



Full wwPDB EM Validation Report ⓘ

Jan 1, 2025 – 12:45 PM EST

PDB ID : 8UPM
EMDB ID : EMD-42452
Title : Pfr state of Stigmatella aurantiaca bacteriophytochrome 2
Authors : Malla, T.N.; Schmidt, M.; Stojkovic, E.A.
Deposited on : 2023-10-23
Resolution : 3.75 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

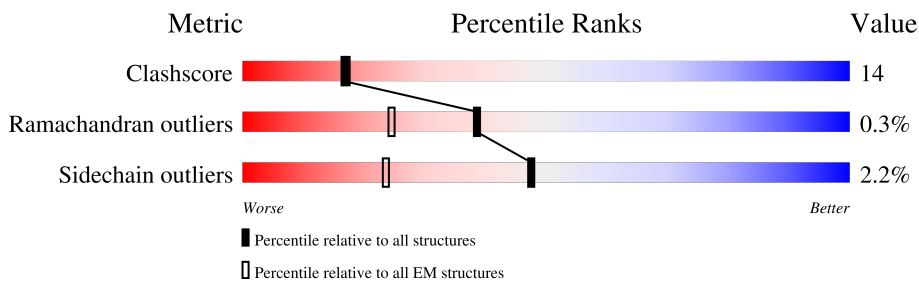
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.75 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	747	
1	B	747	

2 Entry composition [i](#)

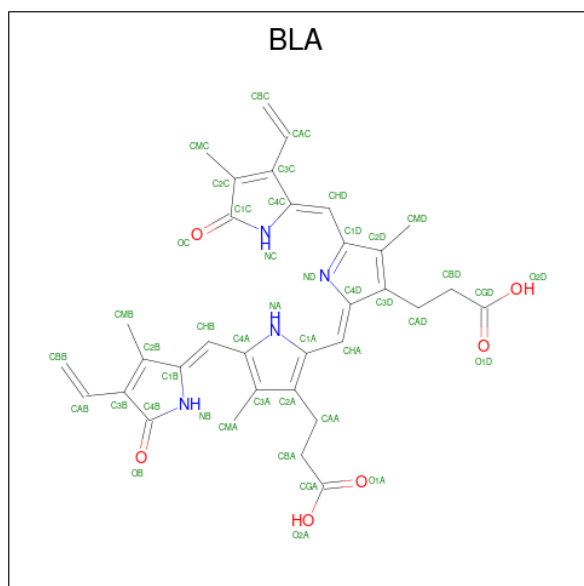
There are 2 unique types of molecules in this entry. The entry contains 7760 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (Light-regulated signal transduction histidine kinase).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	503	Total	C	N	O	S	1	0
			3837	2423	702	703	9		
1	B	503	Total	C	N	O	S	1	0
			3837	2423	702	703	9		

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

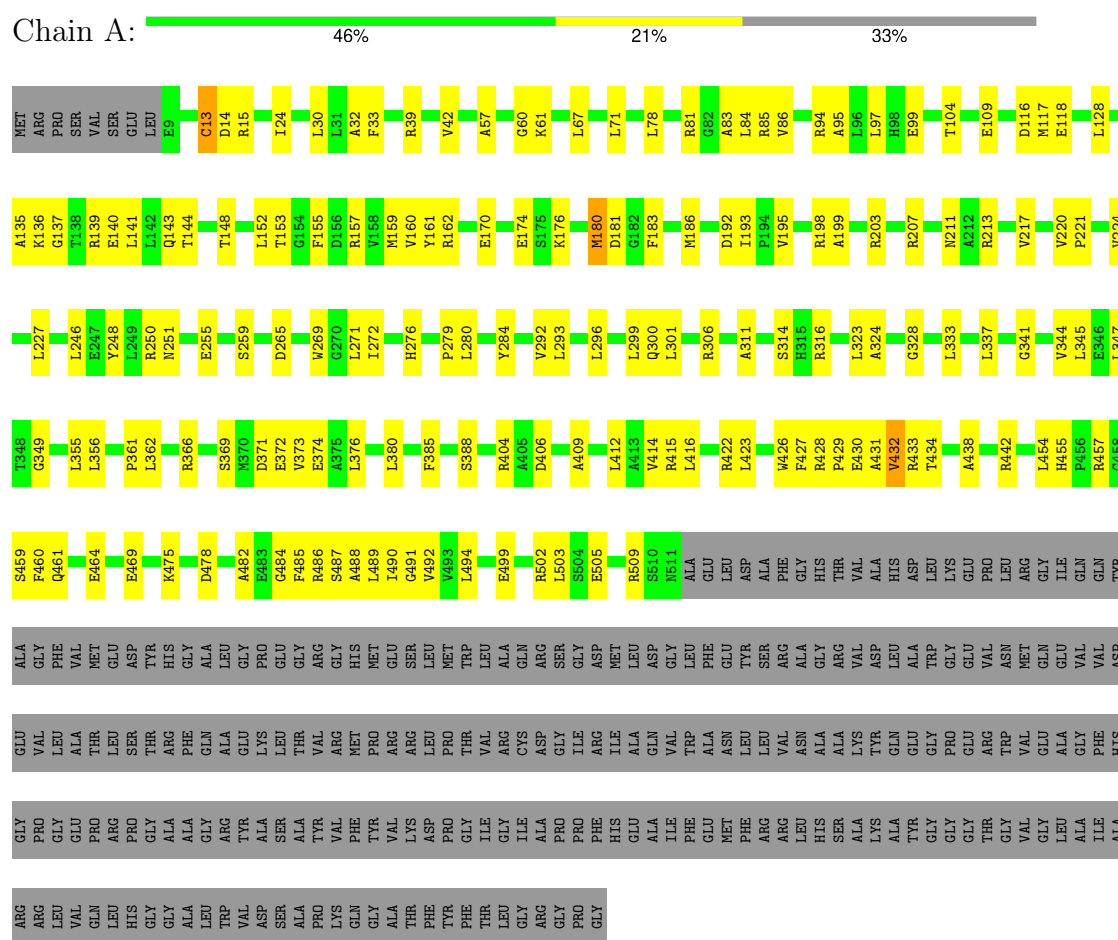


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			43	33	4	6	
2	B	1	Total	C	N	O	0
			43	33	4	6	

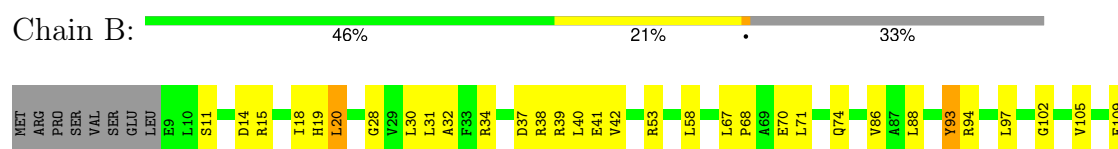
3 Residue-property plots

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 (Light-regulated signal transduction histidine kinase)



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ARG	LEU	GLY	VAL	GLY	W463	L337	P243	E112
LEU	VAL	PHE	ALA	PHE	E464	A338	T244	M117
GLN	VAL	VAL	THR	VAL	E465	R339	T245	E118
LEU	GLN	MET	THR	MET	T466	L347	T246	L128
HIS	LEU	GLU	LEU	GLU	V467	L347	T247	A135
GLY	TRP	ASP	SER	ASP	R468	L347	T248	A136
GLY	THR	THR	THR	THR	L478	T351	T249	L136
GLY	ARG	HIS	ARG	HIS	D478	L351	T250	L139
ALA	ALA	GLY	PHE	GLY	L479	R366	T251	L140
LEU	GLN	ALA	GLN	ALA	A480	L366	T252	L141
TRP	ALA	LEU	ALA	LEU	E483	R370	T253	Q143
VAL	GLU	GLY	GLU	GLY	E483	B371	T254	R152
ASP	LYS	PRO	LYS	PRO	R486	E372	T255	F155
SER	LEU	GLU	LEU	GLU	L486	L376	T256	Y161
PRO	VAL	ARG	VAL	ARG	L489	A377	T257	R162
LYS	VAL	GLY	ARG	GLY	T490	A378	T258	G169
GLN	PHE	MET	MET	HIS	E491	R379	T259	E170
GLY	GLY	PRO	ARG	MET	V492	L380	T260	M180
ALA	VAL	THR	ALA	GLU	V493	A381	T261	M186
THR	ALA	ARG	LYS	SER	L494	P382	T262	H187
PHE	ASP	LEU	LEU	LEU	R495	R385	T263	F188
TYR	PRO	MET	MET	MET	Q496	F386	T264	L200
PHE	THR	THR	THR	THR	L500	T387	T265	Y201
ILE	VAL	VAL	VAL	LEU	E501	L387	T266	T202
LEU	ARG	GLY	ARG	ALA	R502	Y398	T267	R207
GLY	ILE	CYS	CYS	GLN	L503	L401	T268	L208
ALA	ASP	GLY	ASP	ARG	E504	R404	T269	T209
PRO	GLY	GLY	GLY	SER	S504	L401	T270	A210
PRO	PRO	ILE	ILE	GLY	E505	R404	T271	N211
PHE	PHE	ILE	ILE	ASP	A506	V407	T272	A212
HIS	ILE	ILE	ILE	MET	L507	L407	T273	R213
GLU	GLU	ALA	GLN	LEU	S508	V407	T274	P221
ALA	ALA	ILE	VAL	ASP	E511	V414	T275	Y229
ILE	VAL	TRP	TRP	GLY	ALA	R415	T276	L233
PHE	GLU	ALA	ALA	LEU	GLU	L416	T277	S234
GLU	PRO	ASN	ASN	GLU	LEU	L416	T278	G235
PHE	PHE	LEU	LEU	THR	ASP	R422	T279	S236
ARG	ARG	ARG	VAL	SER	ALA	R428	T280	A237
LEU	LEU	ASN	VAL	ARG	PHE	P429	T281	R239
HIS	HIS	ALA	ALA	ALA	GLY	A430	T282	S240
SER	SER	ALA	ALA	ARG	HIS	A431	T283	V241
ALA	ALA	LYS	LYS	VAL	VAL	V432	T284	E242
ALA	ALA	TYR	GLN	ASP	ALA	R440	T285	L243
TYR	TYR	GLU	GLU	ALA	ASP	L440	T286	S244
GLY	GLY	GLY	GLY	TRP	LEU	G450	T287	V245
GLY	GLY	GLU	PRO	TRP	LEU	R451	T288	L246
GLY	GLY	GLU	GLU	GLY	LYS	A452	T289	G247
THR	THR	ARG	ARG	VAL	PRO	R453	T290	L248
GLY	GLY	ASN	ASN	ASN	LEU	L454	T291	S249
VAL	VAL	TRP	TRP	MET	ARG	R455	T292	R250
GLY	GLY	GLU	GLU	MET	GLY	P456	T293	V251
LEU	LEU	ALA	ALA	GLN	ILE	R457	T294	E252
ALA	ALA	GLY	GLY	VAL	GLN	F460	T295	L253
ILE	ILE	PHE	PHE	VAL	GLN	L461	T296	S254
ALA	ALA	HIS	HIS	ASP	TYR	Q462	T297	G255
ASP	ASP	GLY	GLY	ALA	ALA	L462	T298	L256

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.31	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.328	Depositor
Minimum map value	-0.157	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size (\AA)	337.6, 337.6, 337.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84400004, 0.84400004, 0.84400004	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: BLA

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	0.25	0/3920	0.56	0/5339
1	B	0.25	0/3920	0.61	1/5339 (0.0%)
All	All	0.25	0/7840	0.59	1/10678 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	20	LEU	CA-CB-CG	7.93	133.54	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	VAL	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	3837	0	3880	105	0
1	B	3837	0	3880	121	0
2	A	43	0	31	4	0
2	B	43	0	31	3	0
All	All	7760	0	7822	213	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 14.

All (213) 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:A:13:CYS:SG	1:A:14:ASP:N	2.62	0.72
1:A:355:LEU:HD23	1:A:362:LEU:HD21	1.73	0.71
1:A:136:LYS:HZ3	1:B:306:ARG:HD2	1.55	0.70
1:B:251:ASN:ND2	1:B:453:ARG:O	2.25	0.69
1:A:385:PHE:O	1:A:415:ARG:NH2	2.26	0.69
1:A:380:LEU:HD22	1:A:423:LEU:HD11	1.75	0.68
1:A:153:THR:HG23	1:A:155:PHE:H	1.58	0.67
1:B:136:LYS:HA	1:B:136:LYS:HE2	1.77	0.66
1:A:42:VAL:HG22	1:A:221:PRO:HG2	1.77	0.66
1:B:366:ARG:HD2	1:B:407:VAL:HG11	1.77	0.66
1:A:160:VAL:HG22	1:A:272:ILE:HG12	1.77	0.66
1:B:370:MET:HE3	1:B:370:MET:H	1.60	0.65
1:B:128:LEU:HD21	1:B:152:LEU:HD12	1.76	0.65
1:A:484:GLY:O	1:A:488:ALA:N	2.22	0.64
1:B:140:GLU:OE2	1:B:140:GLU:N	2.24	0.64
1:B:88:LEU:HD12	1:B:93:TYR:HD1	1.62	0.64
1:A:137:GLY:O	1:A:141:LEU:N	2.28	0.64
1:A:157:ARG:HH11	1:A:176:LYS:HZ1	1.46	0.64
1:B:276:HIS:ND1	1:B:278:ALA:O	2.31	0.63
1:B:490:ILE:HD12	1:B:493:VAL:HB	1.81	0.63
1:B:94:ARG:HD3	1:B:284:TYR:CZ	2.34	0.62
1:A:299:LEU:HB3	1:B:300:GLN:HE22	1.64	0.62
1:B:162:ARG:HH21	1:B:170:GLU:HG3	1.65	0.61
1:A:371:ASP:OD2	1:A:371:ASP:N	2.33	0.61
1:A:136:LYS:NZ	1:B:306:ARG:HD2	2.16	0.61
1:B:71:LEU:HD11	1:B:86:VAL:HG11	1.81	0.61
1:B:70:GLU:O	1:B:74:GLN:NE2	2.34	0.60
1:A:211:ASN:OD1	1:A:213:ARG:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ILE:HB	1:B:257:SER:H	1.66	0.60
1:B:31:LEU:HB2	1:B:40:LEU:HD11	1.84	0.60
1:A:81:ARG:HH12	1:B:118:GLU:HA	1.67	0.60
1:A:489:LEU:O	1:A:492:VAL:HG12	2.01	0.59
1:B:500:LEU:HD13	1:B:503:LEU:HD21	1.83	0.59
1:A:475:LYS:HA	1:A:475:LYS:HE3	1.84	0.59
1:B:312:GLU:OE2	1:B:316:ARG:NH2	2.35	0.59
1:B:200:LEU:HD23	1:B:239:ARG:HH22	1.67	0.59
1:A:195:VAL:HG22	1:A:198:ARG:HH21	1.68	0.59
1:B:452:ALA:HB3	1:B:453:ARG:HH11	1.68	0.58
1:B:162:ARG:O	1:B:170:GLU:N	2.30	0.58
1:A:349:GLY:O	1:A:428:ARG:NH1	2.37	0.58
1:B:416:LEU:N	1:B:422:ARG:O	2.36	0.58
1:A:71:LEU:HD23	1:A:86:VAL:HG11	1.86	0.58
1:A:161:TYR:HD2	1:A:271:LEU:HB2	1.69	0.58
1:A:176:LYS:NZ	1:A:181:ASP:O	2.35	0.57
1:B:94:ARG:NH2	1:B:112:GLU:H	2.02	0.57
1:B:465:GLU:HA	1:B:468:ARG:HG2	1.85	0.57
1:A:39:ARG:HD2	1:A:60:GLY:HA2	1.87	0.57
1:B:309:GLU:N	1:B:309:GLU:OE1	2.37	0.56
1:A:174:GLU:OE2	1:A:176:LYS:NZ	2.37	0.56
1:A:455:HIS:HD2	2:A:801:BLA:HBB1	1.70	0.56
1:A:455:HIS:CD2	2:A:801:BLA:HBB1	2.40	0.56
1:B:30:LEU:HD11	1:B:105:VAL:HB	1.87	0.56
1:B:213:ARG:HH22	1:B:250:ARG:HB2	1.70	0.56
1:B:53:ARG:HG3	1:B:58:LEU:HD11	1.87	0.56
1:A:162:ARG:NH2	1:A:170:GLU:OE2	2.39	0.56
1:B:455:HIS:HD2	2:B:801:BLA:HBB2	1.71	0.56
1:B:67:LEU:HD13	1:B:71:LEU:HB2	1.87	0.55
1:A:180:MET:SD	1:A:180:MET:N	2.79	0.55
1:A:33:PHE:HZ	1:A:67:LEU:HD11	1.72	0.55
1:A:430:GLU:OE2	1:A:469:GLU:N	2.38	0.55
1:B:11:SER:OG	1:B:15:ARG:NH2	2.39	0.55
1:A:429:PRO:HG2	1:A:434:THR:HB	1.87	0.55
1:B:187:HIS:HB2	1:B:460:PHE:HD1	1.71	0.55
1:A:251:ASN:HB3	1:A:454:LEU:HD13	1.89	0.55
1:B:262:LEU:HD11	1:B:272:ILE:HG13	1.88	0.55
1:A:412:LEU:HD21	1:A:482:ALA:HB2	1.88	0.54
1:A:306:ARG:NH2	1:B:304:GLU:OE2	2.40	0.54
1:A:94:ARG:HB2	1:A:109:GLU:HB3	1.90	0.54
1:B:233:LEU:HB3	1:B:236:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ARG:HH12	1:B:250:ARG:HE	1.57	0.53
1:A:459:SER:OG	1:A:460:PHE:N	2.42	0.53
1:A:193:ILE:HD11	2:A:801:BLA:HMA3	1.90	0.53
1:A:428:ARG:NH2	1:A:478:ASP:OD2	2.41	0.53
1:A:369:SER:OG	1:A:371:ASP:OD2	2.20	0.53
1:A:323:LEU:HD11	1:A:344:VAL:HB	1.91	0.53
1:A:276:HIS:CE1	1:A:280:LEU:HD21	2.44	0.52
1:A:341:GLY:O	1:A:345:LEU:HB3	2.09	0.52
1:B:94:ARG:HG3	1:B:109:GLU:HB3	1.91	0.52
1:A:461:GLN:O	1:A:464:GLU:HG2	2.10	0.52
1:B:387:THR:OG1	1:B:486:ARG:NH2	2.43	0.52
1:A:438:ALA:HA	1:A:442:ARG:HH22	1.74	0.52
1:B:20:LEU:HD21	1:B:229:ARG:HB2	1.92	0.52
1:A:78:LEU:HD13	1:A:84:LEU:HG	1.92	0.52
1:B:428:ARG:NH2	1:B:478:ASP:OD2	2.43	0.52
1:A:128:LEU:HD13	1:A:293:LEU:HD22	1.91	0.51
1:B:70:GLU:HG2	1:B:71:LEU:HD22	1.92	0.51
1:A:406:ASP:OD1	1:A:433:ARG:NH1	2.43	0.51
1:B:303:SER:HA	1:B:306:ARG:HH21	1.76	0.51
1:A:84:LEU:C	1:A:94:ARG:HH12	2.15	0.50
1:A:186:MET:HG3	1:A:455:HIS:HE2	1.77	0.50
1:A:192:ASP:HA	2:A:801:BLA:HMC3	1.93	0.50
1:A:499:GLU:HG2	1:B:503:LEU:HD23	1.94	0.50
1:B:252:MET:HG3	1:B:254:VAL:HG12	1.94	0.50
1:A:509:ARG:NH2	1:B:506:ALA:O	2.45	0.49
1:B:135:ALA:HB1	1:B:141:LEU:HD12	1.94	0.49
1:B:207:ARG:NH1	2:B:801:BLA:O1D	2.45	0.49
1:A:372:GLU:OE2	1:A:404:ARG:NH1	2.46	0.49
1:B:34:ARG:NH1	1:B:102:GLY:O	2.45	0.49
1:A:135:ALA:HA	1:A:140:GLU:OE2	2.11	0.49
1:A:328:GLY:O	1:B:495:ARG:NH1	2.46	0.49
1:B:162:ARG:HB3	1:B:170:GLU:HB2	1.94	0.49
1:A:431:ALA:O	1:A:432:VAL:HB	2.13	0.49
1:B:67:LEU:HD12	1:B:68:PRO:O	2.13	0.49
1:B:463:TRP:O	1:B:467:VAL:HG22	2.12	0.48
1:A:502:ARG:HE	1:A:505:GLU:HG2	1.79	0.48
1:B:315[A]:HIS:CE1	1:B:316:ARG:HE	2.31	0.48
1:B:327:LEU:HD12	1:B:493:VAL:HG12	1.95	0.48
1:A:14:ASP:OD1	1:A:15:ARG:N	2.46	0.48
1:A:199:ALA:O	1:A:203:ARG:HG3	2.14	0.48
1:B:505:GLU:HA	1:B:508:SER:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASN:OD1	1:B:213:ARG:N	2.47	0.48
1:A:490:ILE:HG13	1:A:494:LEU:HD12	1.95	0.48
1:B:32:ALA:HB3	1:B:41:GLU:HB3	1.94	0.48
1:B:88:LEU:HD12	1:B:93:TYR:CD1	2.45	0.48
1:A:246:LEU:O	1:A:250:ARG:HG3	2.14	0.47
1:B:94:ARG:HH21	1:B:112:GLU:H	1.62	0.47
1:B:455:HIS:HB2	1:B:456:PRO:HD3	1.96	0.47
1:A:369:SER:O	1:A:373:VAL:HG12	2.15	0.47
1:B:207:ARG:NH2	1:B:241:VAL:HG12	2.30	0.47
1:A:324:ALA:HB3	1:B:489:LEU:HA	1.97	0.47
1:B:161:TYR:O	1:B:270:GLY:HA2	2.15	0.47
1:A:416:LEU:HB2	1:A:422:ARG:HB2	1.97	0.47
1:B:462:ALA:O	1:B:466:THR:OG1	2.21	0.47
1:B:97:LEU:HD13	1:B:105:VAL:O	2.15	0.46
1:A:489:LEU:O	1:A:491:GLY:N	2.48	0.46
1:B:245:HIS:CE1	1:B:249:LEU:HD11	2.50	0.46
1:B:453:ARG:HD3	1:B:453:ARG:N	2.31	0.46
1:A:248:TYR:CE1	1:A:454:LEU:HA	2.49	0.46
1:A:502:ARG:HB2	1:B:503:LEU:HD22	1.96	0.46
1:B:398:TYR:HE2	1:B:401:LEU:HG	1.79	0.46
1:B:162:ARG:NH2	1:B:170:GLU:HG3	2.29	0.46
1:A:24:ILE:O	1:A:217:VAL:N	2.45	0.46
1:A:78:LEU:HG	1:A:97:LEU:HD23	1.98	0.46
1:A:426:TRP:HH2	1:A:485:PHE:HB3	1.79	0.46
1:B:201:TYR:OH	2:B:801:BLA:O2D	2.33	0.46
1:A:487:SER:HA	1:A:490:ILE:HB	1.97	0.46
1:B:431:ALA:O	1:B:432:VAL:HB	2.16	0.46
1:A:159:MET:HE2	1:A:161:TYR:HE1	1.80	0.46
1:B:276:HIS:HD1	1:B:278:ALA:H	1.63	0.46
1:B:502:ARG:NH2	1:B:505:GLU:OE1	2.49	0.46
1:B:376:LEU:HD12	1:B:377:ALA:N	2.31	0.46
1:B:239:ARG:HD2	1:B:240:SER:O	2.16	0.45
1:B:379:TRP:O	1:B:382:PRO:HD2	2.16	0.45
1:B:492:VAL:O	1:B:496:GLN:HG2	2.16	0.45
1:A:57:ALA:O	1:A:61:LYS:HE2	2.16	0.45
1:B:42:VAL:HG12	1:B:221:PRO:HD2	1.97	0.45
1:B:478:ASP:OD1	1:B:479:LEU:N	2.49	0.45
1:B:19:HIS:CD2	1:B:232:ASP:HB2	2.51	0.45
1:B:28:GLY:HA3	1:B:238:LEU:HD11	1.98	0.45
1:A:224:VAL:HG12	1:A:227:LEU:H	1.82	0.45
1:B:290:CYS:O	1:B:294:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:NH1	1:A:116:ASP:OD2	2.48	0.45
1:A:316:ARG:HD2	1:A:347:LEU:O	2.17	0.45
1:B:37:ASP:HB2	1:B:39:ARG:NH1	2.32	0.45
1:B:454:LEU:HG	1:B:456:PRO:HD2	1.99	0.44
1:A:292:VAL:O	1:A:296:LEU:HD23	2.18	0.44
1:B:380:LEU:HD13	1:B:385:PHE:HZ	1.82	0.44
1:B:407:VAL:HA	1:B:429:PRO:HA	1.98	0.44
1:A:207:ARG:HB3	1:A:259:SER:OG	2.17	0.44
1:A:356:LEU:HB2	1:A:423:LEU:H	1.81	0.44
1:A:213:ARG:NH1	1:A:255:GLU:OE2	2.50	0.44
1:B:315[A]:HIS:HE1	1:B:316:ARG:HH21	1.64	0.44
1:B:319:LEU:O	1:B:322:PRO:HD2	2.17	0.44
1:B:269:TRP:CE3	1:B:301:LEU:HD21	2.53	0.43
1:B:387:THR:O	1:B:414:VAL:HG23	2.18	0.43
1:B:450:GLY:HA3	1:B:453:ARG:CZ	2.48	0.43
1:A:78:LEU:HD21	1:A:95:ALA:HB1	2.00	0.43
1:A:213:ARG:NH2	1:A:250:ARG:HG2	2.33	0.43
1:B:207:ARG:NH2	1:B:239:ARG:HE	2.17	0.43
1:B:500:LEU:O	1:B:503:LEU:HG	2.18	0.43
1:B:335:GLU:C	1:B:339:LYS:HZ2	2.22	0.43
1:B:243:PRO:HA	1:B:246:LEU:HG	2.00	0.43
1:A:81:ARG:HG2	1:A:83:ALA:H	1.82	0.43
1:A:255:GLU:OE1	1:A:279:PRO:HD3	2.19	0.43
1:A:430:GLU:HG2	1:A:432:VAL:HG12	2.01	0.43
1:B:202:THR:HG23	1:B:263:LEU:HD21	1.99	0.43
1:B:480:ALA:O	1:B:483:GLU:HG3	2.19	0.43
1:A:117:MET:SD	1:A:118:GLU:N	2.92	0.42
1:A:388:SER:HB2	1:A:414:VAL:HG12	2.01	0.42
1:B:180:MET:SD	1:B:180:MET:N	2.93	0.42
1:B:186:MET:SD	1:B:187:HIS:N	2.92	0.42
1:B:19:HIS:NE2	1:B:234:SER:HB3	2.34	0.42
1:B:187:HIS:HB2	1:B:460:PHE:CD1	2.53	0.42
1:B:334:GLU:O	1:B:337:LEU:HG	2.20	0.42
1:B:37:ASP:N	1:B:37:ASP:OD1	2.52	0.42
1:B:372:GLU:OE2	1:B:404:ARG:NH2	2.53	0.42
1:B:155:PHE:HA	1:B:276:HIS:HD2	1.84	0.42
1:B:440:ASN:OD1	1:B:440:ASN:N	2.52	0.42
1:A:426:TRP:HZ3	1:A:482:ALA:HA	1.84	0.42
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.80	0.41
1:A:144:THR:O	1:A:148:THR:HG23	2.20	0.41
1:B:207:ARG:CZ	1:B:239:ARG:HH21	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:HD21	1:A:152:LEU:HD13	2.03	0.41
1:B:139:ARG:NH1	1:B:143:GLN:HB2	2.35	0.41
1:B:351:THR:HG22	1:B:429:PRO:HD3	2.01	0.41
1:A:32:ALA:C	1:A:33:PHE:HD2	2.24	0.41
1:A:99:GLU:HG3	1:A:104:THR:HG22	2.02	0.41
1:A:174:GLU:CD	1:A:183:PHE:H	2.23	0.41
1:A:333:LEU:O	1:A:337:LEU:HG	2.21	0.41
1:B:14:ASP:OD1	1:B:15:ARG:HG3	2.21	0.41
1:B:169:GLY:HA3	1:B:188:PHE:CZ	2.56	0.41
1:A:269:TRP:CD2	1:A:301:LEU:HD11	2.56	0.41
1:A:503:LEU:HD22	1:B:503:LEU:HB3	2.03	0.41
1:A:311:ALA:HA	1:B:310:ALA:HB1	2.03	0.40
1:A:316:ARG:HD3	1:A:316:ARG:HA	1.85	0.40
1:A:356:LEU:HD11	1:A:361:PRO:HG3	2.03	0.40
1:B:247:GLU:OE2	1:B:453:ARG:HG3	2.21	0.40
1:A:300:GLN:NE2	1:B:299:LEU:HB3	2.36	0.40
1:A:371:ASP:O	1:A:374:GLU:HG3	2.21	0.40
1:A:139:ARG:HH12	1:A:143:GLN:HB2	1.87	0.40
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.86	0.40
1:A:409:ALA:H	1:A:427:PHE:HE1	1.70	0.40
1:B:18:ILE:HD13	1:B:18:ILE:HA	1.93	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	502/747 (67%)	480 (96%)	19 (4%)	3 (1%)	22	55
1	B	502/747 (67%)	468 (93%)	34 (7%)	0	100	100
All	All	1004/1494 (67%)	948 (94%)	53 (5%)	3 (0%)	38	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	CYS
1	A	432	VAL
1	A	457	ARG

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	390/574 (68%)	383 (98%)	7 (2%)	54	72
1	B	390/574 (68%)	379 (97%)	11 (3%)	38	60
All	All	780/1148 (68%)	762 (98%)	18 (2%)	47	65

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

Mol	Chain	Res	Type
1	A	30	LEU
1	A	180	MET
1	A	265	ASP
1	A	284	TYR
1	A	314	SER
1	A	366	ARG
1	A	486	ARG
1	B	38	ARG
1	B	93	TYR
1	B	117	MET
1	B	136	LYS
1	B	180	MET
1	B	313	ASP
1	B	315[A]	HIS
1	B	315[B]	HIS
1	B	370	MET
1	B	453	ARG
1	B	457	ARG

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

sidechains are listed below:

Mol	Chain	Res	Type
1	B	25	GLN
1	B	74	GLN
1	B	300	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](#)

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	BLA	B	801	1	42,46,46	3.83	21 (50%)	54,67,67	2.19	12 (22%)
2	BLA	A	801	1	42,46,46	3.82	21 (50%)	54,67,67	2.05	10 (18%)

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	BLA	B	801	1	-	19/26/74/74	0/4/4/4
2	BLA	A	801	1	-	14/26/74/74	0/4/4/4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BLA	C4C-NC	9.53	1.54	1.37
2	A	801	BLA	C4C-NC	9.50	1.54	1.37
2	B	801	BLA	C1B-NB	9.48	1.54	1.37
2	A	801	BLA	C1B-NB	9.43	1.53	1.37
2	B	801	BLA	C3C-C2C	7.84	1.53	1.37
2	A	801	BLA	C3C-C2C	7.71	1.52	1.37
2	A	801	BLA	C1C-NC	6.98	1.54	1.38
2	B	801	BLA	C1C-NC	6.91	1.54	1.38
2	A	801	BLA	C4B-NB	6.79	1.53	1.38
2	B	801	BLA	C4B-NB	6.76	1.53	1.38
2	A	801	BLA	C4D-ND	6.06	1.51	1.38
2	B	801	BLA	C4D-ND	5.97	1.51	1.38
2	A	801	BLA	CAC-C3C	-5.83	1.31	1.47
2	B	801	BLA	CAC-C3C	-5.80	1.31	1.47
2	A	801	BLA	C1D-ND	5.41	1.48	1.36
2	B	801	BLA	C1D-ND	5.35	1.48	1.36
2	B	801	BLA	CHD-C1D	5.22	1.52	1.40
2	A	801	BLA	CHD-C1D	5.22	1.52	1.40
2	B	801	BLA	C4D-C3D	5.08	1.53	1.45
2	B	801	BLA	C3D-C2D	5.01	1.47	1.36
2	A	801	BLA	C3D-C2D	4.93	1.47	1.36
2	A	801	BLA	C4D-C3D	4.87	1.53	1.45
2	B	801	BLA	CBC-CAC	4.05	1.49	1.30
2	A	801	BLA	CBC-CAC	4.05	1.49	1.30
2	A	801	BLA	CHA-C4D	-3.04	1.32	1.35
2	B	801	BLA	C1B-C2B	3.01	1.50	1.45
2	A	801	BLA	C4A-CHB	2.99	1.53	1.41
2	B	801	BLA	C1A-CHA	2.97	1.53	1.41
2	B	801	BLA	C4A-CHB	2.96	1.53	1.41
2	A	801	BLA	C1A-CHA	2.90	1.53	1.41
2	B	801	BLA	CHA-C4D	-2.85	1.32	1.35
2	A	801	BLA	C1B-C2B	2.84	1.50	1.45
2	B	801	BLA	C3B-C2B	2.68	1.42	1.37
2	A	801	BLA	C3B-C2B	2.61	1.42	1.37
2	A	801	BLA	CHD-C4C	-2.56	1.31	1.37
2	A	801	BLA	OC-C1C	-2.51	1.18	1.23
2	B	801	BLA	OC-C1C	-2.51	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BLA	CHD-C4C	-2.48	1.31	1.37
2	A	801	BLA	OB-C4B	-2.45	1.18	1.23
2	B	801	BLA	OB-C4B	-2.44	1.18	1.23
2	A	801	BLA	CAB-C3B	2.07	1.52	1.47
2	B	801	BLA	CAB-C3B	2.06	1.52	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	BLA	CMC-C2C-C3C	-7.92	109.26	128.43
2	B	801	BLA	CMC-C2C-C3C	-7.81	109.52	128.43
2	B	801	BLA	C1A-CHA-C4D	-6.91	119.47	128.73
2	A	801	BLA	C1A-CHA-C4D	-6.36	120.22	128.73
2	B	801	BLA	CMC-C2C-C1C	-6.03	108.60	121.21
2	A	801	BLA	CMC-C2C-C1C	-5.60	109.50	121.21
2	B	801	BLA	C4C-CHD-C1D	-3.88	118.52	128.06
2	B	801	BLA	C3D-C4D-ND	-3.23	105.47	110.04
2	A	801	BLA	C3D-C4D-ND	-3.03	105.75	110.04
2	A	801	BLA	C4C-CHD-C1D	-2.88	120.97	128.06
2	A	801	BLA	C1B-NB-C4B	-2.55	107.53	110.66
2	B	801	BLA	C4B-C3B-C2B	2.50	111.13	107.92
2	B	801	BLA	CMB-C2B-C3B	-2.41	122.59	128.43
2	A	801	BLA	C4B-C3B-C2B	2.38	110.98	107.92
2	B	801	BLA	CMB-C2B-C1B	2.33	126.99	124.16
2	B	801	BLA	C4D-C3D-C2D	2.32	109.24	106.73
2	A	801	BLA	C4D-C3D-C2D	2.31	109.22	106.73
2	B	801	BLA	C1B-NB-C4B	-2.26	107.88	110.66
2	A	801	BLA	C3B-C2B-C1B	2.25	110.43	107.92
2	B	801	BLA	C3B-C2B-C1B	2.25	110.42	107.92
2	A	801	BLA	CMB-C2B-C3B	-2.16	123.19	128.43
2	B	801	BLA	CHB-C1B-C2B	2.07	131.10	126.99

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	BLA	NA-C1A-CHA-C4D
2	A	801	BLA	C2A-C1A-CHA-C4D
2	A	801	BLA	NB-C1B-CHB-C4A
2	A	801	BLA	C2B-C1B-CHB-C4A
2	A	801	BLA	ND-C1D-CHD-C4C
2	B	801	BLA	NA-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
2	B	801	BLA	C2A-C1A-CHA-C4D
2	B	801	BLA	NA-C4A-CHB-C1B
2	B	801	BLA	C3A-C4A-CHB-C1B
2	B	801	BLA	C2A-CAA-CBA-CGA
2	B	801	BLA	NB-C1B-CHB-C4A
2	B	801	BLA	C2B-C1B-CHB-C4A
2	B	801	BLA	C2B-C3B-CAB-CBB
2	B	801	BLA	C4B-C3B-CAB-CBB
2	B	801	BLA	C2C-C3C-CAC-CBC
2	B	801	BLA	C4C-C3C-CAC-CBC
2	B	801	BLA	ND-C1D-CHD-C4C
2	A	801	BLA	C2D-C1D-CHD-C4C
2	B	801	BLA	C2D-C1D-CHD-C4C
2	B	801	BLA	C3D-CAD-CBD-CGD
2	A	801	BLA	C3D-CAD-CBD-CGD
2	B	801	BLA	ND-C4D-CHA-C1A
2	A	801	BLA	C4B-C3B-CAB-CBB
2	A	801	BLA	C2B-C3B-CAB-CBB
2	B	801	BLA	CAA-CBA-CGA-O1A
2	A	801	BLA	CAA-CBA-CGA-O1A
2	B	801	BLA	CAA-CBA-CGA-O2A
2	A	801	BLA	CAA-CBA-CGA-O2A
2	B	801	BLA	CAD-CBD-CGD-O1D
2	B	801	BLA	CAD-CBD-CGD-O2D
2	A	801	BLA	CAD-CBD-CGD-O2D
2	A	801	BLA	CAD-CBD-CGD-O1D
2	A	801	BLA	C2A-CAA-CBA-CGA

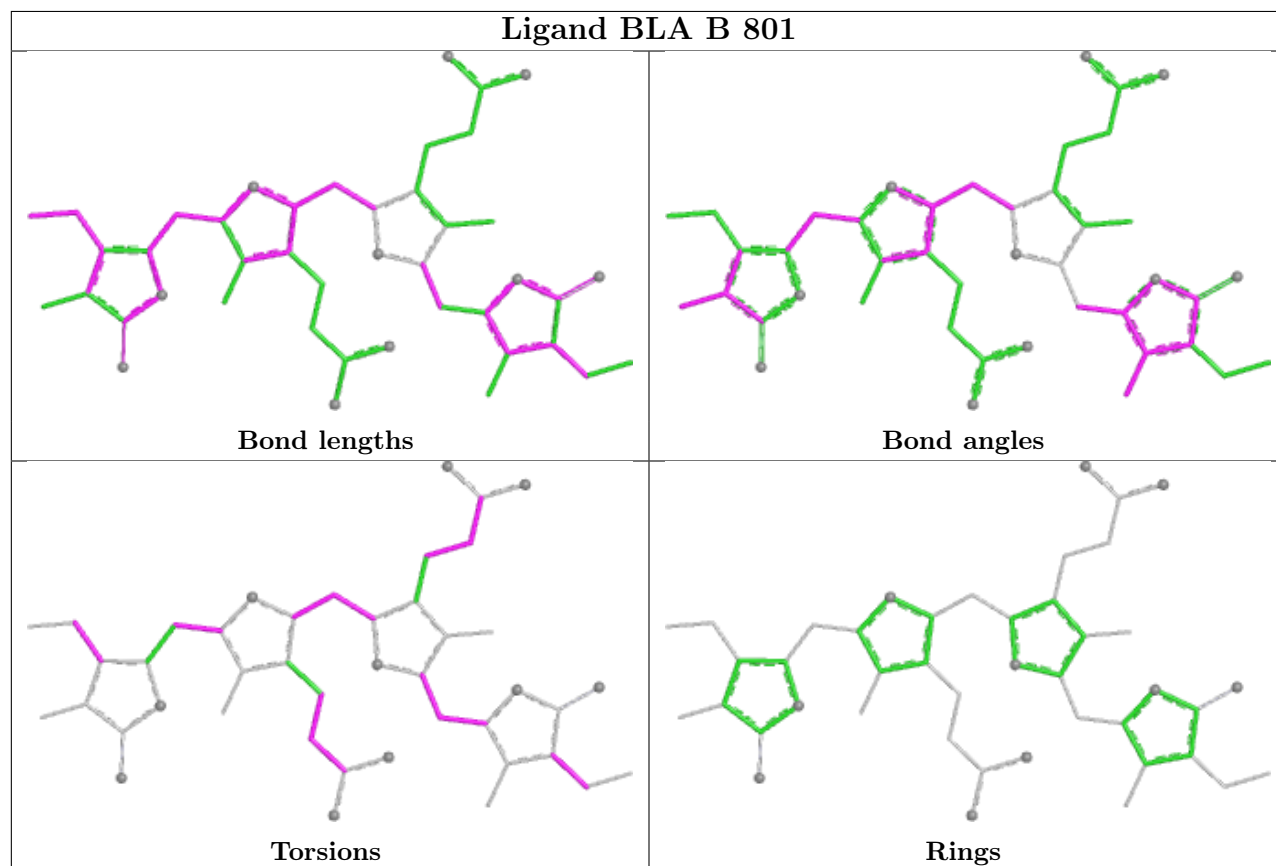
There are no ring outliers.

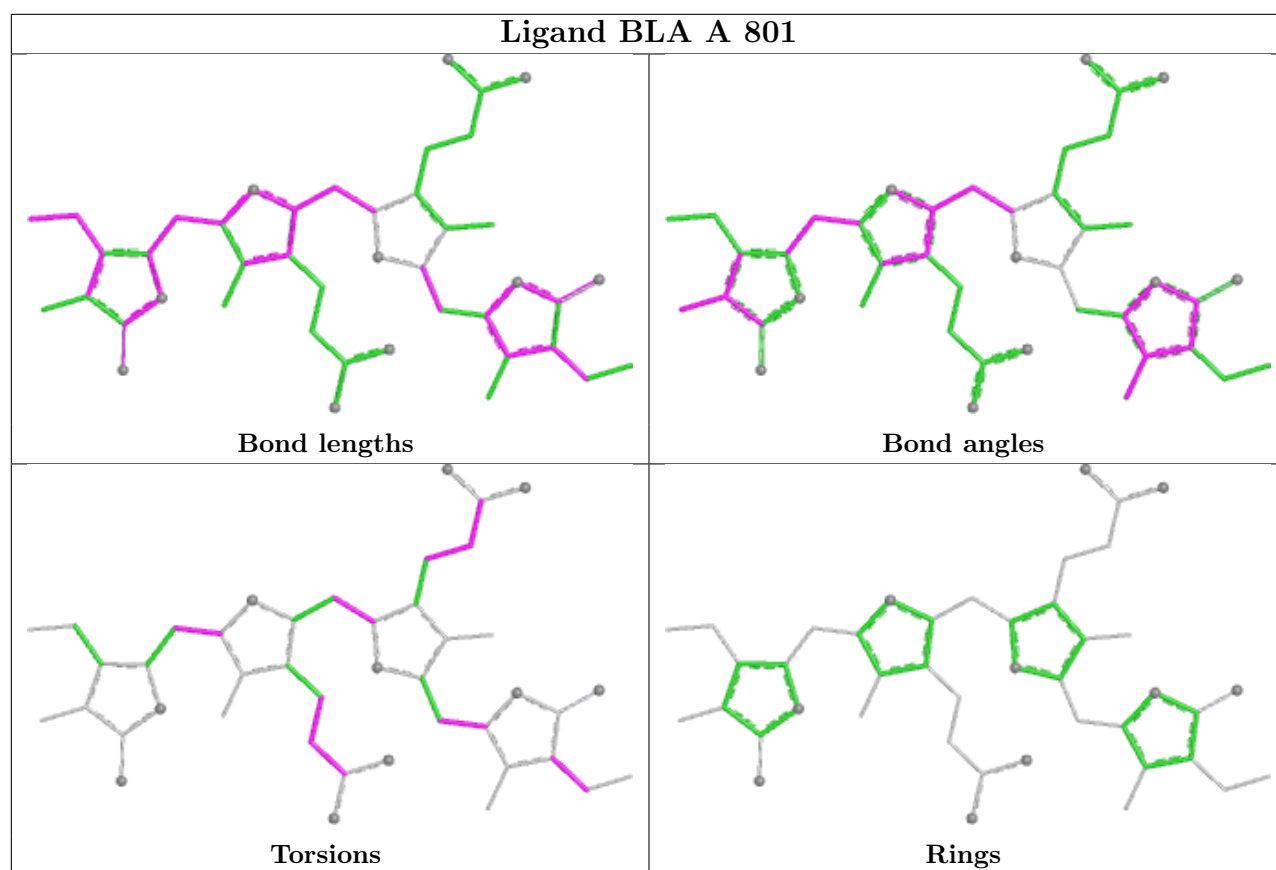
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	BLA	3	0
2	A	801	BLA	4	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.





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.

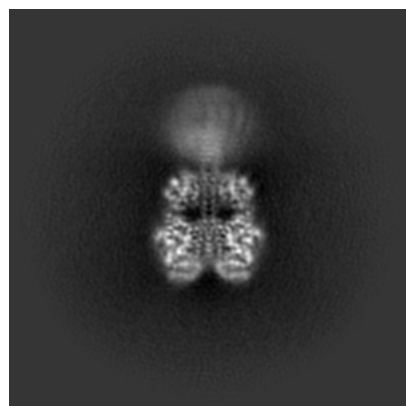
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42452. These allow visual inspection of the internal detail of the map and identification of artifacts.

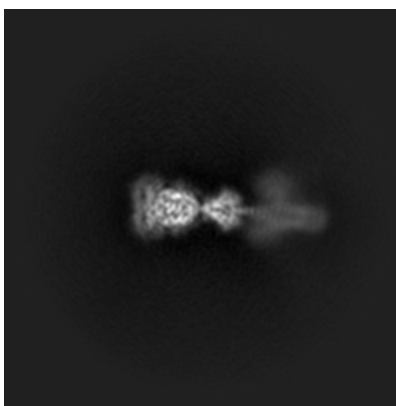
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

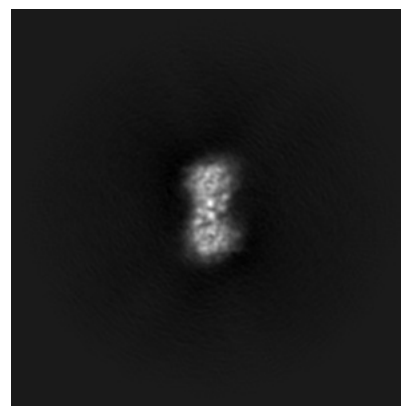
6.1.1 Primary map



X

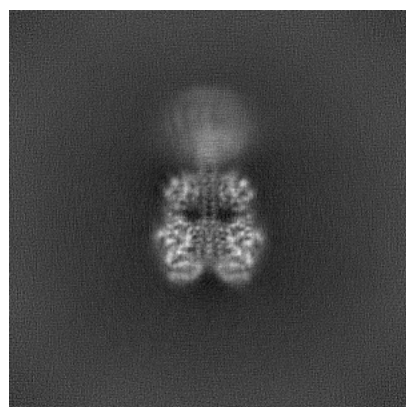


Y

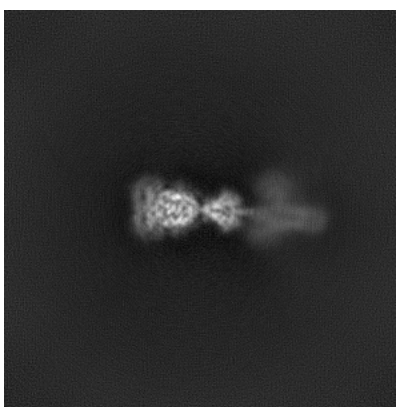


Z

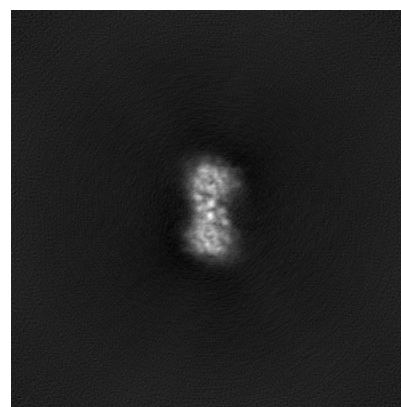
6.1.2 Raw map



X



Y

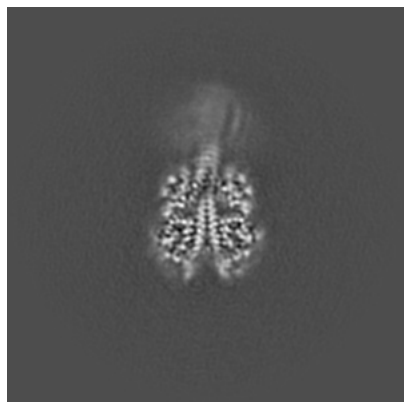


Z

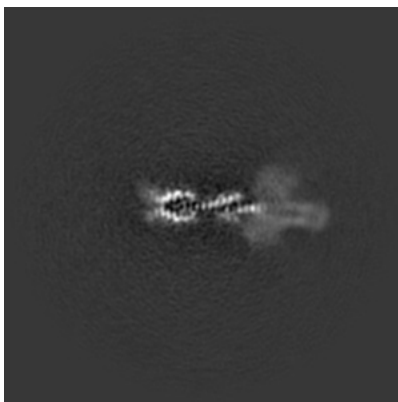
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

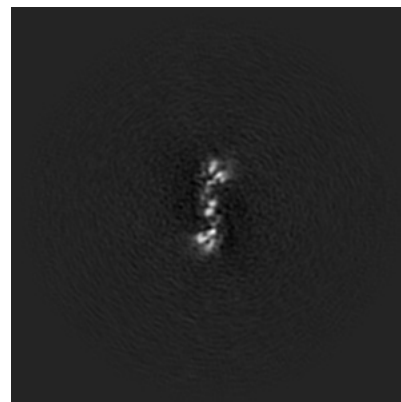
6.2.1 Primary map



X Index: 200

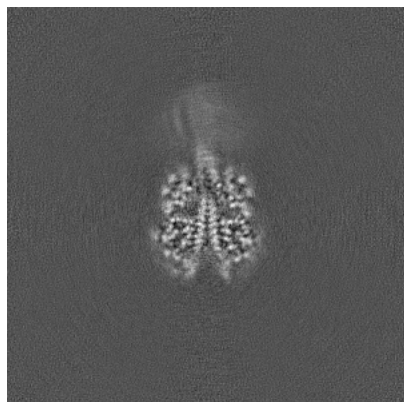


Y Index: 200

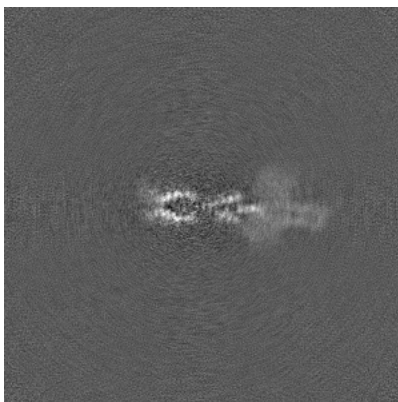


Z Index: 200

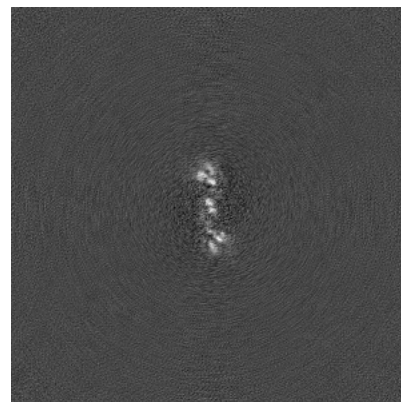
6.2.2 Raw map



X Index: 200



Y Index: 200

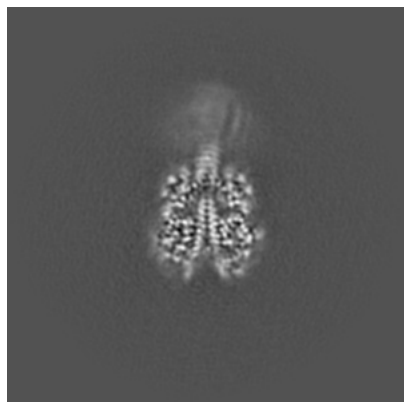


Z Index: 200

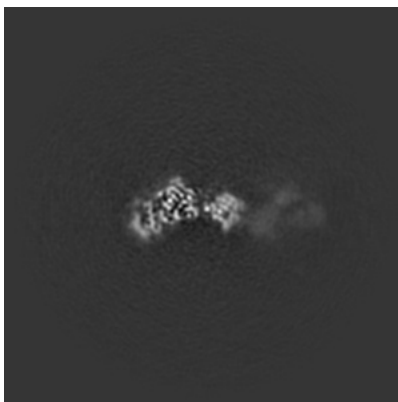
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

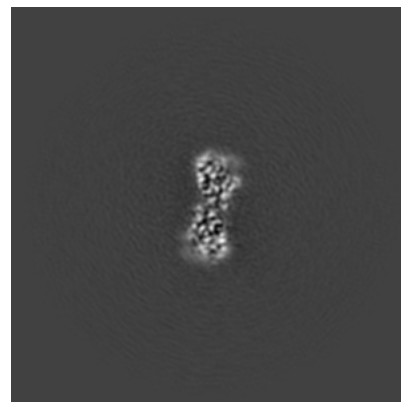
6.3.1 Primary map



X Index: 199

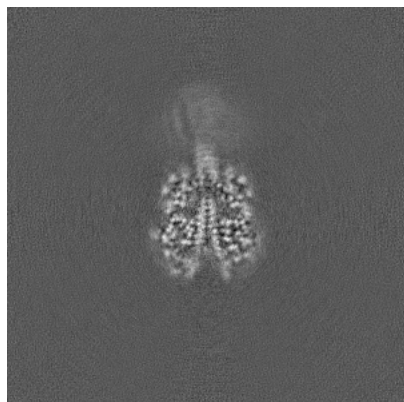


Y Index: 223

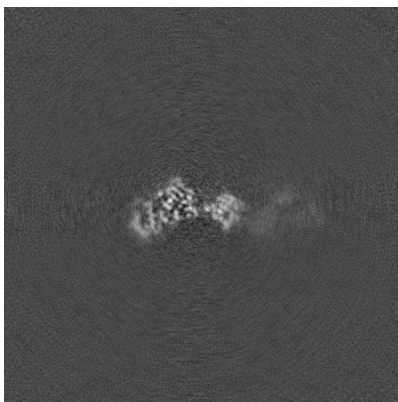


Z Index: 175

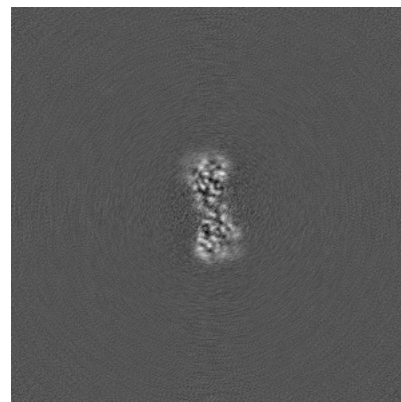
6.3.2 Raw map



X Index: 199



Y Index: 176

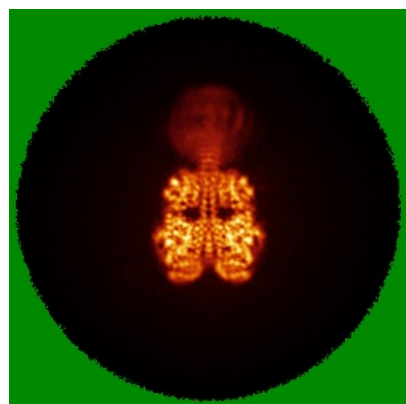


Z Index: 176

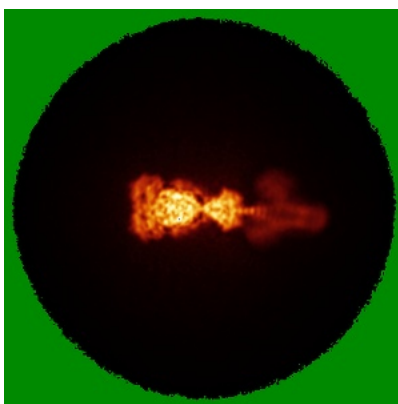
The images above show the largest variance slices of the map in three orthogonal directions.

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

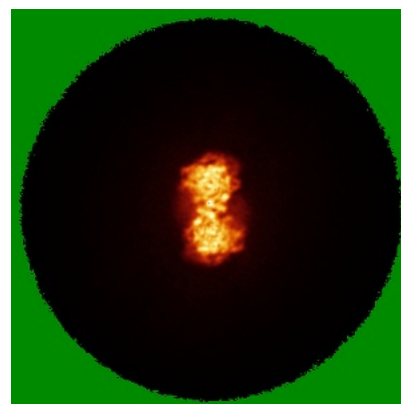
6.4.1 Primary map



X

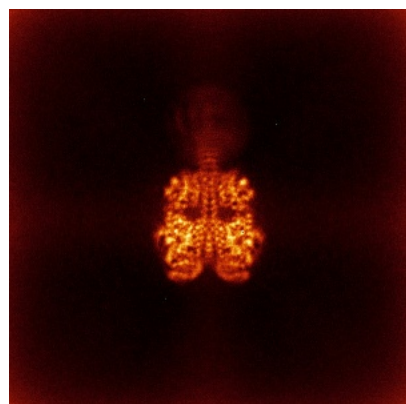


Y

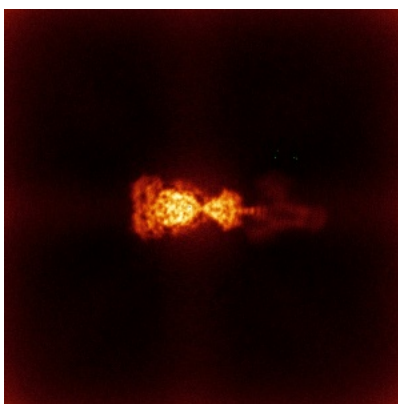


Z

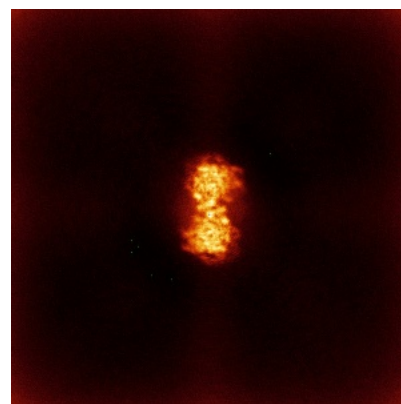
6.4.2 Raw map



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.

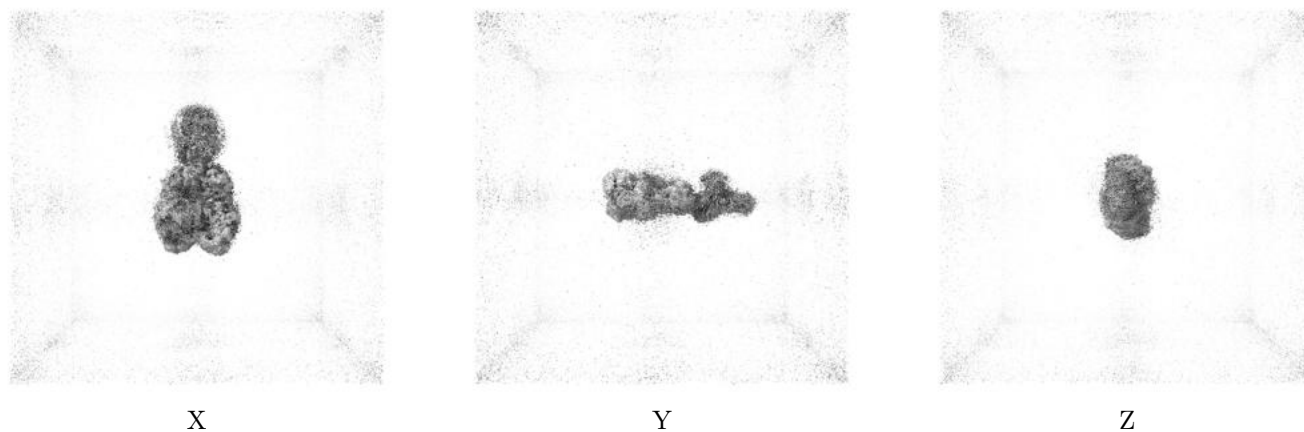
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. 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.

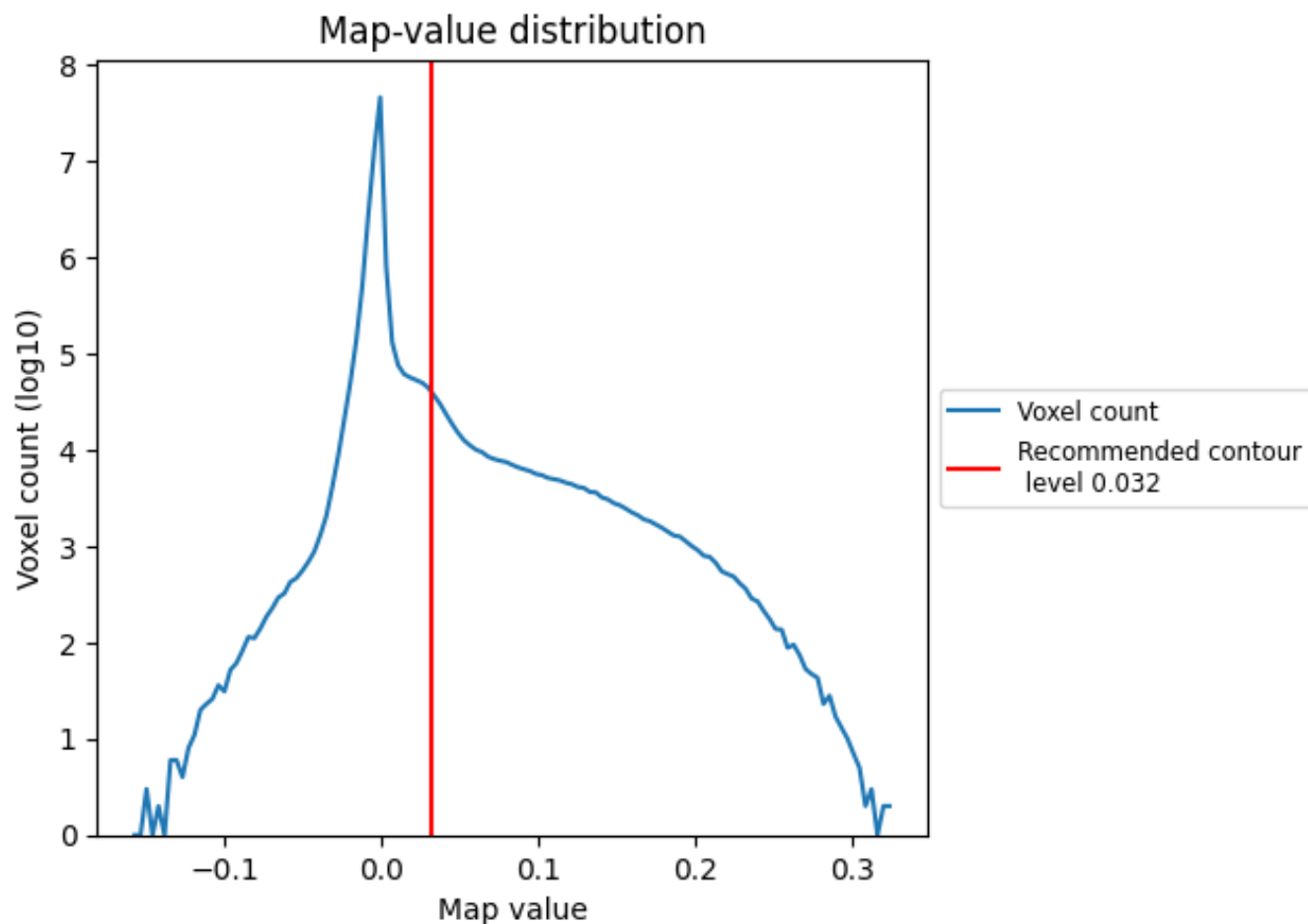
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

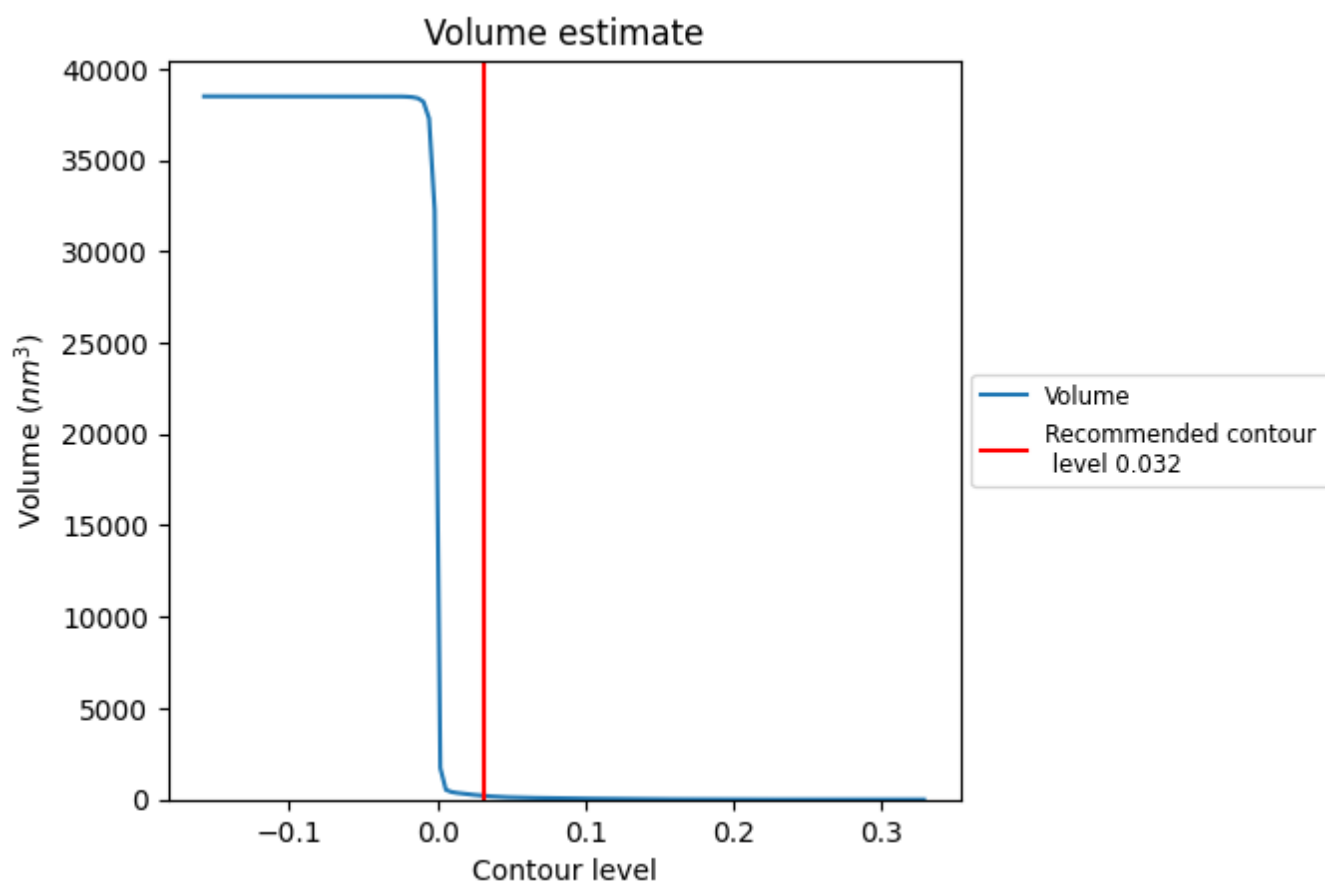
This section contains the results of statistical analysis of the map.

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.

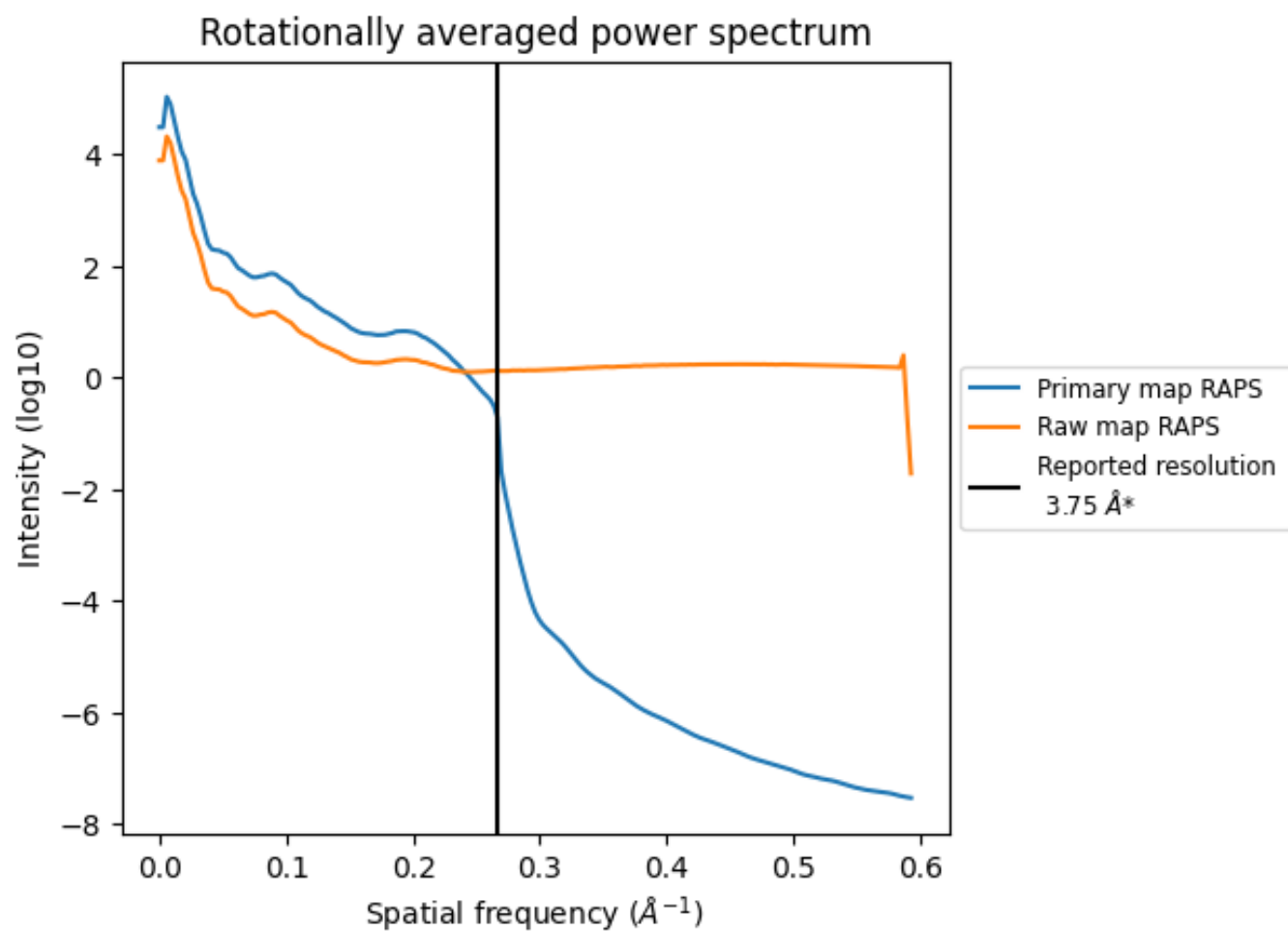
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm³; this corresponds to an approximate mass of 182 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 ⓘ

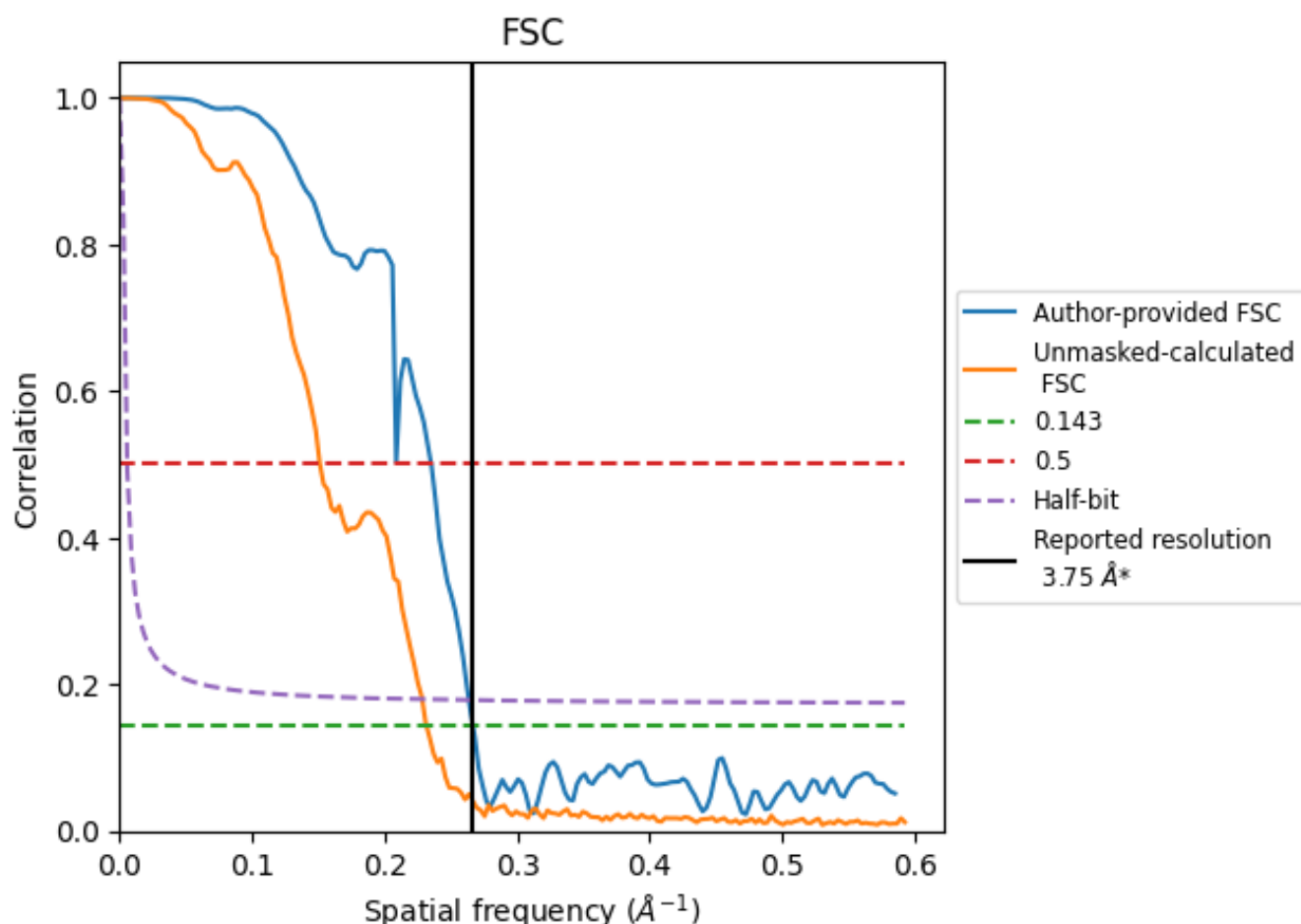


*Reported resolution corresponds to spatial frequency of 0.267 \AA^{-1}

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 0.267 \AA^{-1}

8.2 Resolution estimates [i](#)

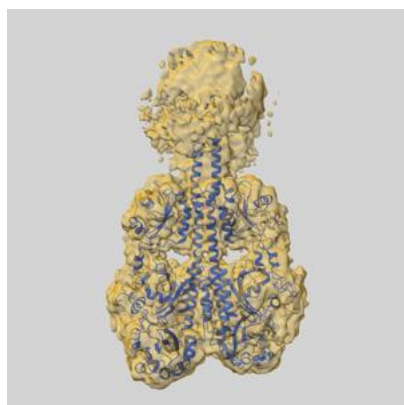
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.75	4.25	3.79
Unmasked-calculated*	4.32	6.62	4.38

*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 4.32 differs from the reported value 3.75 by more than 10 %

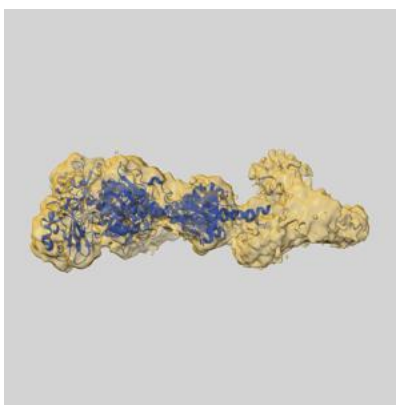
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42452 and PDB model 8UPM. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

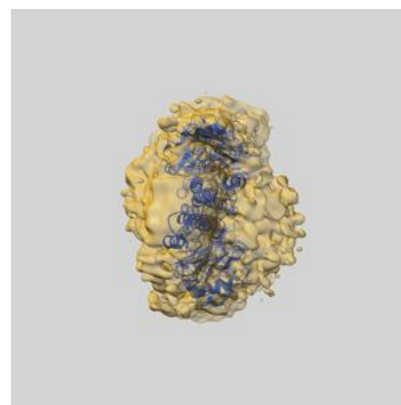
9.1 Map-model overlay [i](#)



X



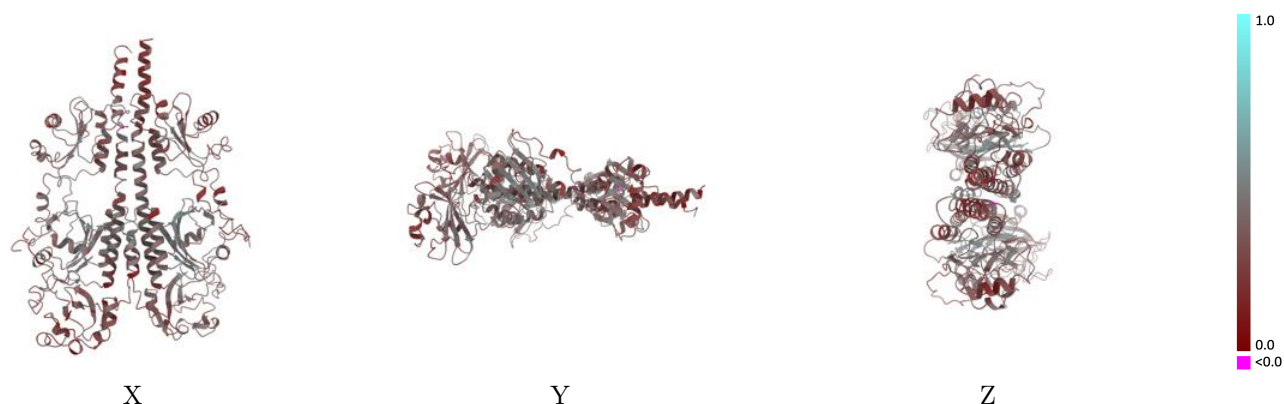
Y



Z

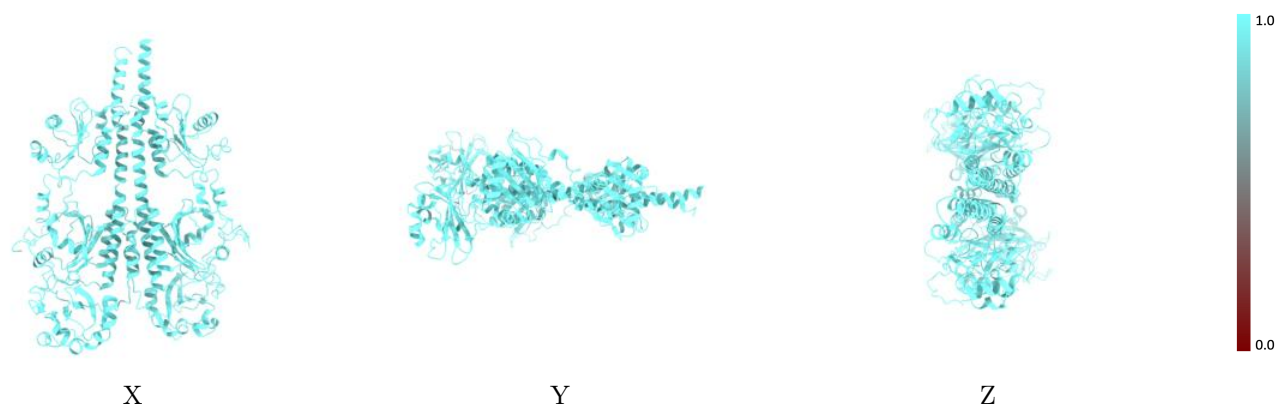
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



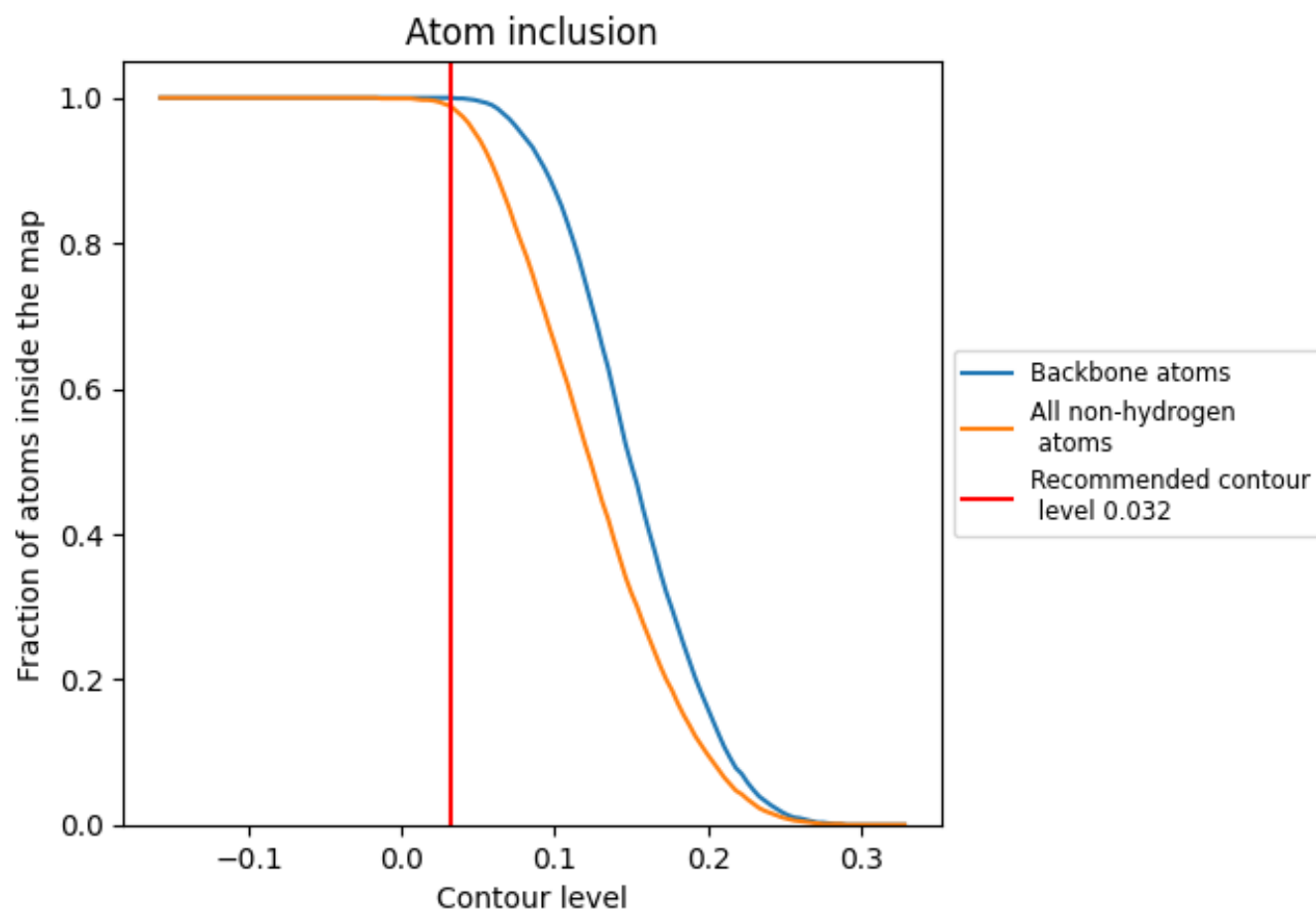
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9880	<div></div> 0.3550
A	<div></div> 0.9900	<div></div> 0.3580
B	<div></div> 0.9860	<div></div> 0.3520

