



Full wwPDB EM Validation Report ⓘ

Jul 4, 2026 – 11:49 AM JST

PDB ID : 8ZKS / pdb_00008zks
EMDB ID : EMD-60207
Title : Structure of Polycystin-1/Polycystin-2 complex
Authors : Chen, M.Y.; Su, Q.; Shi, Y.G.
Deposited on : 2024-05-17
Resolution : 3.21 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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 EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

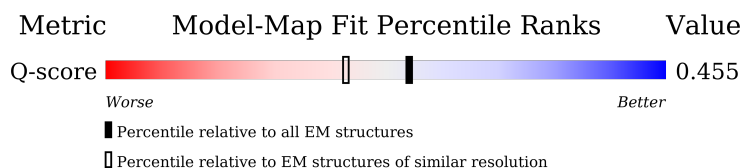
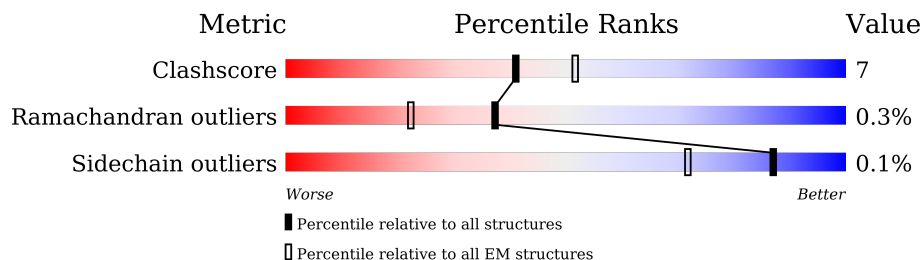
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.21 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	14613 (2.71 - 3.71)

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	1261	
2	B	1007	
2	C	1007	
2	D	1007	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16170 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 Polycystin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	731	Total	C	N	O	S	0	0
			5402	3483	980	923	16		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3043	MET	-	initiating methionine	UNP P98161
A	3044	ASP	-	expression tag	UNP P98161
A	3045	TYR	-	expression tag	UNP P98161
A	3046	LYS	-	expression tag	UNP P98161
A	3047	ASP	-	expression tag	UNP P98161
A	3048	ASP	-	expression tag	UNP P98161
A	3049	ASP	-	expression tag	UNP P98161
A	3050	ASP	-	expression tag	UNP P98161
A	3051	LYS	-	expression tag	UNP P98161

- Molecule 2 is a protein called Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	480	Total	C	N	O	S	0	0
			3959	2607	626	705	21		
2	C	480	Total	C	N	O	S	0	0
			3959	2607	626	705	21		
2	D	481	Total	C	N	O	S	0	0
			2765	1714	508	536	7		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	MET	-	initiating methionine	UNP Q13563
B	-37	GLY	-	expression tag	UNP Q13563
B	-36	ALA	-	expression tag	UNP Q13563
B	-35	SER	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-34	SER	-	expression tag	UNP Q13563
B	-33	ALA	-	expression tag	UNP Q13563
B	-32	TRP	-	expression tag	UNP Q13563
B	-31	SER	-	expression tag	UNP Q13563
B	-30	HIS	-	expression tag	UNP Q13563
B	-29	PRO	-	expression tag	UNP Q13563
B	-28	GLN	-	expression tag	UNP Q13563
B	-27	PHE	-	expression tag	UNP Q13563
B	-26	GLU	-	expression tag	UNP Q13563
B	-25	LYS	-	expression tag	UNP Q13563
B	-24	GLY	-	expression tag	UNP Q13563
B	-23	GLY	-	expression tag	UNP Q13563
B	-22	GLY	-	expression tag	UNP Q13563
B	-21	SER	-	expression tag	UNP Q13563
B	-20	GLY	-	expression tag	UNP Q13563
B	-19	GLY	-	expression tag	UNP Q13563
B	-18	GLY	-	expression tag	UNP Q13563
B	-17	SER	-	expression tag	UNP Q13563
B	-16	GLY	-	expression tag	UNP Q13563
B	-15	GLY	-	expression tag	UNP Q13563
B	-14	SER	-	expression tag	UNP Q13563
B	-13	ALA	-	expression tag	UNP Q13563
B	-12	TRP	-	expression tag	UNP Q13563
B	-11	SER	-	expression tag	UNP Q13563
B	-10	HIS	-	expression tag	UNP Q13563
B	-9	PRO	-	expression tag	UNP Q13563
B	-8	GLN	-	expression tag	UNP Q13563
B	-7	PHE	-	expression tag	UNP Q13563
B	-6	GLU	-	expression tag	UNP Q13563
B	-5	LYS	-	expression tag	UNP Q13563
B	-4	GLY	-	expression tag	UNP Q13563
B	-3	SER	-	linker	UNP Q13563
B	-2	ALA	-	linker	UNP Q13563
B	-1	ALA	-	linker	UNP Q13563
B	0	ALA	-	linker	UNP Q13563
C	-38	MET	-	initiating methionine	UNP Q13563
C	-37	GLY	-	expression tag	UNP Q13563
C	-36	ALA	-	expression tag	UNP Q13563
C	-35	SER	-	expression tag	UNP Q13563
C	-34	SER	-	expression tag	UNP Q13563
C	-33	ALA	-	expression tag	UNP Q13563
C	-32	TRP	-	expression tag	UNP Q13563

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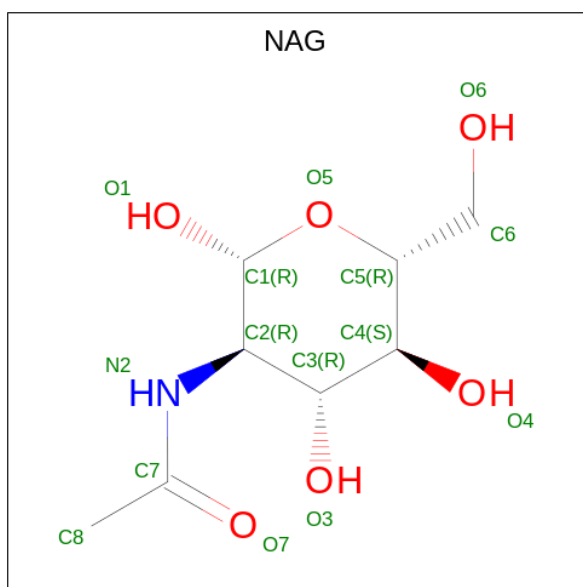
Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	SER	-	expression tag	UNP Q13563
C	-30	HIS	-	expression tag	UNP Q13563
C	-29	PRO	-	expression tag	UNP Q13563
C	-28	GLN	-	expression tag	UNP Q13563
C	-27	PHE	-	expression tag	UNP Q13563
C	-26	GLU	-	expression tag	UNP Q13563
C	-25	LYS	-	expression tag	UNP Q13563
C	-24	GLY	-	expression tag	UNP Q13563
C	-23	GLY	-	expression tag	UNP Q13563
C	-22	GLY	-	expression tag	UNP Q13563
C	-21	SER	-	expression tag	UNP Q13563
C	-20	GLY	-	expression tag	UNP Q13563
C	-19	GLY	-	expression tag	UNP Q13563
C	-18	GLY	-	expression tag	UNP Q13563
C	-17	SER	-	expression tag	UNP Q13563
C	-16	GLY	-	expression tag	UNP Q13563
C	-15	GLY	-	expression tag	UNP Q13563
C	-14	SER	-	expression tag	UNP Q13563
C	-13	ALA	-	expression tag	UNP Q13563
C	-12	TRP	-	expression tag	UNP Q13563
C	-11	SER	-	expression tag	UNP Q13563
C	-10	HIS	-	expression tag	UNP Q13563
C	-9	PRO	-	expression tag	UNP Q13563
C	-8	GLN	-	expression tag	UNP Q13563
C	-7	PHE	-	expression tag	UNP Q13563
C	-6	GLU	-	expression tag	UNP Q13563
C	-5	LYS	-	expression tag	UNP Q13563
C	-4	GLY	-	expression tag	UNP Q13563
C	-3	SER	-	linker	UNP Q13563
C	-2	ALA	-	linker	UNP Q13563
C	-1	ALA	-	linker	UNP Q13563
C	0	ALA	-	linker	UNP Q13563
D	-38	MET	-	initiating methionine	UNP Q13563
D	-37	GLY	-	expression tag	UNP Q13563
D	-36	ALA	-	expression tag	UNP Q13563
D	-35	SER	-	expression tag	UNP Q13563
D	-34	SER	-	expression tag	UNP Q13563
D	-33	ALA	-	expression tag	UNP Q13563
D	-32	TRP	-	expression tag	UNP Q13563
D	-31	SER	-	expression tag	UNP Q13563
D	-30	HIS	-	expression tag	UNP Q13563
D	-29	PRO	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-28	GLN	-	expression tag	UNP Q13563
D	-27	PHE	-	expression tag	UNP Q13563
D	-26	GLU	-	expression tag	UNP Q13563
D	-25	LYS	-	expression tag	UNP Q13563
D	-24	GLY	-	expression tag	UNP Q13563
D	-23	GLY	-	expression tag	UNP Q13563
D	-22	GLY	-	expression tag	UNP Q13563
D	-21	SER	-	expression tag	UNP Q13563
D	-20	GLY	-	expression tag	UNP Q13563
D	-19	GLY	-	expression tag	UNP Q13563
D	-18	GLY	-	expression tag	UNP Q13563
D	-17	SER	-	expression tag	UNP Q13563
D	-16	GLY	-	expression tag	UNP Q13563
D	-15	GLY	-	expression tag	UNP Q13563
D	-14	SER	-	expression tag	UNP Q13563
D	-13	ALA	-	expression tag	UNP Q13563
D	-12	TRP	-	expression tag	UNP Q13563
D	-11	SER	-	expression tag	UNP Q13563
D	-10	HIS	-	expression tag	UNP Q13563
D	-9	PRO	-	expression tag	UNP Q13563
D	-8	GLN	-	expression tag	UNP Q13563
D	-7	PHE	-	expression tag	UNP Q13563
D	-6	GLU	-	expression tag	UNP Q13563
D	-5	LYS	-	expression tag	UNP Q13563
D	-4	GLY	-	expression tag	UNP Q13563
D	-3	SER	-	linker	UNP Q13563
D	-2	ALA	-	linker	UNP Q13563
D	-1	ALA	-	linker	UNP Q13563
D	0	ALA	-	linker	UNP Q13563

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Ca	0
			1	1	

ASN	VAL	HIS	VAL	MET	ARG	GLU	ILE	A612	I524	Q456	S396	G329
GLU	ARG	GLU	ASP	GLU	VAL	ARG	SER	Q613	N525	F457	S396	S330
LEU	ASP	GLU	ASP	LEU	ARG	SER	SER	F619	I526	Q458	T398	C331
VAL	MET	LEU	MET	LEU	ARG	LEU	ARG	E648	Y527	P459	R399	S332
ARG	GLU	ASP	GLU	ASP	GLU	ASP	ARG	E648	T529	L460	E400	P334
GLU	HIS	LEU	HIS	LEU	GLN	LEU	GLN	E651	S530	K461	E401	Q335
GLU	SER	GLU	ILE	GLY	GLY	SER	GLY	G657	N531	L462	T402	D336
GLU	SER	GLU	GLY	GLY	GLY	SER	GLY	G657	E532	I463	A403	L337
TRP	SER	LEU	SER	LEU	LEU	LEU	LEU	F664	V532	R464	A404	R338
GLU	ILE	LEU	VAL	LEU	VAL	PRO	ASP	V665	E533	F469	Q405	D339
GLU	SER	SER	SER	ARG	ARG	ARG	PHE	F669	L535	D470	S408	E340
ASP	LYS	PRO	LYS	ASP	LYS	PRO	ASP	F670	L536	F471	L409	E340
ASP	ILE	ASP	ILE	ASP	ASP	MET	LEU	L671	Q537	F472	K410	K342
ALA	ASP	SER	ALA	SER	ASP	SER	LEU	L672	F538	L473	K411	E343
ALA	VAL	ARG	ALA	ARG	GLN	ARG	GLN	L673	L539	A474	M412	C344
SER	VAL	ARG	SER	ARG	GLN	ARG	GLN	L674	E540	A475	V413	Y345
GLN	ILE	SER	ILE	SER	ASP	SER	ASP	M675	E541	C476	M414	D346
ILE	VAL	PHE	ILE	PHE	LEU	PRO	LEU	F676	D541	E477	L415	V347
SER	VAL	LEU	SER	LEU	GLY	PRO	GLY	L677	Q542	I478	D416	Y348
HIS	LEU	LEU	ARG	SER	GLY	ARG	LYS	N681	N543	I479	R417	S349
GLY	GLU	GLU	SER	GLY	GLY	LEU	GLY	D682	F544	F480	G418	V350
LEU	ILE	LEU	ILE	LEU	GLY	LEU	GLY	Y684	P546	C481	T419	S351
MET	MET	ASP	MET	ASP	HIS	ASP	HIS	Q694	E549	F482	R420	S352
GLY	GLY	GLY	GLY	GLY	THR	ASP	THR	K695	H550	I483	A421	S353
THR	THR	ASP	THR	ASP	THR	ASP	THR	A696	L551	I484	T422	D354
PRO	ARG	ARG	PRO	ARG	ARG	GLU	ARG	E697	A552	F485	F423	R355
VAL	ALA	ALA	VAL	ALA	ALA	GLU	ALA	Q697	E553	Y486	I424	A356
GLY	LYS	LYS	GLY	LYS	GLY	GLU	GLY	MET	Y554	Y487	D425	P357
LEU	LEU	LEU	LEU	LEU	LEU	GLY	LEU	GLU	Q555	V488	F426	F358
LEU	LEU	LEU	LEU	LEU	LEU	SER	LEU	SER	ASP	W489	S427	Q359
ARG	GLY	GLY	GLY	GLY	GLY	ASP	GLY	ASP	ASP	Y428	Y429	R361
ARG	GLY	GLY	GLY	GLY	GLY	ASP	GLY	ASP	ASP	M430	M431	N362
PRO	ASP	ASP	PRO	ASP	ASP	ARG	ARG	ASP	ASP	M432	M432	G363
SER	VAL	VAL	SER	VAL	VAL	GLY	GLN	GLY	TYR	I433	I433	T364
SER	ALA	ALA	SER	ALA	ALA	SER	LEU	ILE	ILE	L500	M434	I367
GLN	GLU	GLU	GLU	GLU	GLU	ILE	GLU	LEU	L561	H501	L435	Y368
SER	ASP	ASP	SER	ASP	ASP	THR	THR	ALA	A562	Y502	F436	T369
THR	ASP	ASP	THR	ASP	ASP	SER	GLU	VAL	L563	F503	C437	S370
GLU	ARG	ARG	GLY	ARG	ARG	GLY	HIS	VAL	A564	S505	V439	E371
GLY	GLY	GLY	GLY	GLY	GLY	VAL	GLY	VAL	T565	R440	L441	K372
MET	GLY	GLY	MET	GLY	GLY	SER	HIS	VAL	V566	F506	L442	S377
GLU	ARG	ARG	GLU	ARG	ARG	TYR	GLN	TYR	R504	V507	V443	S378
GLY	ASP	ASP	GLY	ASP	ASP	LEU	GLN	LEU	V567	N508	V443	H379
ALA												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.720	Depositor
Minimum map value	-1.870	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.32	Depositor
Map size ($\text{\AA}$)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.20	1/5530 (0.0%)	0.43	9/7544 (0.1%)
2	B	0.12	0/4064	0.31	0/5516
2	C	0.11	0/4064	0.30	0/5516
2	D	0.10	0/2787	0.30	1/3843 (0.0%)
All	All	0.15	1/16445 (0.0%)	0.35	10/22419 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3274	ARG	N-CA	-5.83	1.39	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3275	PHE	N-CA-C	-7.34	99.48	109.54
1	A	3310	GLY	CA-C-N	-7.26	111.89	124.82
1	A	3310	GLY	C-N-CA	-7.26	111.89	124.82
1	A	3310	GLY	N-CA-C	6.54	120.58	112.73
1	A	3277	ARG	CA-C-N	5.94	132.65	121.97
1	A	3277	ARG	C-N-CA	5.94	132.65	121.97
1	A	3306	ALA	CA-C-N	5.46	131.96	121.54
1	A	3306	ALA	C-N-CA	5.46	131.96	121.54
1	A	3309	THR	CB-CA-C	-5.29	100.81	109.53
2	D	310	PHE	N-CA-C	5.21	115.89	108.54

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	5402	0	5195	109	0
2	B	3959	0	3900	44	0
2	C	3959	0	3900	56	0
2	D	2765	0	1731	20	0
3	B	42	0	39	0	0
3	C	42	0	39	1	0
4	C	1	0	0	0	0
All	All	16170	0	14804	215	0

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

All (215) 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:3269:ARG:CZ	1:A:3276:THR:HG22	1.41	1.45
1:A:3267:TRP:HA	1:A:3277:ARG:NH2	1.31	1.41
1:A:3275:PHE:CE2	1:A:3280:ARG:HG2	1.54	1.39
1:A:3269:ARG:NH2	1:A:3276:THR:HG22	1.45	1.29
1:A:3095:LEU:CD2	1:A:3277:ARG:HD3	1.65	1.24
1:A:3305:SER:OG	1:A:3308:SER:HB3	1.42	1.16
1:A:3275:PHE:CE2	1:A:3280:ARG:CG	2.31	1.14
1:A:3305:SER:OG	1:A:3308:SER:CB	1.94	1.14
1:A:3275:PHE:HE2	1:A:3280:ARG:CG	1.62	1.12
1:A:3310:GLY:O	1:A:3311:HIS:HB2	1.46	1.11
1:A:3095:LEU:HD22	1:A:3277:ARG:CD	1.84	1.06
1:A:3095:LEU:HD22	1:A:3277:ARG:HD3	1.22	1.06
1:A:3269:ARG:NH2	1:A:3276:THR:CG2	2.19	1.05
1:A:3269:ARG:CZ	1:A:3276:THR:CG2	2.38	1.01
1:A:3095:LEU:CD2	1:A:3277:ARG:CD	2.43	0.97
1:A:3305:SER:O	1:A:3308:SER:N	1.99	0.96
1:A:3267:TRP:CA	1:A:3277:ARG:NH2	2.27	0.96
1:A:3267:TRP:HA	1:A:3277:ARG:HH21	1.25	0.93
1:A:3269:ARG:NH1	1:A:3276:THR:HG22	1.81	0.93
1:A:3266:ILE:O	1:A:3277:ARG:NE	2.06	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3275:PHE:HE2	1:A:3280:ARG:HG2	0.74	0.87
1:A:3267:TRP:HA	1:A:3277:ARG:HH22	1.38	0.86
1:A:3305:SER:OG	1:A:3308:SER:HB2	1.73	0.85
1:A:3095:LEU:HD21	1:A:3277:ARG:HD3	1.60	0.84
1:A:3872:GLU:O	1:A:3879:ALA:HA	1.84	0.77
1:A:3310:GLY:O	1:A:3311:HIS:CB	2.25	0.75
1:A:3305:SER:HG	1:A:3308:SER:HB3	1.52	0.73
1:A:3750:ARG:HB2	1:A:3820:VAL:HG12	1.72	0.70
1:A:3848:ARG:NH1	1:A:3873:PHE:O	2.24	0.70
1:A:4100:ARG:HH21	2:B:677:LEU:HD22	1.56	0.70
2:B:219:SER:O	2:B:221:LEU:N	2.25	0.70
1:A:3275:PHE:HD2	1:A:3280:ARG:NE	1.90	0.70
2:C:681:ASN:HD21	2:D:681:ASN:HD22	1.40	0.69
2:D:431:ALA:HB3	2:D:435:LEU:HA	1.74	0.69
1:A:3754:LEU:HA	1:A:3776:PHE:HA	1.77	0.67
1:A:3269:ARG:NH1	1:A:3276:THR:CG2	2.55	0.66
1:A:3269:ARG:HH22	1:A:3276:THR:CG2	2.09	0.65
2:C:467:THR:HG22	2:C:468:THR:H	1.62	0.65
1:A:3320:VAL:HG22	1:A:3321:ASP:H	1.62	0.64
1:A:3266:ILE:O	1:A:3277:ARG:CZ	2.45	0.64
2:C:462:LEU:HD12	2:C:532:VAL:HG13	1.80	0.64
1:A:3098:LEU:HD13	1:A:3277:ARG:NH1	2.12	0.64
1:A:3884:SER:OG	1:A:3886:ARG:NH1	2.31	0.63
2:B:219:SER:C	2:B:221:LEU:H	2.05	0.63
2:C:430:ASN:ND2	2:C:432:ASN:OD1	2.32	0.63
1:A:3261:HIS:O	1:A:3263:TRP:N	2.32	0.62
1:A:3970:ARG:H	1:A:3973:ARG:HH12	1.47	0.62
2:C:254:SER:O	2:C:258:LEU:HB2	2.00	0.62
2:B:461:LYS:HE2	2:B:464:ARG:HA	1.82	0.61
2:B:322:ARG:NH1	2:B:389:ALA:O	2.32	0.61
1:A:3886:ARG:NH2	1:A:3978:ASP:OD1	2.31	0.60
2:C:570:TRP:NE1	2:D:613:GLN:OE1	2.35	0.60
1:A:3144:GLY:O	1:A:3254:GLN:NE2	2.35	0.59
1:A:3305:SER:C	1:A:3307:TYR:H	2.11	0.59
1:A:3835:ARG:O	1:A:3839:LEU:HB2	2.01	0.58
1:A:3962:GLN:NE2	1:A:3976:SER:O	2.36	0.58
1:A:3275:PHE:CD2	1:A:3280:ARG:CG	2.86	0.57
1:A:3305:SER:C	1:A:3308:SER:H	2.12	0.57
2:C:681:ASN:HD21	2:D:681:ASN:ND2	2.02	0.56
2:C:593:CYS:HB3	2:C:683:THR:HG21	1.87	0.56
1:A:3821:GLN:OE1	1:A:3833:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:GLU:OE1	2:B:432:ASN:ND2	2.38	0.56
2:C:623:VAL:HG12	2:C:625:ASP:H	1.69	0.56
1:A:3261:HIS:HE1	1:A:3605:PRO:HD3	1.70	0.55
2:B:467:THR:OG1	2:B:470:ASP:OD1	2.25	0.55
1:A:3305:SER:C	1:A:3307:TYR:N	2.63	0.55
1:A:3305:SER:O	1:A:3308:SER:CA	2.54	0.55
2:C:619:PHE:HB3	2:C:623:VAL:HG21	1.89	0.55
2:B:492:ILE:HA	2:B:495:ILE:HG22	1.89	0.55
2:C:648:GLU:HA	2:C:651:GLU:HG2	1.89	0.54
1:A:3275:PHE:CD2	1:A:3280:ARG:NE	2.74	0.54
1:A:3274:ARG:HG3	1:A:3274:ARG:O	2.08	0.54
2:C:335:GLN:HA	2:C:338:ARG:HB2	1.90	0.54
1:A:3300:GLY:HA3	1:A:3576:VAL:HG22	1.90	0.53
2:C:319:PRO:HB3	2:C:426:PHE:HB3	1.89	0.53
1:A:3754:LEU:HD13	1:A:3848:ARG:HD3	1.90	0.53
2:B:249:TYR:HE2	2:B:437:CYS:HB2	1.75	0.52
1:A:4022:ALA:HB2	1:A:4109:ARG:HG3	1.92	0.52
2:C:668:MET:SD	2:C:672:LEU:HD12	2.50	0.52
2:C:238:THR:HG21	2:C:566:VAL:HG21	1.91	0.52
1:A:4009:VAL:HB	1:A:4012:TRP:HB2	1.90	0.52
2:B:227:TYR:OH	2:B:569:VAL:O	2.28	0.52
2:B:360:PRO:HG3	2:B:412:ASN:ND2	2.25	0.52
2:D:648:GLU:HA	2:D:651:GLU:HG2	1.91	0.52
1:A:3918:GLU:OE2	1:A:3939:TRP:NE1	2.43	0.52
2:B:431:ALA:HB2	2:C:341:ILE:HD13	1.92	0.51
1:A:3261:HIS:CD2	1:A:3264:LEU:HG	2.46	0.51
2:B:249:TYR:HD1	2:C:448:THR:HB	1.75	0.51
2:B:443:VAL:HG13	2:B:451:VAL:HG13	1.93	0.51
2:B:309:ILE:HD12	2:B:428:VAL:HG11	1.92	0.51
2:C:579:PHE:O	2:C:581:ARG:NH2	2.44	0.51
2:C:320:ARG:NH1	2:C:394:ASP:OD1	2.45	0.51
1:A:3140:ILE:HA	1:A:3184:VAL:HA	1.93	0.50
1:A:3096:HIS:O	1:A:3100:GLN:HG3	2.12	0.50
1:A:3605:PRO:HA	1:A:3608:VAL:HG22	1.93	0.50
2:C:589:THR:HG21	2:C:684:TYR:HD2	1.77	0.50
2:C:415:LEU:HA	2:C:419:THR:HG21	1.93	0.50
2:D:427:SER:HA	2:D:438:VAL:HA	1.94	0.50
2:C:252:MET:HG3	2:C:310:PHE:HE1	1.77	0.50
2:B:577:ILE:HG13	2:B:577:ILE:O	2.12	0.49
1:A:3095:LEU:HD22	1:A:3277:ARG:CB	2.42	0.49
2:B:668:MET:HA	2:B:672:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:589:THR:HG23	2:D:683:THR:HG23	1.95	0.49
2:C:604:PHE:HD1	2:C:672:LEU:HD13	1.77	0.49
2:B:312:GLU:OE2	2:C:417:ARG:NE	2.39	0.49
1:A:3266:ILE:O	1:A:3277:ARG:NH2	2.46	0.49
1:A:3850:VAL:HG22	1:A:3871:LEU:HB2	1.94	0.49
1:A:3261:HIS:CE1	1:A:3605:PRO:HD3	2.47	0.49
1:A:3807:SER:OG	1:A:3870:ARG:NH1	2.43	0.49
2:B:219:SER:C	2:B:221:LEU:N	2.71	0.49
2:B:593:CYS:HB3	2:B:683:THR:HG21	1.95	0.48
2:C:462:LEU:HD11	2:C:535:LEU:HD22	1.95	0.48
1:A:3752:VAL:HG23	1:A:3848:ARG:HB2	1.95	0.48
2:B:487:TYR:O	2:B:490:GLU:HG3	2.12	0.48
2:B:585:GLN:NE2	2:C:596:ASP:OD1	2.46	0.48
2:B:610:ALA:O	2:B:613:GLN:HG3	2.14	0.48
1:A:3098:LEU:HD13	1:A:3277:ARG:HH12	1.76	0.48
1:A:3275:PHE:CE2	1:A:3280:ARG:HG3	2.38	0.48
2:C:374:LEU:HD12	3:C:1002:NAG:H82	1.96	0.47
2:C:499:LYS:O	2:C:502:TYR:HB3	2.14	0.47
1:A:3305:SER:O	1:A:3308:SER:HB2	2.15	0.47
1:A:4104:VAL:HG11	2:D:684:TYR:HB3	1.96	0.47
2:B:325:ARG:HH22	2:B:416:ASP:HB2	1.79	0.47
2:C:664:PHE:O	2:C:668:MET:HB2	2.15	0.47
1:A:3748:ARG:NH2	1:A:3853:GLU:OE2	2.34	0.47
2:B:306:ARG:HG2	2:B:397:ARG:NH2	2.30	0.47
2:B:333:ILE:O	2:B:338:ARG:NH2	2.47	0.47
2:B:525:ASN:O	2:B:529:THR:OG1	2.32	0.47
2:C:538:PHE:HE2	2:C:546:PRO:HB3	1.80	0.47
2:D:325:ARG:HA	2:D:419:THR:HA	1.96	0.46
2:D:597:LEU:HD11	2:D:676:PHE:CE1	2.49	0.46
2:C:288:LEU:HD22	2:C:292:TYR:HE2	1.80	0.46
1:A:3750:ARG:O	1:A:3851:PHE:HB2	2.16	0.46
1:A:3970:ARG:H	1:A:3973:ARG:NH1	2.13	0.46
1:A:3867:VAL:HG22	1:A:3885:VAL:HG22	1.97	0.46
2:D:671:ILE:O	2:D:675:MET:HG2	2.16	0.46
2:C:369:THR:HG21	2:C:392:TYR:HE1	1.81	0.46
2:B:464:ARG:HH22	2:B:528:ARG:HH22	1.62	0.46
2:C:528:ARG:O	2:C:532:VAL:HG23	2.15	0.46
1:A:3699:TYR:O	1:A:3702:GLN:HG3	2.15	0.45
2:C:317:GLY:HA2	2:C:542:GLN:HB3	1.99	0.45
2:C:462:LEU:H	2:C:462:LEU:HD23	1.80	0.45
1:A:3691:ASP:HB2	1:A:3694:CYS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3275:PHE:HD2	1:A:3280:ARG:CZ	2.28	0.45
1:A:3808:TRP:HD1	1:A:3813:VAL:HG22	1.82	0.45
2:C:641:LEU:HD21	2:D:669:PHE:CE2	2.51	0.45
1:A:3269:ARG:HG3	1:A:3280:ARG:NH2	2.32	0.45
2:B:415:LEU:HA	2:B:419:THR:HG21	1.98	0.45
2:C:276:MET:HE3	2:C:276:MET:HB2	1.87	0.45
1:A:3263:TRP:CZ2	1:A:3287:LEU:HD23	2.52	0.44
2:C:667:PHE:HD1	2:C:671:ILE:HD12	1.82	0.44
1:A:3848:ARG:HA	1:A:3873:PHE:HB2	1.99	0.44
2:C:619:PHE:HZ	2:C:657:GLY:HA2	1.82	0.44
1:A:3302:VAL:HG13	1:A:3302:VAL:O	2.17	0.44
2:B:532:VAL:HG12	2:B:532:VAL:O	2.17	0.44
2:C:258:LEU:HB3	2:C:271:LYS:HE3	2.00	0.44
2:D:619:PHE:HZ	2:D:657:GLY:HA2	1.82	0.44
1:A:3263:TRP:HH2	1:A:3288:ILE:HG13	1.82	0.44
2:B:499:LYS:O	2:B:502:TYR:HB2	2.17	0.44
1:A:3095:LEU:HD22	1:A:3277:ARG:HB3	1.99	0.44
1:A:3305:SER:O	1:A:3308:SER:CB	2.66	0.44
2:C:306:ARG:HE	2:C:308:PHE:HB2	1.83	0.43
2:C:324:LEU:HD12	2:C:423:PHE:HE1	1.83	0.43
2:C:567:PHE:O	2:C:571:ILE:HG12	2.17	0.43
2:C:397:ARG:NH1	2:C:542:GLN:OE1	2.51	0.43
1:A:3795:TRP:CH2	1:A:3842:TRP:HD1	2.37	0.43
2:B:234:LEU:HD12	2:B:234:LEU:HA	1.87	0.43
2:C:362:ASN:OD1	2:C:363:GLY:N	2.51	0.43
1:A:4109:ARG:HA	1:A:4109:ARG:HD3	1.90	0.43
1:A:3275:PHE:CD2	1:A:3275:PHE:O	2.72	0.43
2:C:423:PHE:CE2	2:C:442:LEU:HD13	2.53	0.43
1:A:3849:ALA:HA	1:A:3871:LEU:O	2.18	0.43
2:D:665:VAL:HG13	2:D:669:PHE:HD2	1.84	0.43
1:A:3086:VAL:O	1:A:3090:VAL:HG23	2.19	0.42
2:C:615:ALA:HB2	2:C:660:TYR:CZ	2.54	0.42
1:A:3971:PRO:C	1:A:3972:ARG:HG2	2.45	0.42
2:C:316:LEU:HD11	2:C:429:TYR:HB2	2.01	0.42
1:A:4094:ARG:HB3	1:A:4095:LEU:H	1.69	0.42
2:D:611:TYR:CD2	2:D:664:PHE:HD1	2.38	0.42
1:A:4103:ALA:HB1	2:B:677:LEU:HD23	2.01	0.42
1:A:3754:LEU:O	1:A:3754:LEU:HD23	2.20	0.42
2:C:315:LEU:HD21	2:C:319:PRO:HD3	2.01	0.42
2:D:665:VAL:HG13	2:D:669:PHE:CD2	2.54	0.42
2:B:223:GLU:HA	2:B:226:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:258:LEU:HD21	2:C:455:TRP:CD2	2.55	0.42
2:D:581:ARG:O	2:D:585:GLN:HG3	2.20	0.42
1:A:3933:LEU:HG	1:A:3937:ALA:HB2	2.00	0.42
2:B:466:VAL:HG12	2:B:467:THR:HG23	2.01	0.42
1:A:3727:MET:HG2	1:A:3731:LEU:HD22	2.02	0.41
1:A:3332:VAL:O	1:A:3335:PRO:HD2	2.21	0.41
1:A:3691:ASP:OD1	1:A:3691:ASP:N	2.50	0.41
1:A:3754:LEU:O	1:A:3755:GLN:HG3	2.20	0.41
1:A:3754:LEU:HD23	1:A:3756:GLU:HB2	2.02	0.41
2:B:499:LYS:HE3	2:B:502:TYR:H	1.85	0.41
2:C:540:GLU:H	2:C:540:GLU:CD	2.28	0.41
1:A:3256:GLY:HA2	1:A:3259:ASP:OD1	2.21	0.41
1:A:3717:ILE:HG22	1:A:3881:ALA:HB2	2.03	0.41
1:A:4103:ALA:HA	2:B:674:ASN:HB3	2.02	0.41
2:B:619:PHE:HB3	2:B:623:VAL:HG21	2.01	0.41
2:C:489:VAL:HA	2:C:492:ILE:HG12	2.01	0.41
2:B:563:ALA:HB1	2:C:614:LEU:HD12	2.01	0.41
2:C:681:ASN:ND2	2:D:681:ASN:HD22	2.14	0.41
1:A:3095:LEU:HD21	1:A:3266:ILE:HG23	2.02	0.41
2:B:342:LYS:HA	2:B:342:LYS:HD3	1.90	0.41
1:A:3596:PHE:HD2	1:A:3597:LEU:HD12	1.84	0.41
2:D:586:LEU:HD12	2:D:586:LEU:HA	1.90	0.41
2:C:636:GLN:OE1	2:C:660:TYR:OH	2.32	0.40
1:A:3287:LEU:HD13	1:A:3337:TYR:CD1	2.56	0.40
1:A:3783:VAL:HG23	1:A:3836:PHE:HZ	1.86	0.40
2:B:224:LEU:O	2:B:228:LEU:HD23	2.21	0.40
2:B:423:PHE:CE2	2:B:442:LEU:HD13	2.56	0.40
2:B:263:SER:HB2	2:B:266:GLU:HB2	2.03	0.40
2:C:458:GLN:HG2	2:C:552:ALA:HB1	2.01	0.40
2:D:673:LEU:O	2:D:677:LEU:HG	2.21	0.40
2:B:501:HIS:CD2	2:B:504:ARG:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	719/1261 (57%)	643 (89%)	71 (10%)	5 (1%)	18	52
2	B	478/1007 (48%)	431 (90%)	46 (10%)	1 (0%)	43	73
2	C	478/1007 (48%)	440 (92%)	38 (8%)	0	100	100
2	D	479/1007 (48%)	437 (91%)	42 (9%)	0	100	100
All	All	2154/4282 (50%)	1951 (91%)	197 (9%)	6 (0%)	37	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3278	ILE
1	A	3970	ARG
2	B	220	VAL
1	A	3262	ILE
1	A	3307	TYR
1	A	3308	SER

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	499/1041 (48%)	497 (100%)	2 (0%)	84	85
2	B	434/860 (50%)	434 (100%)	0	100	100
2	C	434/860 (50%)	434 (100%)	0	100	100
2	D	104/860 (12%)	104 (100%)	0	100	100
All	All	1471/3621 (41%)	1469 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3278	ILE
1	A	3309	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3668	HIS
1	A	3736	HIS
1	A	3790	ASN
1	A	3840	HIS
1	A	3864	HIS
1	A	3962	GLN
1	A	4111	HIS
2	B	305	ASN
2	B	335	GLN
2	B	430	ASN
2	B	622	GLN
2	B	636	GLN
2	C	323	GLN
2	C	430	ASN
2	C	555	GLN
2	C	681	ASN

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	NAG	B	1003	2	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	C	1004	2	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	B	1001	2	14,14,15	0.22	0	17,19,21	0.38	0
3	NAG	B	1002	2	14,14,15	0.31	0	17,19,21	0.58	0
3	NAG	C	1003	2	14,14,15	0.96	1 (7%)	17,19,21	1.14	1 (5%)
3	NAG	C	1002	2	14,14,15	0.25	0	17,19,21	0.43	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	NAG	B	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1004	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1001	2	-	3/6/23/26	0/1/1/1
3	NAG	B	1002	2	-	3/6/23/26	0/1/1/1
3	NAG	C	1003	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1002	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	NAG	O5-C1	3.34	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1003	NAG	C1-O5-C5	4.46	118.24	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1004	NAG	C4-C5-C6-O6
3	C	1004	NAG	O5-C5-C6-O6
3	B	1002	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1001	NAG	C8-C7-N2-C2
3	B	1001	NAG	O7-C7-N2-C2
3	B	1003	NAG	O5-C5-C6-O6
3	C	1002	NAG	O5-C5-C6-O6
3	B	1002	NAG	O5-C5-C6-O6
3	B	1001	NAG	O5-C5-C6-O6
3	B	1003	NAG	C4-C5-C6-O6
3	B	1002	NAG	C3-C2-N2-C7

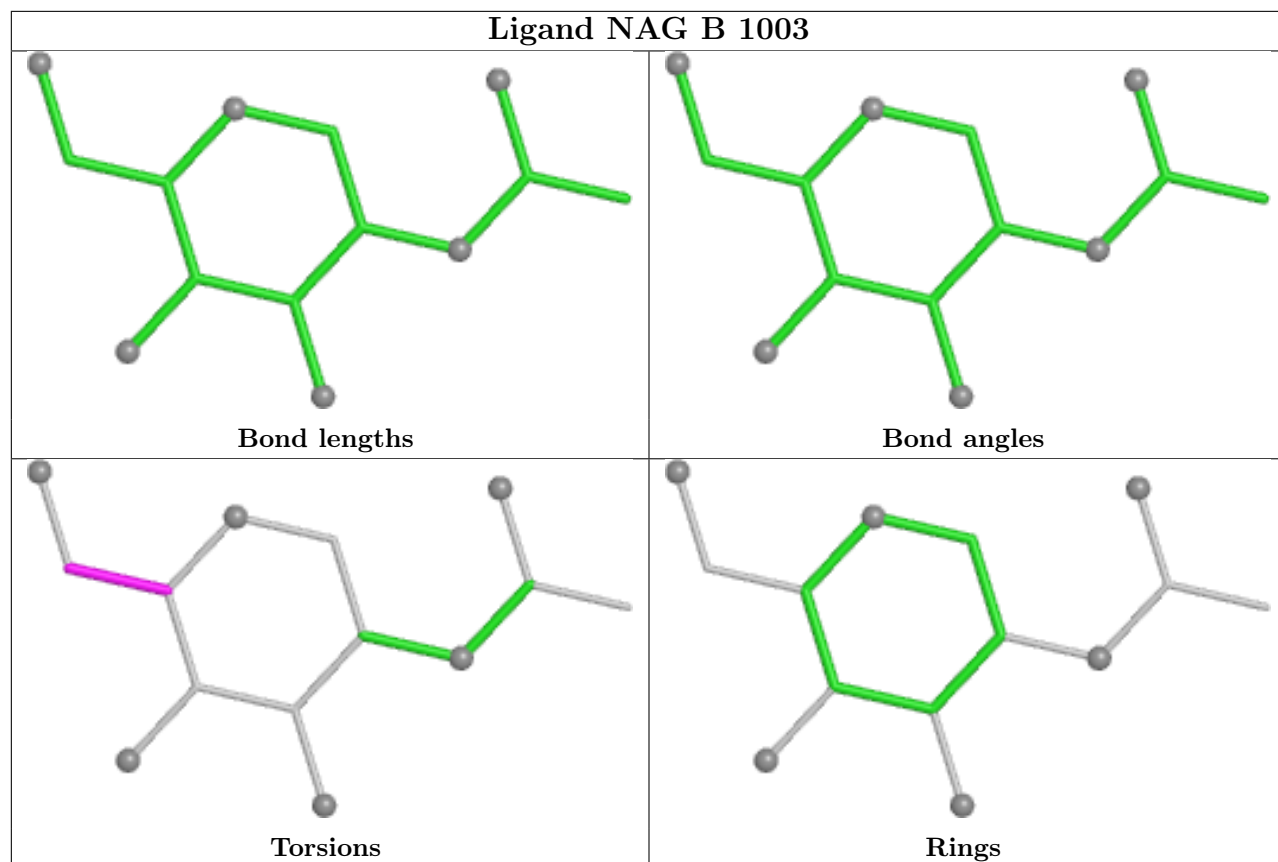
There are no ring outliers.

1 monomer is involved in 1 short contact:

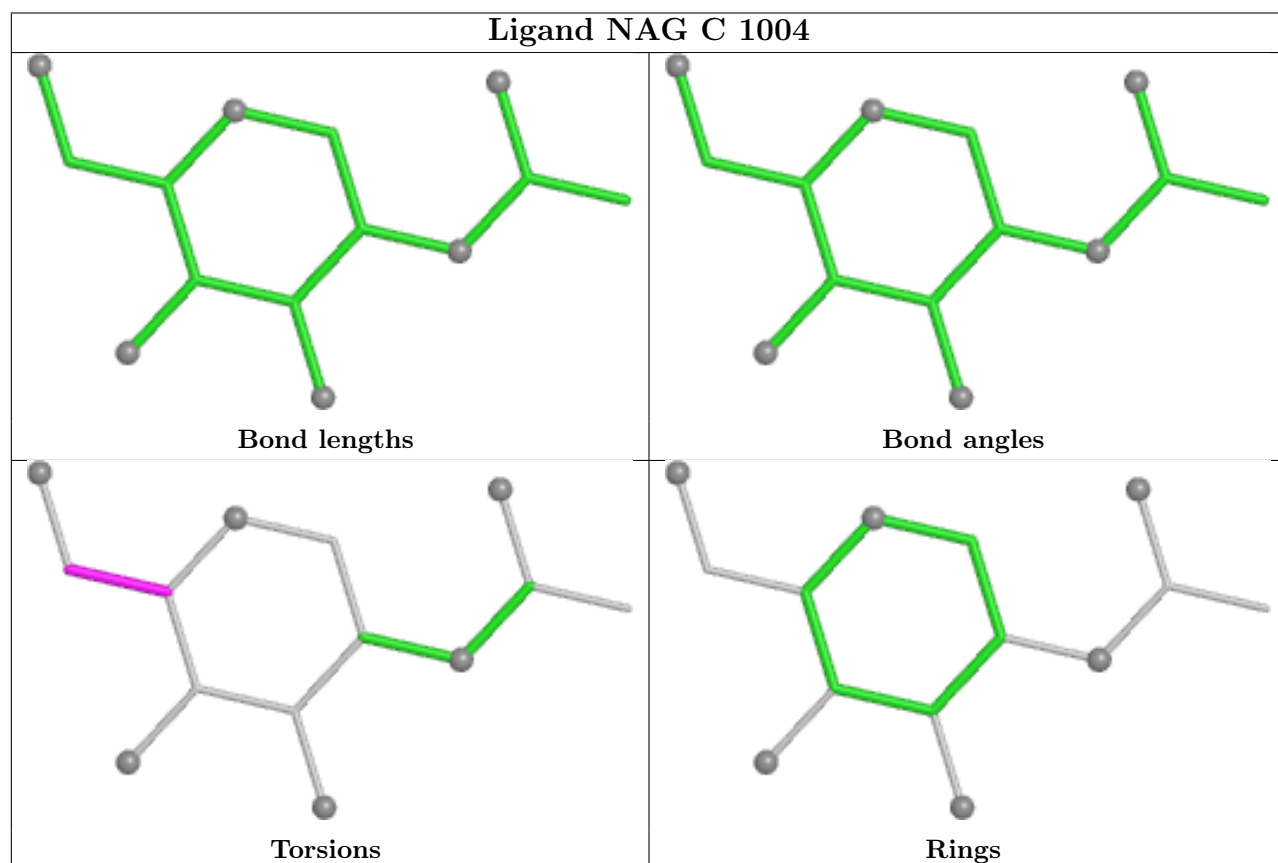
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	NAG	1	0

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.

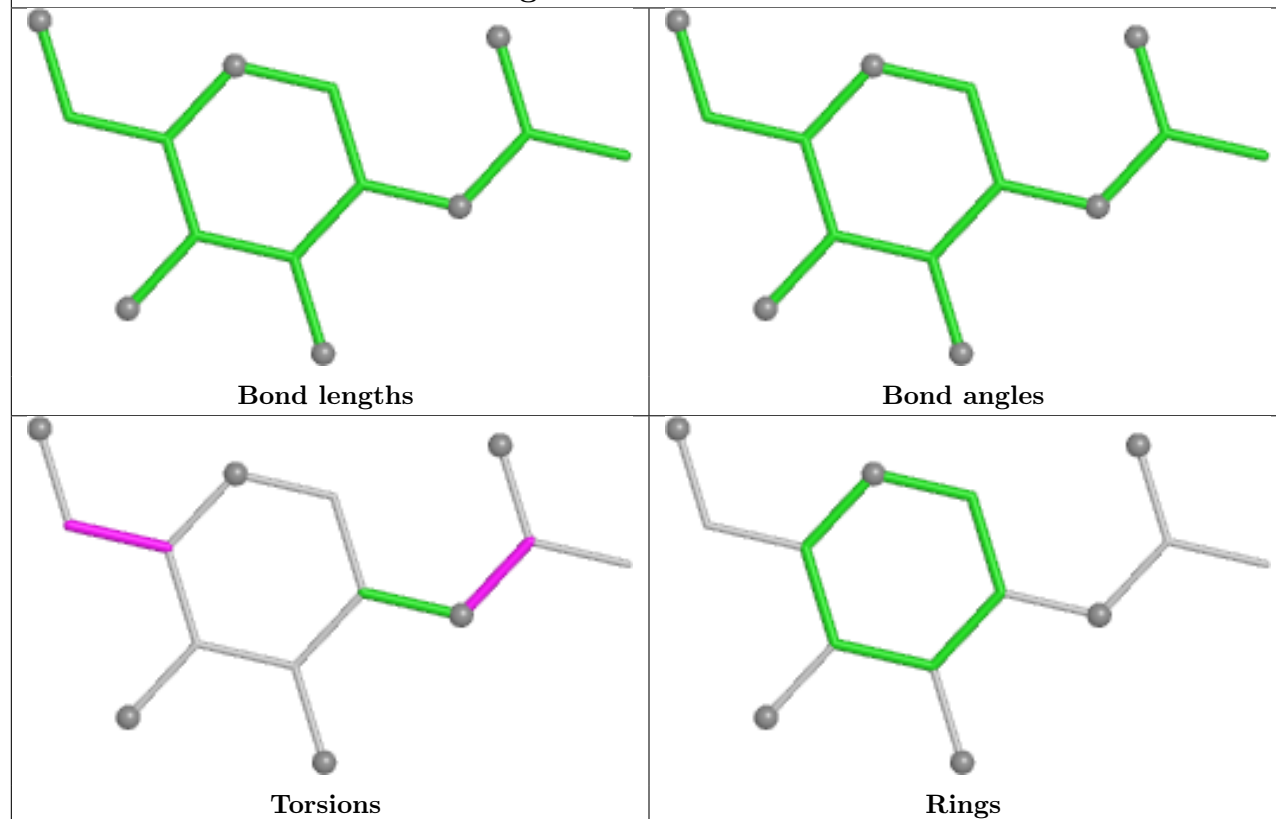
Ligand NAG B 1003



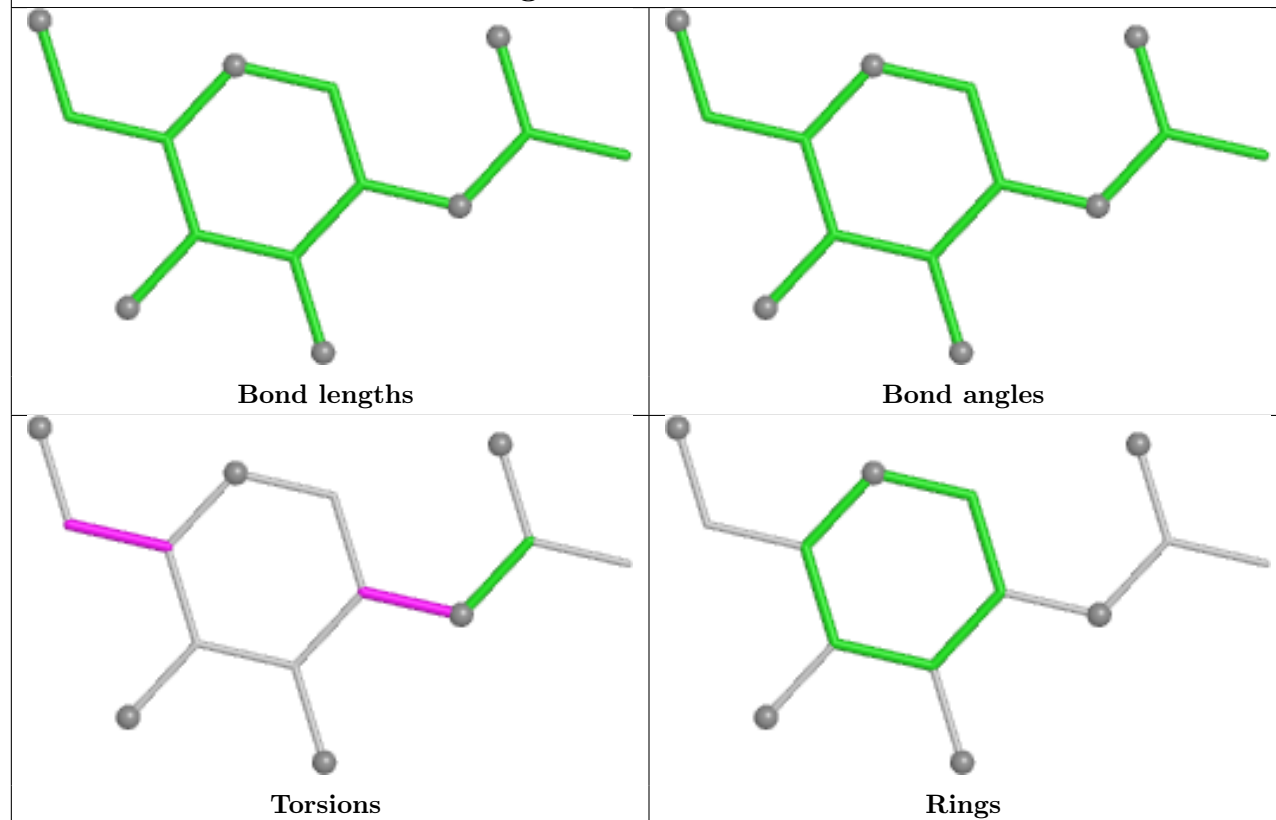
Ligand NAG C 1004



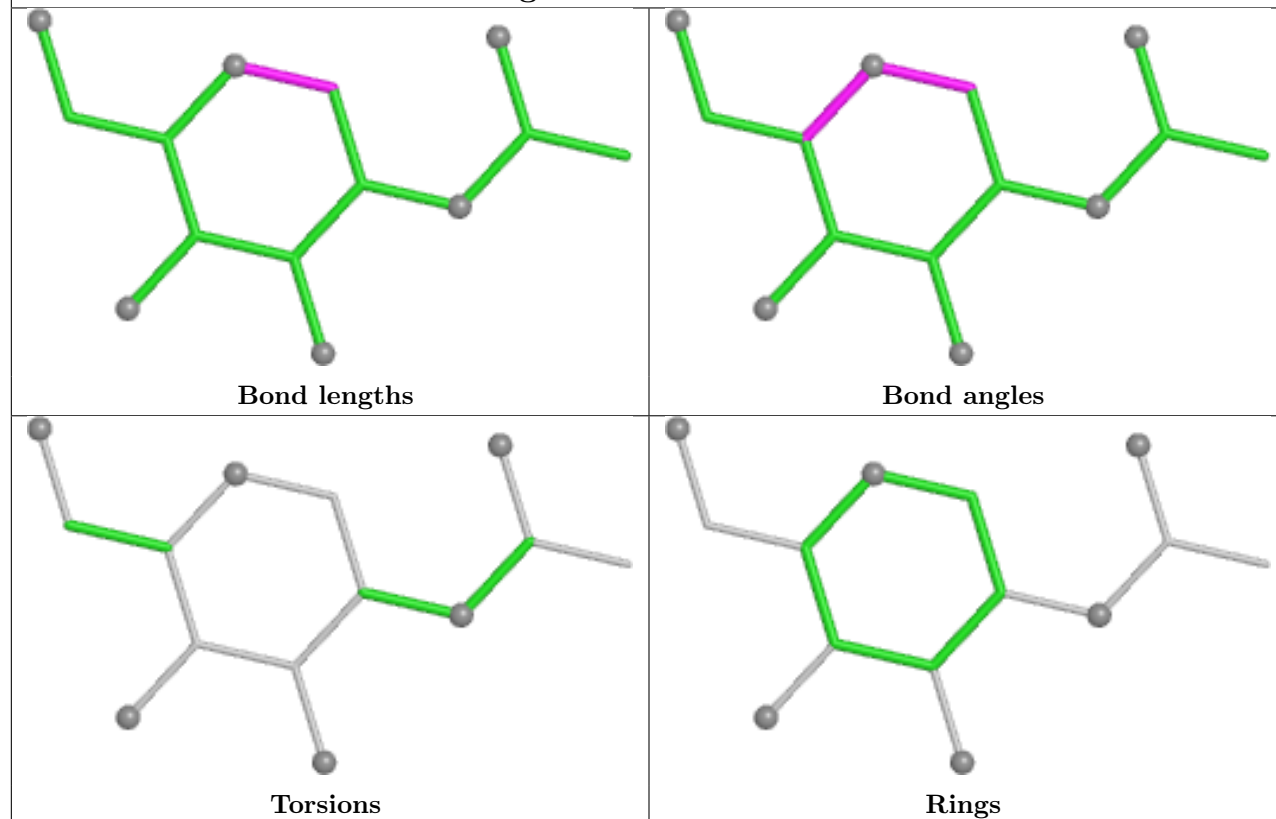
Ligand NAG B 1001



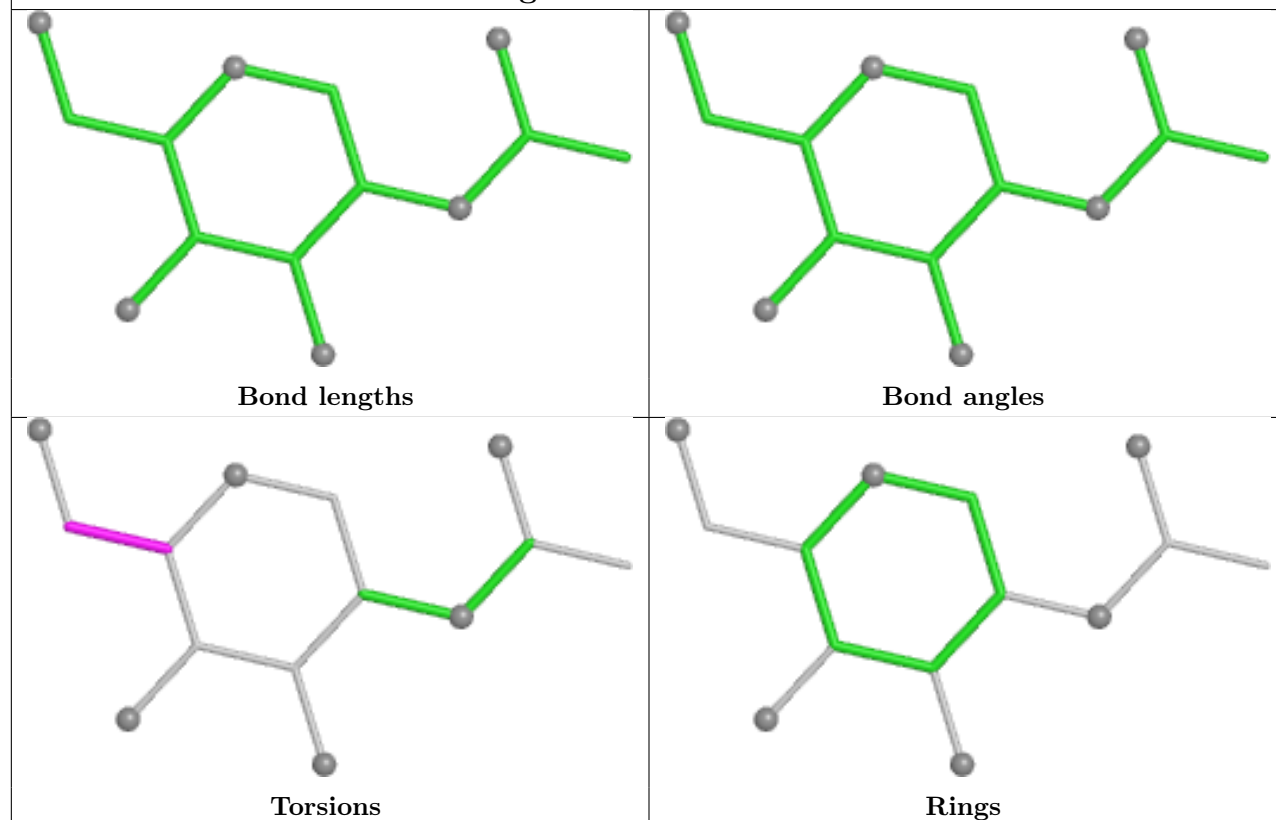
Ligand NAG B 1002



Ligand NAG C 1003



Ligand NAG C 1002



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.

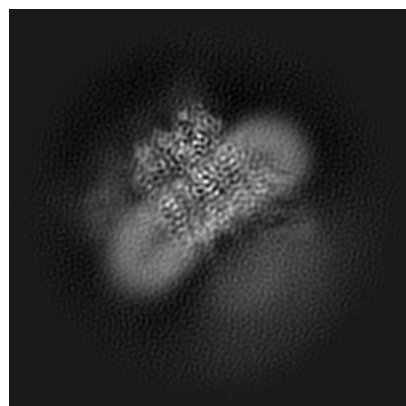
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60207. These allow visual inspection of the internal detail of the map and identification of artifacts.

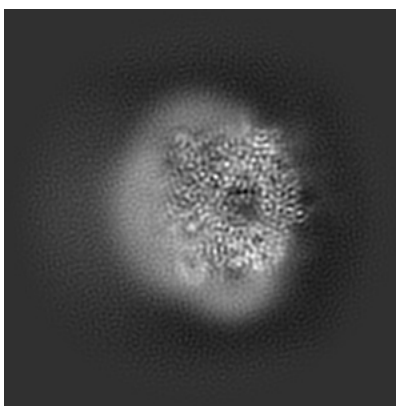
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

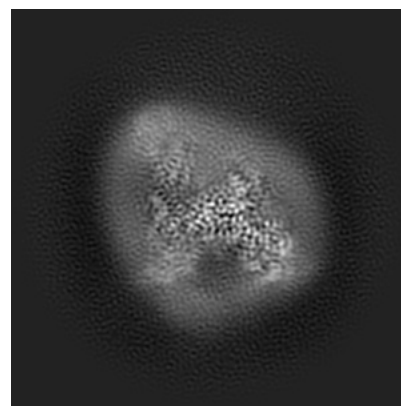
6.1.1 Primary map



X

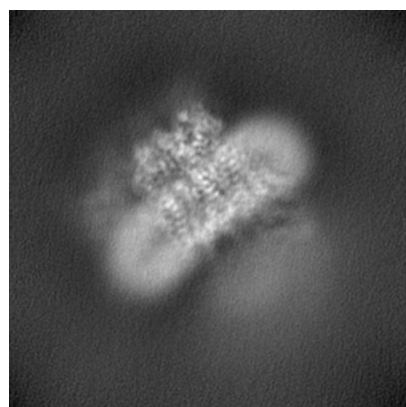


Y

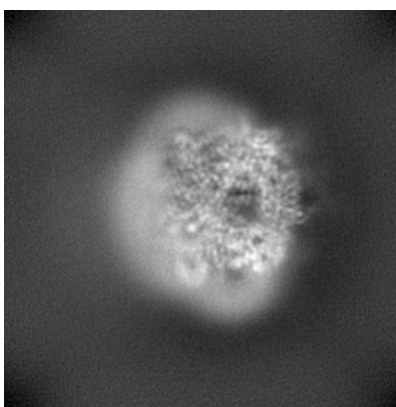


Z

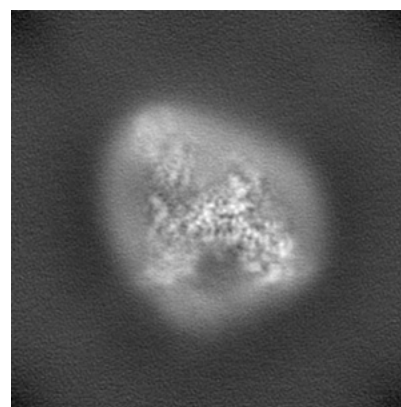
6.1.2 Raw map



X



Y

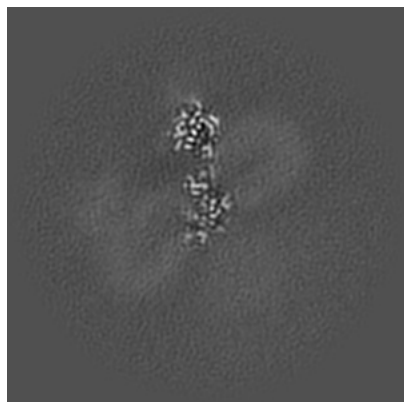


Z

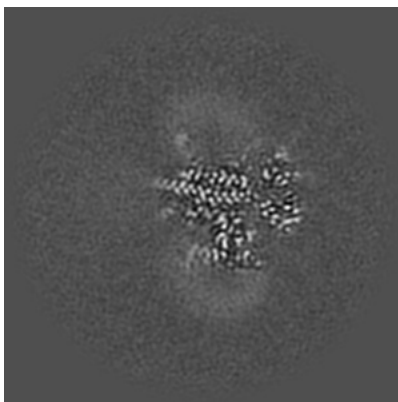
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

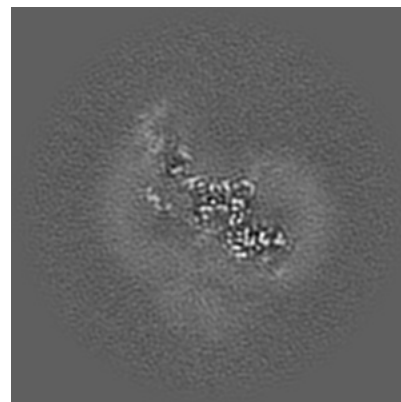
6.2.1 Primary map



X Index: 120

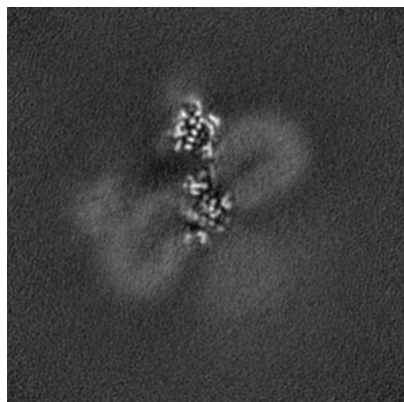


Y Index: 120

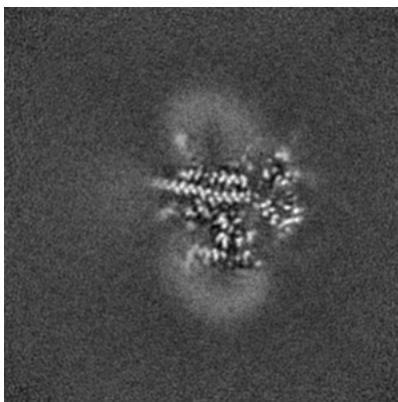


Z Index: 120

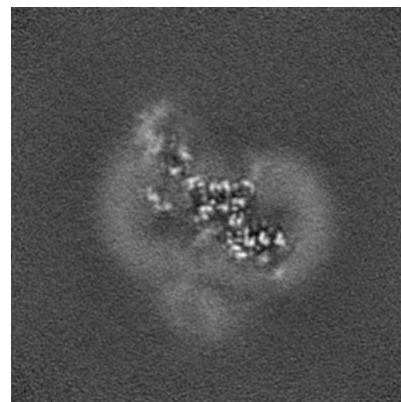
6.2.2 Raw map



X Index: 120



Y Index: 120

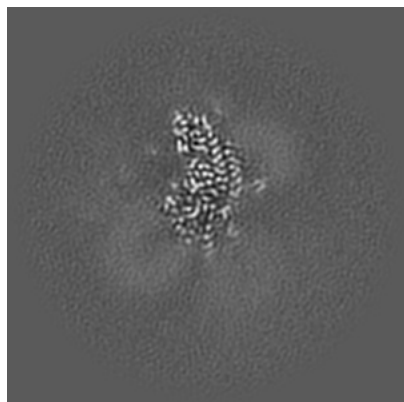


Z Index: 120

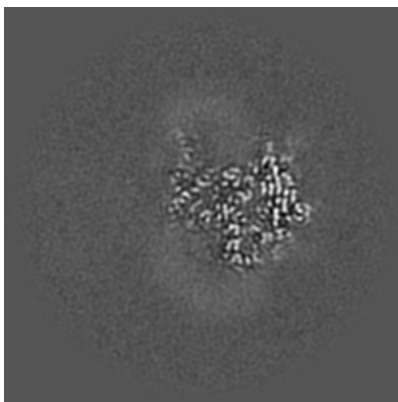
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

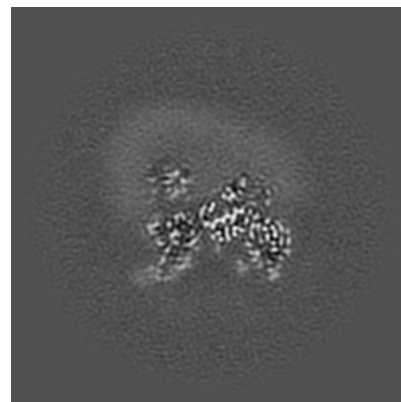
6.3.1 Primary map



X Index: 134

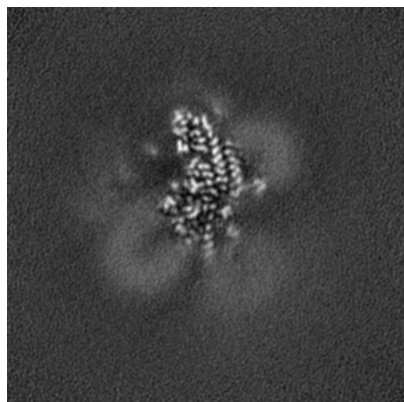


Y Index: 114

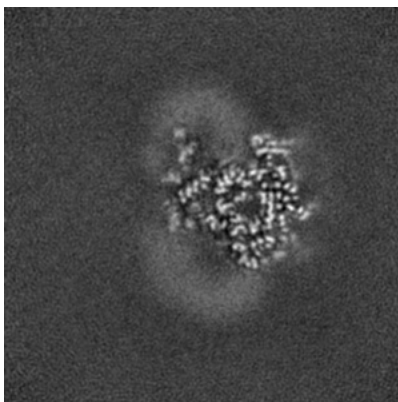


Z Index: 155

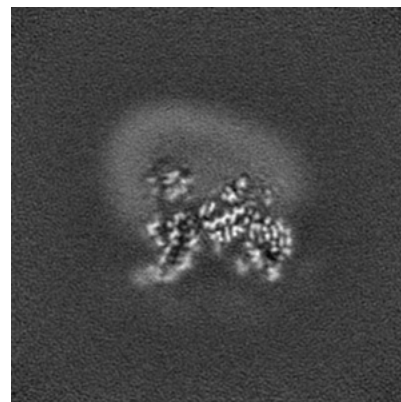
6.3.2 Raw map



X Index: 134



Y Index: 111

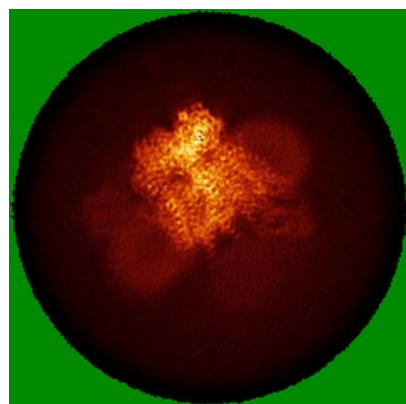


Z Index: 155

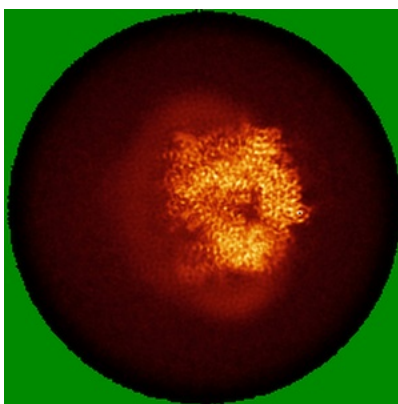
The images above show the largest variance slices of the map in three orthogonal directions.

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

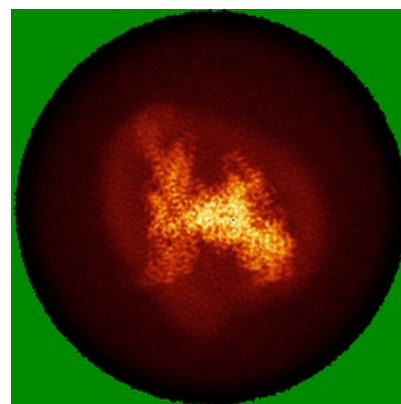
6.4.1 Primary map



X

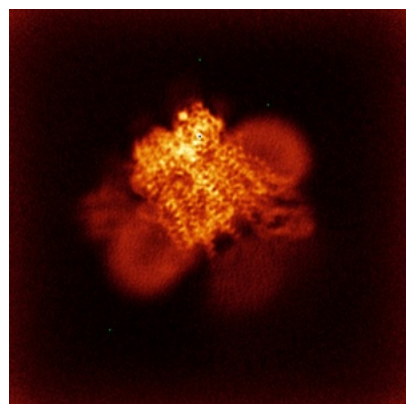


Y

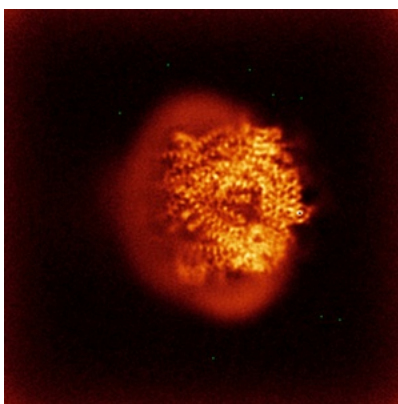


Z

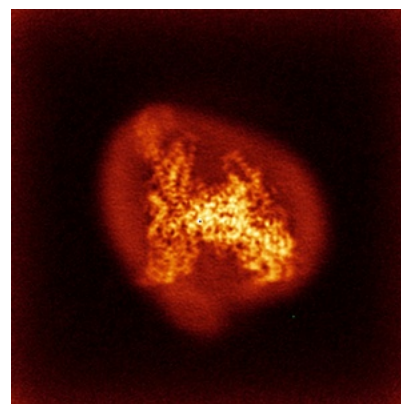
6.4.2 Raw map



X



Y

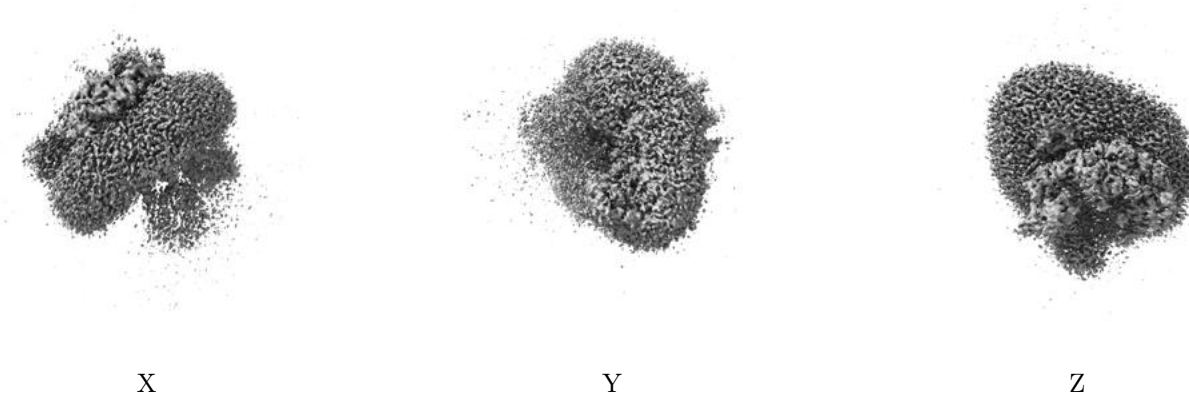


Z

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.

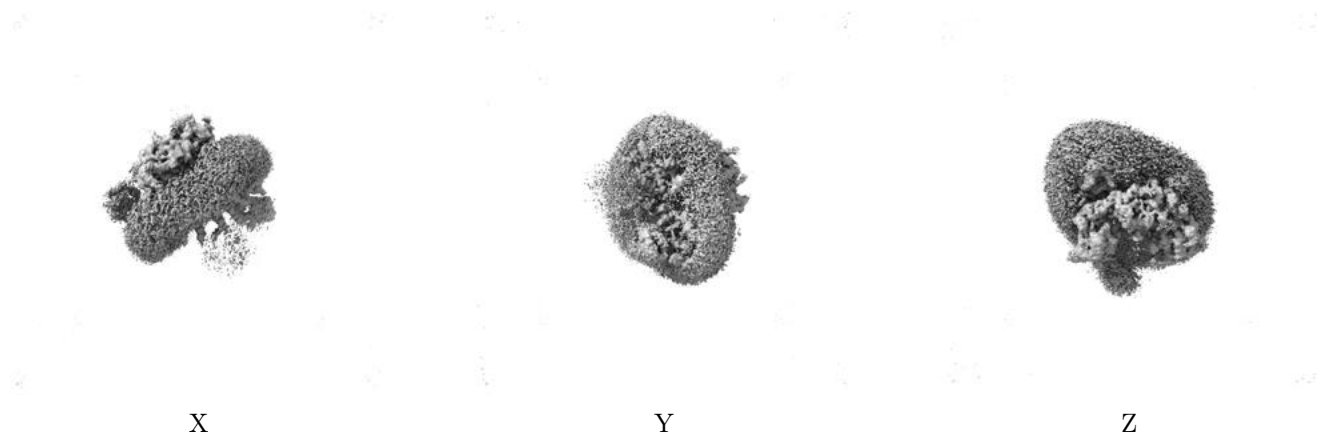
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.32. 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.

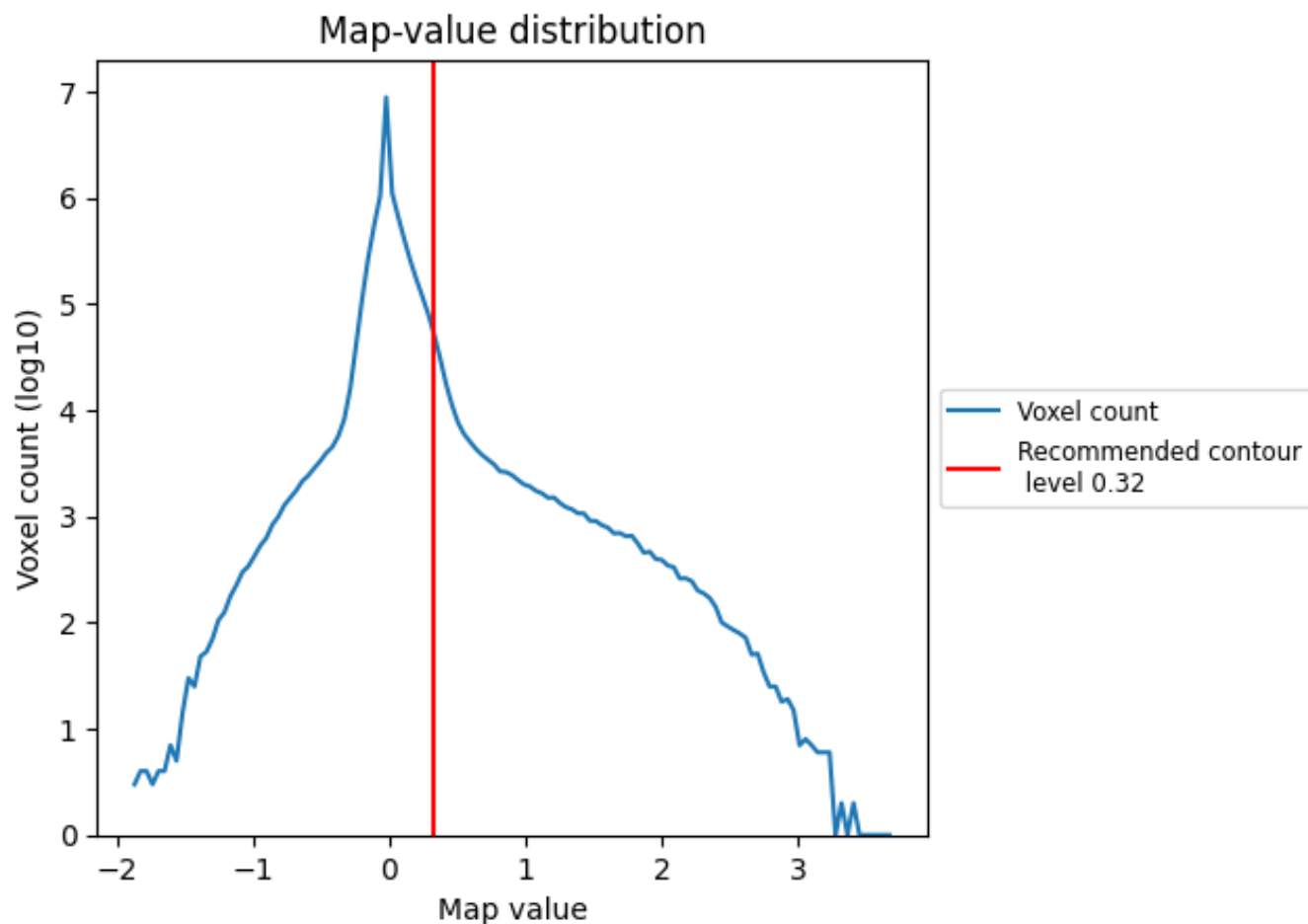
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

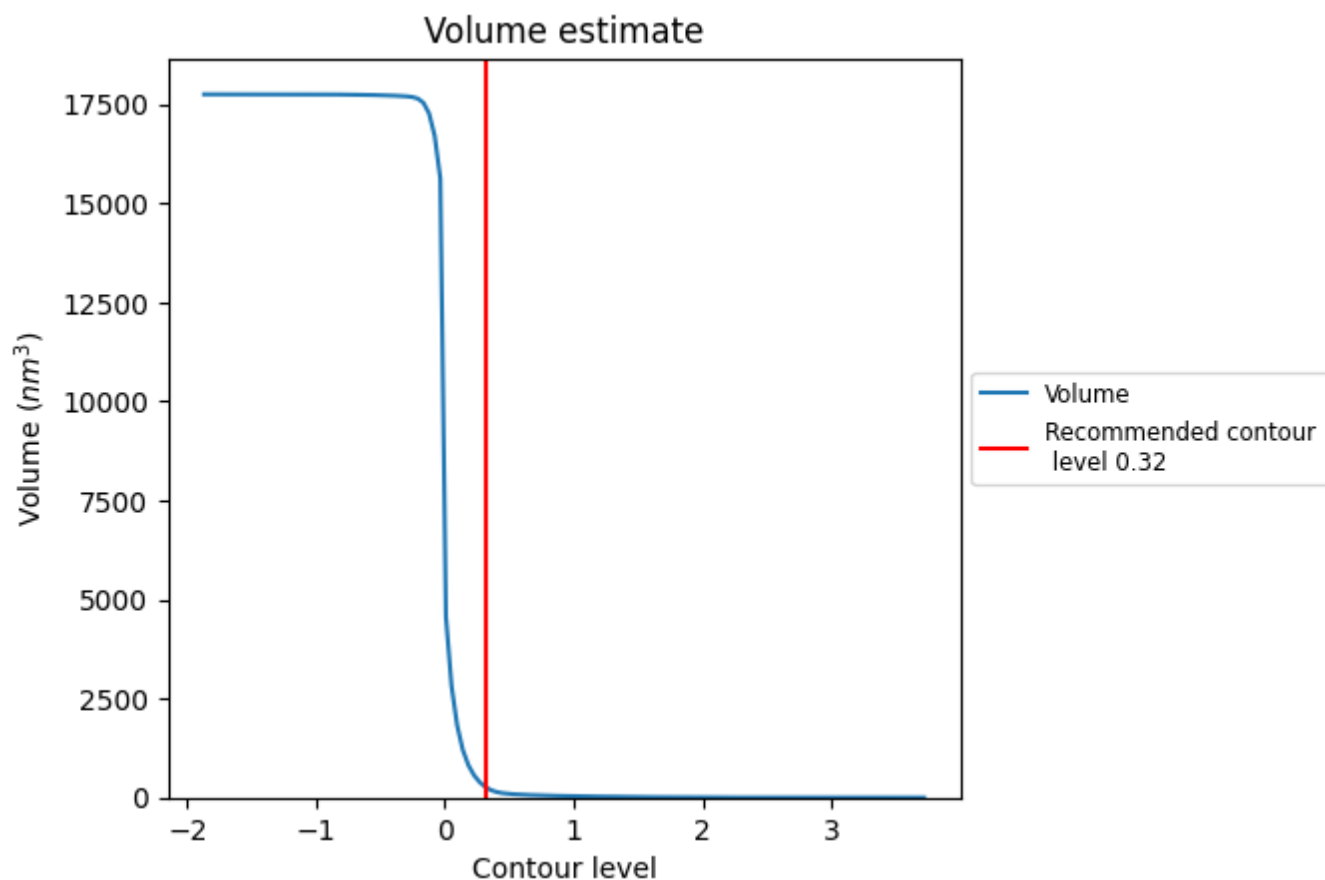
This section contains the results of statistical analysis of the map.

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.

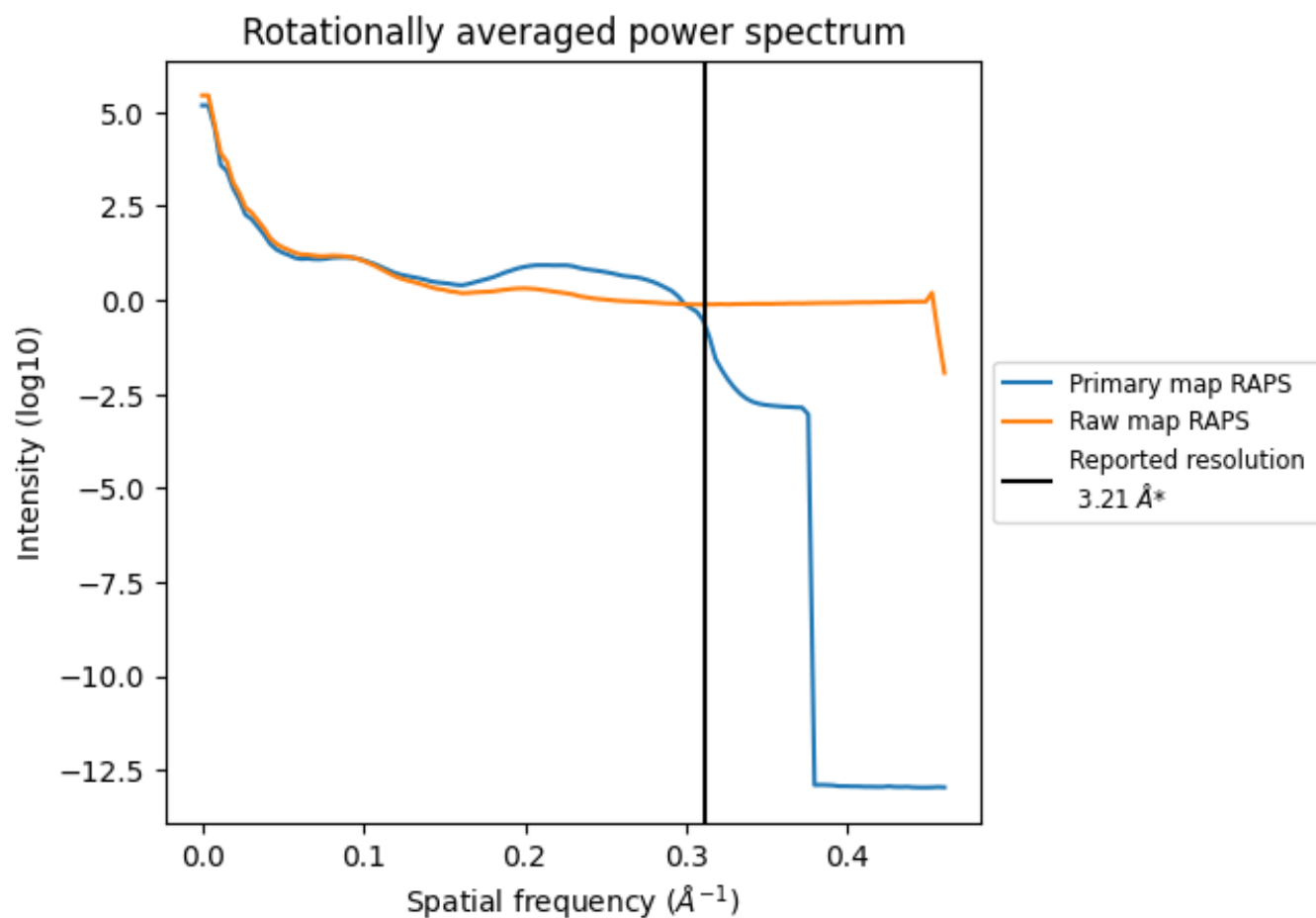
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm³; this corresponds to an approximate mass of 232 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 ⓘ

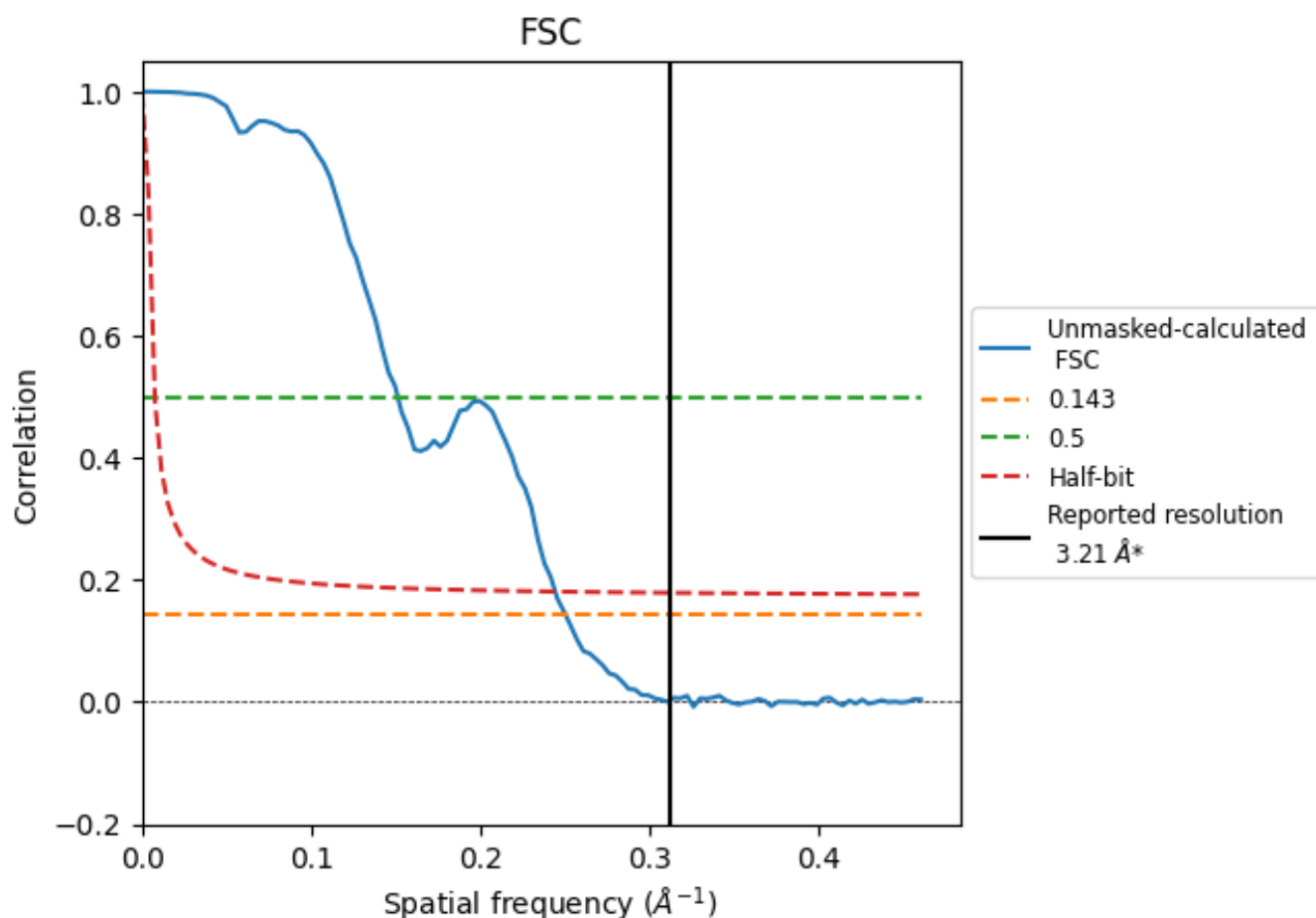


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

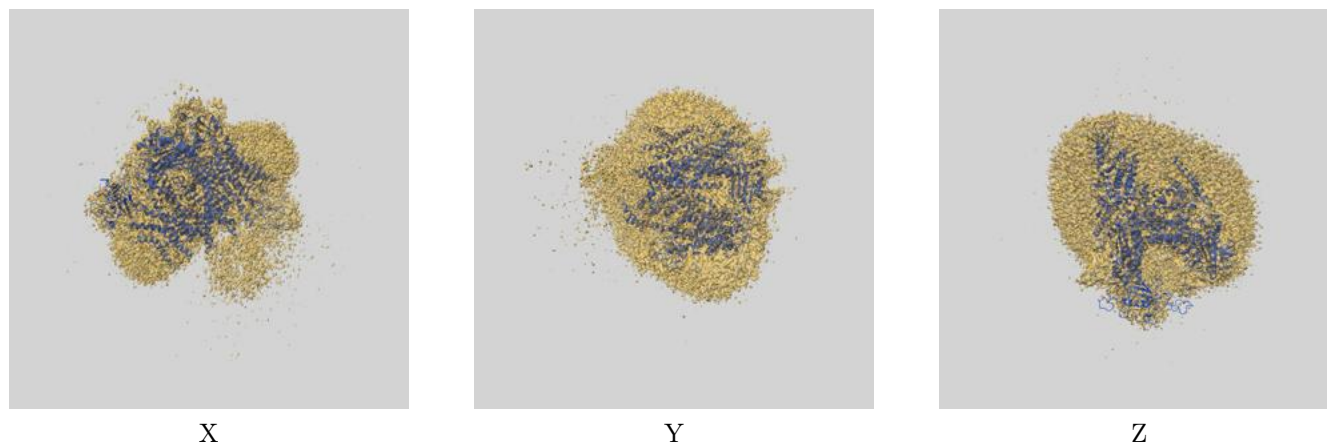
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.00	6.62	4.10

*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 4.00 differs from the reported value 3.21 by more than 10 %

9 Map-model fit [i](#)

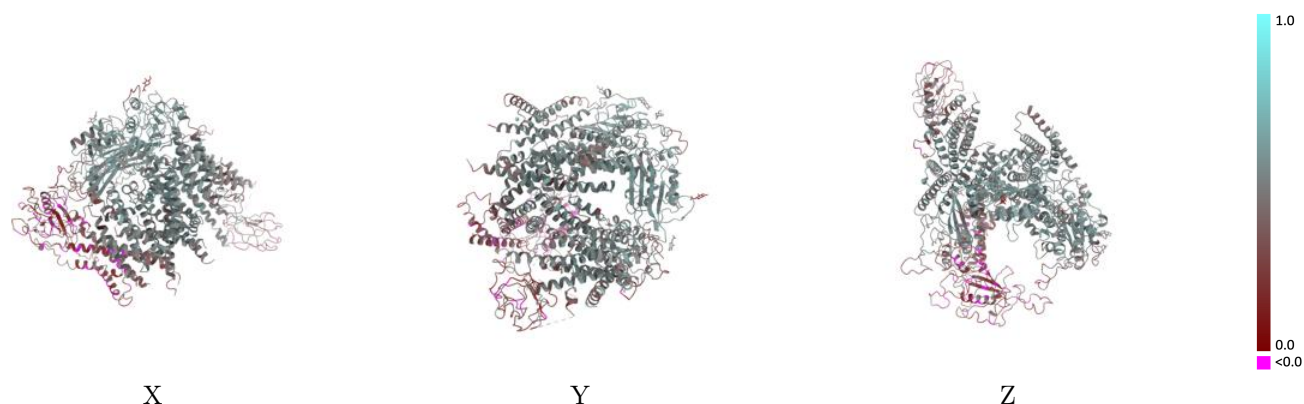
This section contains information regarding the fit between EMDB map EMD-60207 and PDB model 8ZKS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



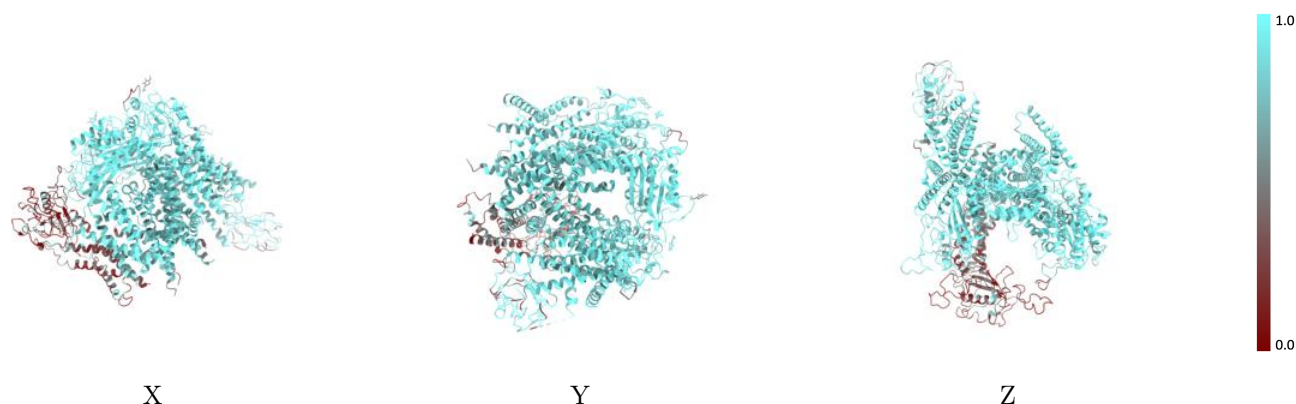
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



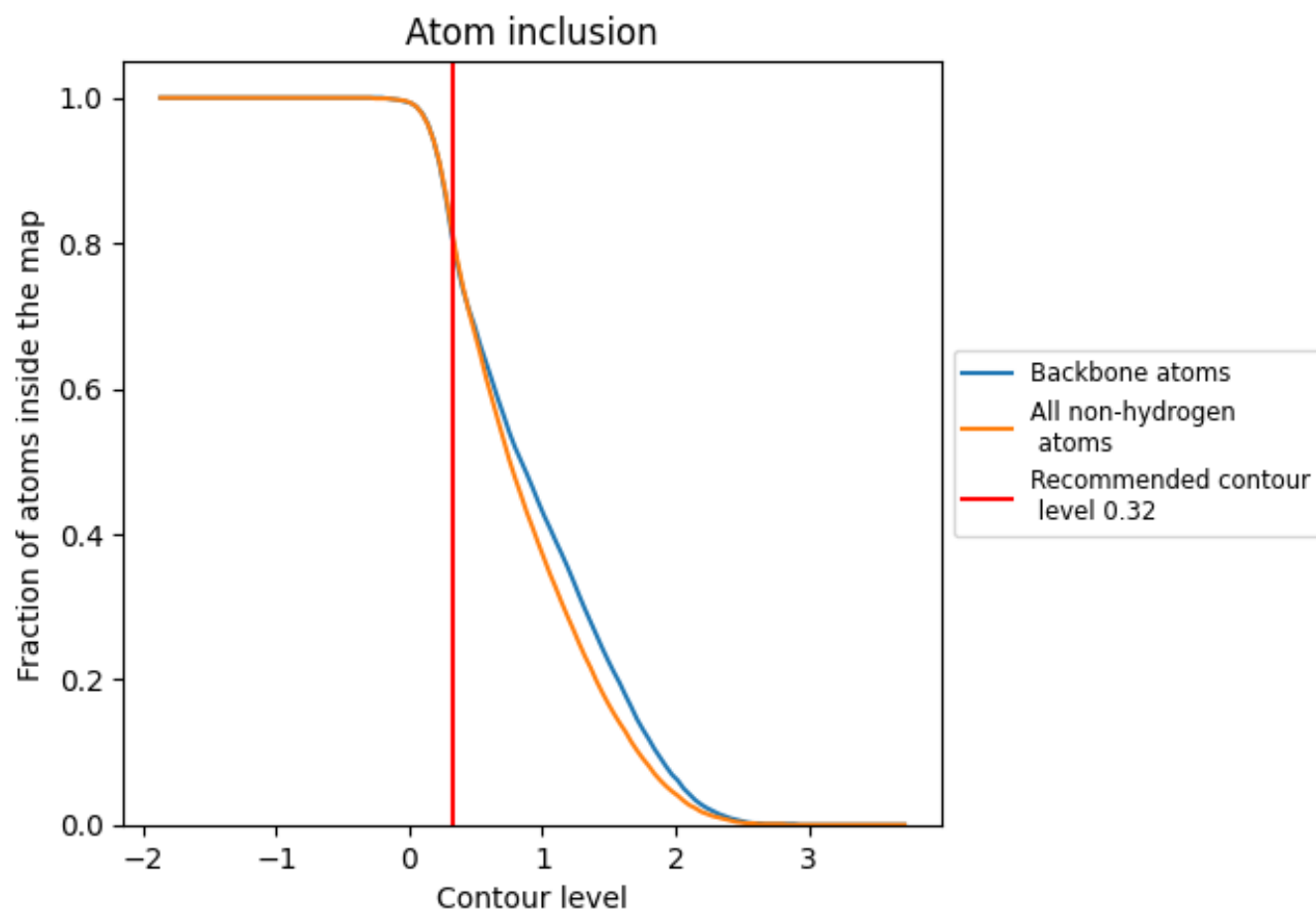
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8170	0.4550
A	0.8670	0.4520
B	0.9150	0.5220
C	0.8940	0.4940
D	0.4700	0.3040

