801	LBV	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
2	B	801	LBV	C2D-C1D-CHD-C4C
2	A	801	LBV	CAC-CBC-CGC-O1C
2	B	801	LBV	CAC-CBC-CGC-O1C
2	A	801	LBV	CAC-CBC-CGC-O2C
2	B	801	LBV	CAC-CBC-CGC-O2C
2	A	801	LBV	CAB-CBB-CGB-O2B
2	B	801	LBV	CAB-CBB-CGB-O2B

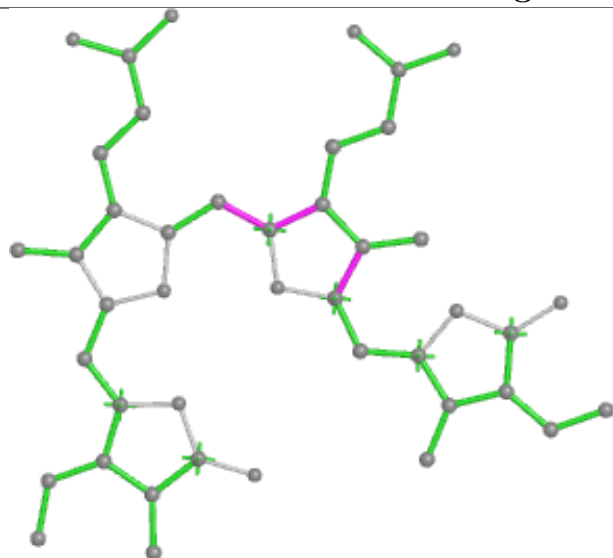
There are no ring outliers.

2 monomers are involved in 4 short contacts:

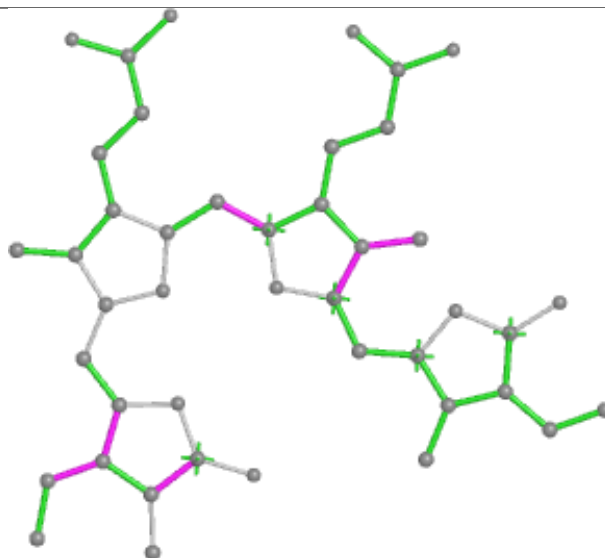
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	LBV	2	0
2	B	801	LBV	2	0

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.

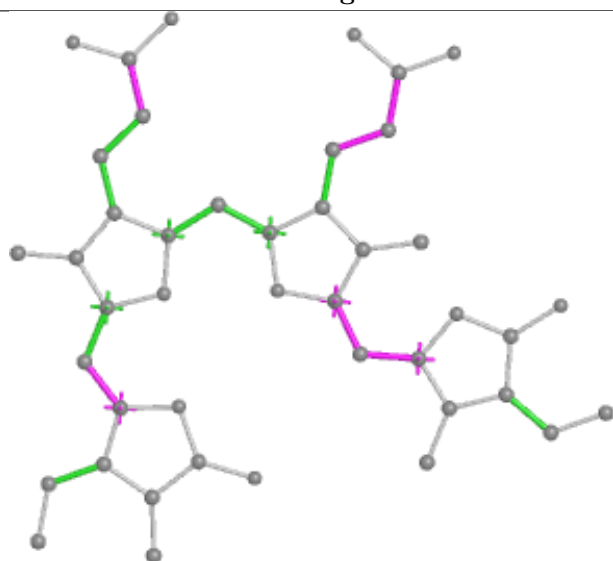
Ligand LBV A 801



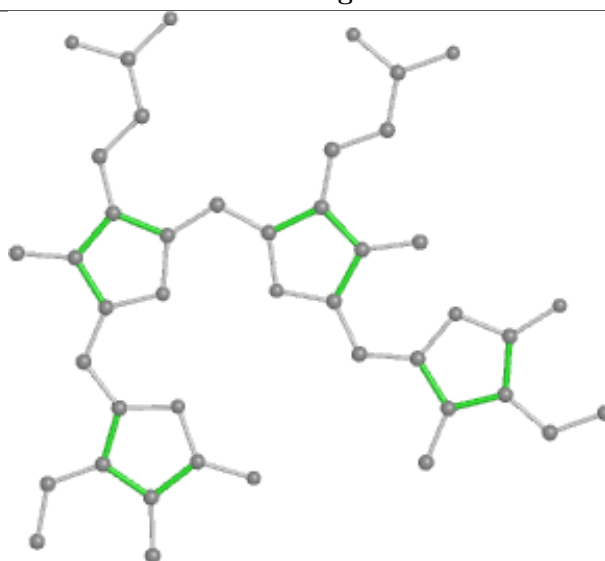
Bond lengths



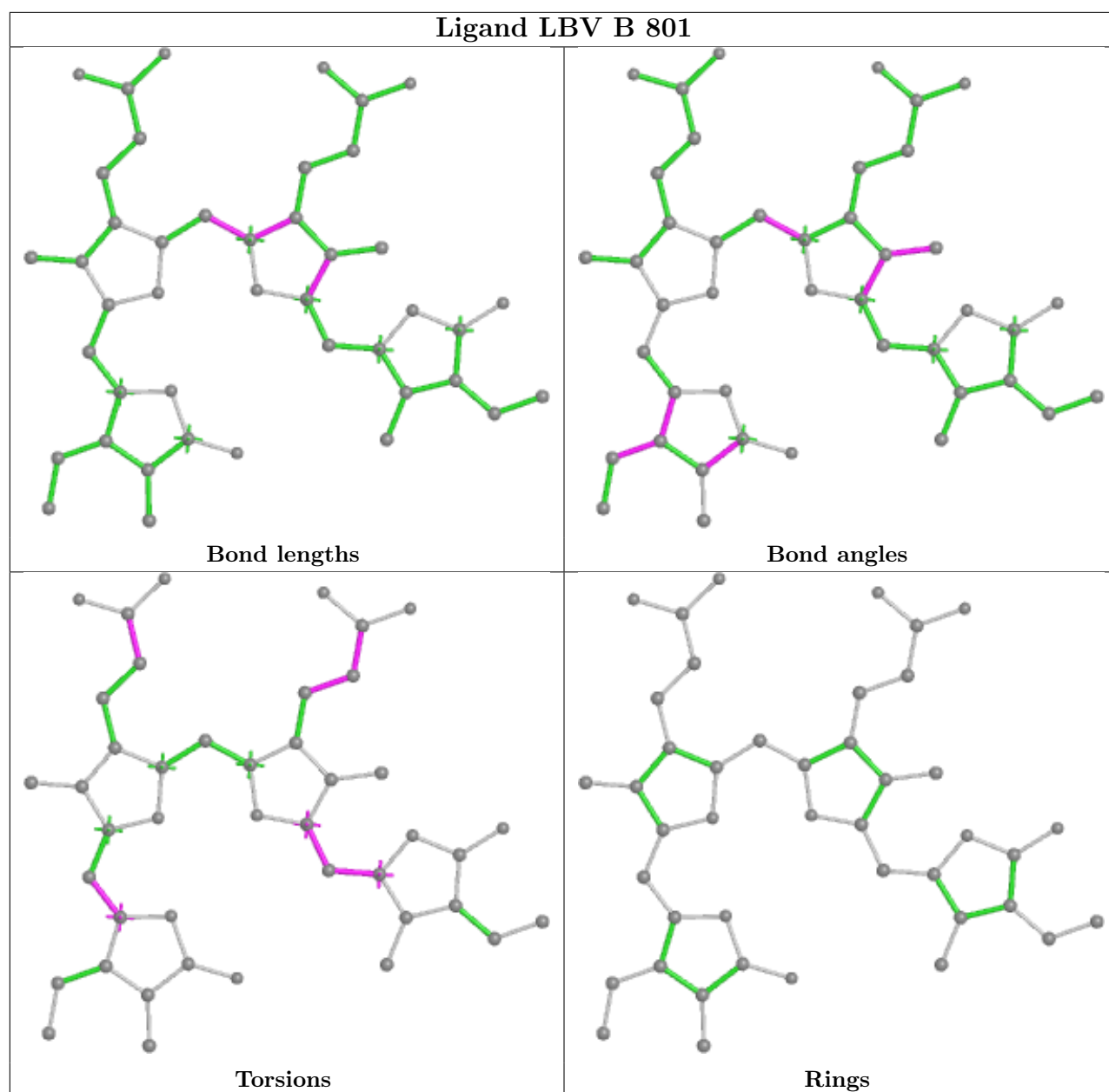
Bond angles



Torsions



Rings



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.

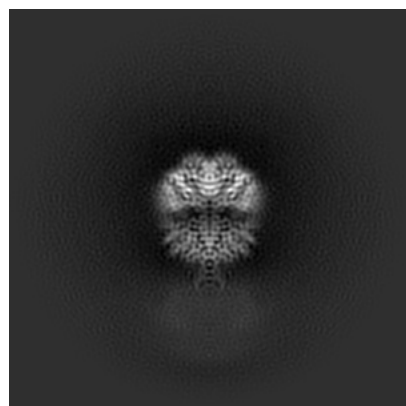
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40458. These allow visual inspection of the internal detail of the map and identification of artifacts.

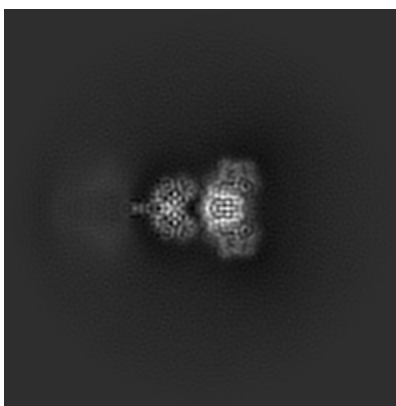
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

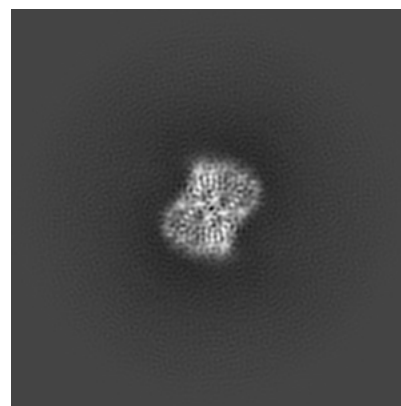
6.1.1 Primary map



X

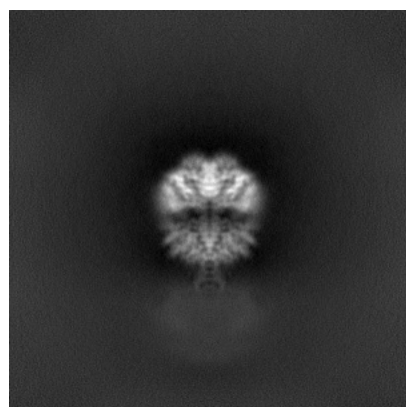


Y

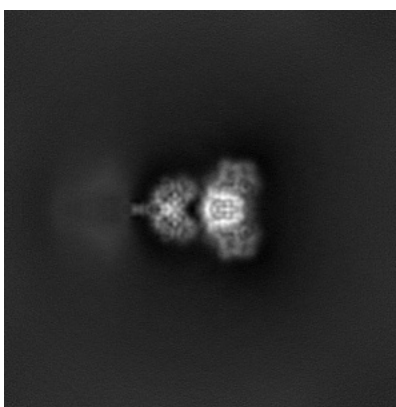


Z

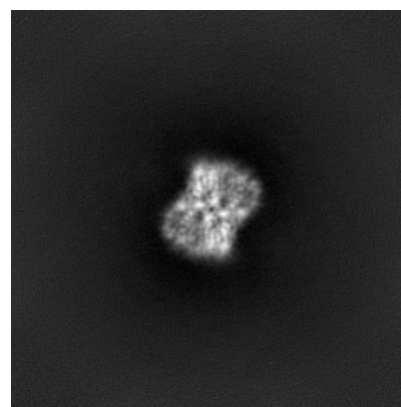
6.1.2 Raw map



X



Y

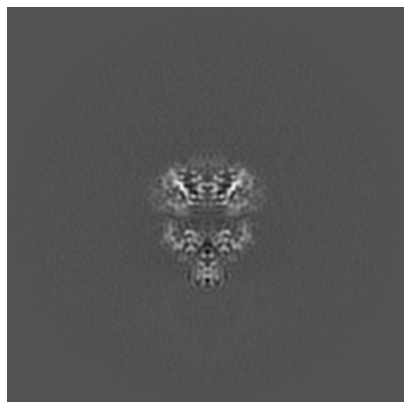


Z

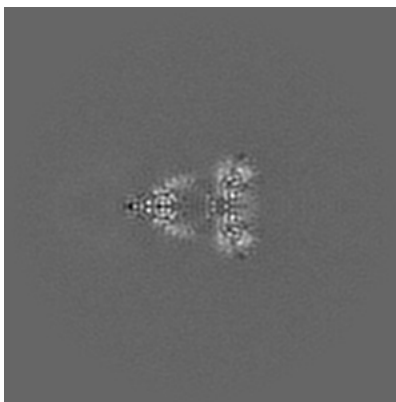
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

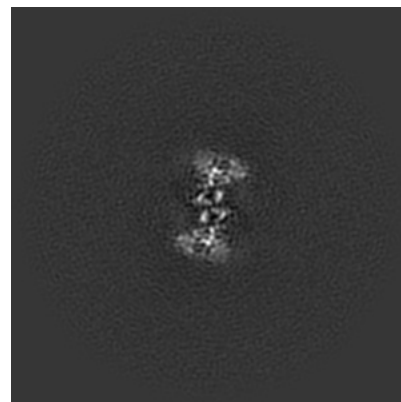
6.2.1 Primary map



X Index: 180

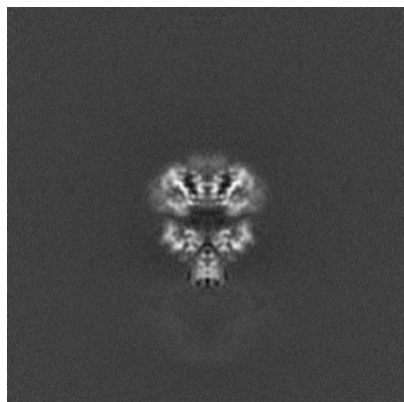


Y Index: 180

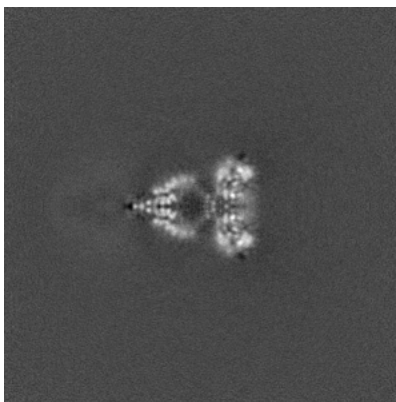


Z Index: 180

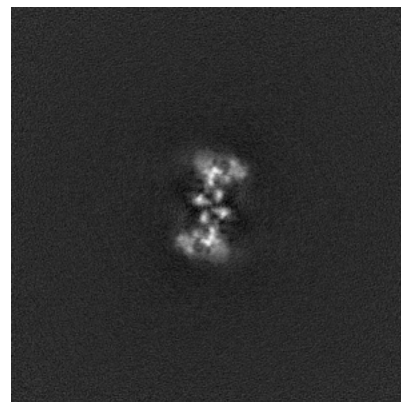
6.2.2 Raw map



X Index: 180



Y Index: 180

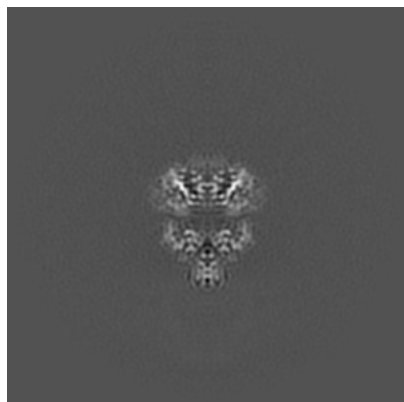


Z Index: 180

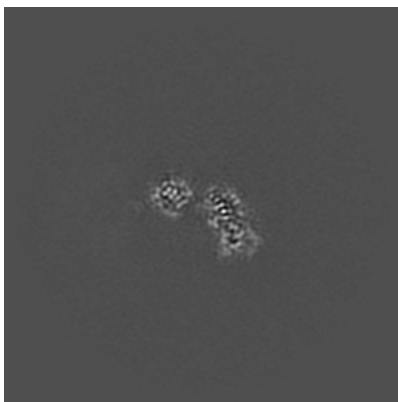
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

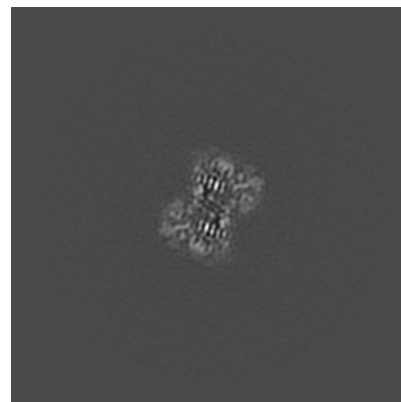
6.3.1 Primary map



X Index: 180

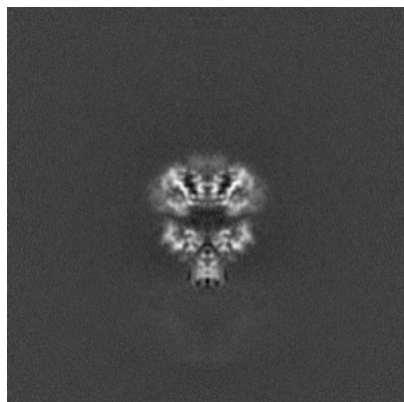


Y Index: 161

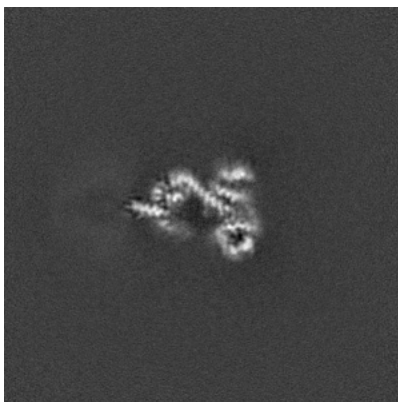


Z Index: 197

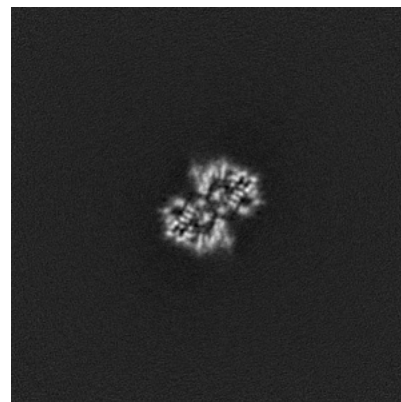
6.3.2 Raw map



X Index: 180



Y Index: 176

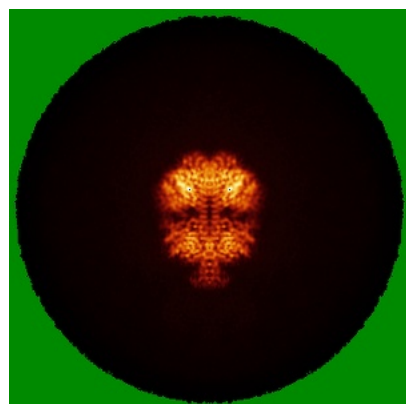


Z Index: 208

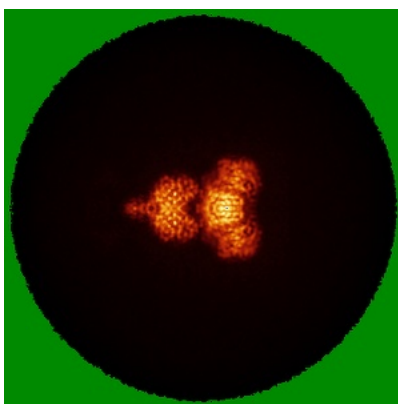
The images above show the largest variance slices of the map in three orthogonal directions.

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

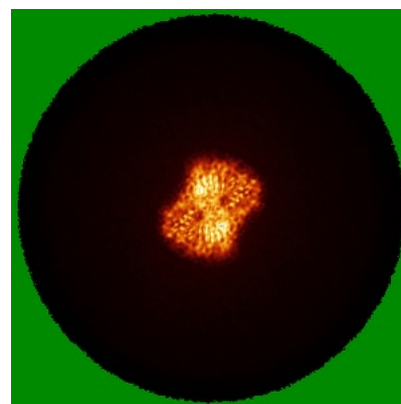
6.4.1 Primary map



X

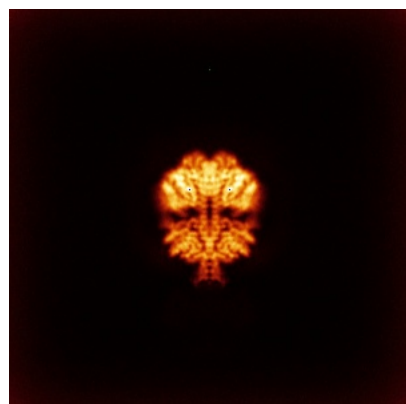


Y

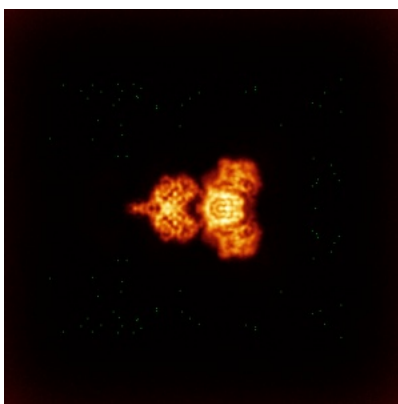


Z

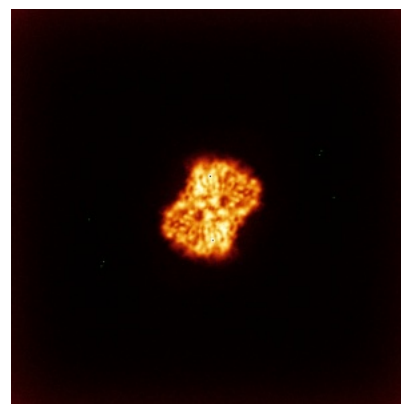
6.4.2 Raw map



X



Y

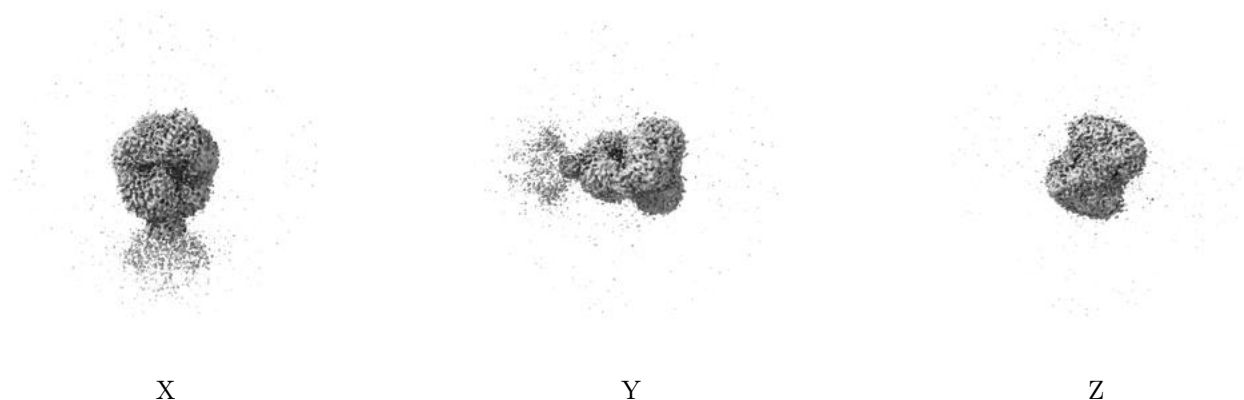


Z

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.

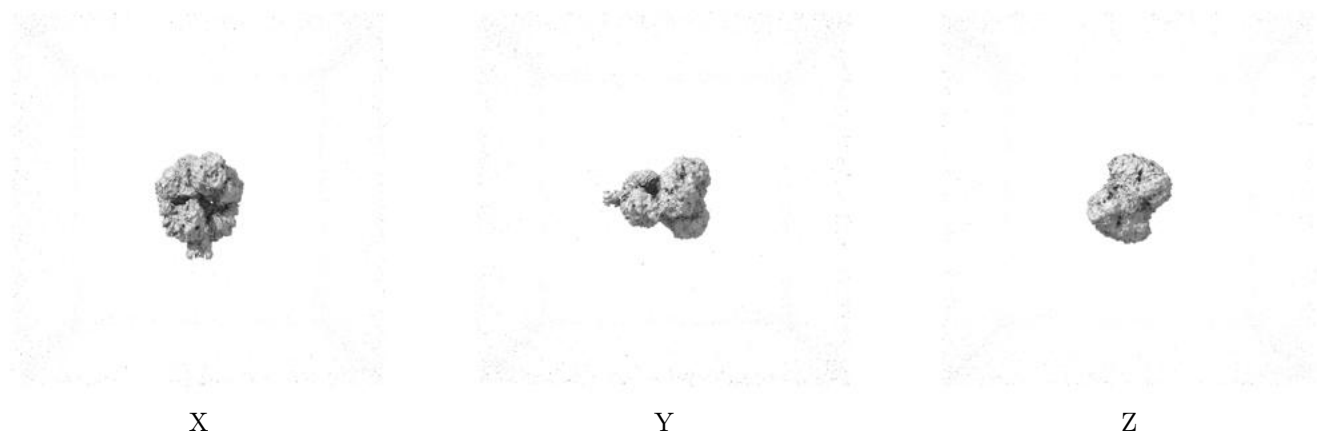
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.063. 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



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.

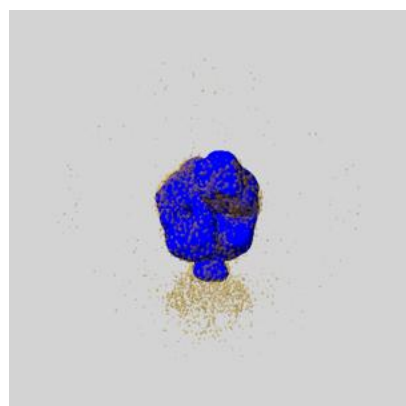
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

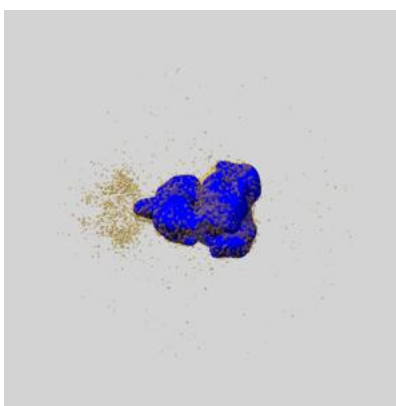
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

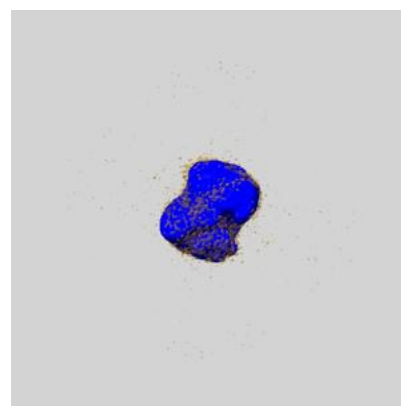
6.6.1 emd_40458_msk_1.map [i](#)



X



Y

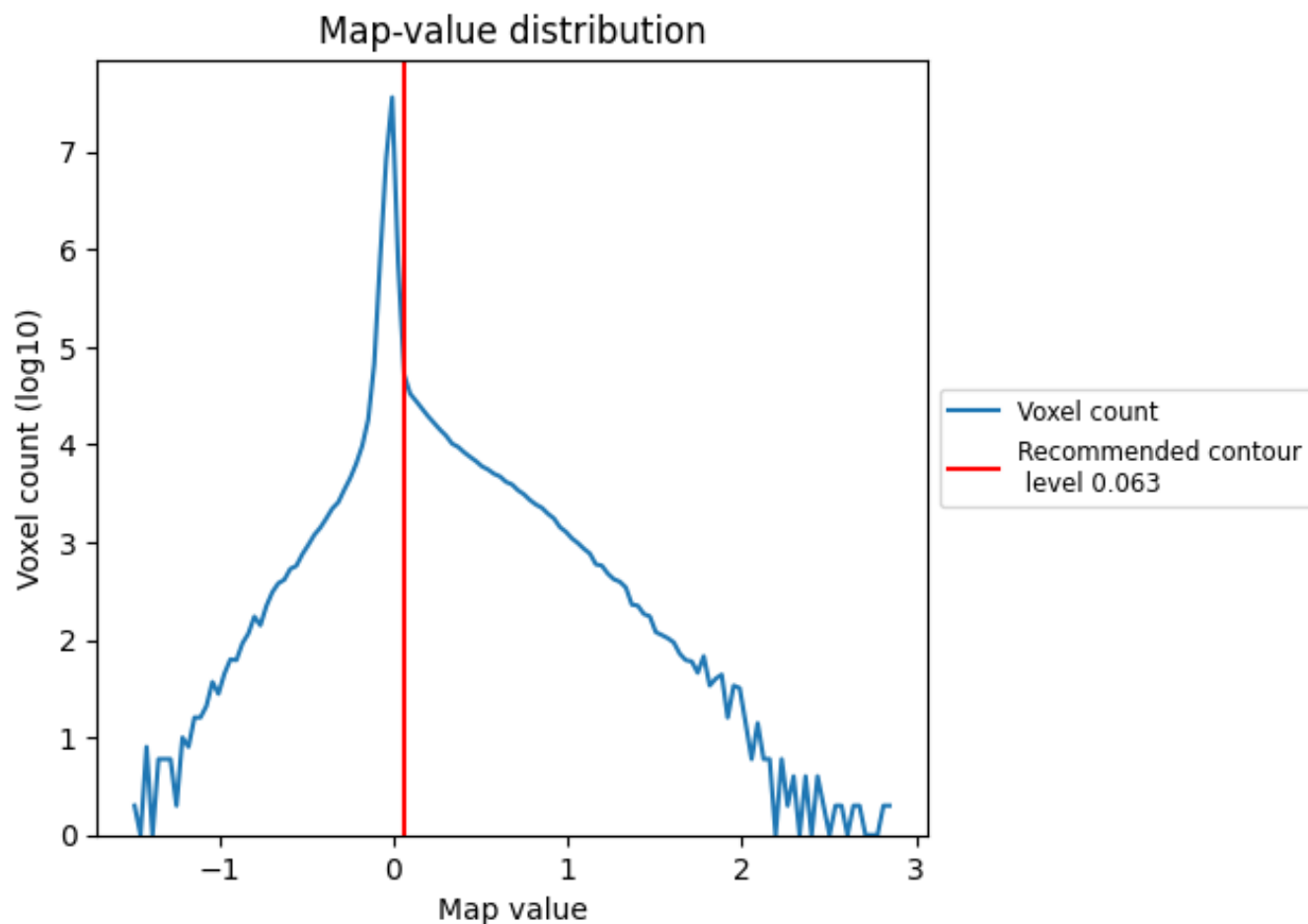


Z

7 Map analysis [i](#)

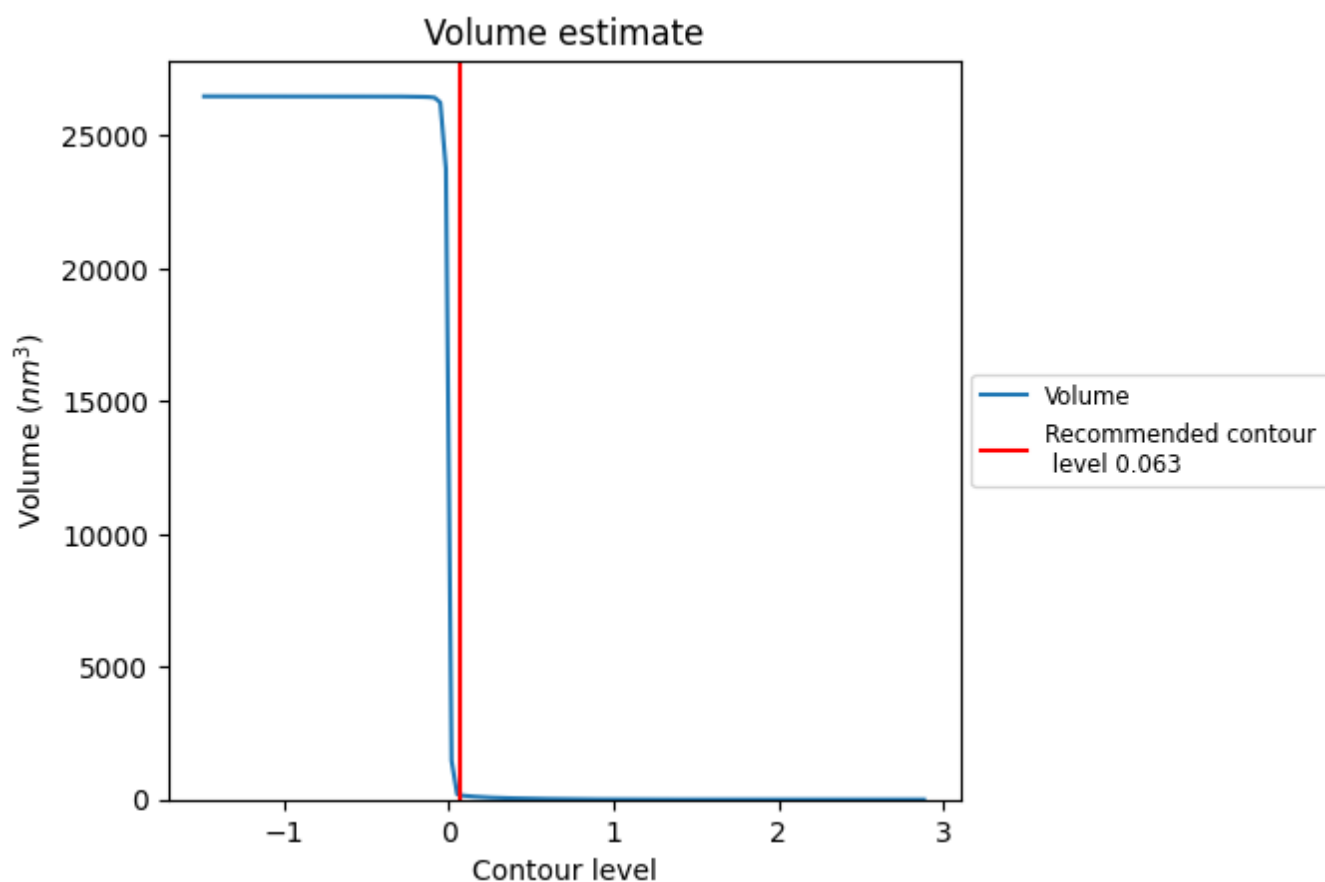
This section contains the results of statistical analysis of the map.

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.

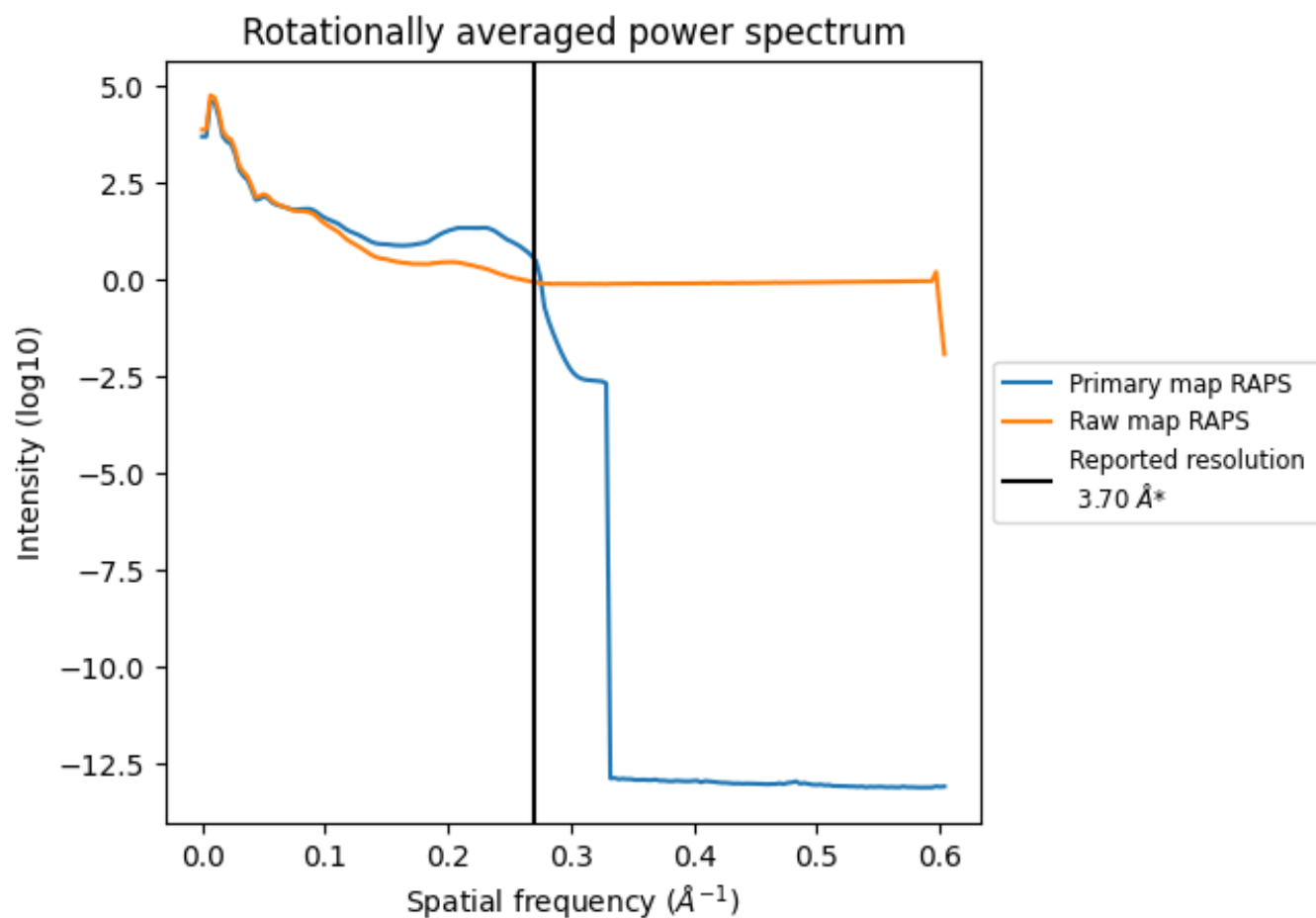
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm^3 ; this corresponds to an approximate mass of 163 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 ⓘ

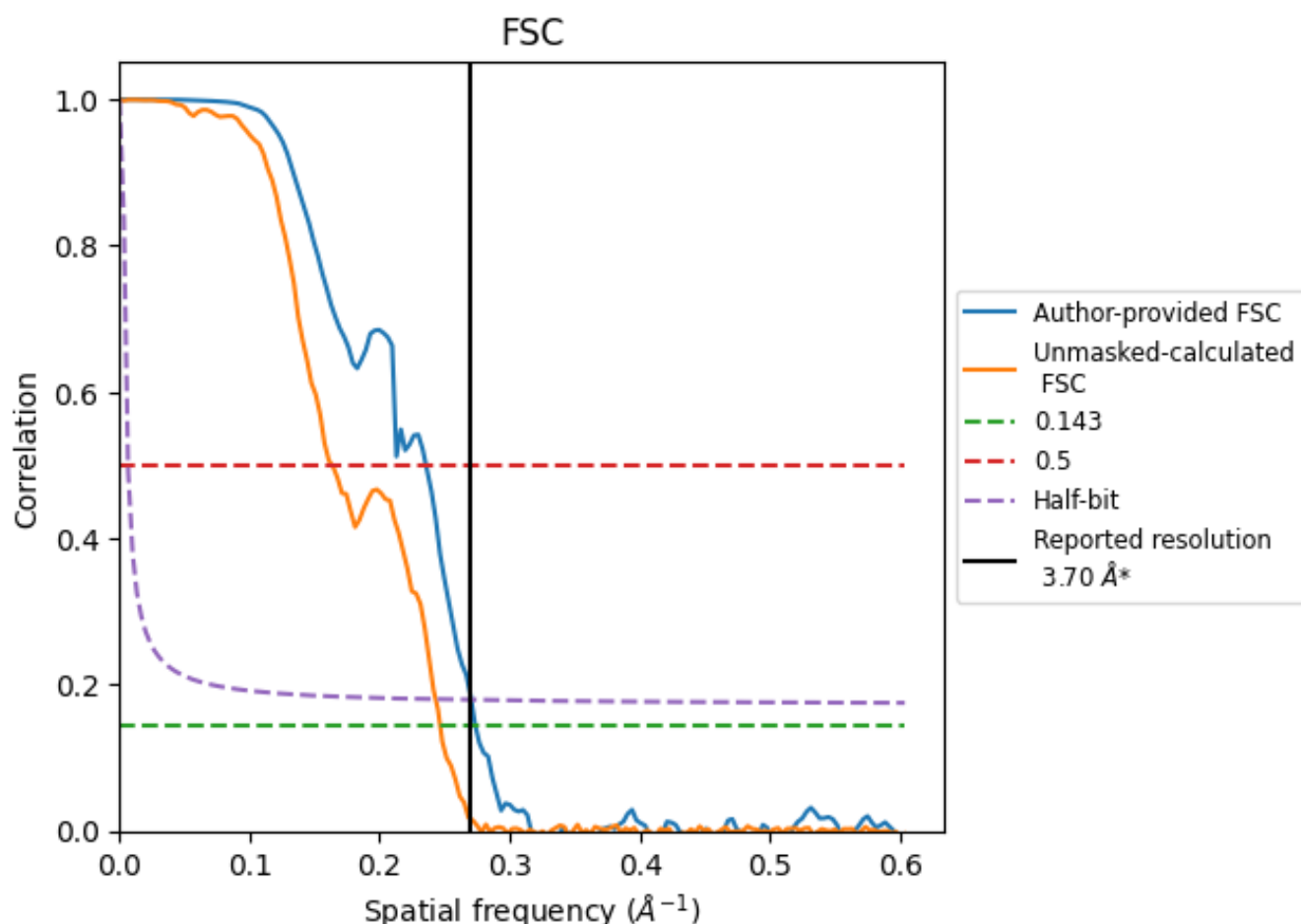


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

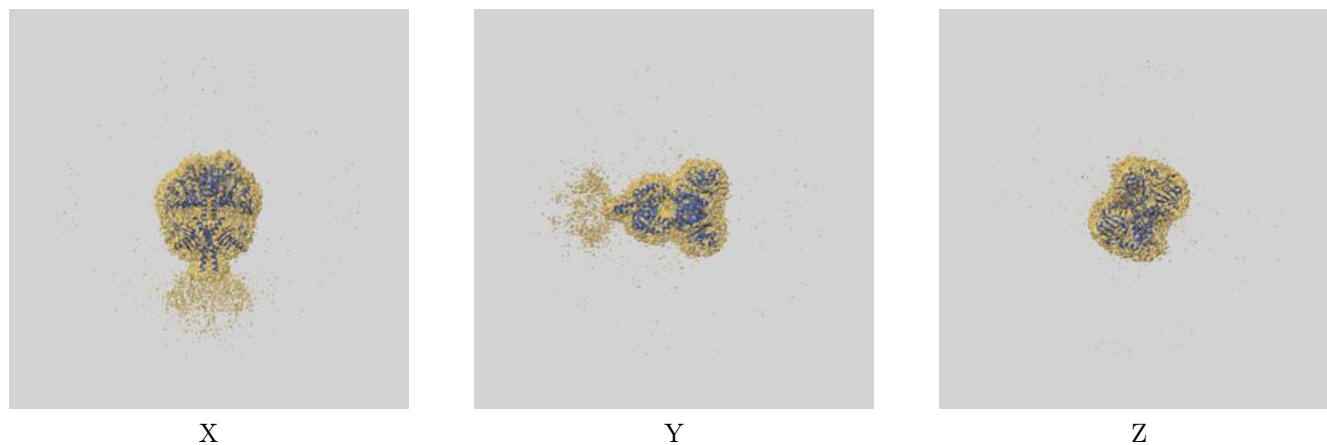
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.65	4.24	3.70
Unmasked-calculated*	4.06	6.12	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

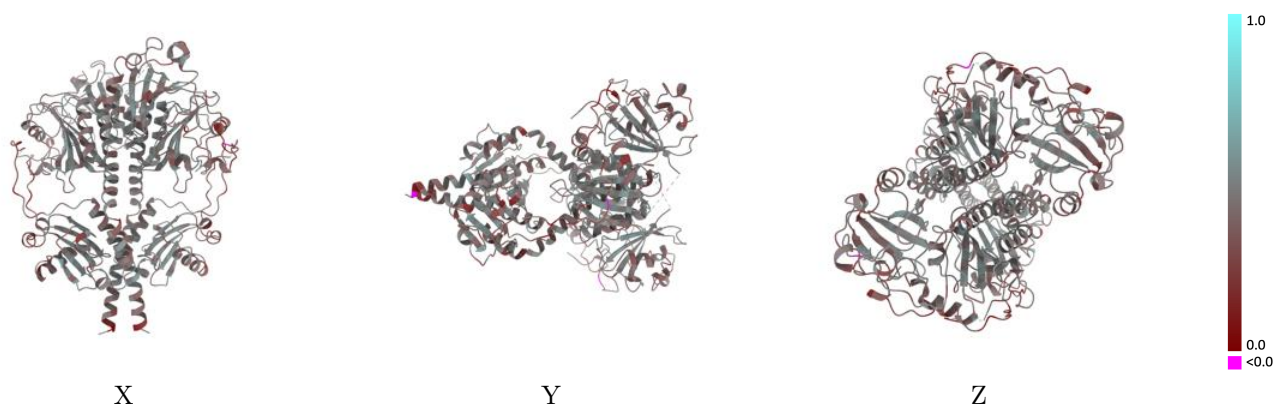
This section contains information regarding the fit between EMDB map EMD-40458 and PDB model 8SGK. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



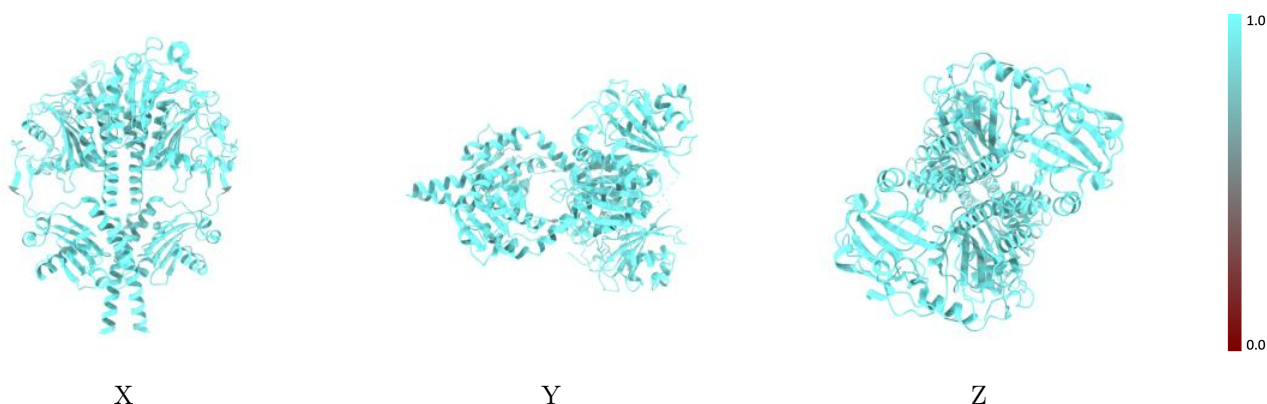
The images above show the 3D surface view of the map at the recommended contour level 0.063 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



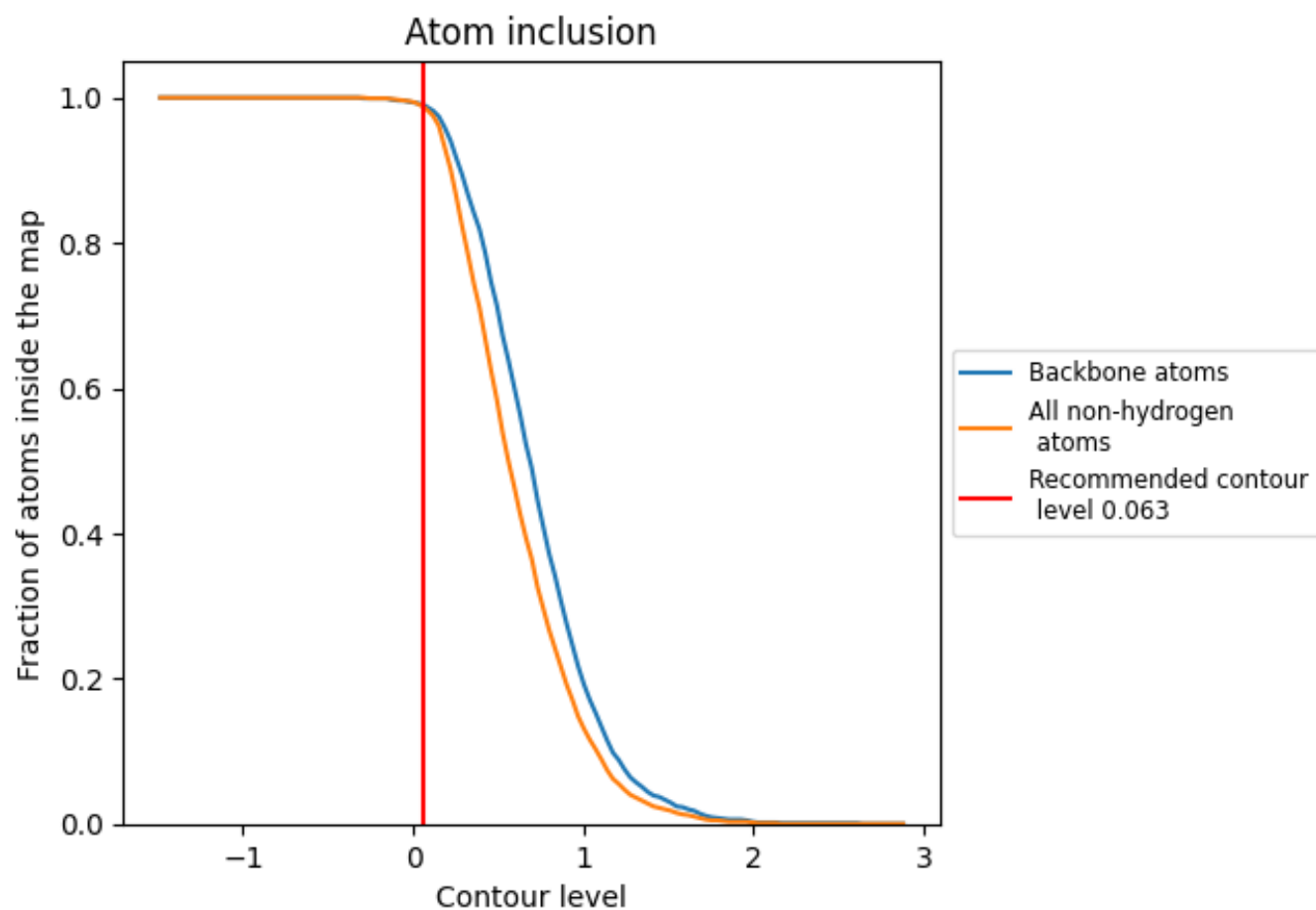
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.063).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.063) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9870	<div></div> 0.4210
A	<div></div> 0.9880	<div></div> 0.4210
B	<div></div> 0.9870	<div></div> 0.4210

