



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 02:28 AM UTC

PDB ID : 7PW6 / pdb_00007pw6
EMDB ID : EMD-13676
Title : Human SMG1-8-9 kinase complex bound to a SMG1 inhibitor - SMG1 body
Authors : Langer, L.M.; Conti, E.
Deposited on : 2021-10-06
Resolution : 3.05 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the 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) : 2.49

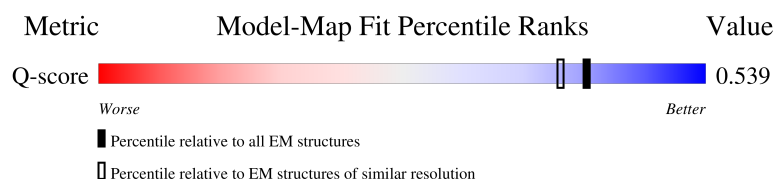
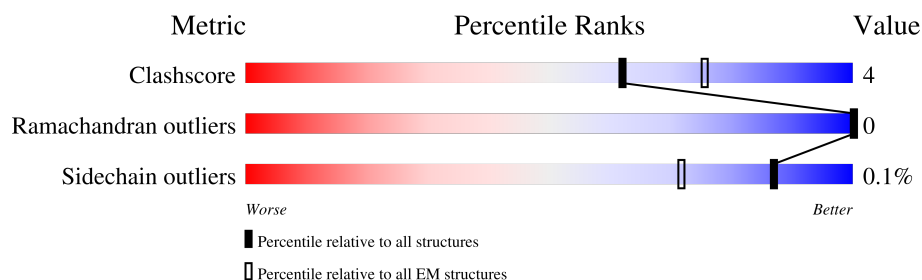
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 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	13971 (2.55 - 3.55)

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	2896	 44% 5% 51%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10393 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.

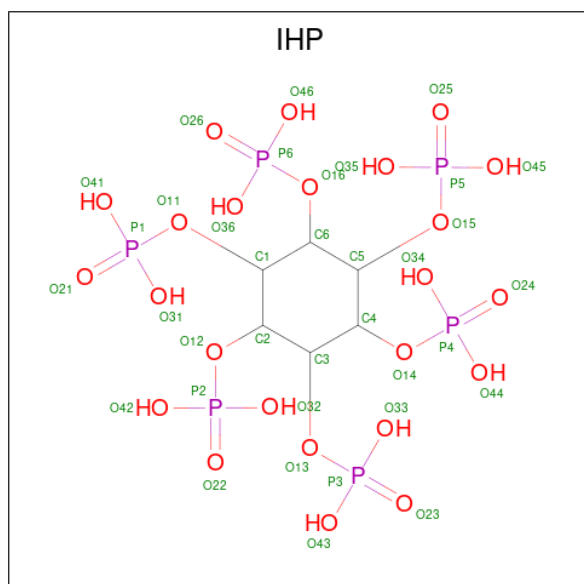
- Molecule 1 is a protein called Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1, Serine/threonine-protein kinase SMG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0
			10318	6612	1844	1810	52		

There are 2 discrepancies between the modelled and reference sequences:

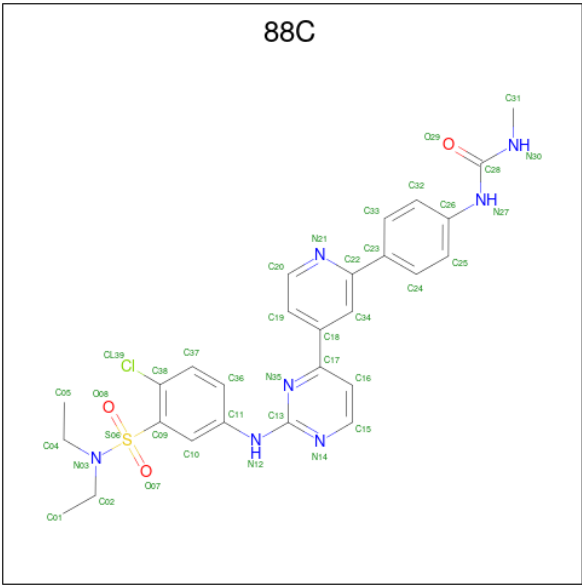
Chain	Residue	Modelled	Actual	Comment	Reference
A	1209	SER	ALA	conflict	UNP Q96Q15
A	1269	ASN	ASP	conflict	UNP Q96Q15

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 3 is 1-[4-[4-[2-[[4-chloranyl-3-(diethylsulfamoyl)phenyl]amino]pyrimidin-4-yl]pyrimidin-2-yl]phenyl]-3-methyl-urea (CCD ID: 88C) (formula: C₂₇H₂₈ClN₇O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	Cl	N	O	S	0
			39	27	1	7	3	1	

ALA	SER	LYS	VAL	GLN	ARG	LEU	THR	THR	TYR	GLN	GLY	SER	R2386	P2137	UNK	UNK	A1924
CYS	SER	ASP	THR	LYS	GLY	ALA	THR	ALA	ALA	GLU	VAL	SER	R2340	P2151	UNK	UNK	Y1930
LEU	CYS	PHE	LEU	LEU	SER	VAL	GLU	THR	VAL	ILE	HIS	ARG	N2341	P2155	UNK	UNK	Y1934
THR	ASP	ALA	ASP	ASP	VAL	ILE	THR	THR	ALA	GLN	THR	ALA	L2342	K2156	P2035	UNK	Y1969
GLN	GLY	THR	GLN	GLY	GLU	THR	GLN	GLN	LEU	ASP	THR	ILE	L2343	L2157	UNK	UNK	VAL
ASN	LEU	ILE	ASP	THR	THR	GLN	GLN	THR	TYR	MET	HIS	LYS	D2344	L2160	UNK	UNK	LEU
VAL	THR	VAL	GLN	GLY	GLY	ASP	GLN	ASP	PRO	GLY	GLN	VAL	G2348	F2169	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	I2353	F2177	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	D2354	N2181	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F2359	P2186	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	P2372	Y2193	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	Q2377	Y2194	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	V2418	V2195	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	A2427	R2201	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	G2202	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	L2204	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	I2205	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	Q2206	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	W2207	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	A2211	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2068	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2071	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2074	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2075	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2076	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2082	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2083	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2006	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2007	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2008	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2009	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2010	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2011	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2012	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2013	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	X2021	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	A2100	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	S2114	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	A2115	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	R2116	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	D2117	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	P2132	UNK	UNK	UNK
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	K2136	UNK	UNK	UNK

GLU ARG ASN	SER	GLU	SER	GLU	ASP	HIS	SER
	THR	HIS	VAL	VAL	PRO	ASN	SER
	ASN	VAL	LYS	LYS	ILE	ILE	ASN
	33607	GLY	HIS	HIS	GLY	ILE	ILE
	33608	GLN	LEU	LEU	SER	SER	PHE
	33609	LYS	LEU	LYS	GLU	GLU	GLU
	33623	THR	GLN	ALA	TRP	SER	SER
		GLN	GLU	ALA	LEU	LEU	ARG
	33627	PRO	ILE	MET	ALA	LEU	LEU
		ASP	THR	ALA	ASP	THR	THR
33640	VAL	PRO	LYS	LYS	SER	SER	
	MET	THR	ASP	ASP	ALA	ARG	
33644	SER	THR	GLU	GLU	HIS	THR	
	GLN	LYS	GLU	ALA	GLN	ALA	
33658	ASN	GLU	ALA	ALA	LEU	ALA	
	ALA	LEU	LEU	LEU	THR	LEU	
33661	ARG	LYS	ALA	ASP	GLN	ASN	
	LYS	THR	ASP	ASP	ASN	LEU	
33662	ILE	GLN	GLY	GLY	MET	ASP	
	GLN	GLN	GLU	GLU	SER	ALA	
33663	LYS	SER	ASP	THR	THR	ALA	
	ASN	ILE	VAL	VAL	ARG	LEU	
33664	LEU	TYR	PRO	TYR	GLU	PHE	
	ALA	ASN	ASN	ASN	ALA	GLU	
33665	THR	ASN	GLU	GLU	ILE	LEU	
	SER	LEU	ASN	LEU	GLN	ILE	
33666	ALA	VAL	SER	SER	THR	LYS	
	ASP	SER	VAL	VAL	GLU	ARG	
33667	THR	PHE	ARG	ARG	LYS	CYS	
	PRO	ALA	GLN	GLN	GLN	GLN	
33668	PRO	SER	PHE	PHE	GLN	GLN	
	SER	PRO	LEU	LEU	GLN	GLN	
33669	THR	THR	GLY	GLY	ILE	CYS	
	VAL	VAL	GLU	GLU	ILE	GLN	
33670	PRO	THR	TYR	TYR	THR	PHE	
	GLY	ALA	SER	LYS	VAL	ALA	
33671	LYS	THR	THR	THR	CYS	SER	
	SER	LYS	ASN	GLN	THR	GLN	
33672	VAL	SER	ASN	ASP	ILE	ASN	
	ALA	CYS	ASN	ASN	GLN	SER	
33673	ALA	SER	ILE	ILE	ASN	SER	
	CYS	SER	GLN	GLN	LEU	VAL	
33674	SER	PRO	THR	THR	VAL	SER	
	PRO	THR	VAL	VAL	ASP	GLU	
33675	LYS	SER	LEU	LEU	ASN	LEU	
	LYS	SER	PHE	PHE	ILE	GLU	
33676	ALA	ALA	THR	THR	LYS	LEU	
	VAL	VAL	TYR	VAL	THR	ARG	
33677	ARG	THR	THR	VAL	VAL	LEU	
	ASP	GLN	GLN	GLN	LEU	LEU	
33678	PRO	PRO	ALA	ALA	THR	GLN	
	LYS	SER	MET	MET	GLY	ARG	
33679	THR	PHE	GLY	GLY	HIS	VAL	
	GLY	ALA	GLN	GLN	ASN	ASP	
33680	LYS	ALA	VAL	VAL	THR	THR	
	ALA	ALA	ARG	ARG	GLN	GLY	
33681	VAL	VAL	ASN	ASN	LEU	GLU	
	GLN	ARG	GLN	GLN	GLY	GLU	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228291	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 ($e^-/\text{\AA}^2$)	89.32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.024	Depositor
Minimum map value	-2.795	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.586	Depositor
Map size ($\text{\AA}$)	326.86078, 326.86078, 326.86078	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8511999, 0.8511999, 0.8511999	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: 88C, IHP

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	0.12	0/10141	0.34	0/13823

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10318	0	9648	87	0
2	A	36	0	6	4	0
3	A	39	0	0	0	0
All	All	10393	0	9654	87	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 4.

All (87) 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:2293:PRO:HB3	1:A:2377:GLN:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:LEU:HD22	1:A:1364:VAL:HG22	1.77	0.67
1:A:2372:PRO:HD2	1:A:3644:ALA:HB2	1.77	0.66
1:A:963:GLN:O	1:A:979:ARG:NH2	2.28	0.65
1:A:2193:TYR:OH	1:A:2353:ILE:O	2.15	0.64
1:A:1530:LYS:NZ	2:A:3701:IHP:O25	2.31	0.63
1:A:2211:ALA:HB1	1:A:2342:LEU:HB3	1.81	0.63
1:A:2160:LEU:HD12	1:A:2203:GLY:HA3	1.81	0.62
1:A:2344:ASP:O	1:A:2348:GLY:N	2.33	0.62
1:A:1571:LEU:HD12	1:A:1572:PRO:HD2	1.83	0.61
1:A:3623:ARG:HB3	1:A:3627:PRO:HA	1.83	0.61
1:A:991:GLU:OE1	1:A:1049:ARG:NH2	2.30	0.60
1:A:1401:MET:O	1:A:1405:GLN:HG2	2.03	0.59
1:A:2254:TYR:HA	1:A:2257:ILE:HG22	1.83	0.58
1:A:1834:GLU:HB3	1:A:1837:VAL:HB	1.85	0.57
1:A:1200:TRP:CG	1:A:1235:SER:HG	2.22	0.57
1:A:845:LEU:O	1:A:849:MET:HG3	2.05	0.56
1:A:3658:THR:HG22	1:A:3661:VAL:HG12	1.87	0.56
1:A:1625:TRP:HD1	1:A:1628:ARG:HH21	1.54	0.56
1:A:804:VAL:HG21	1:A:837:GLU:HB3	1.89	0.55
1:A:2186:PRO:HB2	1:A:2319:ARG:HD2	1.89	0.54
1:A:1120:LYS:HE3	1:A:1148:THR:HG22	1.90	0.54
1:A:2257:ILE:HD12	1:A:2283:VAL:HG21	1.90	0.53
1:A:2344:ASP:O	1:A:2348:GLY:CA	2.58	0.52
1:A:1133:THR:HG21	1:A:1213:LEU:HD11	1.91	0.52
1:A:876:ARG:HH12	1:A:886:LEU:HD13	1.75	0.52
1:A:1525:ILE:HG21	1:A:1608:SER:HB2	1.92	0.52
1:A:1206:TRP:CZ2	1:A:1210:ILE:HD11	2.44	0.51
1:A:1324:LEU:HD13	1:A:1361:GLU:HA	1.92	0.51
1:A:1044:PRO:HB2	1:A:1083:LEU:HG	1.92	0.51
1:A:1325:LYS:NZ	1:A:1361:GLU:OE2	2.43	0.51
1:A:1054:LEU:HG	1:A:1058:MET:HE3	1.93	0.51
1:A:1026:TRP:HE3	1:A:1027:LEU:HD22	1.76	0.51
1:A:2169:PHE:CE1	1:A:2331:ILE:HD11	2.46	0.51
1:A:1106:TRP:O	1:A:1109:SER:OG	2.17	0.50
1:A:1816:THR:HB	1:A:1848:VAL:HG22	1.94	0.49
1:A:1617:LYS:NZ	2:A:3701:IHP:O43	2.42	0.49
1:A:2137:PRO:HB3	1:A:2155:LYS:HD3	1.95	0.49
1:A:1484:ASP:O	1:A:1488:THR:HG23	2.13	0.48
1:A:1017:TYR:O	1:A:1020:ARG:NH1	2.42	0.48
1:A:1375:ILE:HG22	1:A:1377:LEU:H	1.79	0.48
1:A:1031:ARG:O	1:A:1035:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1489:LYS:NZ	2:A:3701:IHP:O21	2.47	0.47
1:A:2358:CYS:SG	1:A:2359:PHE:N	2.88	0.47
1:A:2372:PRO:HG2	1:A:3640:VAL:HG13	1.95	0.47
1:A:807:VAL:HG22	1:A:909:ASP:HB2	1.96	0.47
1:A:1849:ALA:HB2	1:A:1856:ILE:HD11	1.97	0.47
1:A:2193:TYR:HE1	1:A:2353:ILE:HA	1.79	0.46
1:A:773:VAL:HG13	1:A:813:ILE:HD11	1.96	0.46
1:A:1360:LEU:HA	1:A:1363:THR:HG22	1.97	0.46
1:A:2195:VAL:HG12	1:A:2205:ILE:HG12	1.97	0.46
1:A:2353:ILE:HG13	1:A:2354:ASP:H	1.81	0.46
1:A:1184:ASN:OD1	1:A:1188:ASN:ND2	2.49	0.45
1:A:943:ILE:HG21	1:A:987:LEU:HD21	1.97	0.45
1:A:2344:ASP:O	1:A:2348:GLY:HA2	2.15	0.45
1:A:1489:LYS:NZ	2:A:3701:IHP:O22	2.39	0.45
1:A:1844:LEU:O	1:A:1848:VAL:HG23	2.16	0.45
1:A:975:ASN:O	1:A:979:ARG:HG3	2.17	0.45
1:A:2336:ARG:NH1	1:A:2340:ASN:HB3	2.31	0.45
1:A:807:VAL:HG13	1:A:807:VAL:O	2.17	0.45
1:A:839:GLN:O	1:A:843:LEU:HG	2.17	0.44
1:A:1831:ASN:C	1:A:1831:ASN:HD22	2.25	0.44
1:A:1368:LEU:HD13	1:A:1407:LEU:HD13	2.00	0.44
1:A:1864:THR:HG21	1:A:1934:VAL:HG21	2.00	0.44
1:A:1517:ALA:HB1	1:A:1521:VAL:HG23	2.00	0.44
1:A:2132:PRO:HA	1:A:2136:LYS:NZ	2.32	0.43
1:A:2195:VAL:HG12	1:A:2205:ILE:HG23	1.99	0.43
1:A:2157:LEU:HA	1:A:2201:ARG:HB3	2.01	0.43
1:A:1445:LEU:HD23	1:A:1487:LYS:HG2	2.01	0.43
1:A:1823:ILE:HG21	1:A:1856:ILE:HG22	2.01	0.42
1:A:1754:PHE:O	1:A:1758:ASN:ND2	2.48	0.42
1:A:1590:VAL:O	1:A:1594:VAL:HB	2.20	0.42
1:A:887:PHE:O	1:A:891:GLN:HG2	2.20	0.41
1:A:1592:ILE:O	1:A:1592:ILE:HG13	2.20	0.41
1:A:1360:LEU:O	1:A:1364:VAL:HG23	2.19	0.41
1:A:1834:GLU:O	1:A:1838:ARG:NE	2.52	0.41
1:A:2132:PRO:HA	1:A:2136:LYS:HZ3	1.85	0.41
1:A:1027:LEU:HB3	1:A:1031:ARG:HH21	1.85	0.41
1:A:1811:LEU:HD12	1:A:1844:LEU:HD22	2.02	0.41
1:A:2151:PRO:HG2	1:A:2207:TRP:HB3	2.01	0.41
1:A:1257:ILE:H	1:A:1257:ILE:HD12	1.85	0.41
1:A:1293:LEU:HD22	1:A:1360:LEU:HD12	2.02	0.41
1:A:1863:GLY:HA3	1:A:1930:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1810:GLY:O	1:A:1814:THR:HG23	2.20	0.40
1:A:2177:PHE:O	1:A:2181:ASN:ND2	2.55	0.40
1:A:2186:PRO:HG2	1:A:2319:ARG:NH1	2.36	0.40
1:A:2418:VAL:HG22	1:A:3609:ALA:HB1	2.03	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	1298/2896 (45%)	1261 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	964/2393 (40%)	963 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1831	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	839	GLN
1	A	914	GLN
1	A	973	HIS
1	A	1019	ASN
1	A	1043	GLN
1	A	1204	GLN
1	A	1344	GLN
1	A	1542	GLN
1	A	1825	GLN
1	A	2168	GLN
1	A	2183	GLN
1	A	2206	GLN
1	A	2278	HIS
1	A	2315	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
3	88C	A	3702	-	42,42,42	1.39	6 (14%)	57,59,59	1.97	13 (22%)
2	IHP	A	3701	-	36,36,36	1.58	6 (16%)	60,60,60	0.94	3 (5%)

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	88C	A	3702	-	-	3/34/34/34	0/4/4/4
2	IHP	A	3701	-	-	5/30/54/54	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3701	IHP	P5-O15	3.60	1.65	1.59
2	A	3701	IHP	P3-O13	3.49	1.65	1.59
2	A	3701	IHP	P4-O14	3.41	1.65	1.59
3	A	3702	88C	C28-N27	3.32	1.44	1.37
2	A	3701	IHP	P2-O12	3.26	1.65	1.59
2	A	3701	IHP	P6-O16	3.25	1.65	1.59
2	A	3701	IHP	P1-O11	3.22	1.65	1.59
3	A	3702	88C	C13-N14	3.18	1.39	1.34
3	A	3702	88C	S06-N03	3.06	1.67	1.63
3	A	3702	88C	C28-N30	2.84	1.42	1.35
3	A	3702	88C	C13-N12	2.72	1.42	1.36
3	A	3702	88C	C26-N27	2.47	1.46	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3702	88C	C37-C38-C09	6.54	124.30	120.04
3	A	3702	88C	C10-C09-S06	5.45	124.28	117.53
3	A	3702	88C	C10-C09-C38	-5.27	112.81	118.33
3	A	3702	88C	N27-C28-N30	4.58	120.66	114.68
3	A	3702	88C	C32-C26-C25	-3.12	114.90	119.04
3	A	3702	88C	C16-C17-C18	-2.99	116.43	121.97
3	A	3702	88C	C18-C17-N35	2.80	120.09	116.04
3	A	3702	88C	O08-S06-O07	-2.76	115.28	119.59
2	A	3701	IHP	C5-C6-C1	2.59	116.11	110.43
3	A	3702	88C	C36-C11-C10	-2.35	116.81	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3701	IHP	O13-C3-C4	2.29	113.62	108.76
3	A	3702	88C	C09-S06-N03	2.21	110.79	106.69
3	A	3702	88C	N14-C13-N35	-2.17	124.32	126.42
3	A	3702	88C	C09-C38-CL39	-2.09	120.01	121.52
2	A	3701	IHP	C6-C1-C2	2.06	114.96	110.43
3	A	3702	88C	C33-C32-C26	2.01	122.61	120.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

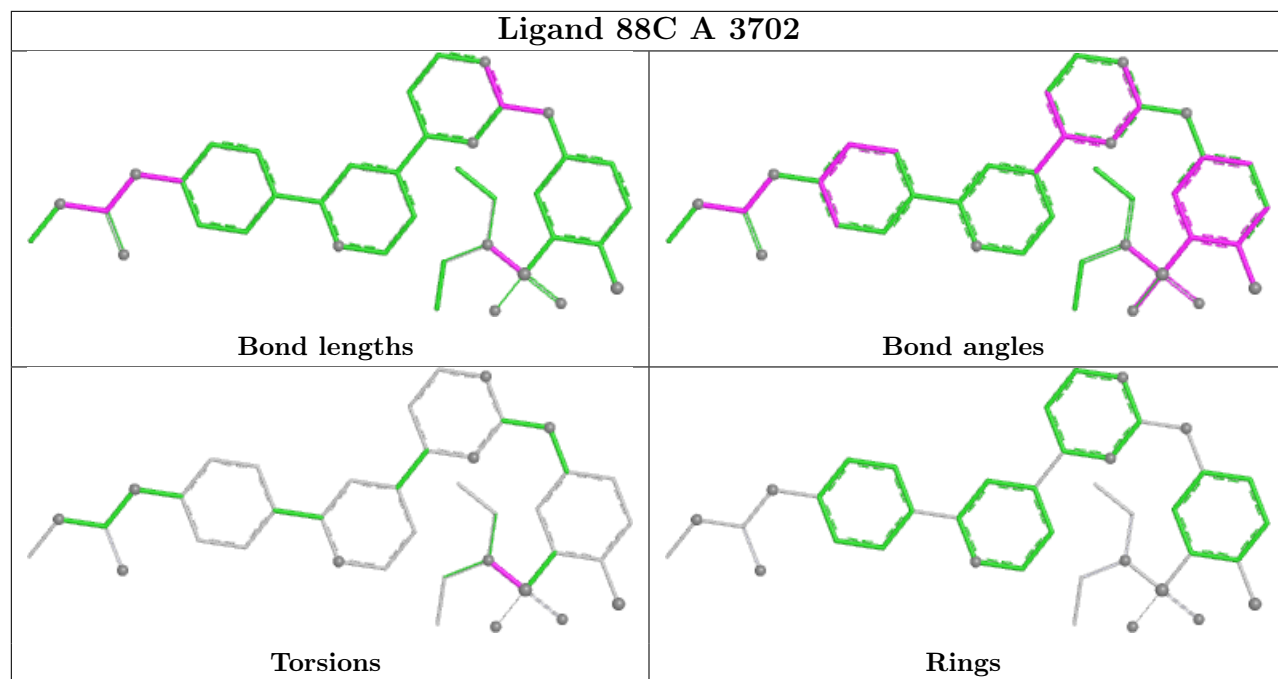
Mol	Chain	Res	Type	Atoms
2	A	3701	IHP	C4-C3-O13-P3
2	A	3701	IHP	C6-C5-O15-P5
3	A	3702	88C	C04-N03-S06-O08
2	A	3701	IHP	C2-C3-O13-P3
3	A	3702	88C	C04-N03-S06-C09
3	A	3702	88C	C04-N03-S06-O07
2	A	3701	IHP	C3-O13-P3-O33
2	A	3701	IHP	C4-O14-P4-O24

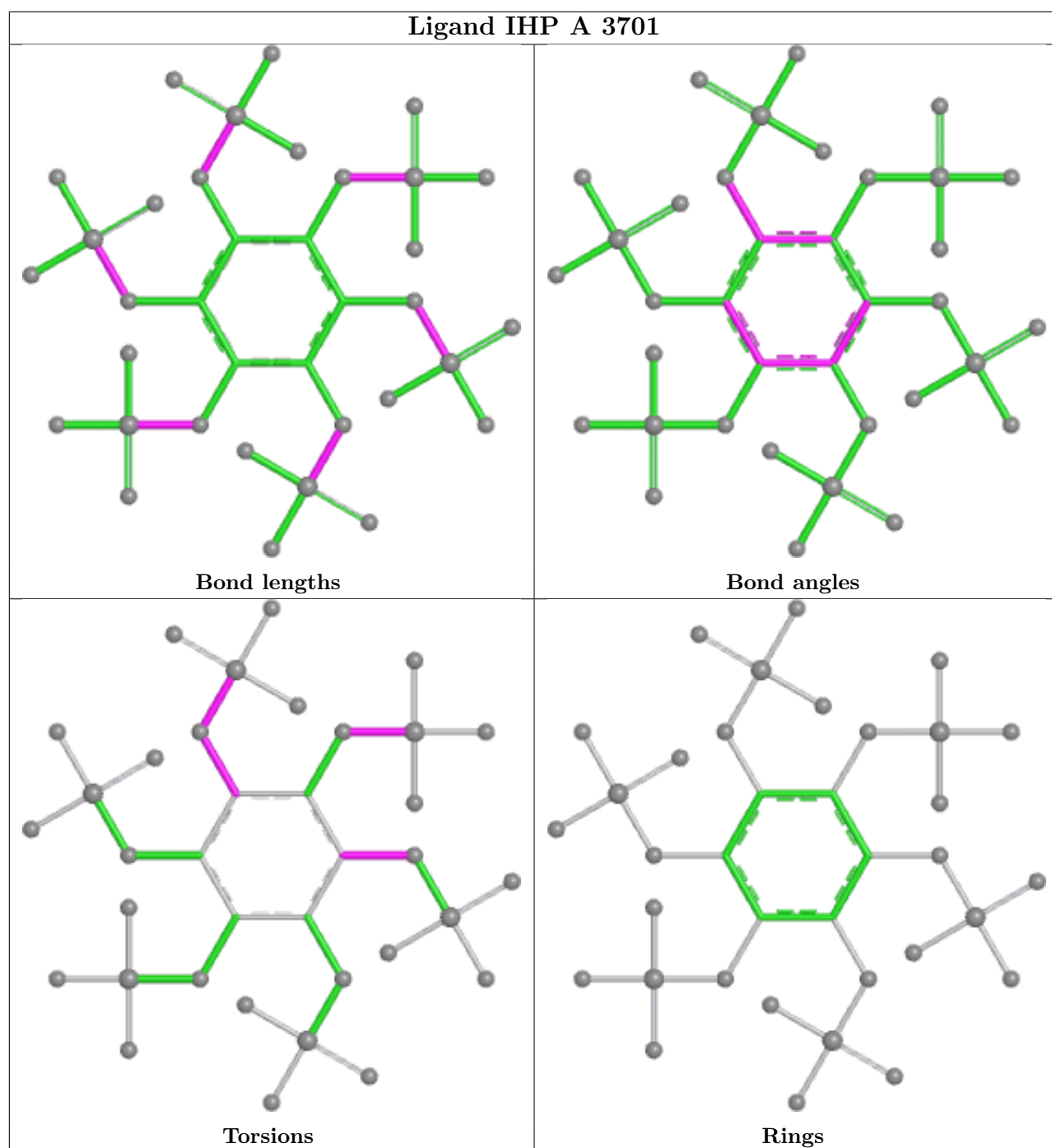
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3701	IHP	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.

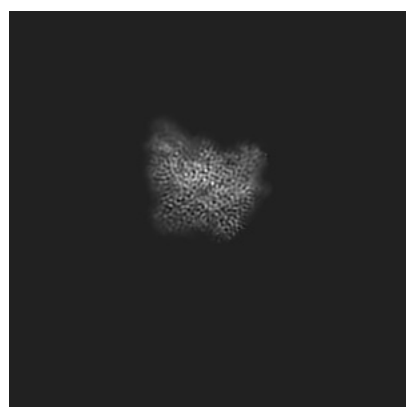
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13676. These allow visual inspection of the internal detail of the map and identification of artifacts.

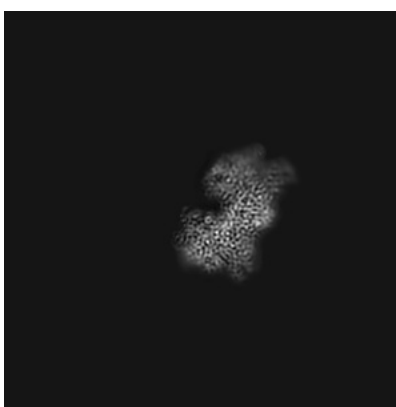
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

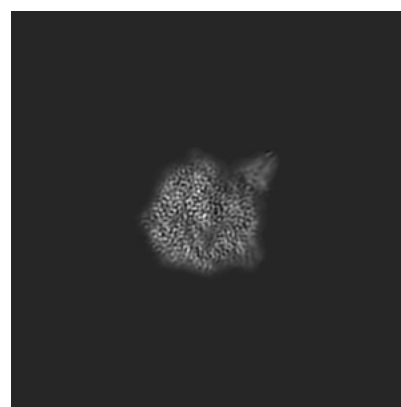
6.1.1 Primary map



X



Y

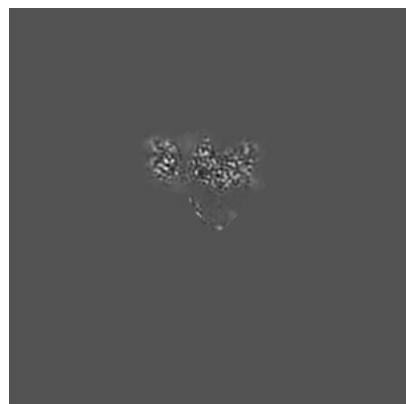


Z

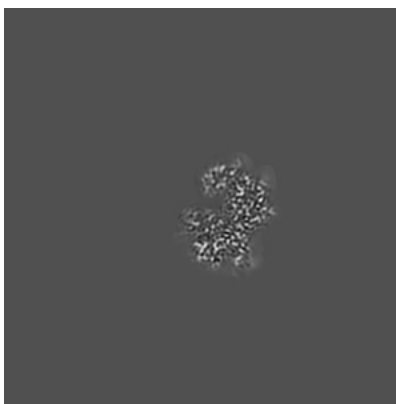
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

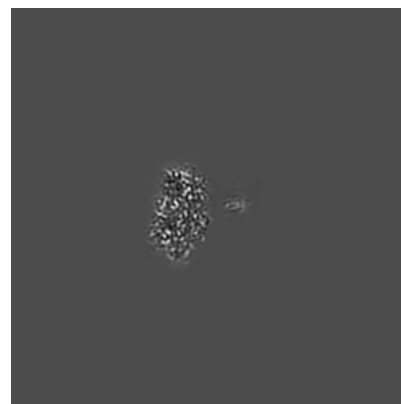
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices [i](#)

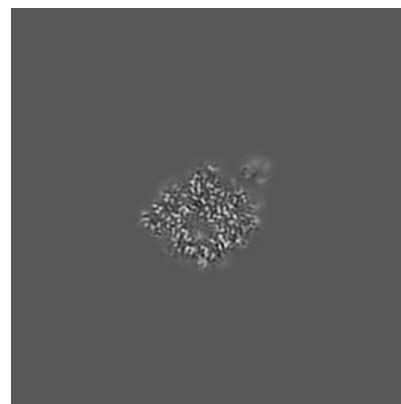
6.3.1 Primary map



X Index: 176



Y Index: 200

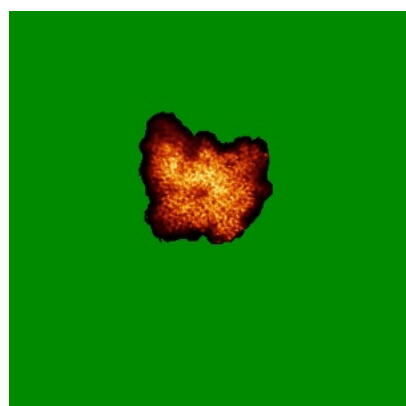


Z Index: 225

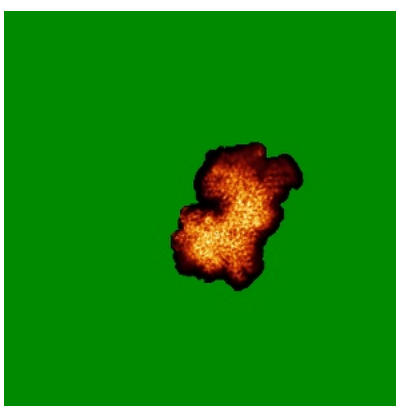
The images above show the largest variance slices of the map in three orthogonal directions.

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

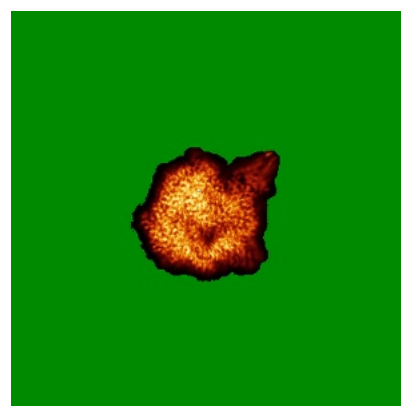
6.4.1 Primary map



X



Y

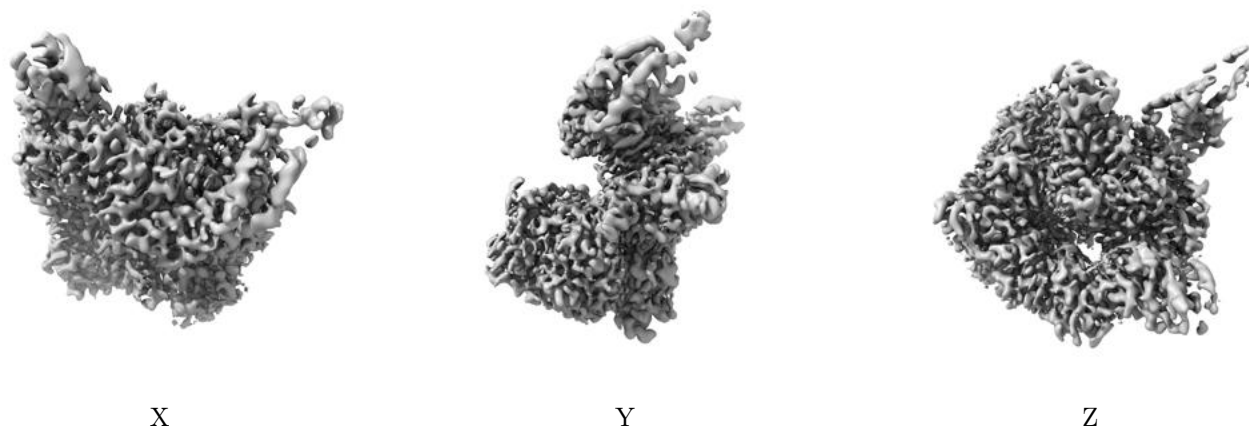


Z

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 0.586. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

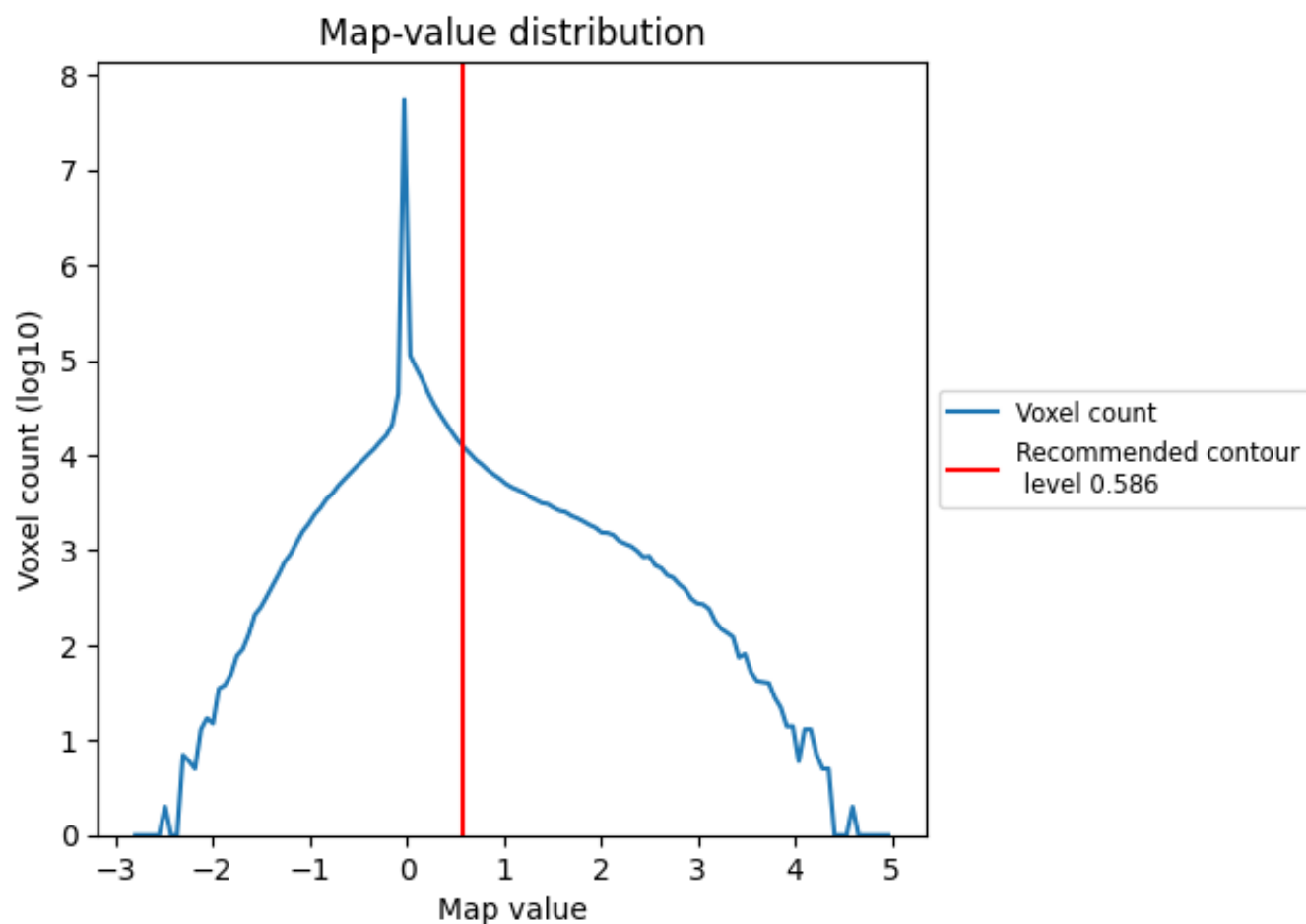
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

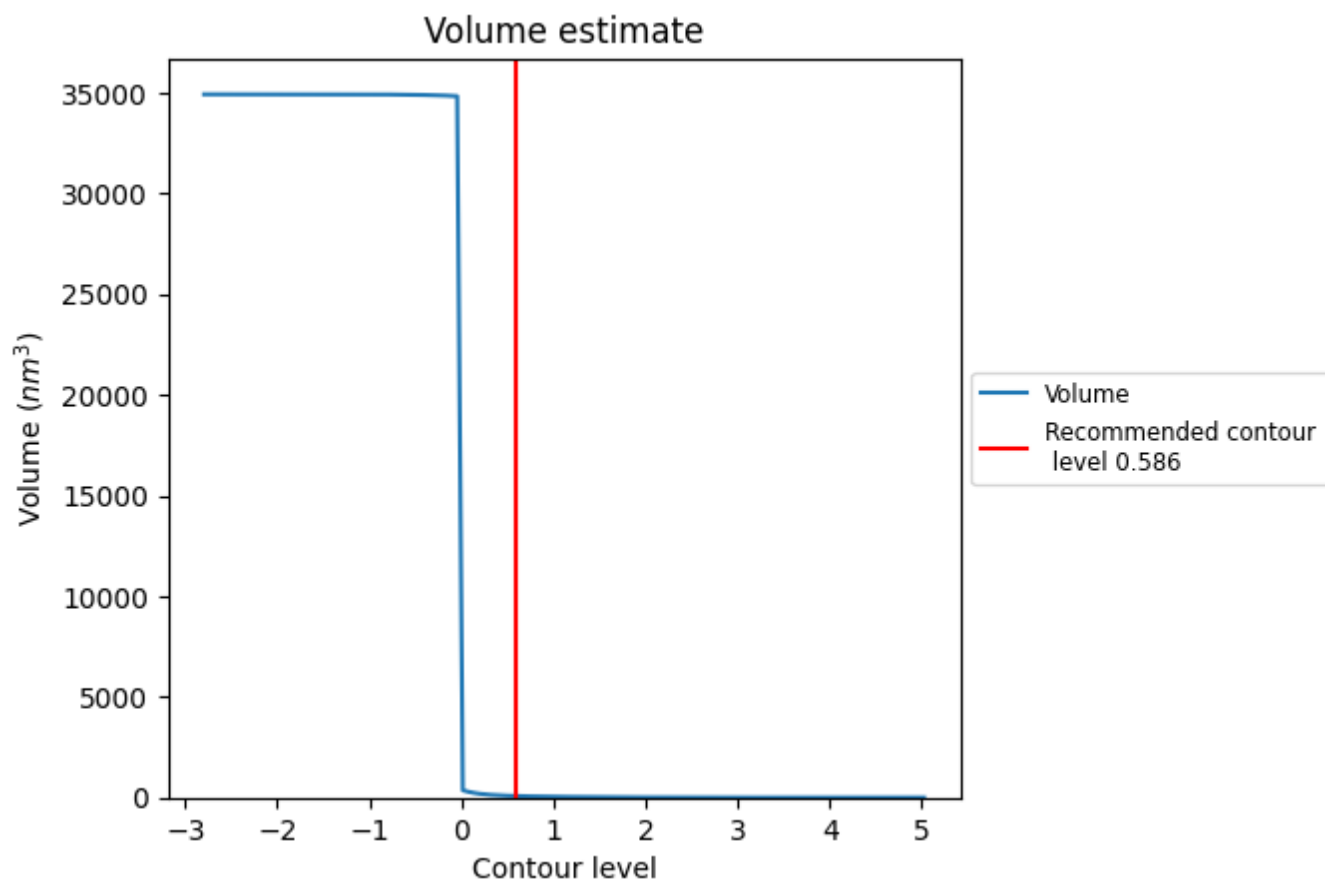
This section contains the results of statistical analysis of the map.

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.

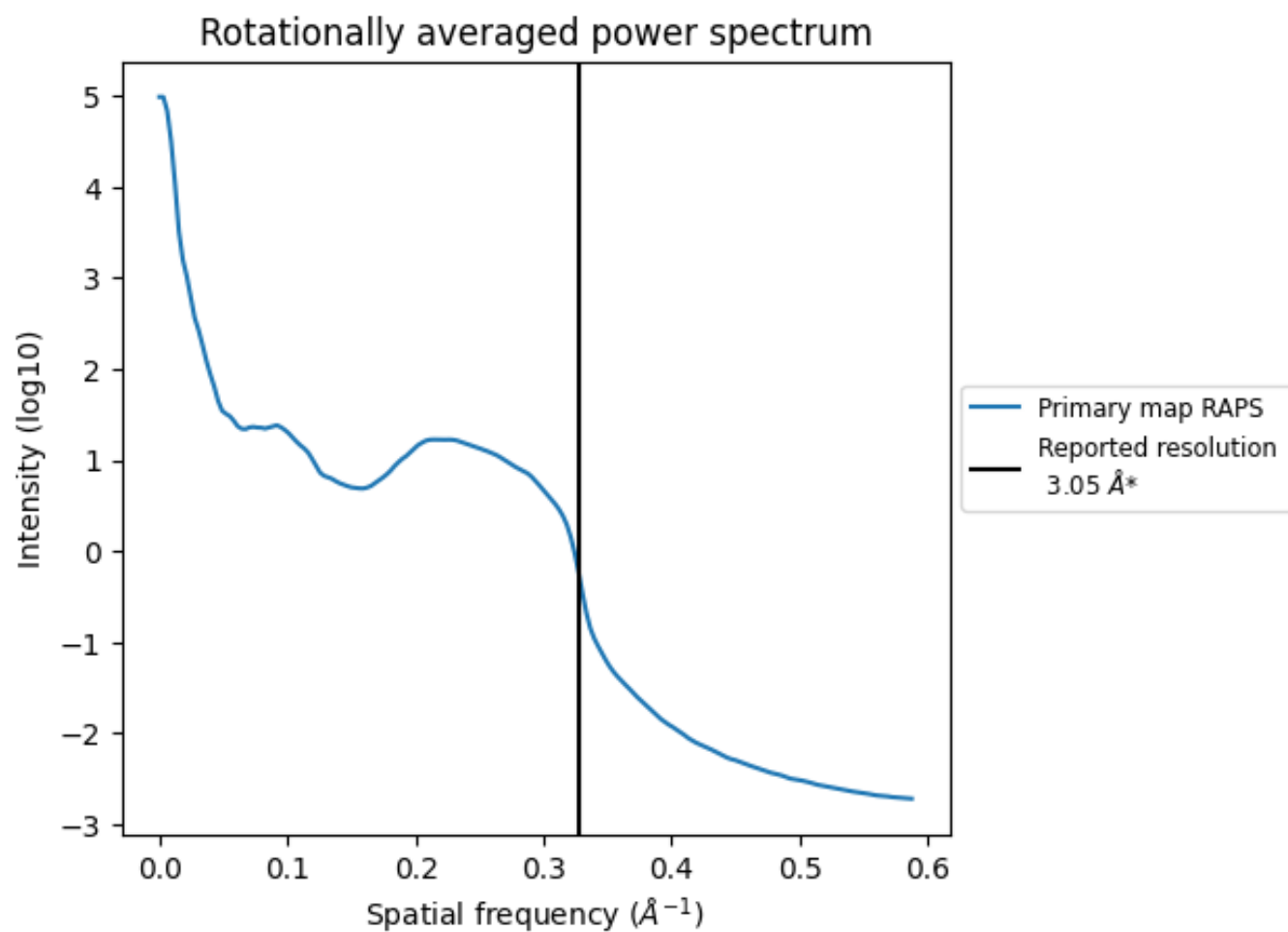
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm^3 ; this corresponds to an approximate mass of 69 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 0.328 Å⁻¹

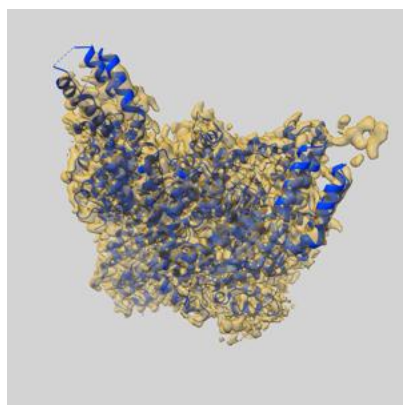
8 Fourier-Shell correlation

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

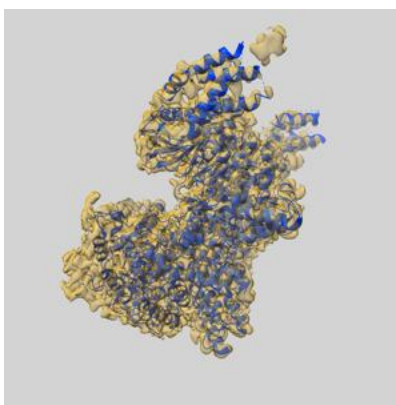
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13676 and PDB model 7PW6. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

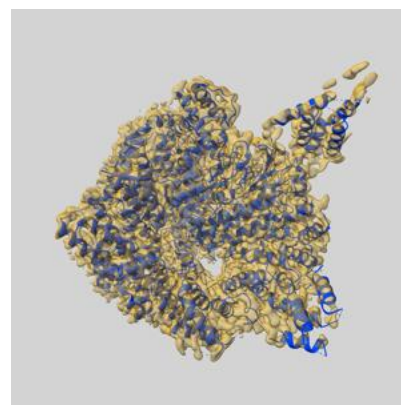
9.1 Map-model overlay [i](#)



X



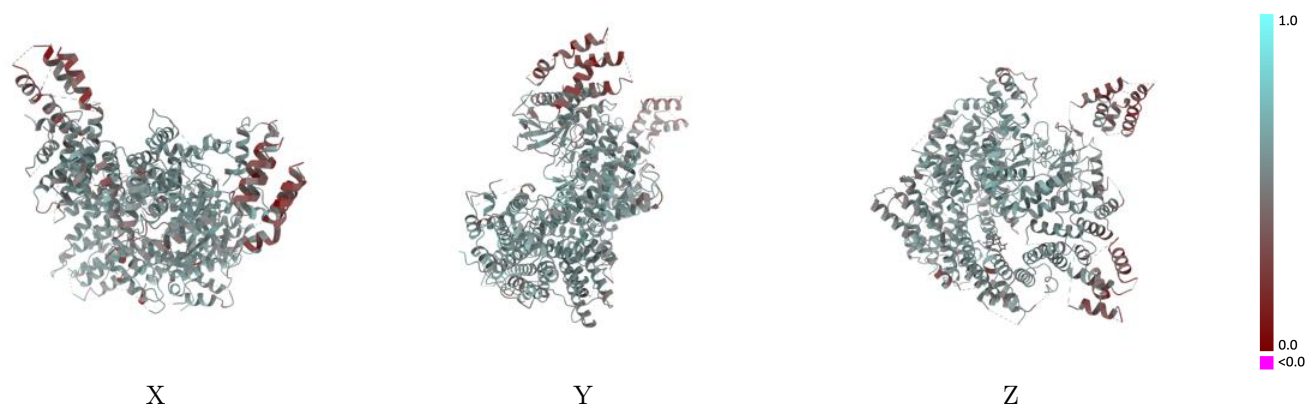
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.586 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](#)



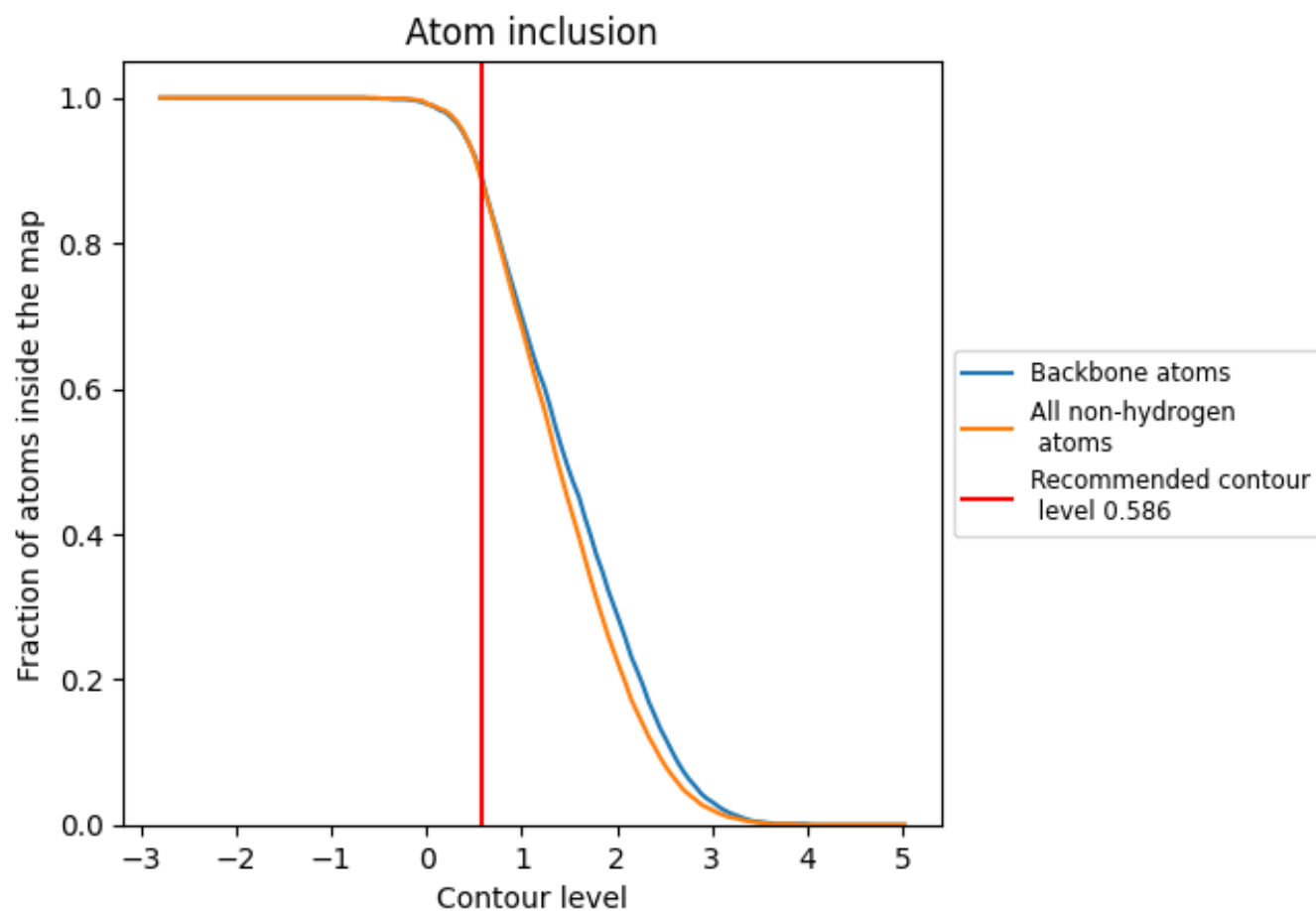
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.586).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.586) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.5390
A	0.8840	0.5390

