



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:27 AM UTC

PDB ID : 9CAF / pdb_00009caf
EMDB ID : EMD-45389
Title : Cryo-EM structure of the reconstituted TRRAP lobe of the human TIP60 complex (composite structure)
Authors : Louder, R.K.; Park, G.; Patel, A.B.
Deposited on : 2024-06-17
Resolution : 2.35 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

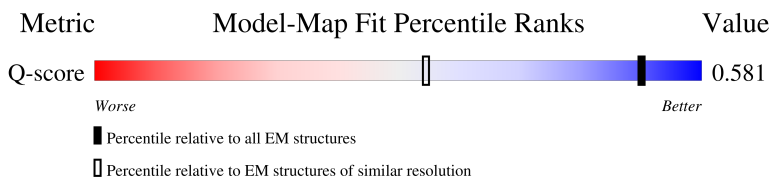
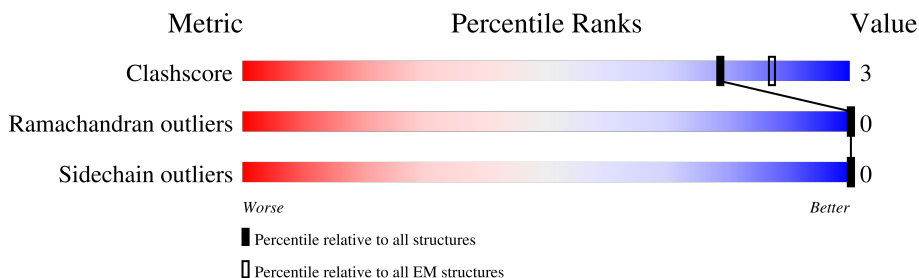
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 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	4607 (1.85 - 2.85)

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	1122	 13% 86%
2	D	3811	 6% 86% 8% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29921 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 E1A-binding protein p400,Haloalkane dehalogenase chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	154	Total	C	N	O	S	0	0
			1235	779	222	230	4		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2132	PRO	-	linker	UNP Q96L91
A	2133	GLY	-	linker	UNP Q96L91
A	2364	ASP	-	insertion	UNP Q96L91
A	?	-	GLY	deletion	UNP Q96L91
A	2443	LEU	-	insertion	UNP Q96L91
A	?	-	SER	deletion	UNP Q96L91
A	2492	PRO	-	insertion	UNP Q96L91
A	2531	ASP	-	linker	UNP Q96L91
A	2532	GLY	-	linker	UNP Q96L91
A	2533	SER	-	linker	UNP Q96L91
A	2534	GLY	-	linker	UNP Q96L91
A	2535	GLY	-	linker	UNP Q96L91
A	2536	SER	-	linker	UNP Q96L91
A	2537	GLY	-	linker	UNP Q96L91
A	2538	GLU	-	linker	UNP Q96L91
A	2539	ASP	-	linker	UNP Q96L91
A	2540	LEU	-	linker	UNP Q96L91
A	2541	TYR	-	linker	UNP Q96L91
A	2542	PHE	-	linker	UNP Q96L91
A	2543	GLN	-	linker	UNP Q96L91
A	2544	SER	-	linker	UNP Q96L91
A	2545	GLY	-	linker	UNP Q96L91
A	2546	GLY	-	linker	UNP Q96L91
A	2547	SER	-	linker	UNP Q96L91
A	2548	MET	-	linker	UNP Q96L91
A	2549	ALA	-	linker	UNP Q96L91
A	2594	VAL	LEU	conflict	UNP P0A3G4
A	2605	THR	SER	conflict	UNP P0A3G4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2625	GLY	ASP	conflict	UNP P0A3G4
A	2634	PHE	TYR	conflict	UNP P0A3G4
A	2635	MET	LEU	conflict	UNP P0A3G4
A	2675	PHE	CYS	conflict	UNP P0A3G4
A	2702	THR	ALA	conflict	UNP P0A3G4
A	2707	LYS	GLU	conflict	UNP P0A3G4
A	2714	VAL	ALA	conflict	UNP P0A3G4
A	2719	THR	ALA	conflict	UNP P0A3G4
A	2722	MET	LYS	conflict	UNP P0A3G4
A	2723	GLY	CYS	conflict	UNP P0A3G4
A	2742	ASN	LYS	conflict	UNP P0A3G4
A	2771	GLU	ALA	conflict	UNP P0A3G4
A	2774	ASP	ASN	conflict	UNP P0A3G4
A	2804	LYS	GLU	conflict	UNP P0A3G4
A	2811	ALA	THR	conflict	UNP P0A3G4
A	2819	ASN	HIS	conflict	UNP P0A3G4
A	2820	LEU	TYR	conflict	UNP P0A3G4
A	2838	SER	-	expression tag	UNP P0A3G4
A	2839	THR	-	expression tag	UNP P0A3G4
A	2840	LEU	-	expression tag	UNP P0A3G4
A	2841	GLU	-	expression tag	UNP P0A3G4
A	2842	ILE	-	expression tag	UNP P0A3G4
A	2843	SER	-	expression tag	UNP P0A3G4
A	2844	GLY	-	expression tag	UNP P0A3G4
A	2845	GLY	-	expression tag	UNP P0A3G4
A	2846	GLY	-	expression tag	UNP P0A3G4
A	2847	HIS	-	expression tag	UNP P0A3G4
A	2848	HIS	-	expression tag	UNP P0A3G4
A	2849	HIS	-	expression tag	UNP P0A3G4
A	2850	HIS	-	expression tag	UNP P0A3G4
A	2851	HIS	-	expression tag	UNP P0A3G4
A	2852	HIS	-	expression tag	UNP P0A3G4

- Molecule 2 is a protein called Isoform 2 of Transformation/transcription domain-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	3570	Total	C	N	O	S	0	0
			28650	18360	4952	5140	198		

There are 60 discrepancies between the modelled and reference sequences:

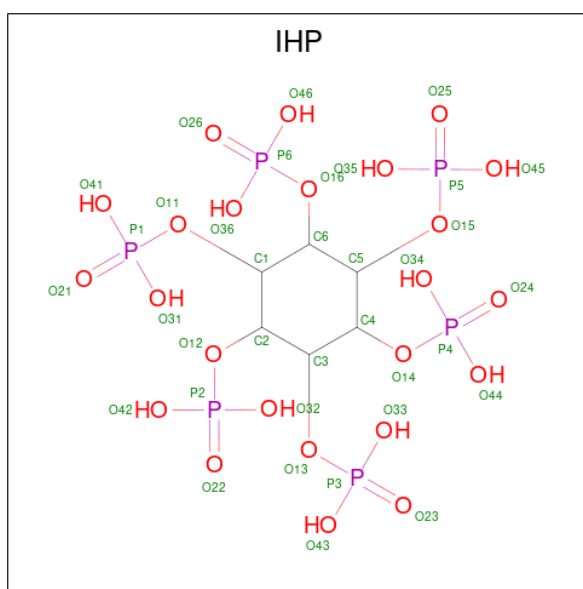
Chain	Residue	Modelled	Actual	Comment	Reference
D	521	SER	VAL	conflict	UNP Q9Y4A5
D	522	GLY	PRO	conflict	UNP Q9Y4A5
D	523	GLY	THR	conflict	UNP Q9Y4A5
D	524	GLY	ALA	conflict	UNP Q9Y4A5
D	525	ALA	PRO	conflict	UNP Q9Y4A5
D	526	SER	ALA	conflict	UNP Q9Y4A5
D	527	GLY	ALA	conflict	UNP Q9Y4A5
D	528	GLY	PRO	conflict	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	ALA	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	SER	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	ALA	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	VAL	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	ALA	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	ALA	deletion	UNP Q9Y4A5
D	?	-	THR	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	VAL	deletion	UNP Q9Y4A5
D	?	-	THR	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	ALA	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	VAL	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PRO	deletion	UNP Q9Y4A5
D	?	-	PHE	deletion	UNP Q9Y4A5
D	?	-	GLU	deletion	UNP Q9Y4A5
D	?	-	LYS	deletion	UNP Q9Y4A5
D	530	SER	GLN	conflict	UNP Q9Y4A5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2007N	GLY	-	insertion	UNP Q9Y4A5
D	2007O	ASP	-	insertion	UNP Q9Y4A5
D	2007P	TYR	-	insertion	UNP Q9Y4A5
D	2007Q	LYS	-	insertion	UNP Q9Y4A5
D	2007R	ASP	-	insertion	UNP Q9Y4A5
D	2007S	HIS	-	insertion	UNP Q9Y4A5
D	2007T	ASP	-	insertion	UNP Q9Y4A5
D	2007U	ILE	-	insertion	UNP Q9Y4A5
D	2007V	ASP	-	insertion	UNP Q9Y4A5
D	2007W	TYR	-	insertion	UNP Q9Y4A5
D	2007X	LYS	-	insertion	UNP Q9Y4A5
D	2007Y	ASP	-	insertion	UNP Q9Y4A5
D	2007Z	ASP	-	insertion	UNP Q9Y4A5
D	2008A	ASP	-	insertion	UNP Q9Y4A5
D	2008B	ASP	-	insertion	UNP Q9Y4A5
D	2008C	LYS	VAL	conflict	UNP Q9Y4A5
D	2008D	GLY	ASN	conflict	UNP Q9Y4A5

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

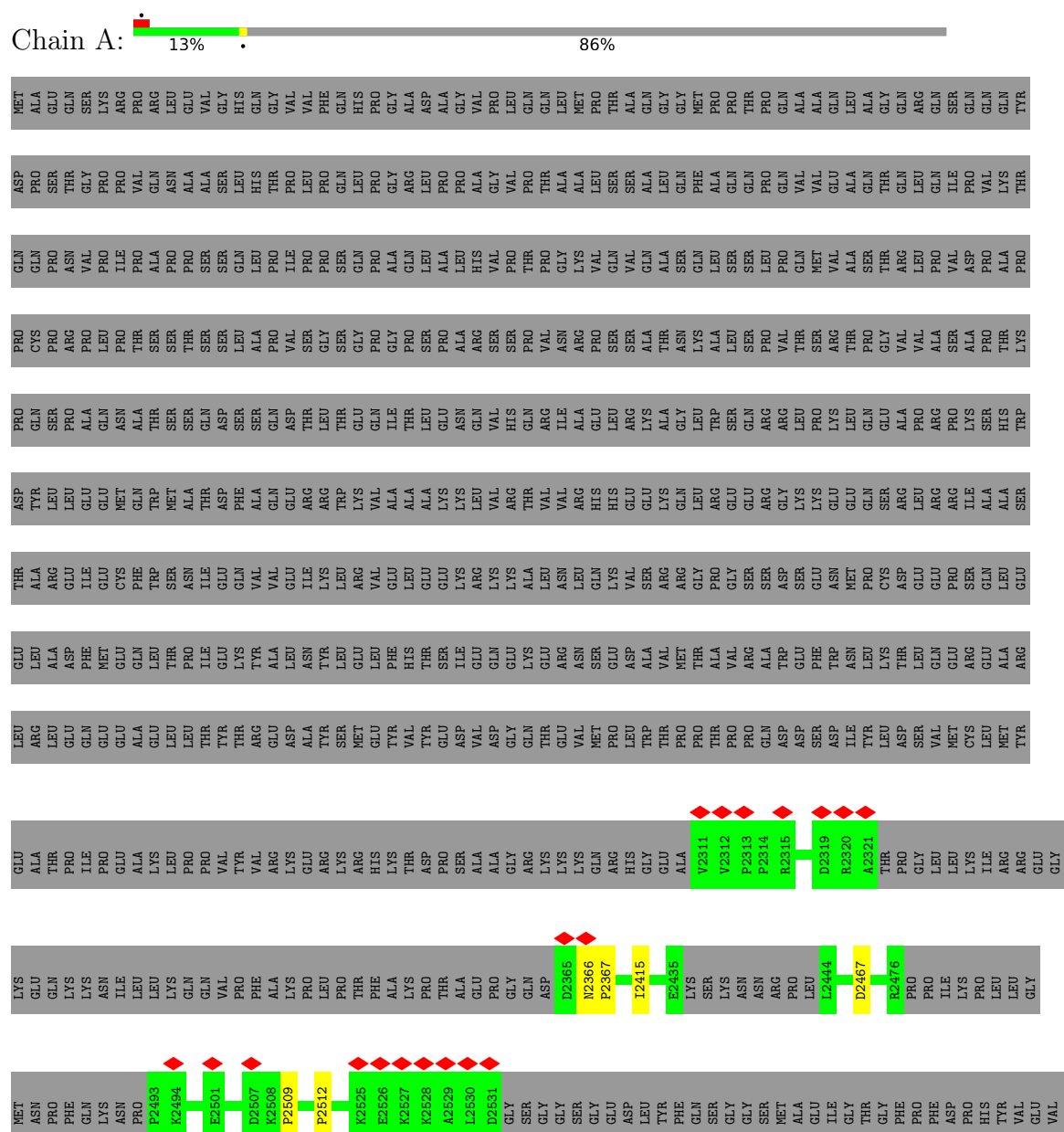


Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	O	P	0
			36	6	24	6	

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: E1A-binding protein p400,Haloalkane dehalogenase chimera







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141352	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.099	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	371.712, 371.712, 371.712	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.726, 0.726, 0.726	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: 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	0.14	0/1259	0.32	0/1707
2	D	0.16	0/29263	0.35	0/39628
All	All	0.16	0/30522	0.35	0/41335

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	1235	0	1242	5	0
2	D	28650	0	29217	167	0
3	D	36	0	6	1	0
All	All	29921	0	30465	169	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 3.

All (169) 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)
2:D:2868:MET:HE1	2:D:2921:GLN:HB3	1.59	0.85
2:D:3432:ILE:HG23	2:D:3436:CYS:HB2	1.64	0.77
2:D:2327:ASN:O	2:D:2331:ALA:HB3	1.86	0.75
2:D:2426:LEU:HD12	2:D:2467:ALA:HB3	1.70	0.72
2:D:361:ILE:HD13	2:D:372:ARG:HG2	1.73	0.70
2:D:1906:MET:HE2	2:D:1948:LEU:HD13	1.74	0.68
2:D:124:GLU:OE2	2:D:128:ASN:ND2	2.20	0.66
2:D:707:SER:OG	2:D:755:ASN:ND2	2.29	0.66
2:D:1145:LEU:HD13	2:D:1163:SER:HB3	1.81	0.62
2:D:2886:ILE:HG21	2:D:2929:ALA:HB2	1.83	0.61
2:D:918:GLU:HA	2:D:3628:HIS:NE2	2.17	0.60
2:D:935:LEU:HD22	2:D:2617:ARG:HB3	1.84	0.59
2:D:3703:THR:HG22	2:D:3704:PRO:HD2	1.85	0.59
2:D:1859:PRO:HB2	2:D:1898:ALA:HB2	1.84	0.58
2:D:2279:LEU:HA	2:D:2282:MET:HE3	1.86	0.58
2:D:1126:LEU:HD12	2:D:1132:ALA:HA	1.87	0.57
2:D:3054:VAL:HG13	2:D:3099:PHE:HE2	1.69	0.57
2:D:818:SER:HA	2:D:821:LEU:HD23	1.86	0.57
2:D:861:LEU:O	2:D:865:ILE:HG23	2.03	0.57
2:D:148:THR:H	2:D:151:ILE:HD12	1.70	0.56
2:D:357:GLU:HG3	2:D:361:ILE:HD12	1.86	0.56
2:D:2283:VAL:HG21	2:D:2332:ILE:HG23	1.89	0.55
2:D:1430:LEU:HD11	2:D:1444:VAL:HG13	1.86	0.55
2:D:967:ILE:HD13	2:D:1024:GLY:HA3	1.89	0.54
2:D:629:LYS:NZ	2:D:633:GLU:OE2	2.33	0.54
2:D:3054:VAL:HG13	2:D:3099:PHE:CE2	2.42	0.54
2:D:3178:SER:OG	2:D:3746:ARG:NH1	2.40	0.54
2:D:1168:MET:O	2:D:1216:ARG:NH1	2.38	0.54
2:D:3025:VAL:HG11	2:D:3060:LEU:HG	1.90	0.54
2:D:2491:ILE:HD11	2:D:2592:LEU:HD13	1.89	0.54
1:A:2367:PRO:HG2	1:A:2415:ILE:HG21	1.89	0.53
2:D:1872:ILE:HG22	2:D:1878:ILE:HD11	1.90	0.53
2:D:1646:VAL:HG21	2:D:1685:TYR:CD1	2.42	0.53
1:A:2366:ASN:HB2	1:A:2367:PRO:HD3	1.91	0.53
2:D:1940:PRO:HA	2:D:1943:VAL:HG22	1.91	0.53
2:D:2840:ARG:HB3	2:D:2975:MET:SD	2.49	0.53
2:D:261:GLN:OE1	2:D:319:ASN:ND2	2.41	0.53
2:D:254:ILE:HG21	2:D:291:LEU:HB2	1.91	0.52
2:D:3693:ASP:OD1	2:D:3694:ALA:N	2.36	0.52
2:D:1662:HIS:CD2	2:D:1675:PRO:HD3	2.45	0.52
2:D:2838:ALA:HB3	2:D:2847:MET:HG2	1.92	0.52
2:D:639:PHE:HA	2:D:642:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2793:PRO:HA	2:D:2796:PHE:CD2	2.45	0.51
2:D:2445:ASP:OD2	2:D:2450:ARG:NH1	2.42	0.51
2:D:406:ILE:HD12	2:D:420:CYS:SG	2.50	0.51
2:D:1567:SER:O	2:D:1571:MET:HG2	2.11	0.51
2:D:593:VAL:HG12	2:D:597:MET:HE2	1.93	0.51
2:D:2401:ASP:OD1	2:D:2439:LYS:NZ	2.33	0.50
2:D:2251:PHE:O	2:D:2255:MET:HG2	2.11	0.50
2:D:1184:LEU:HD22	2:D:1241:VAL:HG13	1.92	0.50
2:D:2338:GLU:OE2	2:D:2384:TYR:OH	2.23	0.50
2:D:255:MET:HG3	2:D:305:TYR:HB3	1.94	0.50
2:D:2158:PHE:O	2:D:2161:THR:HG22	2.12	0.50
2:D:402:PHE:O	2:D:406:ILE:HG12	2.13	0.49
2:D:314:LEU:HD11	2:D:350:CYS:SG	2.51	0.49
2:D:66:ILE:HG21	2:D:109:HIS:HB3	1.94	0.49
2:D:2083:LEU:HD21	2:D:2111:LEU:HD23	1.94	0.49
2:D:1434:LEU:HD22	2:D:1448:LEU:HD11	1.95	0.49
2:D:2853:GLN:O	2:D:2856:VAL:HG22	2.13	0.49
2:D:3582:PRO:HB2	2:D:3829:TRP:CZ2	2.48	0.49
2:D:1946:LEU:HD13	2:D:1991:LEU:HD11	1.95	0.48
2:D:2868:MET:HE2	2:D:2872:TYR:CE1	2.47	0.48
2:D:3529:LYS:HD2	3:D:3901:IHP:O36	2.14	0.48
1:A:2467:ASP:OD1	2:D:2783:LYS:NZ	2.42	0.48
2:D:3381:ASP:HB3	2:D:3384:PHE:HB3	1.96	0.48
2:D:1619:ASP:O	2:D:1623:GLN:HG2	2.13	0.48
2:D:2441:PHE:CE1	2:D:2479:GLU:HG2	2.48	0.48
2:D:2638:LEU:HD11	2:D:2661:MET:HE1	1.96	0.48
2:D:3302:ASN:HD21	2:D:3426:LEU:HD13	1.79	0.48
2:D:1342:LEU:HD23	2:D:1369:ALA:HB2	1.97	0.47
2:D:2202:MET:HE1	2:D:2228:VAL:HG11	1.96	0.47
2:D:2449:LYS:HD2	2:D:2454:GLU:HG2	1.97	0.47
2:D:3251:GLN:HB2	2:D:3268:MET:HE1	1.95	0.47
2:D:62:LEU:HD22	2:D:66:ILE:HD11	1.96	0.47
2:D:3742:LYS:HG3	2:D:3786:VAL:HG21	1.96	0.47
2:D:254:ILE:HG23	2:D:287:THR:HG22	1.97	0.47
2:D:1732:ARG:HG3	2:D:1775:LEU:HD12	1.96	0.47
2:D:831:LEU:HD21	2:D:849:LEU:HD13	1.96	0.47
2:D:1571:MET:HE1	2:D:1627:ILE:HG13	1.97	0.46
2:D:1662:HIS:NE2	2:D:1675:PRO:HD3	2.30	0.46
2:D:862:TYR:O	2:D:865:ILE:HG12	2.16	0.46
2:D:2759:ALA:HB2	2:D:2774:SER:HB2	1.96	0.46
2:D:65:ILE:HG13	2:D:66:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1907:ALA:HA	2:D:1952:HIS:NE2	2.30	0.46
2:D:3657:LEU:O	2:D:3659:LEU:N	2.49	0.46
2:D:583:PRO:HB3	2:D:1531:GLU:HB2	1.99	0.45
2:D:3679:ALA:HA	2:D:3680:TYR:CG	2.51	0.45
2:D:1051:MET:HE1	2:D:2577:HIS:CG	2.51	0.45
2:D:1168:MET:HE1	2:D:1213:LEU:HB2	1.97	0.45
1:A:2509:PRO:HG3	2:D:3111:LYS:HG2	1.98	0.45
2:D:1427:MET:HE2	2:D:1451:VAL:HG21	1.98	0.45
2:D:2113:LYS:HA	2:D:2158:PHE:CZ	2.52	0.45
2:D:2637:PHE:O	2:D:2643:HIS:NE2	2.45	0.45
2:D:2978:GLN:NE2	2:D:3011:ALA:HB3	2.32	0.45
2:D:1409:MET:HG2	2:D:1454:LEU:HD13	1.99	0.44
2:D:224:VAL:O	2:D:228:LEU:HG	2.17	0.44
2:D:3202:TRP:CZ2	2:D:3224:LEU:HD11	2.53	0.44
2:D:455:LYS:HG3	2:D:553:LEU:HD11	2.00	0.44
2:D:3309:ARG:HG3	2:D:3482:THR:HG22	1.99	0.44
2:D:3098:MET:SD	2:D:3129:MET:HE2	2.58	0.44
2:D:3160:HIS:CE1	2:D:3162:ASN:HB3	2.52	0.44
2:D:690:VAL:CG1	2:D:717:VAL:HG11	2.48	0.43
2:D:1679:ALA:HB1	2:D:1714:LEU:HD11	1.99	0.43
2:D:1005:HIS:ND1	2:D:1143:GLU:OE1	2.34	0.43
2:D:1471:LEU:HB2	2:D:1499:ILE:HG21	2.00	0.43
2:D:974:MET:HB3	2:D:1018:PHE:CZ	2.52	0.43
2:D:2829:ILE:HG22	2:D:2831:PRO:HD3	1.99	0.43
2:D:3705:ASN:HB2	2:D:3830:LEU:O	2.18	0.43
2:D:2195:HIS:ND1	2:D:2259:SER:OG	2.52	0.43
2:D:2287:LEU:HD13	2:D:2339:LYS:HE3	2.01	0.43
2:D:3703:THR:HG22	2:D:3704:PRO:CD	2.48	0.43
2:D:1464:CYS:HB3	2:D:1513:LEU:HD11	1.99	0.43
2:D:2328:PHE:HA	2:D:2332:ILE:HD12	2.01	0.43
2:D:1227:ALA:HB3	2:D:1230:ILE:HG22	2.00	0.43
2:D:2692:LEU:HD12	2:D:2733:LEU:HD12	1.99	0.43
2:D:1515:LYS:HB3	2:D:1516:PRO:HD3	2.00	0.43
1:A:2512:PRO:HG2	2:D:3149:SER:HB3	2.01	0.43
2:D:386:VAL:HG12	2:D:390:LEU:HG	2.00	0.43
2:D:447:ARG:NH1	2:D:450:GLU:OE1	2.50	0.42
2:D:2441:PHE:CZ	2:D:2479:GLU:HG2	2.54	0.42
2:D:2615:PHE:HB3	2:D:2660:ALA:HB1	2.01	0.42
2:D:3811:ALA:HA	2:D:3814:ASN:ND2	2.33	0.42
2:D:3135:GLU:HG3	2:D:3176:LEU:HD21	2.02	0.42
2:D:1177:LEU:HD22	2:D:1234:GLN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2858:CYS:SG	2:D:2862:MET:HB3	2.59	0.42
2:D:686:ALA:O	2:D:690:VAL:HG22	2.19	0.42
2:D:724:PHE:HB2	2:D:728:ASN:ND2	2.34	0.42
2:D:1096:ILE:O	2:D:1100:MET:HG2	2.19	0.42
2:D:1107:LEU:O	2:D:1110:ILE:HG22	2.20	0.42
2:D:725:ALA:HB1	2:D:729:GLU:OE2	2.20	0.42
2:D:1931:ILE:HG12	2:D:1945:ILE:HD11	2.01	0.42
2:D:3230:ARG:HG2	2:D:3281:LEU:HD22	2.02	0.42
2:D:464:LEU:HD21	2:D:602:ILE:HB	2.00	0.42
2:D:862:TYR:HA	2:D:865:ILE:HG12	2.02	0.41
2:D:336:LYS:O	2:D:340:THR:HG23	2.20	0.41
2:D:460:ALA:HA	2:D:464:LEU:HD12	2.02	0.41
2:D:2923:ILE:HG13	2:D:2924:GLU:N	2.34	0.41
2:D:3572:CYS:O	2:D:3576:GLY:N	2.54	0.41
2:D:61:PHE:O	2:D:65:ILE:HG12	2.19	0.41
2:D:229:PRO:HB3	2:D:290:PHE:HB2	2.02	0.41
2:D:284:GLN:HB3	2:D:316:LEU:HD21	2.03	0.41
2:D:981:LYS:HB3	2:D:981:LYS:HE2	1.96	0.41
2:D:1138:PHE:CE1	2:D:1171:LEU:HD21	2.55	0.41
2:D:1702:ALA:HA	2:D:1707:PHE:HE2	1.85	0.41
2:D:651:PHE:HA	2:D:654:THR:OG1	2.20	0.41
2:D:1015:ARG:NH1	2:D:1088:ASP:OD1	2.54	0.41
2:D:1015:ARG:NH2	2:D:1094:ASP:OD2	2.54	0.41
2:D:348:ILE:HG12	2:D:386:VAL:HG13	2.02	0.41
2:D:464:LEU:HD11	2:D:599:ALA:HA	2.03	0.41
2:D:804:ASP:HA	2:D:841:LEU:HD11	2.03	0.41
2:D:1420:VAL:HA	2:D:1423:ILE:HD12	2.03	0.41
2:D:1571:MET:HG3	2:D:1626:LYS:HE3	2.02	0.41
2:D:2134:LEU:O	2:D:2137:THR:OG1	2.36	0.41
2:D:3199:PRO:HG3	2:D:3231:VAL:HG21	2.02	0.41
2:D:3387:LEU:HD21	2:D:3422:LYS:HE3	2.03	0.41
2:D:1939:VAL:N	2:D:1940:PRO:HD2	2.36	0.41
2:D:1702:ALA:HA	2:D:1707:PHE:CE2	2.56	0.40
2:D:3289:LEU:O	2:D:3293:VAL:HG23	2.21	0.40
2:D:3531:LYS:HG2	2:D:3532:GLU:H	1.86	0.40
2:D:721:VAL:HG21	2:D:732:LEU:HD22	2.03	0.40
2:D:2158:PHE:O	2:D:2162:VAL:HG23	2.21	0.40
2:D:2756:THR:OG1	2:D:2802:TRP:NE1	2.49	0.40
2:D:2908:VAL:HA	2:D:2912:HIS:CE1	2.56	0.40
2:D:3054:VAL:HG11	2:D:3095:LEU:HD13	2.03	0.40
2:D:636:ALA:HB2	2:D:671:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2202:MET:SD	2:D:2260:ALA:HA	2.61	0.40
2:D:2956:TRP:O	2:D:2977:ARG:NH1	2.55	0.40
2:D:3606:ARG:NH1	2:D:3817:ASP:OD1	2.55	0.40
2:D:3648:ALA:HB2	2:D:3719:LEU:HD12	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	146/1122 (13%)	145 (99%)	1 (1%)	0	100	100
2	D	3544/3811 (93%)	3488 (98%)	56 (2%)	0	100	100
All	All	3690/4933 (75%)	3633 (98%)	57 (2%)	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	138/974 (14%)	138 (100%)	0	100	100
2	D	3187/3377 (94%)	3187 (100%)	0	100	100
All	All	3325/4351 (76%)	3325 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2455	ASN
1	A	2465	HIS
2	D	57	GLN
2	D	98	HIS
2	D	140	HIS
2	D	212	HIS
2	D	307	GLN
2	D	346	GLN
2	D	457	HIS
2	D	610	ASN
2	D	612	GLN
2	D	755	ASN
2	D	874	GLN
2	D	920	GLN
2	D	1234	GLN
2	D	1504	HIS
2	D	1562	ASN
2	D	1634	ASN
2	D	1824	HIS
2	D	1951	GLN
2	D	2280	GLN
2	D	2496	GLN
2	D	2683	ASN
2	D	2694	HIS
2	D	2765	HIS
2	D	2772	GLN
2	D	2853	GLN
2	D	2939	ASN
2	D	2982	GLN
2	D	3000	ASN
2	D	3278	GLN
2	D	3302	ASN
2	D	3686	ASN

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	IHP	D	3901	-	36,36,36	2.04	7 (19%)	60,60,60	1.29	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IHP	D	3901	-	-	4/30/54/54	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3901	IHP	P4-O14	4.77	1.67	1.59
3	D	3901	IHP	P5-O15	4.69	1.67	1.59
3	D	3901	IHP	P6-O16	4.42	1.67	1.59
3	D	3901	IHP	P2-O12	4.40	1.67	1.59
3	D	3901	IHP	P1-O11	4.39	1.67	1.59
3	D	3901	IHP	P3-O13	4.08	1.66	1.59
3	D	3901	IHP	O16-C6	-3.14	1.33	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3901	IHP	C5-C6-C1	5.04	121.49	110.43
3	D	3901	IHP	C6-C5-C4	3.80	118.76	110.43
3	D	3901	IHP	C5-C4-C3	2.41	115.71	110.43
3	D	3901	IHP	C6-C1-C2	2.36	115.59	110.43
3	D	3901	IHP	C4-C3-C2	2.14	115.12	110.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

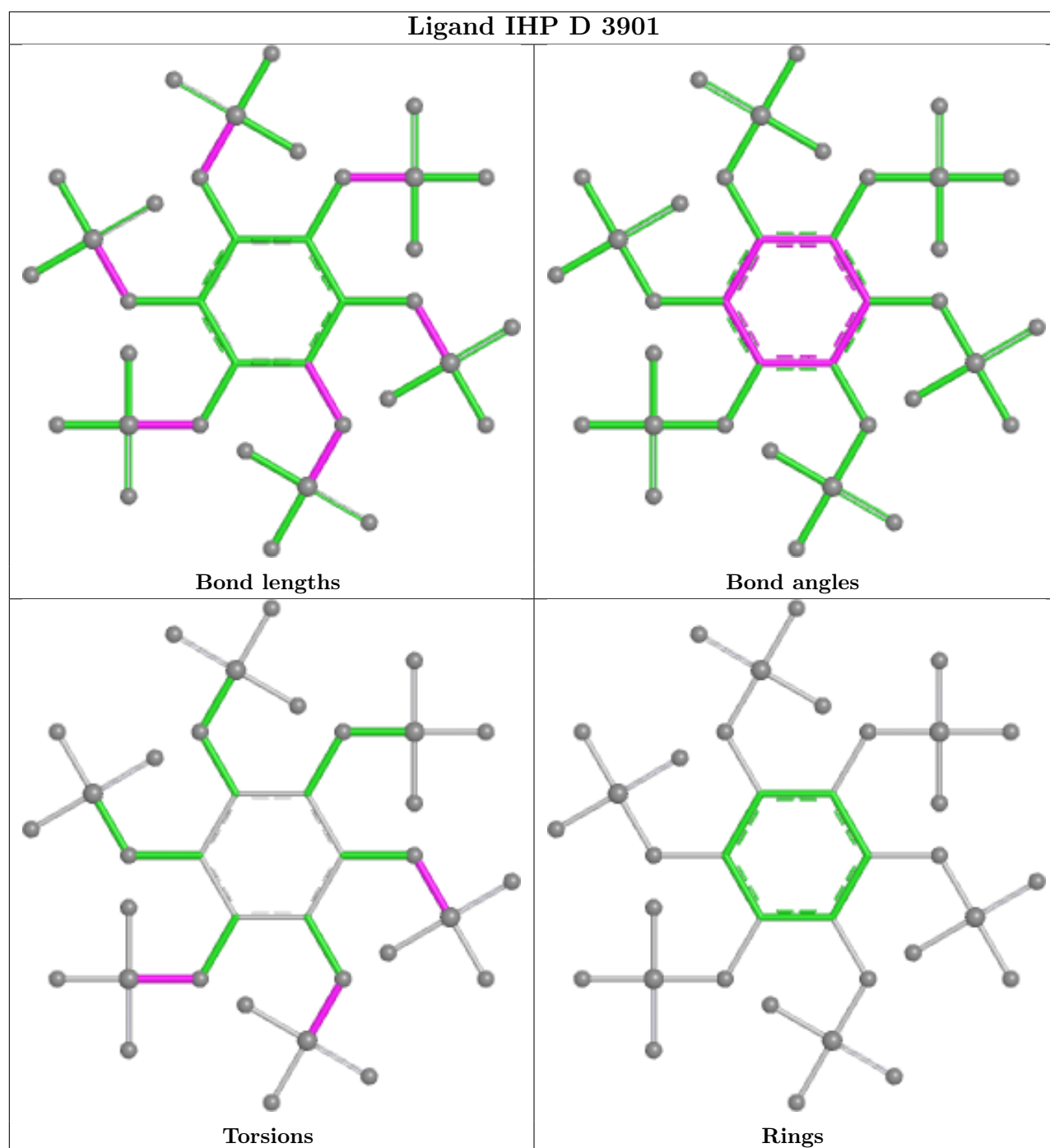
Mol	Chain	Res	Type	Atoms
3	D	3901	IHP	C1-O11-P1-O21
3	D	3901	IHP	C5-O15-P5-O35
3	D	3901	IHP	C6-O16-P6-O46
3	D	3901	IHP	C6-O16-P6-O26

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3901	IHP	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.



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.

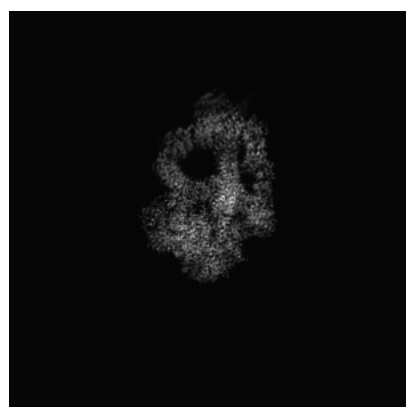
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45389. These allow visual inspection of the internal detail of the map and identification of artifacts.

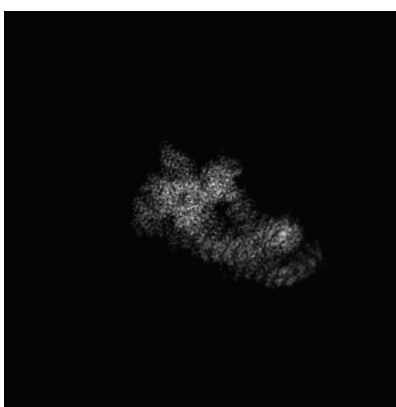
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

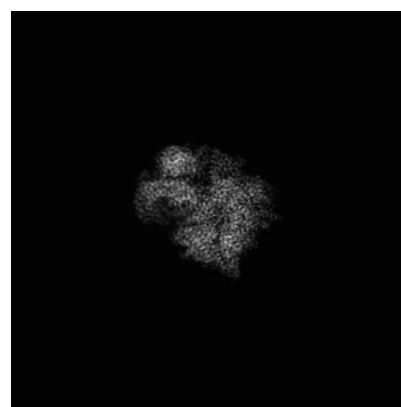
6.1.1 Primary map



X



Y

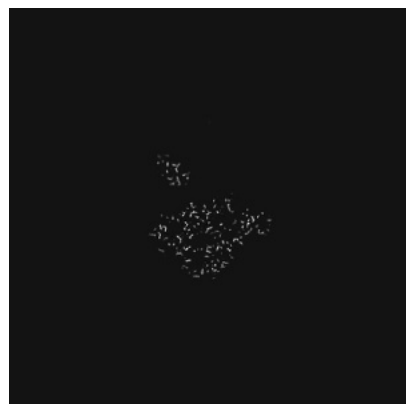


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

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: 274



Y Index: 282

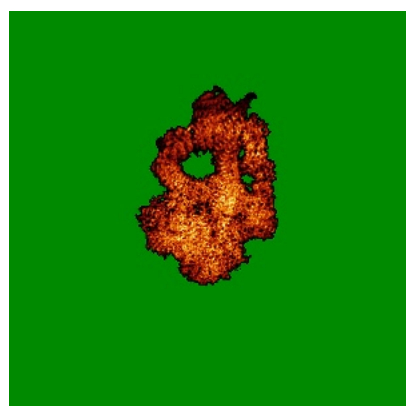


Z Index: 240

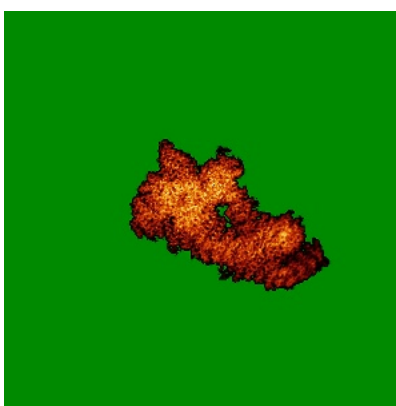
The images above show the largest variance slices of the map in three orthogonal directions.

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

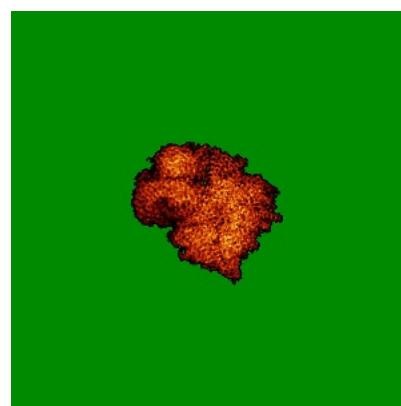
6.4.1 Primary map



X



Y

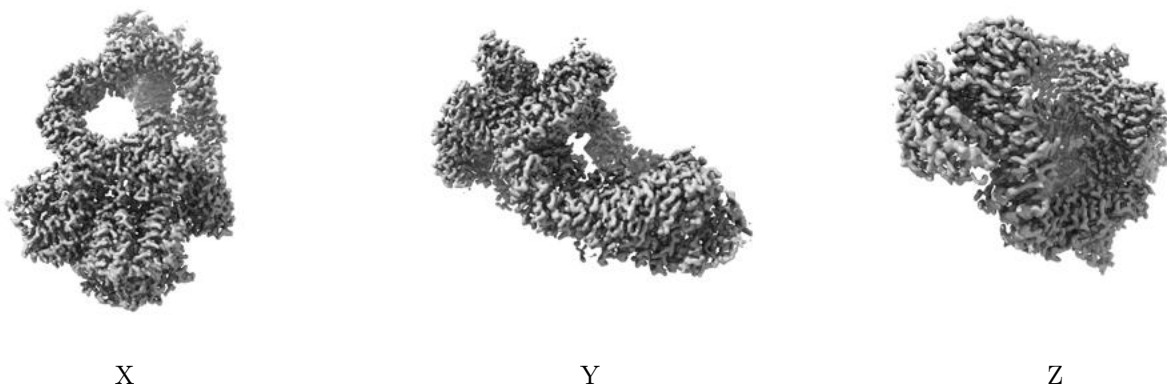


Z

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

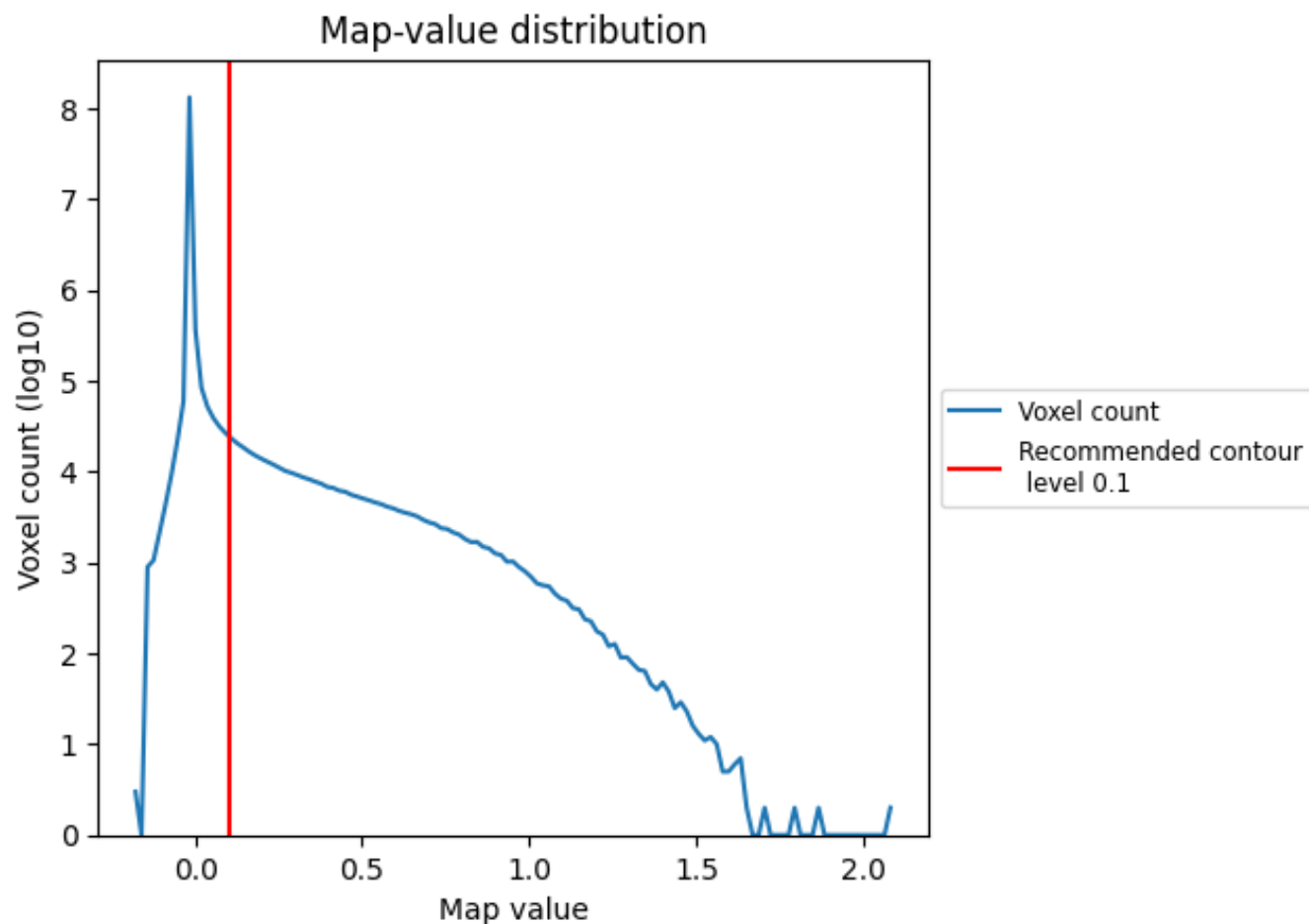
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

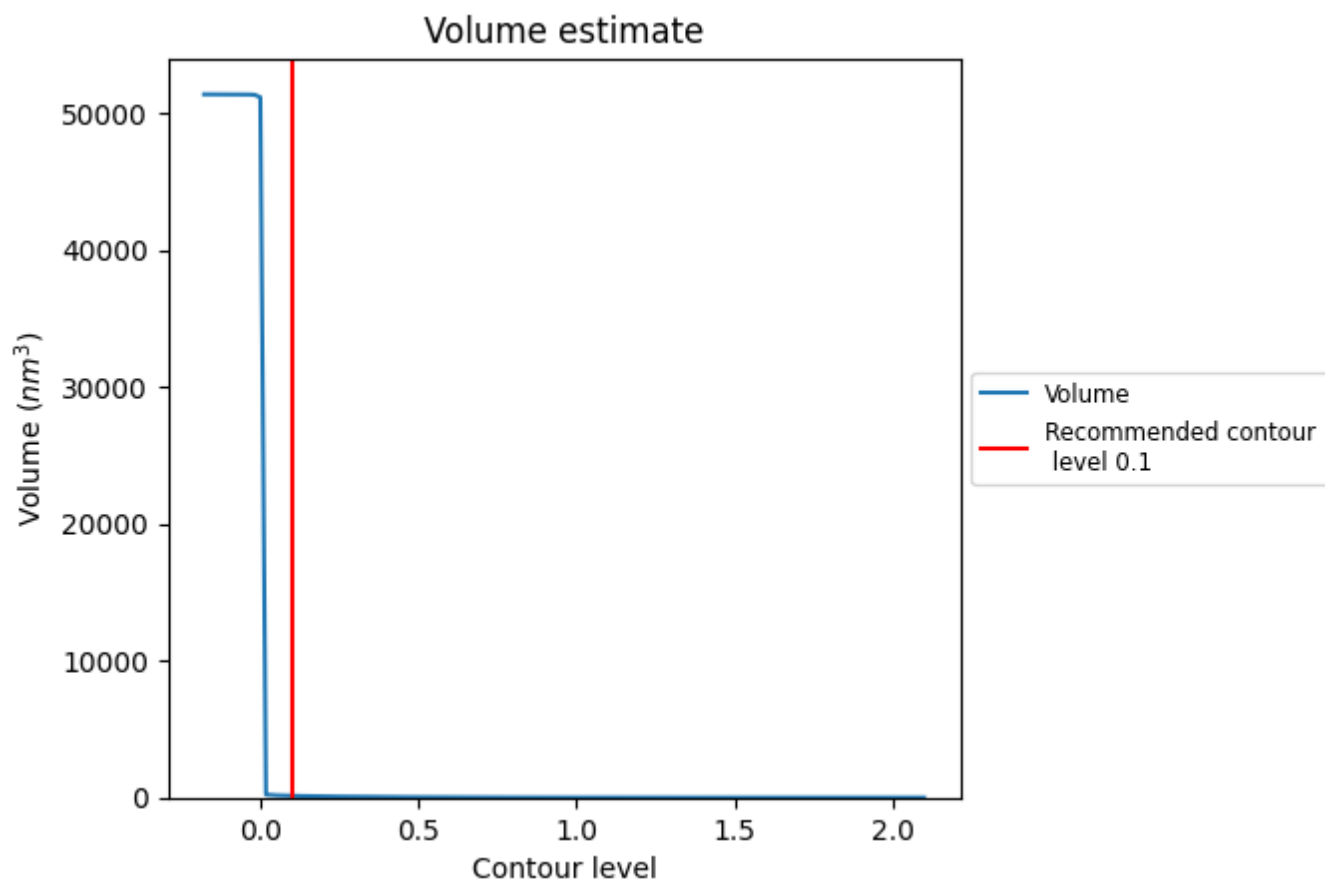
This section contains the results of statistical analysis of the map.

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.

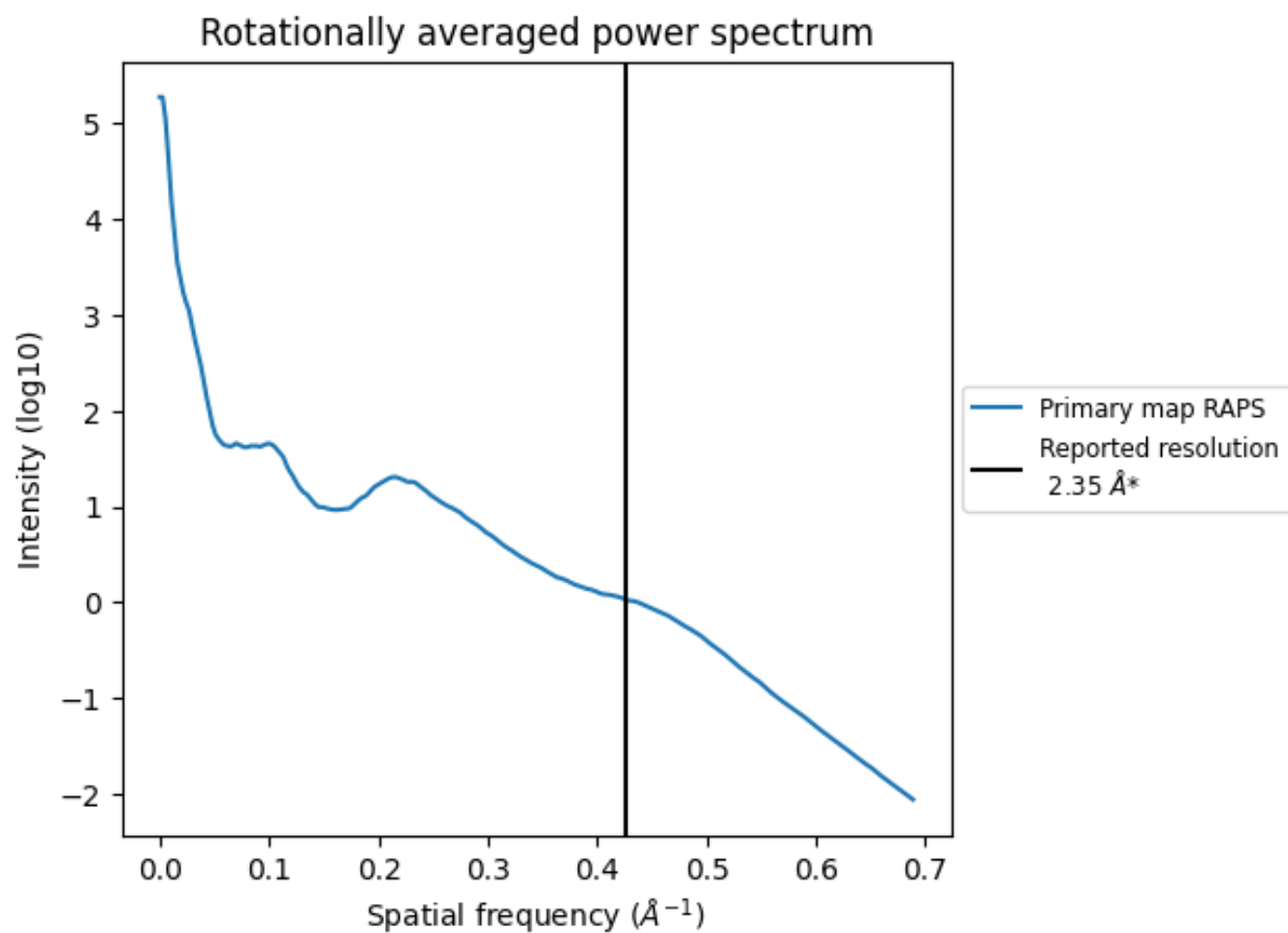
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 115 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 0.426 Å⁻¹

8 Fourier-Shell correlation

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

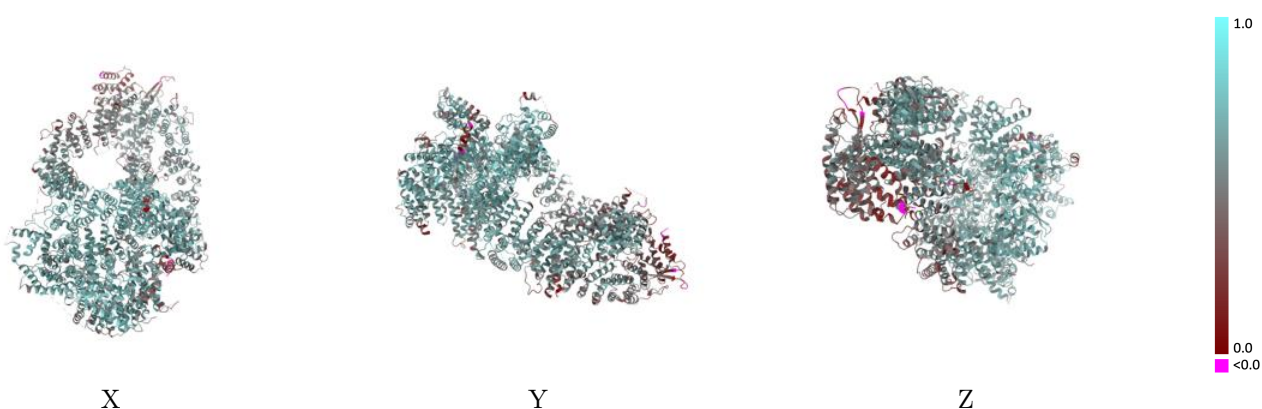
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45389 and PDB model 9CAF. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

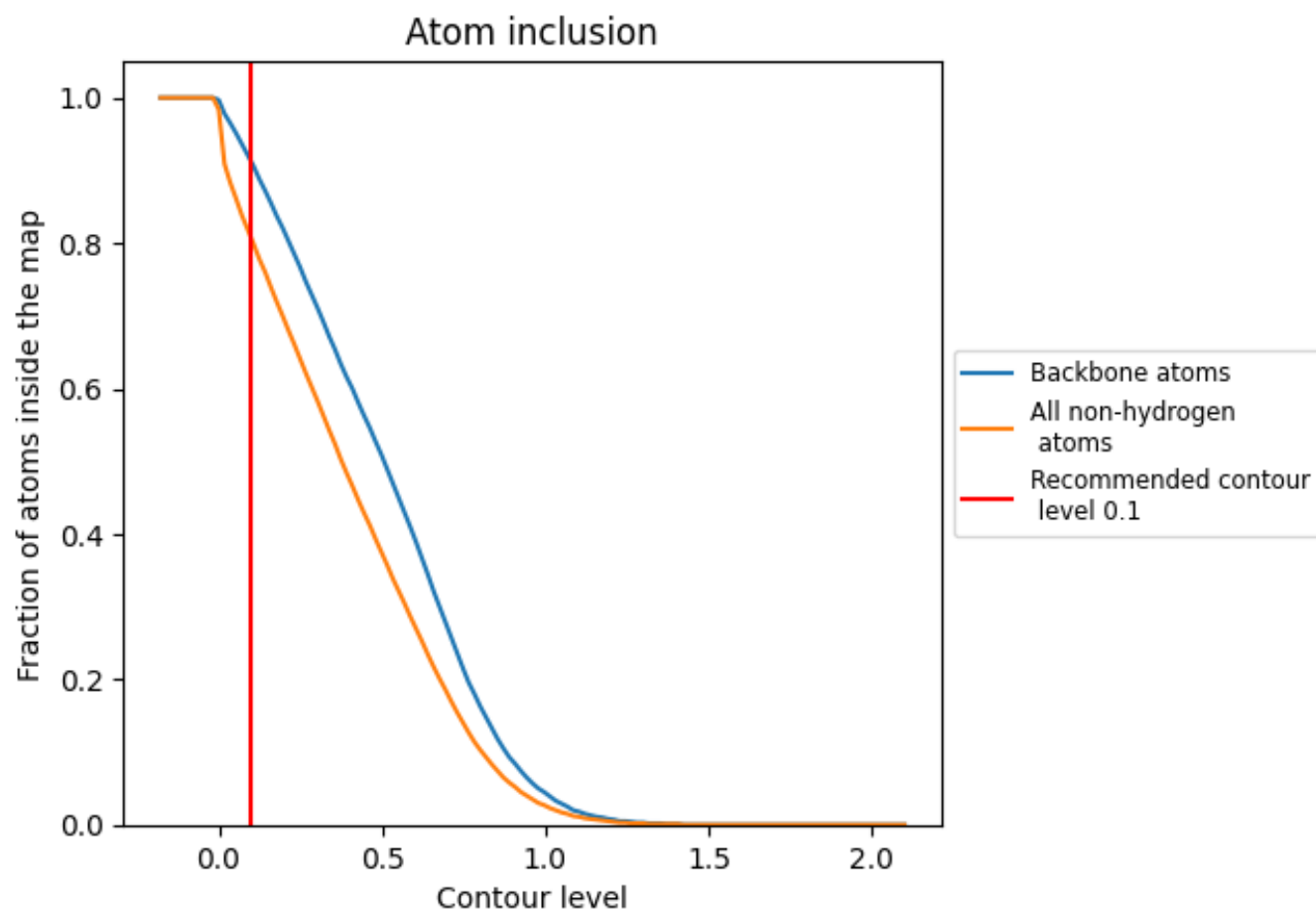


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 81% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8060	0.5810
A	0.7460	0.5730
D	0.8090	0.5810

