



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 09:25 PM UTC

PDB ID : 9OOU / pdb_00009oou
EMDB ID : EMD-70673
Title : Glycine/Glutamate/EU 1622-240 rGluN1a-2B NMDAR
Authors : Steigerwald, R.; Furukawa, H.
Deposited on : 2025-05-16
Resolution : 3.34 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

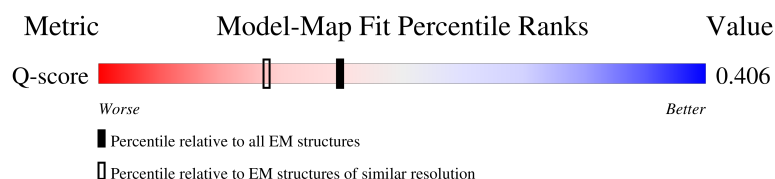
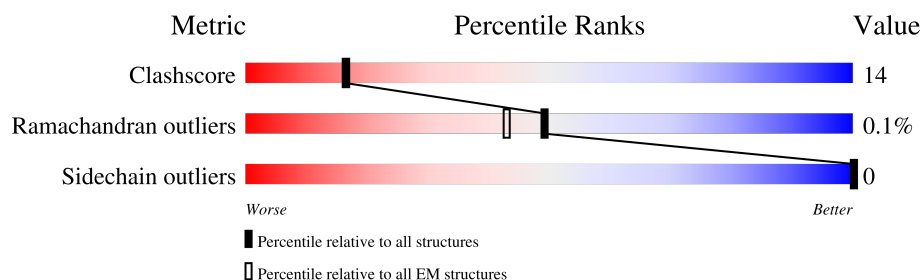
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.34 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	14446 (2.84 - 3.84)

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	847	26% 36% 15% 50%
1	C	847	26% 36% 14% 50%
2	B	862	22% 32% 17% 51%
2	D	862	23% 32% 16% 51%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13198 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	426	Total	C	N	O	S	0	0
			3295	2128	551	593	23		
1	C	426	Total	C	N	O	S	0	0
			3299	2130	551	595	23		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	CYS	conflict	UNP P35439
A	61	GLN	ASN	engineered mutation	UNP P35439
A	239	ASP	ASN	engineered mutation	UNP P35439
A	350	GLN	ASN	engineered mutation	UNP P35439
A	471	GLN	ASN	engineered mutation	UNP P35439
A	491	GLN	ASN	engineered mutation	UNP P35439
A	771	GLN	ASN	engineered mutation	UNP P35439
A	844	ASN	ARG	engineered mutation	UNP P35439
A	845	GLY	ARG	engineered mutation	UNP P35439
A	846	ALA	LYS	engineered mutation	UNP P35439
C	22	SER	CYS	conflict	UNP P35439
C	61	GLN	ASN	engineered mutation	UNP P35439
C	239	ASP	ASN	engineered mutation	UNP P35439
C	350	GLN	ASN	engineered mutation	UNP P35439
C	471	GLN	ASN	engineered mutation	UNP P35439
C	491	GLN	ASN	engineered mutation	UNP P35439
C	771	GLN	ASN	engineered mutation	UNP P35439
C	844	ASN	ARG	engineered mutation	UNP P35439
C	845	GLY	ARG	engineered mutation	UNP P35439
C	846	ALA	LYS	engineered mutation	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	421	Total 3155	C 2043	N 509	O 579	S 24	0	0
2	D	421	Total 3155	C 2043	N 509	O 579	S 24	0	0

There are 74 discrepancies between the modelled and reference sequences:

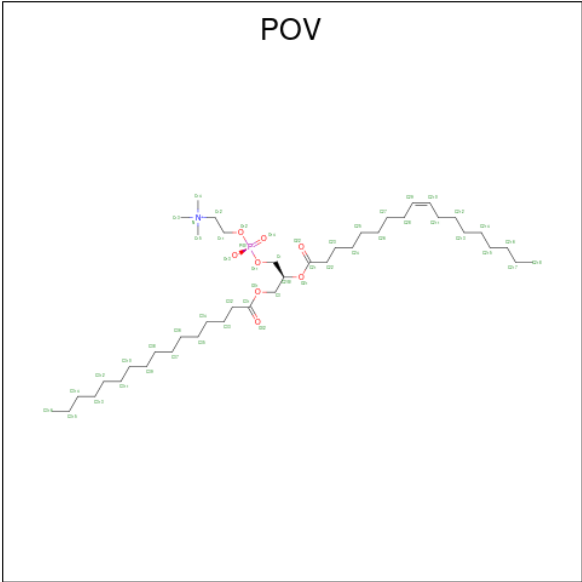
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLY	-	expression tag	UNP Q00960
B	-8	TRP	-	expression tag	UNP Q00960
B	-7	SER	-	expression tag	UNP Q00960
B	-6	HIS	-	expression tag	UNP Q00960
B	-5	PRO	-	expression tag	UNP Q00960
B	-4	GLN	-	expression tag	UNP Q00960
B	-3	PHE	-	expression tag	UNP Q00960
B	-2	GLU	-	expression tag	UNP Q00960
B	-1	LYS	-	expression tag	UNP Q00960
B	0	GLY	-	expression tag	UNP Q00960
B	1	GLY	-	expression tag	UNP Q00960
B	2	GLY	-	expression tag	UNP Q00960
B	3	SER	-	expression tag	UNP Q00960
B	4	GLY	-	expression tag	UNP Q00960
B	5	GLY	-	expression tag	UNP Q00960
B	6	GLY	-	expression tag	UNP Q00960
B	7	SER	-	expression tag	UNP Q00960
B	8	GLY	-	expression tag	UNP Q00960
B	9	GLY	-	expression tag	UNP Q00960
B	10	SER	-	expression tag	UNP Q00960
B	11	ALA	-	expression tag	UNP Q00960
B	12	TRP	-	expression tag	UNP Q00960
B	13	SER	-	expression tag	UNP Q00960
B	14	HIS	-	expression tag	UNP Q00960
B	15	PRO	-	expression tag	UNP Q00960
B	16	GLN	-	expression tag	UNP Q00960
B	17	PHE	-	expression tag	UNP Q00960
B	18	GLU	-	expression tag	UNP Q00960
B	19	LYS	-	expression tag	UNP Q00960
B	20	GLY	-	expression tag	UNP Q00960
B	21	ALA	-	expression tag	UNP Q00960
B	22	LEU	-	expression tag	UNP Q00960
B	23	VAL	-	expression tag	UNP Q00960
B	24	PRO	-	expression tag	UNP Q00960
B	25	ARG	-	expression tag	UNP Q00960

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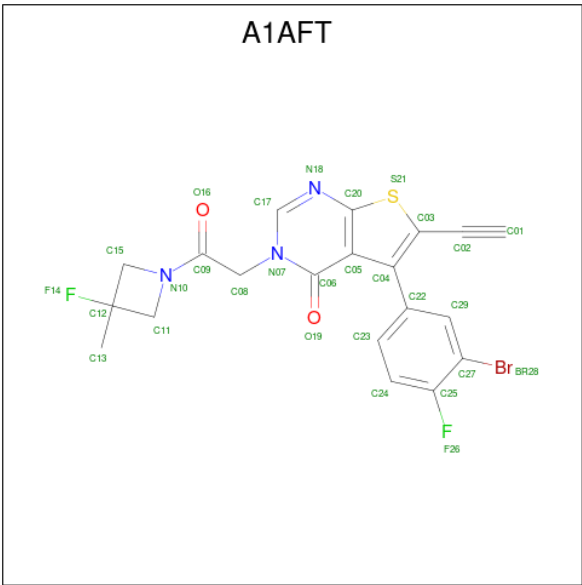
Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLY	-	expression tag	UNP Q00960
B	849	SER	CYS	conflict	UNP Q00960
D	-9	GLY	-	expression tag	UNP Q00960
D	-8	TRP	-	expression tag	UNP Q00960
D	-7	SER	-	expression tag	UNP Q00960
D	-6	HIS	-	expression tag	UNP Q00960
D	-5	PRO	-	expression tag	UNP Q00960
D	-4	GLN	-	expression tag	UNP Q00960
D	-3	PHE	-	expression tag	UNP Q00960
D	-2	GLU	-	expression tag	UNP Q00960
D	-1	LYS	-	expression tag	UNP Q00960
D	0	GLY	-	expression tag	UNP Q00960
D	1	GLY	-	expression tag	UNP Q00960
D	2	GLY	-	expression tag	UNP Q00960
D	3	SER	-	expression tag	UNP Q00960
D	4	GLY	-	expression tag	UNP Q00960
D	5	GLY	-	expression tag	UNP Q00960
D	6	GLY	-	expression tag	UNP Q00960
D	7	SER	-	expression tag	UNP Q00960
D	8	GLY	-	expression tag	UNP Q00960
D	9	GLY	-	expression tag	UNP Q00960
D	10	SER	-	expression tag	UNP Q00960
D	11	ALA	-	expression tag	UNP Q00960
D	12	TRP	-	expression tag	UNP Q00960
D	13	SER	-	expression tag	UNP Q00960
D	14	HIS	-	expression tag	UNP Q00960
D	15	PRO	-	expression tag	UNP Q00960
D	16	GLN	-	expression tag	UNP Q00960
D	17	PHE	-	expression tag	UNP Q00960
D	18	GLU	-	expression tag	UNP Q00960
D	19	LYS	-	expression tag	UNP Q00960
D	20	GLY	-	expression tag	UNP Q00960
D	21	ALA	-	expression tag	UNP Q00960
D	22	LEU	-	expression tag	UNP Q00960
D	23	VAL	-	expression tag	UNP Q00960
D	24	PRO	-	expression tag	UNP Q00960
D	25	ARG	-	expression tag	UNP Q00960
D	26	GLY	-	expression tag	UNP Q00960
D	849	SER	CYS	conflict	UNP Q00960

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 4 is (5M)-5-(3-bromo-4-fluorophenyl)-6-ethynyl-3-[2-(3-fluoro-3-methylazetidin-1-yl)-2-oxoethyl]thieno[2,3-d]pyrimidin-4(3H)-one (CCD ID: A1AFT) (formula: C₂₀H₁₄BrF₂N₃O₂S) (labeled as "Ligand of Interest" by depositor).

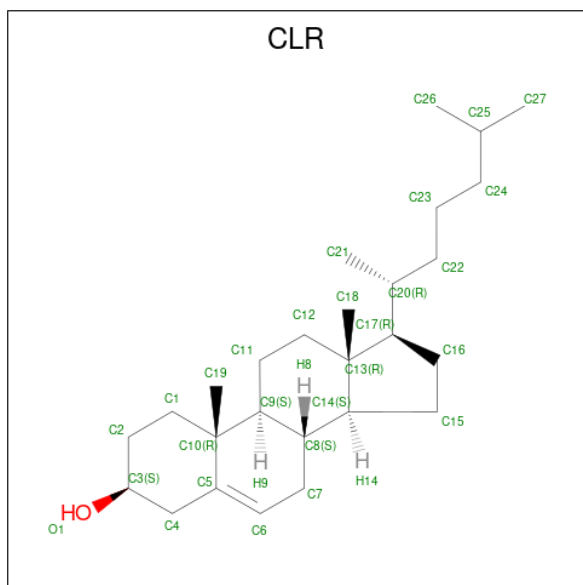


Mol	Chain	Residues	Atoms							AltConf
4	A	1	Total	Br	C	F	N	O	S	0
			29	1	20	2	3	2	1	

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Mol	Chain	Residues	Atoms							AltConf
4	B	1	Total	Br	C	F	N	O	S	0
			29	1	20	2	3	2	1	
4	C	1	Total	Br	C	F	N	O	S	0
			29	1	20	2	3	2	1	
4	D	1	Total	Br	C	F	N	O	S	0
			29	1	20	2	3	2	1	

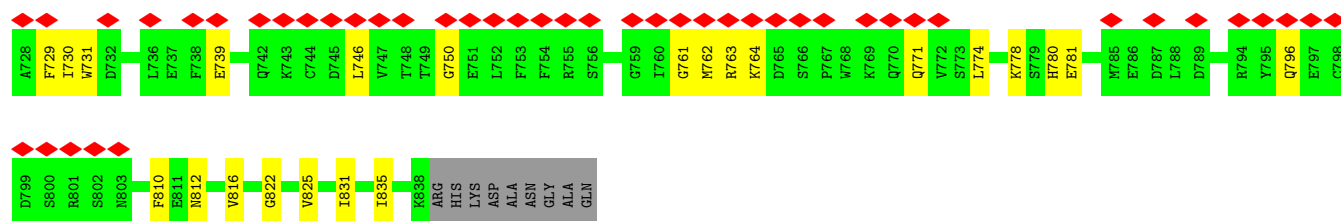
- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



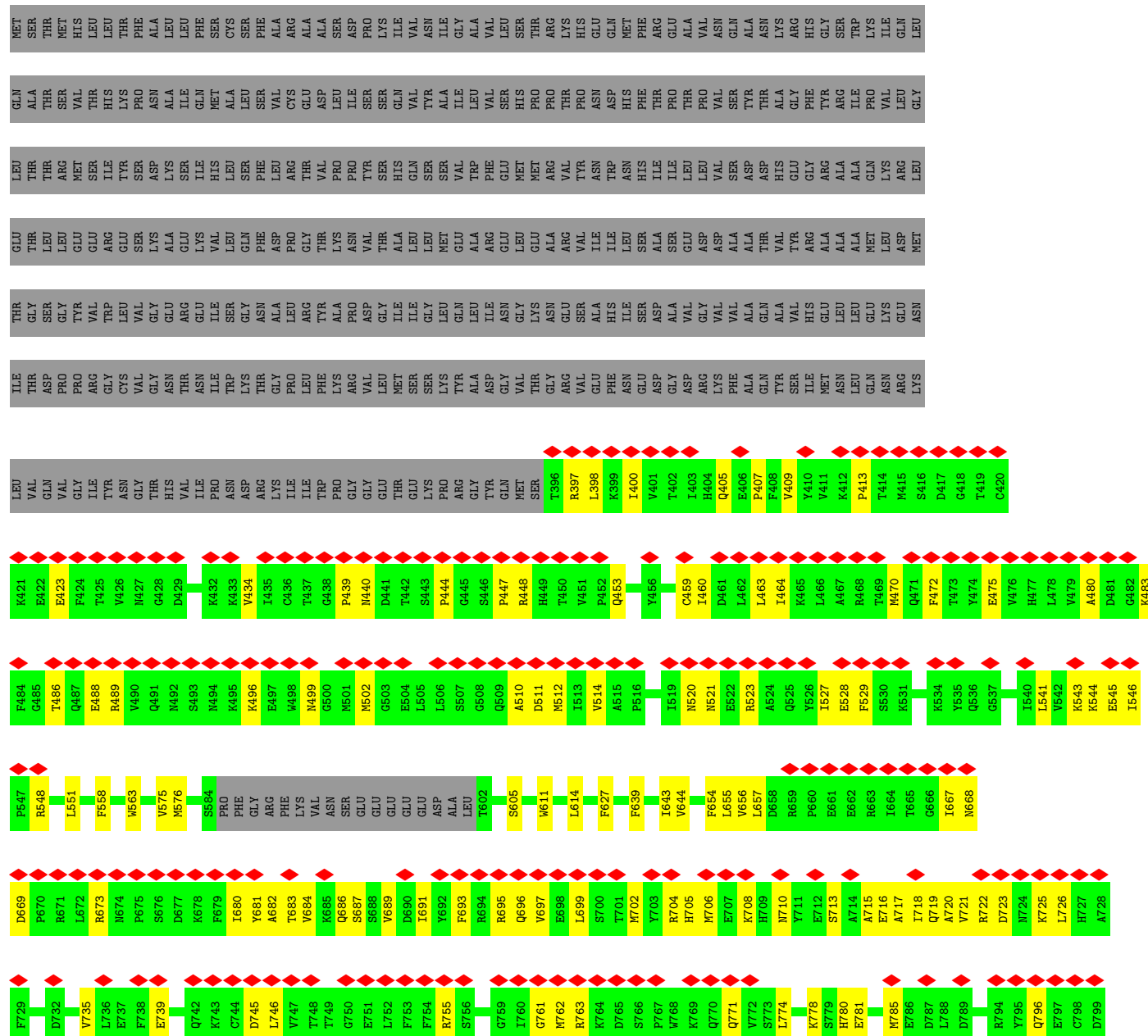
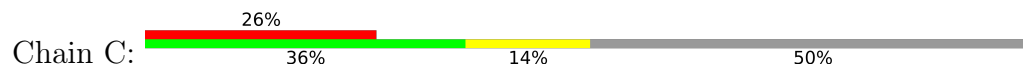
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			28	27	1	
5	D	1	Total	C	O	0
			28	27	1	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	3	Total	O	0
			3	3	
6	B	6	Total	O	0
			6	6	
6	C	3	Total	O	0
			3	3	
6	D	6	Total	O	0
			6	6	

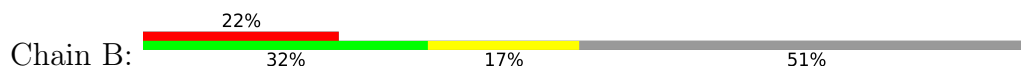


• Molecule 1: Glutamate receptor ionotropic, NMDA 1





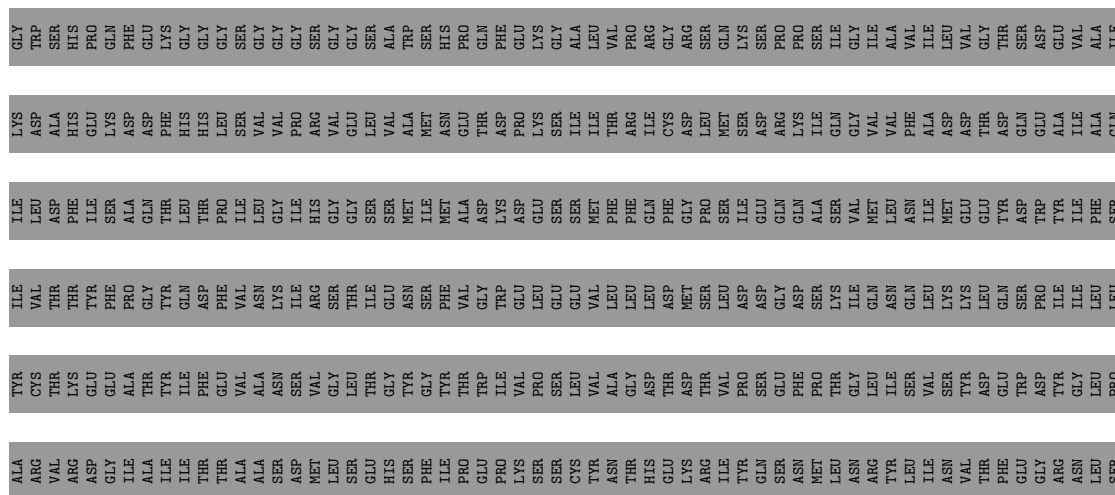
• Molecule 2: Glutamate receptor ionotropic, NMDA 2B



GLY	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	GLY	SER	GLY	G822	V825	V816	F817	F810	N803	S800
LYS	ASP	ALA	HIS	GLU	LYS	ASP	ASP	PHE	HIS	GLY	LEU	SER	VAL	GLY	V825	V816	F817	F810	N803	S800	
ILE	LEU	ASP	PHE	ILE	SER	ALA	GLN	THR	THR	THR	PRO	ILE	LEU	GLY	V825	V816	F817	F810	N803	S800	
ILE	VAL	THR	THR	TYR	PHE	PRO	GLY	THR	THR	THR	ASP	PHE	VAL	ASN	V825	V816	F817	F810	N803	S800	
TYR	CYS	THR	LYS	GLU	GLU	ALA	ALA	THR	PHE	THR	VAL	ALA	VAL	ASN	V825	V816	F817	F810	N803	S800	
ALA	ARG	VAL	VAL	ASP	GLY	ILE	ALA	THR	THR	THR	VAL	ALA	VAL	ASN	V825	V816	F817	F810	N803	S800	

PHE	SER	GLU	ASP	GLY	TYR	GLN	MET	HIS	PRO	LYS	LEU	VAL	ILE	ILE	LEU	LEU	ASN	LYS	GLU	ARG	LYS	TRP	GLU	GLN	GLY	VAL	GLY	LYS	LYS	LYS	ASP	LYS	LYS	SER	LEU	SER	GLM	MET	LYS	TYR	TYR	VAL	TRP	PRO	ARG	MET	CYS	PRO	GLU	THR	GLU	GLU	GLN	GLU	D403	D404	H405	L406	S407	I408	V409	T410																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
L411	E412	E413	A414	P415	F416	V417	I418	V419	E420	S421	V422	D423	P424	L425	S426	G427	T428	C429	M430	R431	N432	T433	M434	V435	P436	C437	K438	R439	I440	I441	S442	E443	N444	K445	T446	D447	E448	E449	P450	G451	Y452	I453	K454	K455	C456	C457	K458	C461	I462	D463	I464	L465	K466	K467	I468	S469	K470	S471																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
V472	K473	F474	T475	Y476	D477	L478	Y479	L480	V481	M483	G484	K485	H486	G487	K488	K489	I490	M491	G492	T493	M494	N495	G496	M497	I498	V502	M503	K504	R505	A506	V507	M508	A509	G511	S512	N516	E517	E518	R519	S520	E521	V522	V523	D524	F525	S526	V527	P528	F529	I530	E531	I534	S535	V536																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
M537	V538	S539	B540	V545	S546	P547	L551	M561	V564	M565	L566	L567	I568	A573	V574	F575	V576	F577	E578	P579	PHE	SER	PRO	VAL	GLY	TYR	ASN	ARG	CYS	LEU	ALA	ASP	GLY	ARG	GLU	PRO	GLY	PRO	S599	I602	M610	V613	G625	T626	T627	I630	M631																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															

• Molecule 2: Glutamate receptor ionotropic, NMDA 2B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	382882	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 ($e^-/\text{\AA}^2$)	58.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.345	Depositor
Minimum map value	-0.949	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.101	Depositor
Map size (Å)	363.88, 363.88, 363.88	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	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: POV, CLR, A1AFT

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	0.43	0/3373	0.43	0/4574
1	C	0.42	0/3377	0.42	0/4579
2	B	0.45	0/3221	0.46	0/4373
2	D	0.45	0/3221	0.45	0/4373
All	All	0.44	0/13192	0.44	0/17899

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	3295	0	3234	88	0
1	C	3299	0	3238	91	0
2	B	3155	0	3073	107	0
2	D	3155	0	3073	101	0
3	A	52	0	82	2	0
3	C	52	0	82	1	0
4	A	29	0	0	0	0
4	B	29	0	0	5	0
4	C	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	29	0	0	5	0
5	B	28	0	46	2	0
5	D	28	0	46	3	0
6	A	3	0	0	0	0
6	B	6	0	0	0	0
6	C	3	0	0	0	0
6	D	6	0	0	0	0
All	All	13198	0	12874	368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (368) 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:551:LEU:HD21	1:A:654:PHE:HB3	1.53	0.90
1:C:551:LEU:HD21	1:C:654:PHE:HB3	1.53	0.88
2:D:498:ILE:HD11	2:D:519:ARG:HG2	1.59	0.83
1:A:397:ARG:HH22	1:A:475:GLU:HG2	1.47	0.80
2:B:565:MET:HE1	1:C:817:PHE:CD1	2.18	0.79
1:C:696:GLN:HB3	1:C:699:LEU:HB2	1.63	0.79
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.67	0.76
1:A:696:GLN:HB3	1:A:699:LEU:HB2	1.69	0.75
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.68	0.74
2:B:439:ARG:HG3	2:B:450:PRO:HB3	1.70	0.73
2:D:516:ASN:HD21	2:D:519:ARG:HD2	1.54	0.71
1:C:668:ASN:HA	1:C:673:ARG:HH22	1.54	0.71
2:B:437:GLN:HE22	2:B:452:TYR:HA	1.56	0.70
2:D:436:CYS:SG	2:D:457:CYS:N	2.62	0.70
1:C:720:ALA:HA	1:C:725:LYS:HE3	1.74	0.69
1:C:413:PRO:HA	1:C:453:GLN:HG2	1.75	0.69
2:D:687:PRO:HD3	2:D:710:ASN:HB2	1.75	0.68
5:B:902:CLR:H211	5:B:902:CLR:H273	1.75	0.68
1:A:720:ALA:HA	1:A:725:LYS:HE3	1.75	0.68
2:D:508:MET:HE2	2:D:764:ILE:HG22	1.76	0.67
1:C:488:GLU:OE2	1:C:499:ASN:ND2	2.28	0.67
1:C:704:ARG:HH12	1:C:708:LYS:HD3	1.58	0.67
2:D:423:ASP:HB2	2:D:430:MET:HE1	1.77	0.66
1:A:683:THR:HG21	1:A:689:VAL:HG11	1.78	0.66
1:A:696:GLN:HG2	1:A:699:LEU:HD13	1.77	0.65
2:D:510:VAL:HG22	2:D:764:ILE:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:VAL:HG22	3:A:901:POV:H315	1.78	0.65
2:B:439:ARG:HH12	2:B:479:TYR:HB2	1.61	0.65
1:C:644:VAL:HG22	3:C:901:POV:H315	1.78	0.65
1:A:704:ARG:HH12	1:A:708:LYS:HD3	1.61	0.65
1:C:796:GLN:NE2	1:C:800:SER:OG	2.29	0.65
2:D:521:GLU:HG3	2:D:522:VAL:HG13	1.80	0.64
1:C:695:ARG:HD2	2:D:431:ARG:HH12	1.61	0.64
2:B:687:PRO:HD3	2:B:710:ASN:HB2	1.79	0.64
2:B:498:ILE:HD11	2:B:519:ARG:HG2	1.80	0.63
1:C:696:GLN:HG2	1:C:699:LEU:HD13	1.82	0.62
2:B:457:CYS:C	2:B:458:LYS:HD2	2.25	0.62
2:B:521:GLU:HG3	2:B:522:VAL:HG13	1.80	0.62
2:B:538:VAL:HG12	2:B:728:ALA:HA	1.81	0.62
2:B:627:THR:HG21	1:C:831:ILE:HD13	1.82	0.62
1:C:683:THR:HG21	1:C:689:VAL:HG11	1.82	0.61
1:A:668:ASN:HA	1:A:673:ARG:HH22	1.65	0.60
2:B:423:ASP:HB2	2:B:430:MET:HE1	1.82	0.60
2:D:522:VAL:HG23	2:D:523:VAL:HG23	1.81	0.60
2:B:561:MET:HA	2:B:564:VAL:HG12	1.84	0.60
1:A:413:PRO:HA	1:A:453:GLN:HG2	1.83	0.59
2:D:433:THR:HA	2:D:458:LYS:HE2	1.84	0.59
2:D:678:SER:HB2	2:D:679:PRO:HD2	1.84	0.59
2:B:671:PHE:HB3	2:B:702:MET:HE2	1.86	0.58
2:B:522:VAL:HG23	2:B:523:VAL:HG23	1.85	0.58
2:D:525:PHE:O	2:D:773:LYS:NZ	2.37	0.58
2:B:436:CYS:SG	2:B:457:CYS:N	2.74	0.57
2:D:671:PHE:HB3	2:D:702:MET:HE2	1.87	0.57
2:B:692:GLU:HA	2:B:695:ILE:HG22	1.86	0.57
2:B:462:ILE:O	2:B:466:LYS:HG2	2.04	0.57
1:C:510:ALA:O	1:C:763:ARG:NH1	2.38	0.57
2:D:610:TRP:HZ2	4:D:901:A1AFT:BR28	2.42	0.57
1:A:470:MET:HE1	1:A:771:GLN:HG3	1.87	0.57
2:B:463:ASP:OD1	2:B:464:ILE:N	2.38	0.57
2:D:692:GLU:HA	2:D:695:ILE:HG22	1.87	0.57
1:A:459:CYS:HB2	1:A:514:VAL:HG12	1.85	0.57
1:A:713:SER:N	1:A:716:GLU:OE2	2.37	0.57
2:B:610:TRP:HZ2	4:B:901:A1AFT:BR28	2.43	0.57
1:A:722:ARG:HA	1:A:746:LEU:HD21	1.86	0.56
2:D:508:MET:HE1	2:D:766:ILE:HG12	1.87	0.56
2:B:517:GLU:HG3	1:C:774:LEU:HG	1.87	0.56
2:B:537:MET:HA	2:B:750:THR:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:ILE:HD12	1:C:761:GLY:HA3	1.87	0.56
2:D:693:ARG:HA	2:D:696:ARG:HE	1.70	0.56
1:A:780:HIS:ND1	2:D:759:SER:O	2.38	0.56
2:B:693:ARG:HA	2:B:696:ARG:HE	1.71	0.55
1:C:528:GLU:O	1:C:762:MET:N	2.39	0.55
1:A:470:MET:HB2	1:A:472:PHE:HD1	1.72	0.55
1:C:463:LEU:HD21	1:C:514:VAL:HG21	1.89	0.55
2:B:678:SER:HB2	2:B:679:PRO:HD2	1.86	0.55
2:D:438:LYS:HE3	2:D:453:ILE:HD11	1.87	0.55
2:D:537:MET:HA	2:D:750:THR:HA	1.88	0.55
1:A:400:ILE:HG12	1:A:512:MET:HB3	1.90	0.54
1:C:470:MET:HE1	1:C:771:GLN:HG3	1.89	0.54
1:C:722:ARG:HA	1:C:746:LEU:HD21	1.88	0.54
1:A:528:GLU:O	1:A:762:MET:N	2.39	0.54
1:A:643:ILE:HD13	2:B:818:MET:HE1	1.89	0.54
1:A:831:ILE:HD13	2:D:627:THR:HG21	1.89	0.54
2:D:518:GLU:OE1	2:D:693:ARG:NE	2.39	0.54
2:B:525:PHE:O	2:B:773:LYS:NZ	2.40	0.54
2:D:703:HIS:HA	2:D:706:MET:HG2	1.89	0.54
1:C:489:ARG:HB3	1:C:496:LYS:HD3	1.90	0.54
1:C:543:LYS:HG2	1:C:545:GLU:H	1.73	0.54
1:A:489:ARG:HB3	1:A:496:LYS:HD3	1.89	0.54
1:A:414:THR:OG1	1:A:452:PRO:O	2.20	0.53
1:A:543:LYS:HG2	1:A:545:GLU:H	1.73	0.53
2:B:439:ARG:HH22	2:B:479:TYR:HD2	1.55	0.53
1:C:667:ILE:O	1:C:673:ARG:NH1	2.39	0.53
2:B:536:VAL:HG22	2:B:730:ILE:HG12	1.90	0.53
1:C:444:PRO:HB3	1:C:448:ARG:HA	1.90	0.53
2:D:458:LYS:HD3	2:D:462:ILE:HG21	1.90	0.53
1:C:459:CYS:HB2	1:C:514:VAL:HG12	1.89	0.53
2:D:413:GLU:OE1	2:D:414:ALA:N	2.41	0.53
1:C:470:MET:HB2	1:C:472:PHE:HD1	1.71	0.53
2:D:547:PRO:HB2	5:D:902:CLR:H3	1.89	0.53
1:C:713:SER:N	1:C:716:GLU:OE2	2.39	0.53
1:A:717:ALA:O	1:A:721:VAL:HG23	2.09	0.52
2:D:423:ASP:HB3	2:D:426:SER:HB2	1.91	0.52
2:D:573:ALA:HA	2:D:576:VAL:HG22	1.91	0.52
2:B:518:GLU:OE1	2:B:693:ARG:NE	2.42	0.52
1:C:460:ILE:O	1:C:464:ILE:HG13	2.10	0.52
1:A:718:ILE:HD13	1:A:739:GLU:HG3	1.92	0.52
1:C:717:ALA:O	1:C:721:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LEU:HD21	1:A:514:VAL:HG21	1.91	0.52
1:C:669:ASP:H	1:C:673:ARG:HH12	1.57	0.52
1:C:681:TYR:HA	1:C:726:LEU:HD11	1.91	0.52
1:A:499:ASN:OD1	1:A:500:GLY:N	2.43	0.51
2:B:703:HIS:HA	2:B:706:MET:HG2	1.90	0.51
1:A:774:LEU:HG	2:D:517:GLU:HG3	1.92	0.51
1:A:831:ILE:O	1:A:835:ILE:HG12	2.11	0.51
2:B:574:VAL:HG12	2:B:574:VAL:O	2.10	0.51
1:C:831:ILE:O	1:C:835:ILE:HG12	2.11	0.51
1:A:527:ILE:HD12	1:A:761:GLY:HA3	1.92	0.51
1:A:706:MET:SD	1:A:706:MET:N	2.79	0.51
1:C:489:ARG:HH21	1:C:496:LYS:HE2	1.76	0.51
2:D:548:SER:HB3	5:D:902:CLR:H6	1.92	0.51
1:A:681:TYR:HA	1:A:726:LEU:HD11	1.91	0.51
1:A:470:MET:HB2	1:A:472:PHE:CD1	2.47	0.50
2:B:508:MET:HE2	2:B:764:ILE:HG22	1.93	0.50
2:D:732:ASP:OD2	2:D:762:TYR:OH	2.24	0.50
1:A:655:LEU:C	1:A:657:LEU:H	2.19	0.50
1:C:470:MET:HB2	1:C:472:PHE:CD1	2.46	0.50
1:A:667:ILE:HD11	1:A:699:LEU:HD11	1.92	0.50
2:B:565:MET:HE1	1:C:817:PHE:CG	2.47	0.50
2:D:527:VAL:HG11	2:D:781:LEU:HD21	1.93	0.50
1:C:718:ILE:HD13	1:C:739:GLU:HG3	1.93	0.50
1:C:397:ARG:HH22	1:C:475:GLU:HG2	1.76	0.50
1:C:520:ASN:HB3	1:C:523:ARG:HG3	1.93	0.50
2:D:574:VAL:HG12	2:D:574:VAL:O	2.12	0.50
1:A:611:TRP:O	1:A:614:LEU:N	2.44	0.50
1:A:483:LYS:HG2	1:A:686:GLN:HB2	1.94	0.49
2:B:534:ILE:HD11	2:B:730:ILE:HG22	1.93	0.49
1:A:510:ALA:O	1:A:763:ARG:NH1	2.44	0.49
1:A:639:PHE:CD2	2:B:821:VAL:HG12	2.48	0.49
2:B:495:ASN:OD1	2:B:496:GLY:N	2.44	0.49
1:A:397:ARG:NH2	1:A:475:GLU:HG2	2.22	0.49
2:D:534:ILE:HD11	2:D:730:ILE:HG22	1.94	0.49
2:B:547:PRO:O	2:B:820:GLY:HA3	2.12	0.49
1:C:486:THR:OG1	1:C:488:GLU:OE2	2.28	0.49
2:B:573:ALA:HA	2:B:576:VAL:HG22	1.94	0.49
2:D:538:VAL:HG12	2:D:728:ALA:HA	1.94	0.49
1:A:674:ASN:HB3	2:B:742:ARG:HH21	1.77	0.49
2:B:732:ASP:OD2	2:B:762:TYR:OH	2.26	0.49
2:B:815:ILE:O	2:B:819:ALA:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:436:CYS:HB2	2:D:455:LYS:HB2	1.94	0.49
2:D:551:LEU:HD22	4:D:901:A1AFT:O19	2.13	0.49
1:A:520:ASN:HB3	1:A:523:ARG:HG3	1.95	0.48
2:B:577:PHE:HE1	2:B:625:GLY:H	1.60	0.48
1:A:699:LEU:HA	1:A:702:MET:HE1	1.94	0.48
2:B:631:MET:HA	2:B:634:VAL:HG12	1.94	0.48
2:D:723:THR:OG1	2:D:725:LYS:NZ	2.40	0.48
1:C:529:PHE:HA	1:C:761:GLY:HA2	1.95	0.48
1:C:669:ASP:H	1:C:673:ARG:NH1	2.10	0.48
2:D:523:VAL:HG11	2:D:765:ALA:HB1	1.96	0.48
1:C:397:ARG:NH2	1:C:475:GLU:HG2	2.28	0.48
2:D:715:ASP:OD1	2:D:716:ASP:N	2.47	0.48
1:C:611:TRP:O	1:C:614:LEU:N	2.44	0.48
2:B:527:VAL:HG11	2:B:781:LEU:HD21	1.96	0.48
1:C:605:SER:O	1:C:605:SER:OG	2.30	0.48
1:A:719:GLN:HG2	1:A:722:ARG:HH22	1.78	0.47
2:B:510:VAL:HG22	2:B:764:ILE:HD12	1.96	0.47
2:B:715:ASP:OD1	2:B:716:ASP:N	2.47	0.47
1:C:656:VAL:O	1:C:656:VAL:HG12	2.14	0.47
2:D:433:THR:CA	2:D:458:LYS:HE2	2.44	0.47
2:B:472:VAL:HB	2:B:474:PHE:CD1	2.49	0.47
1:A:489:ARG:HH21	1:A:496:LYS:HE2	1.80	0.47
1:A:558:PHE:HB2	1:A:563:TRP:NE1	2.30	0.47
1:A:529:PHE:HA	1:A:761:GLY:HA2	1.95	0.47
2:B:690:SER:HA	2:B:693:ARG:HB3	1.97	0.47
1:C:719:GLN:HG2	1:C:722:ARG:HH22	1.78	0.47
1:A:796:GLN:O	1:A:796:GLN:HG3	2.14	0.47
2:B:436:CYS:HB2	2:B:455:LYS:HB2	1.96	0.47
2:B:610:TRP:CZ2	4:B:901:A1AFT:BR28	3.22	0.47
1:C:558:PHE:HB2	1:C:563:TRP:NE1	2.30	0.47
2:D:408:ILE:HG12	2:D:476:TYR:HB2	1.95	0.47
2:D:464:ILE:HA	2:D:467:LYS:NZ	2.30	0.47
2:D:610:TRP:CZ2	4:D:901:A1AFT:BR28	3.21	0.47
2:D:772:TRP:HA	2:D:775:GLN:HE21	1.78	0.47
1:A:515:ALA:O	1:A:517:LEU:N	2.47	0.47
1:A:557:PRO:O	1:A:650:ASN:ND2	2.48	0.47
2:B:408:ILE:HB	2:B:478:LEU:HD23	1.96	0.47
2:B:613:VAL:O	2:B:643:LEU:HD21	2.14	0.47
1:C:400:ILE:HG12	1:C:512:MET:HB3	1.96	0.47
2:B:565:MET:HA	2:B:568:ILE:HG12	1.97	0.46
1:A:723:ASP:HB2	1:A:725:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:GLY:HA2	1:A:825:VAL:HG22	1.97	0.46
1:C:705:HIS:O	1:C:708:LYS:HG2	2.15	0.46
2:D:547:PRO:O	2:D:820:GLY:HA3	2.15	0.46
1:C:715:ALA:O	1:C:719:GLN:HG3	2.15	0.46
2:D:489:LYS:HB2	2:D:494:TRP:CZ3	2.50	0.46
2:D:682:ARG:N	2:D:727:ASP:OD1	2.49	0.46
2:B:433:THR:HA	2:B:458:LYS:HE2	1.97	0.46
2:B:772:TRP:HA	2:B:775:GLN:HE21	1.80	0.46
2:D:438:LYS:HB3	2:D:453:ILE:HD11	1.98	0.46
2:D:731:TYR:CG	2:D:732:ASP:N	2.84	0.46
1:A:693:PHE:HZ	1:A:730:ILE:HD12	1.81	0.46
2:B:693:ARG:O	2:B:693:ARG:NH1	2.36	0.46
2:B:693:ARG:HA	2:B:696:ARG:NE	2.31	0.46
2:B:731:TYR:CG	2:B:732:ASP:N	2.84	0.46
1:C:639:PHE:CD2	2:D:821:VAL:HG12	2.51	0.46
1:C:723:ASP:HB2	1:C:725:LYS:HE2	1.97	0.46
1:A:702:MET:HG2	1:A:706:MET:HE1	1.96	0.46
1:C:697:VAL:HG22	2:D:432:ASN:HD21	1.80	0.46
2:D:818:MET:HE3	2:D:818:MET:HB3	1.75	0.46
2:D:613:VAL:O	2:D:643:LEU:HD21	2.14	0.46
2:B:566:LEU:HD13	2:B:610:TRP:HE3	1.81	0.46
2:B:682:ARG:N	2:B:727:ASP:OD1	2.48	0.46
2:B:759:SER:O	1:C:780:HIS:ND1	2.49	0.45
2:D:563:PHE:O	2:D:567:LEU:HD23	2.15	0.45
2:D:693:ARG:HA	2:D:696:ARG:NE	2.31	0.45
1:A:764:LYS:HE3	2:D:774:ARG:HH21	1.81	0.45
2:D:479:TYR:OH	2:D:506:ALA:HB2	2.17	0.45
1:A:486:THR:HG22	1:A:691:ILE:HD11	1.99	0.45
2:D:477:ASP:N	2:D:477:ASP:OD1	2.48	0.45
1:A:605:SER:O	1:A:605:SER:OG	2.31	0.45
1:A:715:ALA:O	1:A:719:GLN:HG3	2.15	0.45
2:B:489:LYS:HB2	2:B:494:TRP:CZ3	2.52	0.45
1:A:816:VAL:HB	2:D:638:PHE:HD1	1.81	0.45
1:C:483:LYS:HG2	1:C:686:GLN:HB2	1.99	0.45
2:D:439:ARG:CZ	2:D:439:ARG:HA	2.47	0.45
1:A:665:THR:HA	1:A:750:GLY:HA2	1.98	0.45
2:B:626:THR:O	2:B:630:ILE:HG12	2.16	0.45
1:A:691:ILE:O	1:A:695:ARG:HB2	2.17	0.45
1:C:489:ARG:NH1	2:D:425:LEU:O	2.50	0.45
2:D:545:VAL:HG22	2:D:657:GLU:HG2	1.98	0.45
2:D:631:MET:HA	2:D:634:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LYS:HZ1	1:A:420:CYS:HB2	1.82	0.44
1:C:541:LEU:HD11	1:C:746:LEU:HB3	1.98	0.44
1:C:546:ILE:HG22	1:C:548:ARG:H	1.82	0.44
1:C:575:VAL:HG12	1:C:575:VAL:O	2.18	0.44
1:C:682:ALA:HB1	1:C:710:ASN:HA	2.00	0.44
2:D:602:ILE:HD12	2:D:602:ILE:H	1.82	0.44
4:D:901:A1AFT:C02	4:D:901:A1AFT:C29	2.95	0.44
2:B:409:VAL:HA	2:B:479:TYR:O	2.18	0.44
2:B:523:VAL:HG11	2:B:765:ALA:HB1	1.99	0.44
1:C:439:PRO:HG3	1:C:480:ALA:HA	2.00	0.44
1:A:398:LEU:HD12	1:A:472:PHE:CD2	2.53	0.44
2:B:440:ILE:HG22	2:B:451:GLY:N	2.32	0.44
2:B:779:ALA:O	2:B:782:GLN:HG2	2.17	0.44
4:B:901:A1AFT:C02	4:B:901:A1AFT:C29	2.95	0.44
1:C:822:GLY:HA2	1:C:825:VAL:HG22	2.00	0.44
2:D:626:THR:O	2:D:630:ILE:HG12	2.18	0.44
2:D:721:LEU:HD23	2:D:726:LEU:O	2.18	0.44
1:C:778:LYS:HA	1:C:781:GLU:HG2	1.98	0.44
2:B:781:LEU:O	1:C:521:ASN:ND2	2.46	0.44
1:C:440:ASN:HD22	1:C:447:PRO:HG3	1.83	0.44
2:D:565:MET:O	2:D:569:VAL:HG23	2.18	0.44
5:D:902:CLR:H8	5:D:902:CLR:H182	1.77	0.44
1:A:434:VAL:HG21	1:A:460:ILE:HD12	1.99	0.43
2:B:721:LEU:HD23	2:B:726:LEU:O	2.18	0.43
1:C:695:ARG:HD2	2:D:431:ARG:NH1	2.30	0.43
1:C:810:PHE:C	1:C:812:ASN:H	2.25	0.43
2:D:690:SER:HA	2:D:693:ARG:HB3	1.99	0.43
2:B:551:LEU:HD22	4:B:901:A1AFT:O19	2.18	0.43
4:D:901:A1AFT:O19	4:D:901:A1AFT:C23	2.66	0.43
1:A:695:ARG:O	2:B:431:ARG:NH2	2.44	0.43
2:B:738:TYR:CZ	2:B:742:ARG:HD2	2.53	0.43
4:B:901:A1AFT:O19	4:B:901:A1AFT:C23	2.66	0.43
1:C:699:LEU:HA	1:C:702:MET:HE1	2.00	0.43
1:C:655:LEU:C	1:C:657:LEU:H	2.24	0.43
2:D:679:PRO:HA	2:D:680:PRO:HD3	1.88	0.43
1:A:575:VAL:HG12	1:A:575:VAL:O	2.18	0.43
2:B:471:SER:OG	2:B:782:GLN:NE2	2.52	0.43
2:D:577:PHE:HE1	2:D:625:GLY:H	1.65	0.43
1:A:680:ILE:HG22	1:A:705:HIS:HE1	1.84	0.43
1:A:695:ARG:HD2	2:B:431:ARG:NH1	2.33	0.43
2:B:561:MET:HE3	2:B:561:MET:HB3	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:LEU:HD12	1:C:472:PHE:CD2	2.53	0.43
1:A:546:ILE:HG22	1:A:548:ARG:H	1.82	0.43
2:D:567:LEU:HD13	2:D:606:ILE:HD11	2.00	0.43
1:A:778:LYS:HA	1:A:781:GLU:HG2	2.00	0.43
2:D:465:LEU:HA	2:D:468:ILE:HG12	2.01	0.43
1:A:810:PHE:C	1:A:812:ASN:H	2.25	0.43
2:B:463:ASP:O	2:B:467:LYS:HG2	2.19	0.43
2:D:469:SER:HA	2:D:474:PHE:CE2	2.54	0.43
2:D:693:ARG:HH12	2:D:697:ASN:HB2	1.84	0.43
1:A:511:ASP:HA	1:A:763:ARG:HH12	1.83	0.43
2:B:818:MET:HB3	2:B:818:MET:HE3	1.74	0.43
2:D:663:VAL:HB	2:D:751:ILE:HD13	2.01	0.43
2:B:693:ARG:HH12	2:B:697:ASN:HB2	1.84	0.42
2:D:489:LYS:HD2	2:D:494:TRP:CZ2	2.54	0.42
2:B:472:VAL:HB	2:B:474:PHE:HD1	1.84	0.42
2:B:602:ILE:HD12	2:B:602:ILE:H	1.82	0.42
2:B:638:PHE:HD1	1:C:816:VAL:HB	1.83	0.42
1:C:434:VAL:HG21	1:C:460:ILE:HD12	2.00	0.42
1:C:511:ASP:HA	1:C:763:ARG:HH12	1.85	0.42
2:B:545:VAL:HG22	2:B:657:GLU:HG2	2.00	0.42
2:D:776:VAL:O	2:D:780:ILE:HG13	2.19	0.42
1:A:409:VAL:HG22	1:A:459:CYS:SG	2.60	0.42
2:B:469:SER:HA	2:B:474:PHE:CE1	2.55	0.42
2:B:477:ASP:OD1	2:B:477:ASP:N	2.51	0.42
1:C:405:GLN:H	1:C:409:VAL:HB	1.84	0.42
1:C:423:GLU:OE1	1:C:423:GLU:N	2.44	0.42
2:B:434:VAL:O	2:B:458:LYS:NZ	2.51	0.42
2:D:469:SER:HB2	2:D:470:LYS:NZ	2.35	0.42
2:D:504:LYS:C	2:D:506:ALA:H	2.28	0.42
2:B:831:LEU:O	2:B:835:THR:HG22	2.18	0.42
1:C:502:MET:HE1	1:C:523:ARG:HB3	2.01	0.42
1:C:680:ILE:HG22	1:C:705:HIS:HE1	1.85	0.42
1:A:502:MET:HE1	1:A:523:ARG:HB3	2.02	0.42
1:A:658:ASP:O	1:A:660:PRO:HD3	2.19	0.42
1:A:666:GLY:H	1:A:750:GLY:HA3	1.84	0.42
2:B:439:ARG:NH2	2:B:480:LEU:O	2.53	0.42
1:C:693:PHE:CD1	1:C:699:LEU:HD23	2.55	0.42
2:D:655:ILE:HD13	2:D:655:ILE:HG21	1.82	0.42
2:D:831:LEU:O	2:D:835:THR:HG22	2.19	0.42
1:A:436:CYS:HA	1:A:476:VAL:O	2.20	0.42
2:B:545:VAL:HG21	2:B:817:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:VAL:O	2:B:739:MET:HG2	2.20	0.42
1:C:576:MET:HE2	1:C:576:MET:HB3	1.69	0.42
2:B:516:ASN:HD21	2:B:519:ARG:HD2	1.85	0.41
2:B:668:ASP:OD2	2:B:670:LYS:HB3	2.19	0.41
2:D:537:MET:HG2	2:D:736:LEU:HD22	2.02	0.41
2:B:454:LYS:O	2:B:454:LYS:HD2	2.21	0.41
2:B:685:THR:OG1	2:B:686:VAL:N	2.53	0.41
1:C:470:MET:HE1	1:C:771:GLN:CG	2.50	0.41
1:C:691:ILE:O	1:C:695:ARG:N	2.50	0.41
2:D:550:PHE:HB3	2:D:654:MET:HE1	2.02	0.41
2:D:685:THR:OG1	2:D:686:VAL:N	2.53	0.41
2:D:721:LEU:HA	2:D:726:LEU:O	2.20	0.41
1:A:602:THR:HG23	1:A:605:SER:H	1.85	0.41
1:C:785:MET:HE2	1:C:785:MET:HB3	1.83	0.41
2:D:735:VAL:O	2:D:739:MET:HG2	2.19	0.41
2:D:440:ILE:HD12	2:D:440:ILE:HA	1.96	0.41
1:A:643:ILE:HD13	2:B:818:MET:CE	2.50	0.41
2:B:663:VAL:HB	2:B:751:ILE:HD13	2.03	0.41
2:D:668:ASP:OD2	2:D:670:LYS:HB3	2.21	0.41
1:A:697:VAL:HG22	2:B:432:ASN:HD21	1.85	0.41
1:C:755:ARG:HB2	1:C:755:ARG:CZ	2.51	0.41
2:D:654:MET:O	2:D:817:ASN:ND2	2.53	0.41
2:B:413:GLU:OE2	2:B:512:SER:HB2	2.20	0.41
2:B:504:LYS:C	2:B:506:ALA:H	2.28	0.41
2:B:650:LEU:HA	2:B:650:LEU:HD12	1.82	0.41
2:D:532:THR:OG1	2:D:732:ASP:OD1	2.39	0.41
2:B:428:THR:HA	2:B:454:LYS:NZ	2.35	0.41
2:B:834:ILE:HD13	2:B:834:ILE:HA	1.87	0.41
1:C:486:THR:H	1:C:499:ASN:ND2	2.19	0.41
1:C:627:PHE:HB3	2:D:839:GLU:OE2	2.20	0.41
2:D:430:MET:N	2:D:430:MET:HE2	2.36	0.41
2:D:495:ASN:OD1	2:D:496:GLY:N	2.52	0.41
2:D:544:THR:OG1	2:D:658:GLU:O	2.38	0.41
2:D:608:LEU:O	2:D:610:TRP:N	2.54	0.41
2:D:693:ARG:NH1	2:D:697:ASN:HB2	2.36	0.41
1:A:423:GLU:OE1	1:A:423:GLU:N	2.46	0.41
5:B:902:CLR:H191	5:B:902:CLR:H8	1.84	0.41
1:C:544:LYS:HB3	1:C:745:ASP:O	2.21	0.41
1:A:627:PHE:HB3	2:B:839:GLU:OE2	2.21	0.40
1:A:729:PHE:CE2	1:A:731:TRP:HB2	2.56	0.40
2:B:489:LYS:HD2	2:B:494:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:679:PRO:HA	2:B:680:PRO:HD3	1.87	0.40
2:B:723:THR:OG1	2:B:725:LYS:NZ	2.43	0.40
1:A:444:PRO:HB3	1:A:448:ARG:HA	2.03	0.40
1:C:706:MET:SD	1:C:706:MET:N	2.94	0.40
1:A:656:VAL:O	1:A:656:VAL:HG12	2.22	0.40
1:A:675:PRO:HG3	1:A:702:MET:HB2	2.02	0.40
2:B:705:TYR:O	2:B:708:LYS:HG2	2.22	0.40
1:C:643:ILE:HD13	1:C:643:ILE:HA	1.96	0.40
1:C:684:VAL:O	1:C:687:SER:OG	2.36	0.40
1:A:408:PHE:CG	1:A:516:PRO:HG3	2.56	0.40
1:A:608:TRP:CH2	3:A:901:POV:H217	2.57	0.40
2:B:670:LYS:HG2	2:B:681:PHE:CE2	2.57	0.40
1:C:407:PRO:CG	1:C:735:VAL:HA	2.52	0.40
2:D:566:LEU:HD13	2:D:610:TRP:HE3	1.85	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	422/847 (50%)	390 (92%)	32 (8%)	0	100	100
1	C	422/847 (50%)	392 (93%)	30 (7%)	0	100	100
2	B	417/862 (48%)	380 (91%)	37 (9%)	0	100	100
2	D	417/862 (48%)	382 (92%)	34 (8%)	1 (0%)	43	71
All	All	1678/3418 (49%)	1544 (92%)	133 (8%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	542	ASN

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	347/728 (48%)	347 (100%)	0	100	100
1	C	348/728 (48%)	348 (100%)	0	100	100
2	B	328/745 (44%)	328 (100%)	0	100	100
2	D	328/745 (44%)	328 (100%)	0	100	100
All	All	1351/2946 (46%)	1351 (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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	GLN
1	A	453	GLN
1	A	696	GLN
1	A	742	GLN
1	A	771	GLN
1	A	796	GLN
2	B	437	GLN
2	B	694	ASN
2	B	775	GLN
2	B	782	GLN
1	C	405	GLN
1	C	440	ASN
1	C	650	ASN
1	C	709	HIS
1	C	771	GLN
1	C	796	GLN
2	D	516	ASN
2	D	694	ASN
2	D	711	GLN
2	D	775	GLN
2	D	817	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
5	CLR	B	902	-	31,31,31	0.60	0	48,48,48	1.61	9 (18%)
4	A1AFT	B	901	-	31,32,32	0.82	1 (3%)	38,49,49	1.81	10 (26%)
4	A1AFT	D	901	-	31,32,32	0.82	1 (3%)	38,49,49	1.80	10 (26%)
3	POV	C	901	-	51,51,51	0.50	0	57,59,59	0.57	0
4	A1AFT	C	902	-	31,32,32	0.97	2 (6%)	38,49,49	1.27	6 (15%)
4	A1AFT	A	902	-	31,32,32	0.95	2 (6%)	38,49,49	1.28	6 (15%)
5	CLR	D	902	-	31,31,31	0.65	0	48,48,48	1.36	9 (18%)
3	POV	A	901	-	51,51,51	0.50	0	57,59,59	0.57	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
5	CLR	B	902	-	-	6/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1AFT	B	901	-	-	6/10/24/24	0/4/4/4
4	A1AFT	D	901	-	-	6/10/24/24	0/4/4/4
3	POV	C	901	-	-	21/55/55/55	-
4	A1AFT	C	902	-	-	1/10/24/24	0/4/4/4
4	A1AFT	A	902	-	-	0/10/24/24	0/4/4/4
5	CLR	D	902	-	-	5/10/68/68	0/4/4/4
3	POV	A	901	-	-	21/55/55/55	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	902	A1AFT	F14-C12	-3.06	1.37	1.43
4	C	902	A1AFT	C13-C12	-3.03	1.48	1.51
4	A	902	A1AFT	F14-C12	-3.02	1.37	1.43
4	A	902	A1AFT	C13-C12	-2.90	1.49	1.51
4	D	901	A1AFT	F14-C12	-2.62	1.38	1.43
4	B	901	A1AFT	F14-C12	-2.61	1.38	1.43

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	902	CLR	C10-C9-C8	-4.54	106.09	112.71
4	B	901	A1AFT	C09-C08-N07	4.12	116.30	110.73
5	B	902	CLR	C13-C17-C20	4.08	125.79	119.50
4	D	901	A1AFT	C09-C08-N07	4.05	116.20	110.73
4	D	901	A1AFT	C15-C12-C11	-3.90	86.22	89.54
4	B	901	A1AFT	C15-C12-C11	-3.89	86.22	89.54
5	B	902	CLR	C17-C13-C14	-3.59	95.98	100.10
4	D	901	A1AFT	C13-C12-C11	-3.57	112.06	115.67
4	B	901	A1AFT	C13-C12-C11	-3.56	112.07	115.67
4	B	901	A1AFT	C06-C05-C20	-3.49	116.09	118.12
4	D	901	A1AFT	C06-C05-C20	-3.40	116.14	118.12
4	B	901	A1AFT	N07-C17-N18	-3.36	123.17	126.45
4	D	901	A1AFT	N07-C17-N18	-3.26	123.27	126.45
5	B	902	CLR	C21-C20-C17	-3.10	108.24	112.88
4	D	901	A1AFT	C08-N07-C17	3.06	122.56	119.55
4	B	901	A1AFT	C08-N07-C17	3.00	122.50	119.55
5	D	902	CLR	C21-C20-C17	2.99	117.38	112.88
5	D	902	CLR	C8-C7-C6	-2.96	108.67	112.76
5	B	902	CLR	C14-C8-C9	2.90	112.87	109.09
4	B	901	A1AFT	C11-N10-C15	-2.83	92.65	95.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	A1AFT	C08-C09-N10	2.83	120.48	117.04
5	D	902	CLR	C1-C10-C5	-2.83	103.86	108.74
4	D	901	A1AFT	C11-N10-C15	-2.79	92.69	95.12
4	C	902	A1AFT	C08-C09-N10	2.78	120.41	117.04
5	B	902	CLR	C1-C10-C9	2.69	112.30	108.74
5	B	902	CLR	C12-C13-C14	-2.66	103.27	107.25
4	C	902	A1AFT	C17-N07-C06	-2.66	121.16	123.06
5	D	902	CLR	C13-C14-C8	-2.63	110.68	114.41
5	D	902	CLR	C13-C17-C20	2.63	123.56	119.50
4	A	902	A1AFT	C17-N07-C06	-2.62	121.19	123.06
4	C	902	A1AFT	N07-C17-N18	-2.58	123.93	126.45
4	A	902	A1AFT	N07-C17-N18	-2.56	123.95	126.45
4	D	901	A1AFT	C08-N07-C06	-2.52	115.53	117.38
5	D	902	CLR	C11-C9-C8	-2.48	108.31	111.78
4	B	901	A1AFT	C08-N07-C06	-2.46	115.57	117.38
5	D	902	CLR	C9-C10-C5	2.45	113.24	109.65
5	D	902	CLR	C12-C13-C14	-2.31	103.78	107.25
4	D	901	A1AFT	C04-C05-C20	-2.30	111.77	113.31
4	B	901	A1AFT	C04-C05-C20	-2.29	111.77	113.31
5	D	902	CLR	C1-C10-C9	2.28	111.75	108.74
4	A	902	A1AFT	C13-C12-C11	2.24	117.93	115.67
4	C	902	A1AFT	C13-C12-C11	2.20	117.89	115.67
5	B	902	CLR	C11-C12-C13	-2.18	109.06	112.74
4	A	902	A1AFT	C04-C05-C20	-2.15	111.87	113.31
4	C	902	A1AFT	C04-C05-C20	-2.14	111.87	113.31
4	C	902	A1AFT	C09-C08-N07	2.13	113.61	110.73
4	D	901	A1AFT	C02-C03-S21	-2.08	114.18	119.02
5	B	902	CLR	C22-C20-C17	2.08	114.64	110.33
4	B	901	A1AFT	C02-C03-S21	-2.07	114.21	119.02
4	A	902	A1AFT	C09-C08-N07	2.02	113.47	110.73

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	POV	C1-O11-P-O14
3	A	901	POV	O12-C11-C12-N
3	A	901	POV	C22-C21-O21-C2
3	C	901	POV	C1-O11-P-O14
3	C	901	POV	O12-C11-C12-N
3	C	901	POV	C22-C21-O21-C2
4	B	901	A1AFT	C09-C08-N07-C17

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Mol	Chain	Res	Type	Atoms
4	B	901	A1AFT	C09-C08-N07-C06
4	D	901	A1AFT	C09-C08-N07-C17
4	D	901	A1AFT	C09-C08-N07-C06
3	A	901	POV	O22-C21-O21-C2
3	C	901	POV	O22-C21-O21-C2
5	B	902	CLR	C13-C17-C20-C21
4	D	901	A1AFT	C05-C04-C22-C23
4	B	901	A1AFT	C05-C04-C22-C23
5	B	902	CLR	C13-C17-C20-C22
5	B	902	CLR	C16-C17-C20-C21
4	D	901	A1AFT	C05-C04-C22-C29
4	B	901	A1AFT	C05-C04-C22-C29
3	A	901	POV	C32-C31-O31-C3
5	D	902	CLR	C22-C23-C24-C25
3	C	901	POV	C32-C31-O31-C3
3	C	901	POV	O32-C31-O31-C3
3	A	901	POV	O32-C31-O31-C3
3	A	901	POV	C34-C35-C36-C37
3	C	901	POV	C34-C35-C36-C37
3	A	901	POV	C26-C27-C28-C29
3	C	901	POV	C26-C27-C28-C29
4	B	901	A1AFT	C03-C04-C22-C23
4	B	901	A1AFT	C03-C04-C22-C29
4	D	901	A1AFT	C03-C04-C22-C23
4	D	901	A1AFT	C03-C04-C22-C29
5	D	902	CLR	C21-C20-C22-C23
5	D	902	CLR	C13-C17-C20-C21
3	A	901	POV	C313-C314-C315-C316
3	C	901	POV	C313-C314-C315-C316
3	C	901	POV	C24-C25-C26-C27
5	D	902	CLR	C16-C17-C20-C22
3	A	901	POV	C23-C24-C25-C26
4	C	902	A1AFT	C09-C08-N07-C17
3	C	901	POV	C310-C311-C312-C313
3	A	901	POV	C1-C2-C3-O31
3	C	901	POV	C1-C2-C3-O31
5	B	902	CLR	C23-C24-C25-C27
3	A	901	POV	C310-C311-C312-C313
3	A	901	POV	C311-C312-C313-C314
3	C	901	POV	C311-C312-C313-C314
3	C	901	POV	C23-C24-C25-C26
3	A	901	POV	C24-C25-C26-C27

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Continued from previous page...

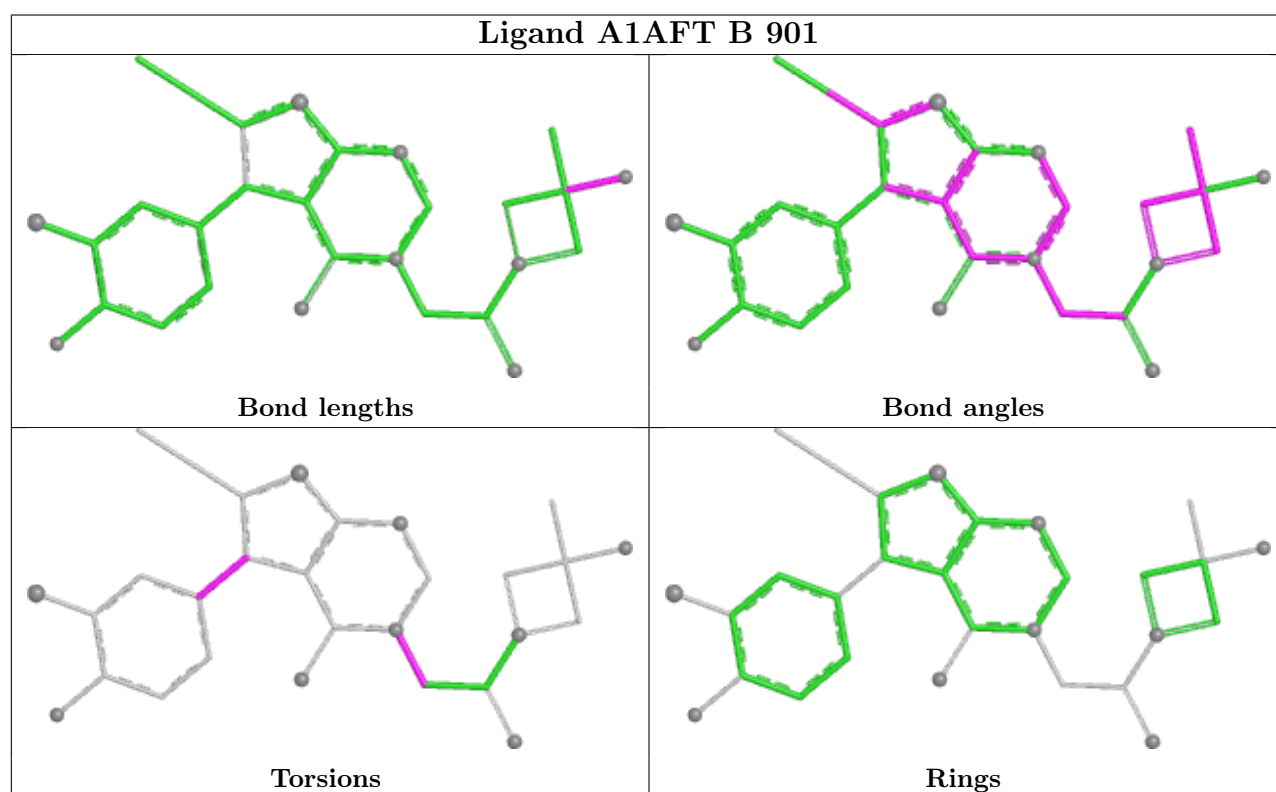
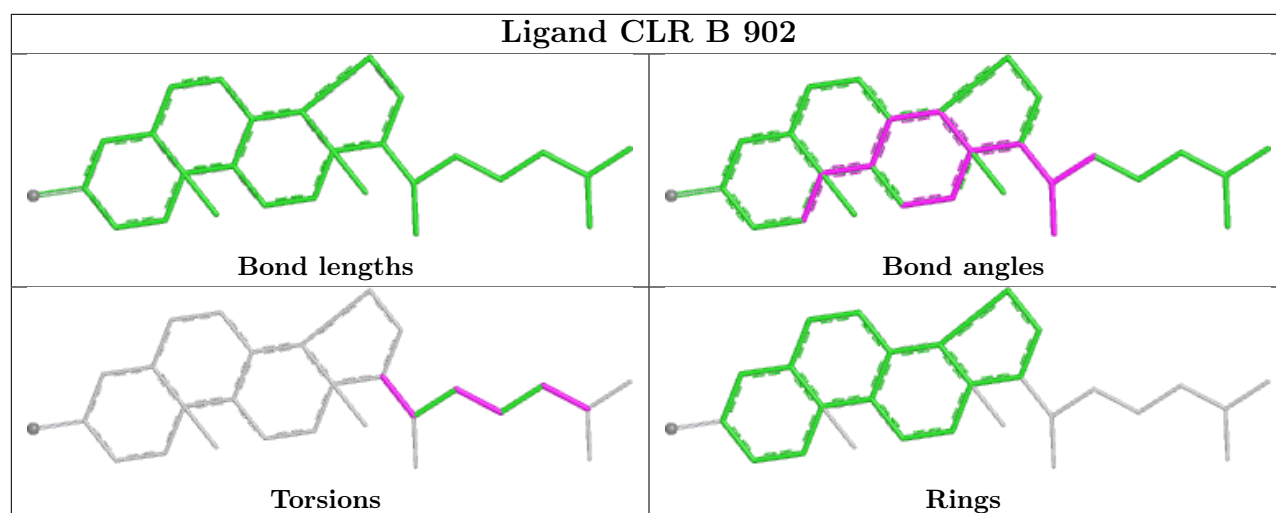
Mol	Chain	Res	Type	Atoms
3	A	901	POV	C1-O11-P-O12
3	C	901	POV	C1-O11-P-O12
3	A	901	POV	C3-C2-O21-C21
3	C	901	POV	C3-C2-O21-C21
3	A	901	POV	C22-C23-C24-C25
5	B	902	CLR	C20-C22-C23-C24
3	A	901	POV	C210-C211-C212-C213
3	C	901	POV	C22-C23-C24-C25
3	C	901	POV	O11-C1-C2-O21
3	C	901	POV	C311-C310-C39-C38
3	A	901	POV	C311-C310-C39-C38
5	B	902	CLR	C23-C24-C25-C26
3	A	901	POV	O11-C1-C2-O21
3	A	901	POV	C32-C33-C34-C35
3	C	901	POV	C210-C211-C212-C213
3	C	901	POV	C32-C33-C34-C35
5	D	902	CLR	C16-C17-C20-C21

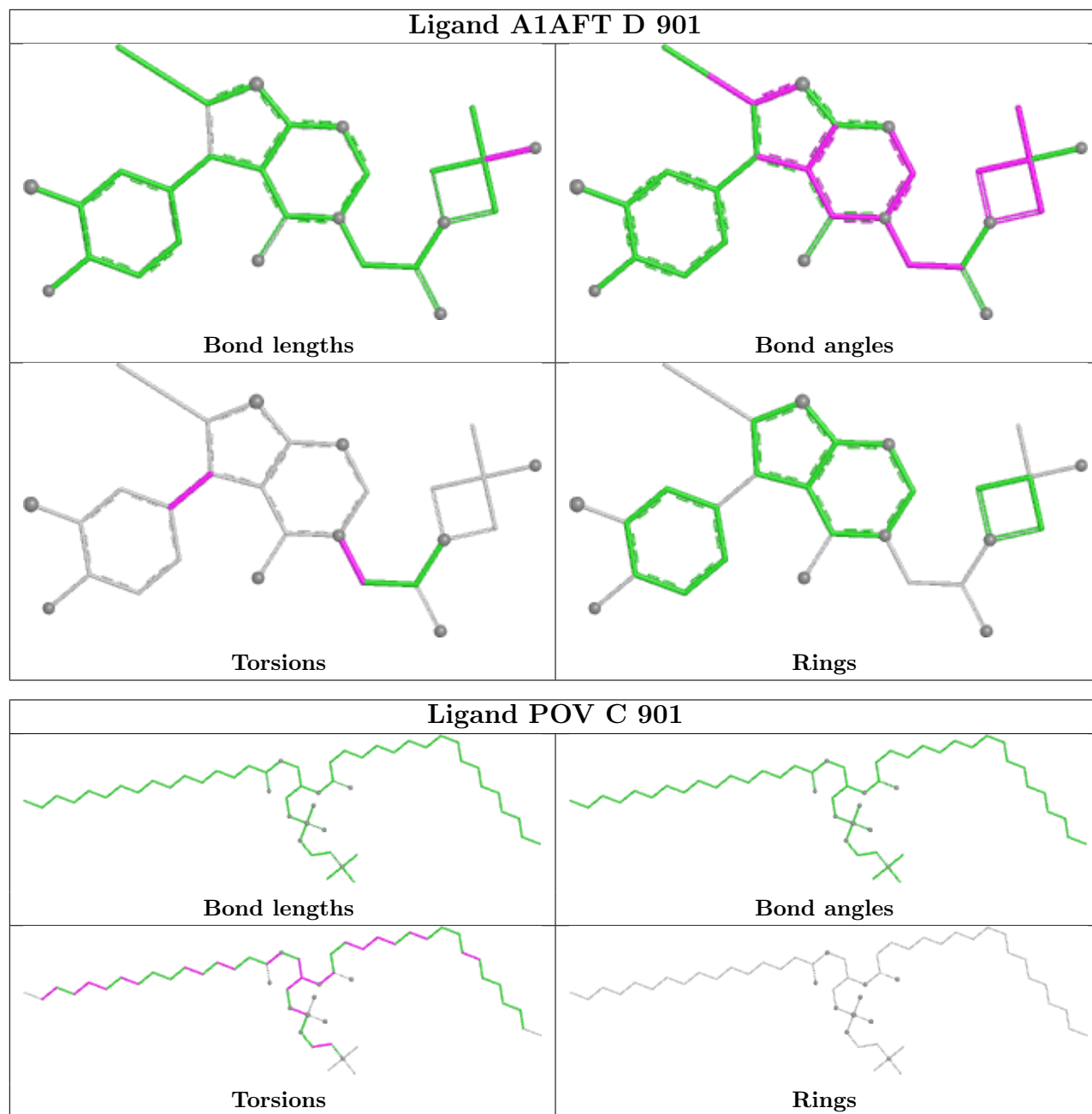
There are no ring outliers.

6 monomers are involved in 18 short contacts:

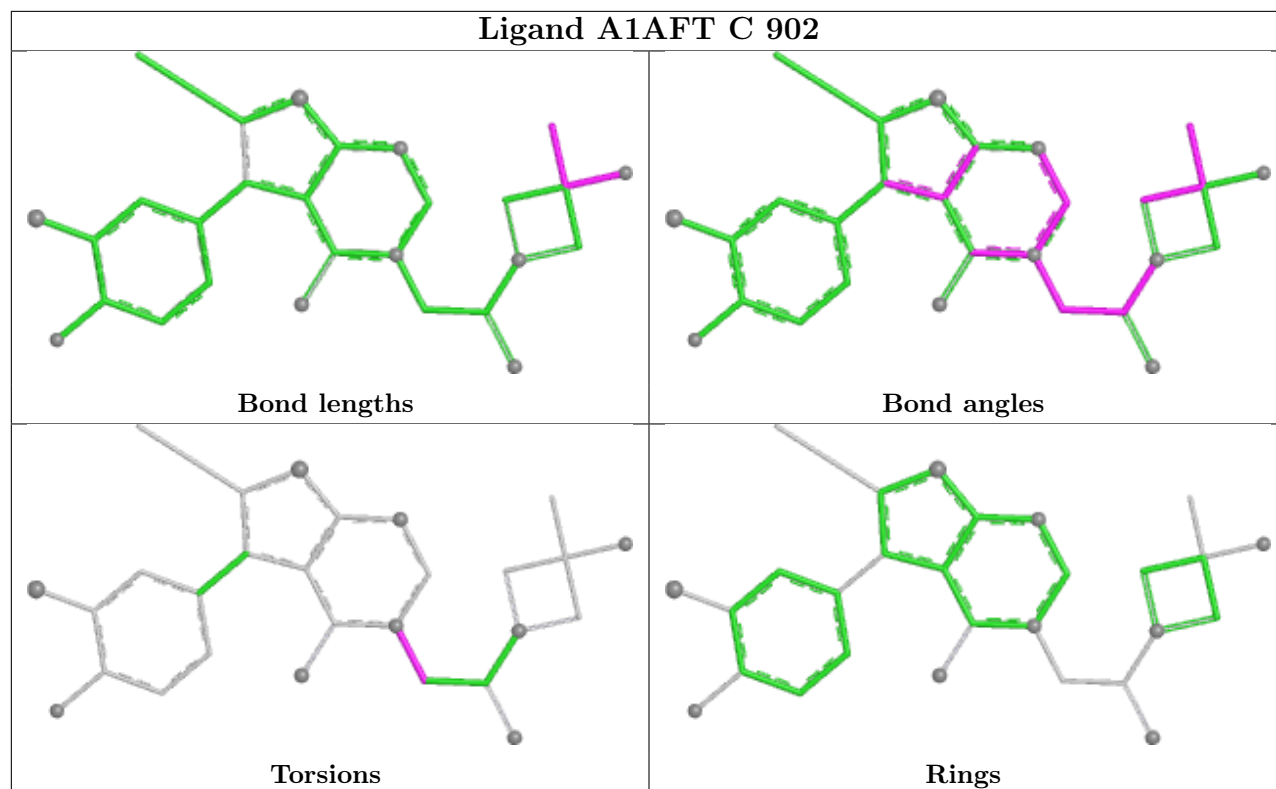
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	CLR	2	0
4	B	901	A1AFT	5	0
4	D	901	A1AFT	5	0
3	C	901	POV	1	0
5	D	902	CLR	3	0
3	A	901	POV	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

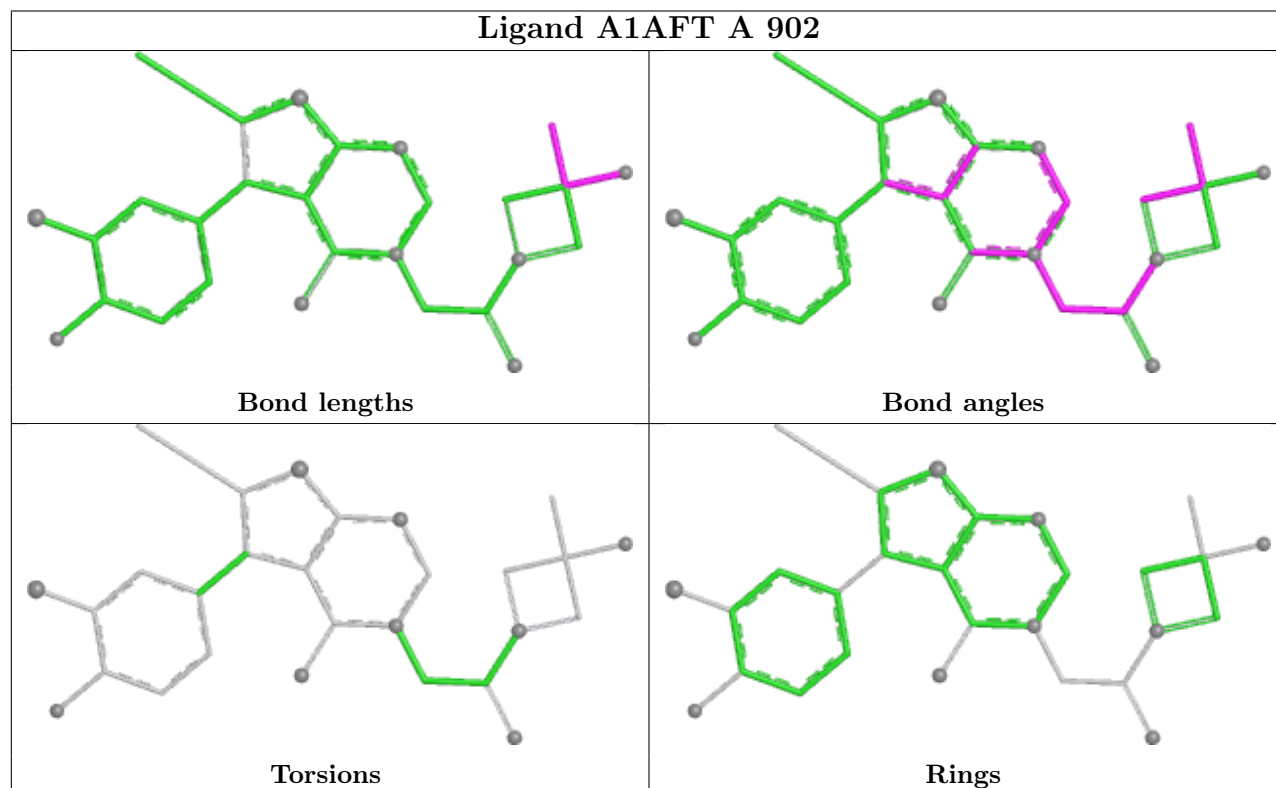


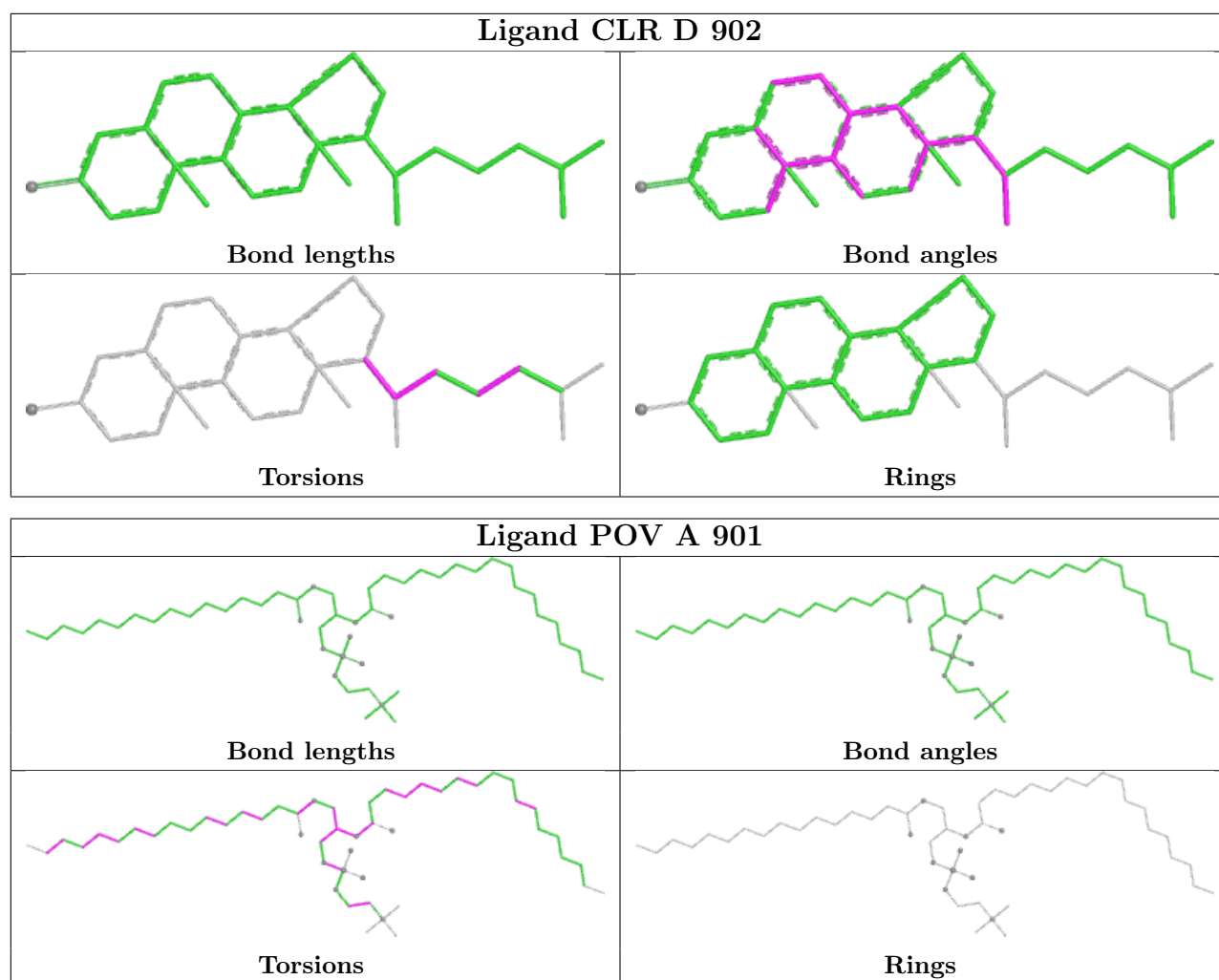


Ligand A1AFT C 902



Ligand A1AFT A 902





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.

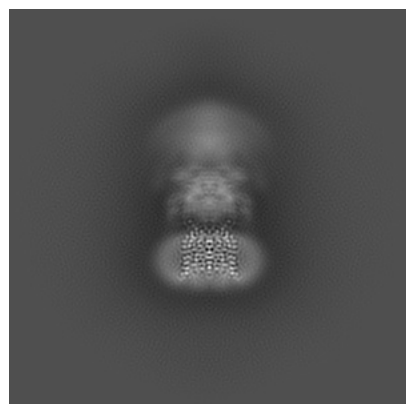
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70673. These allow visual inspection of the internal detail of the map and identification of artifacts.

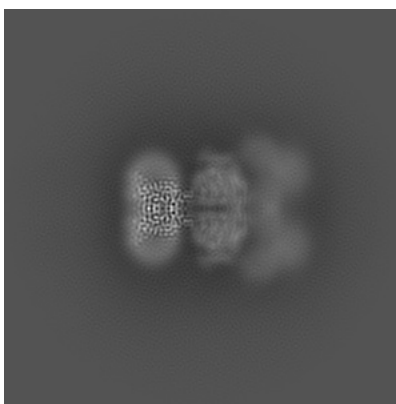
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

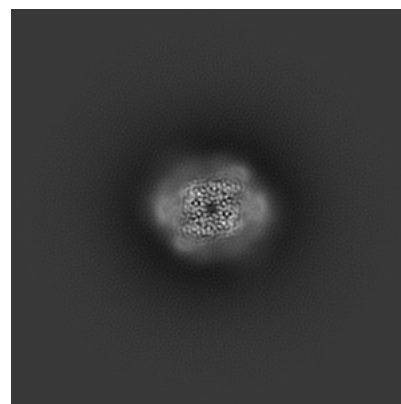
6.1.1 Primary map



X

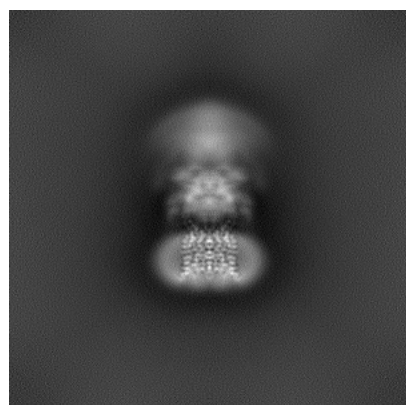


Y

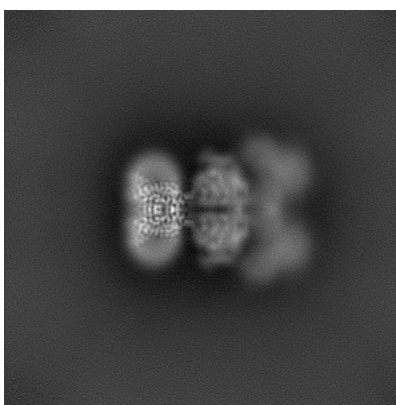


Z

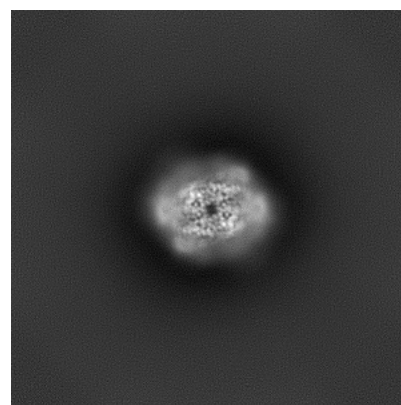
6.1.2 Raw map



X



Y

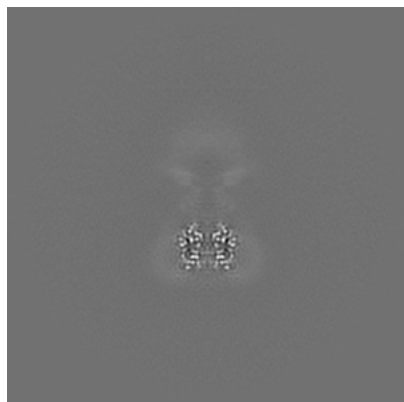


Z

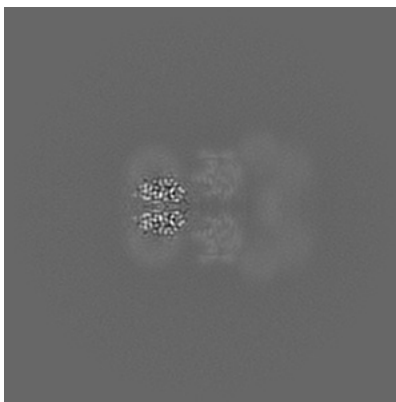
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

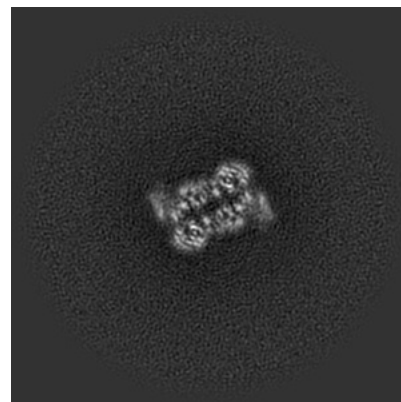
6.2.1 Primary map



X Index: 220

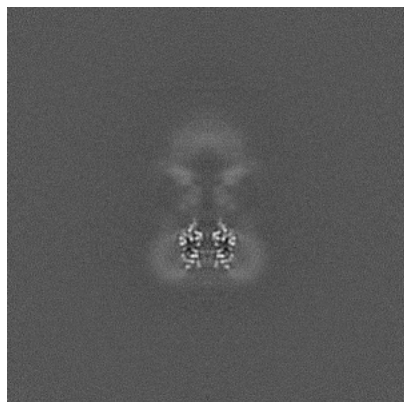


Y Index: 220

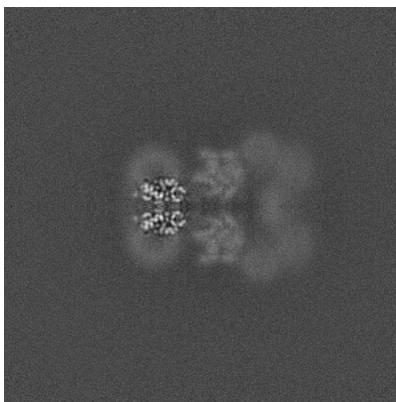


Z Index: 220

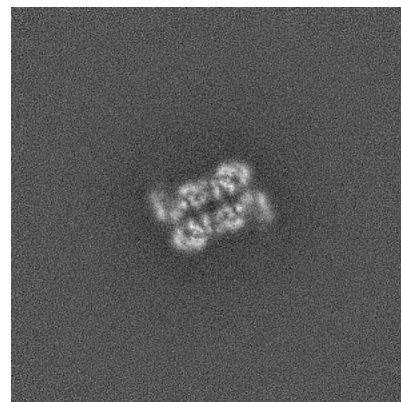
6.2.2 Raw map



X Index: 220



Y Index: 220

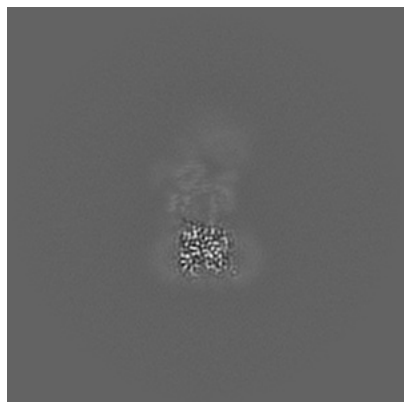


Z Index: 220

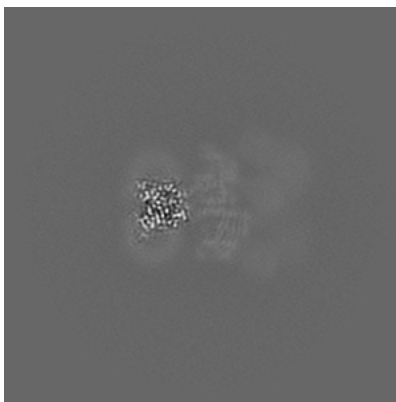
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

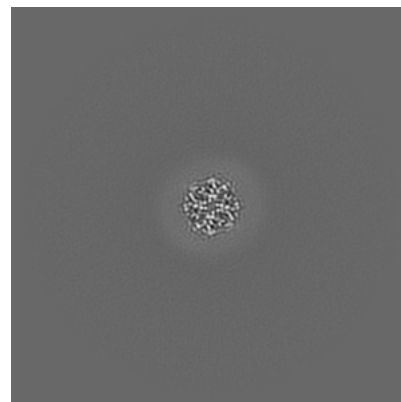
6.3.1 Primary map



X Index: 210



Y Index: 206

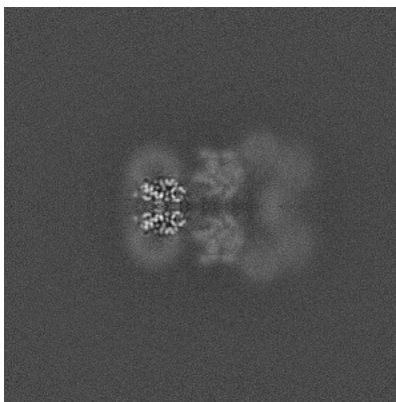


Z Index: 184

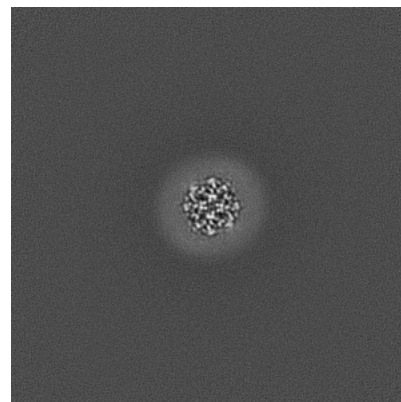
6.3.2 Raw map



X Index: 230



Y Index: 220

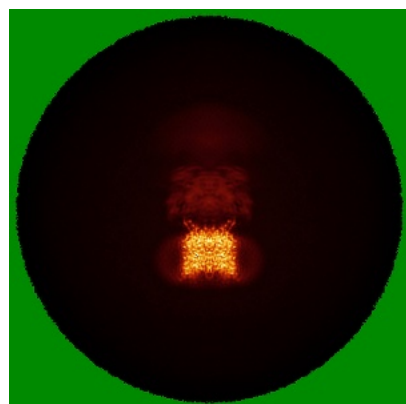


Z Index: 185

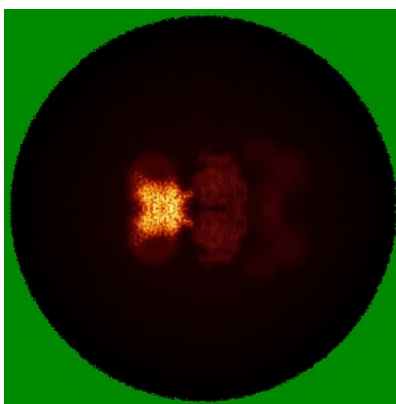
The images above show the largest variance slices of the map in three orthogonal directions.

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

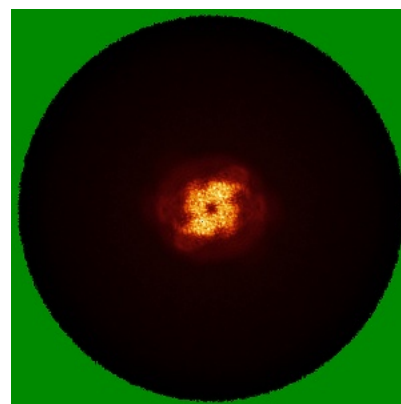
6.4.1 Primary map



X

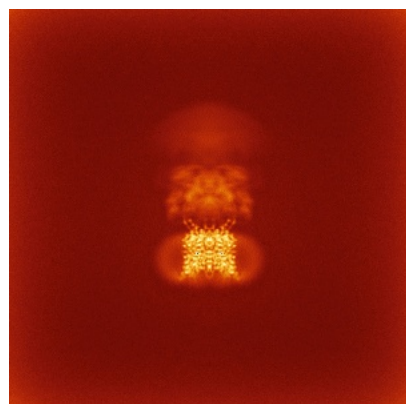


Y

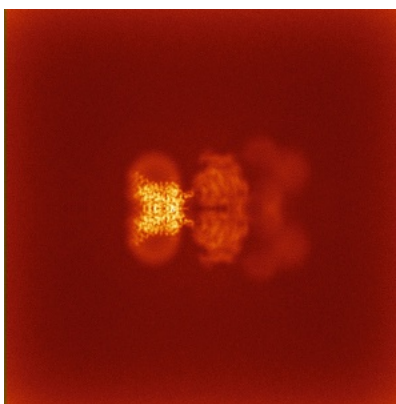


Z

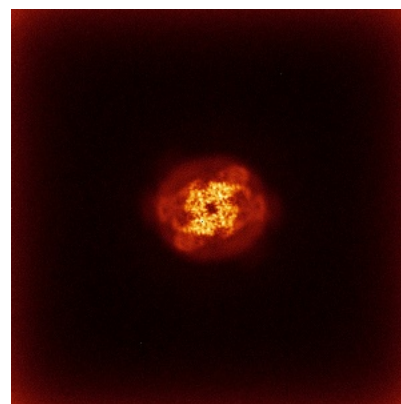
6.4.2 Raw map



X



Y

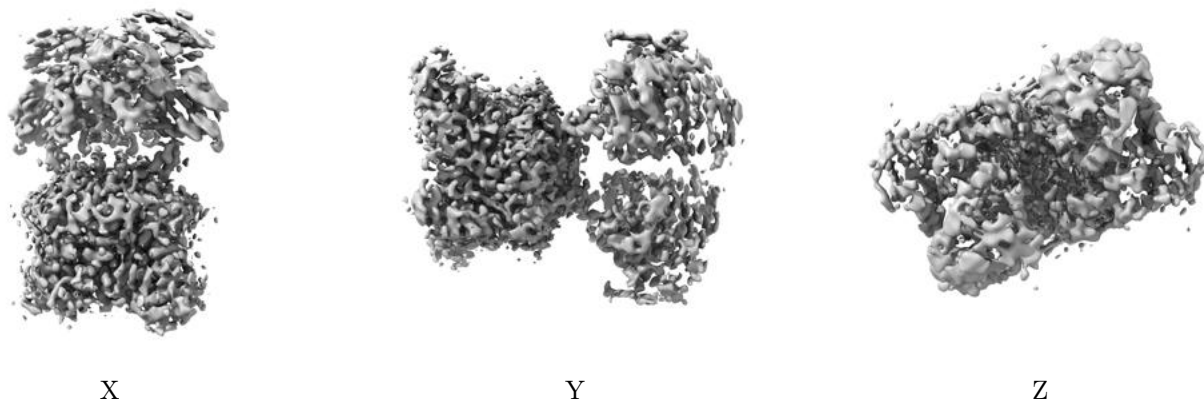


Z

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.

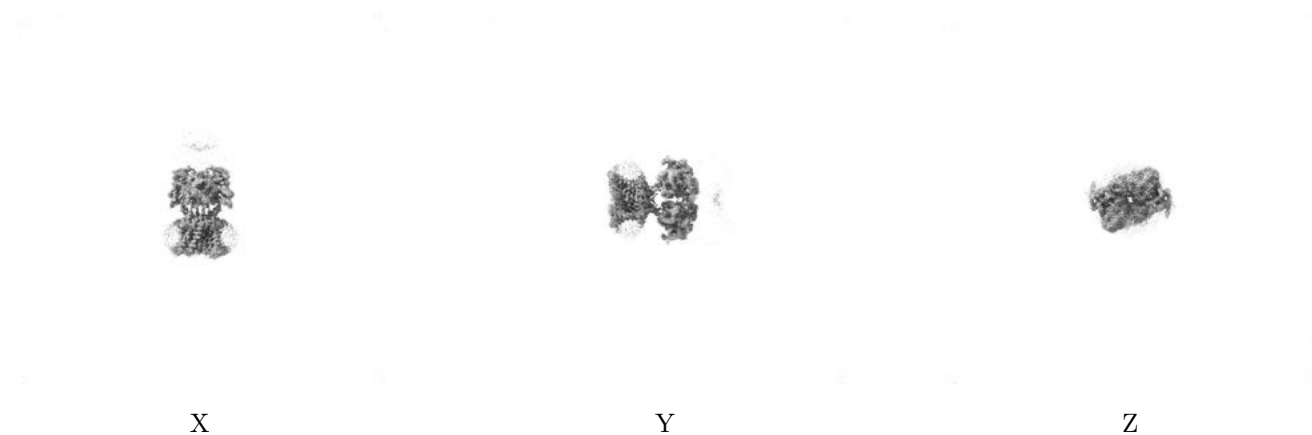
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.101. 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.

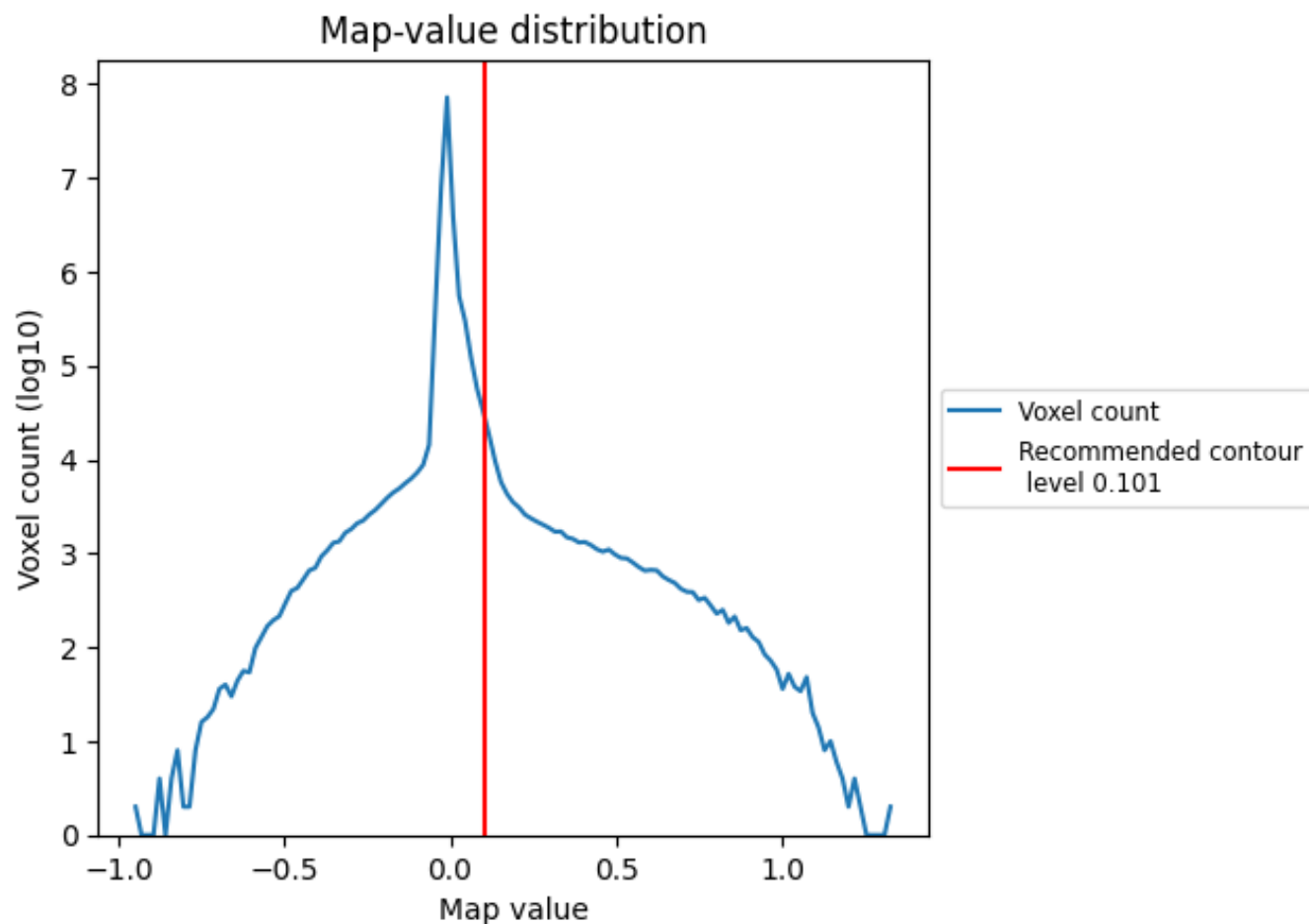
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

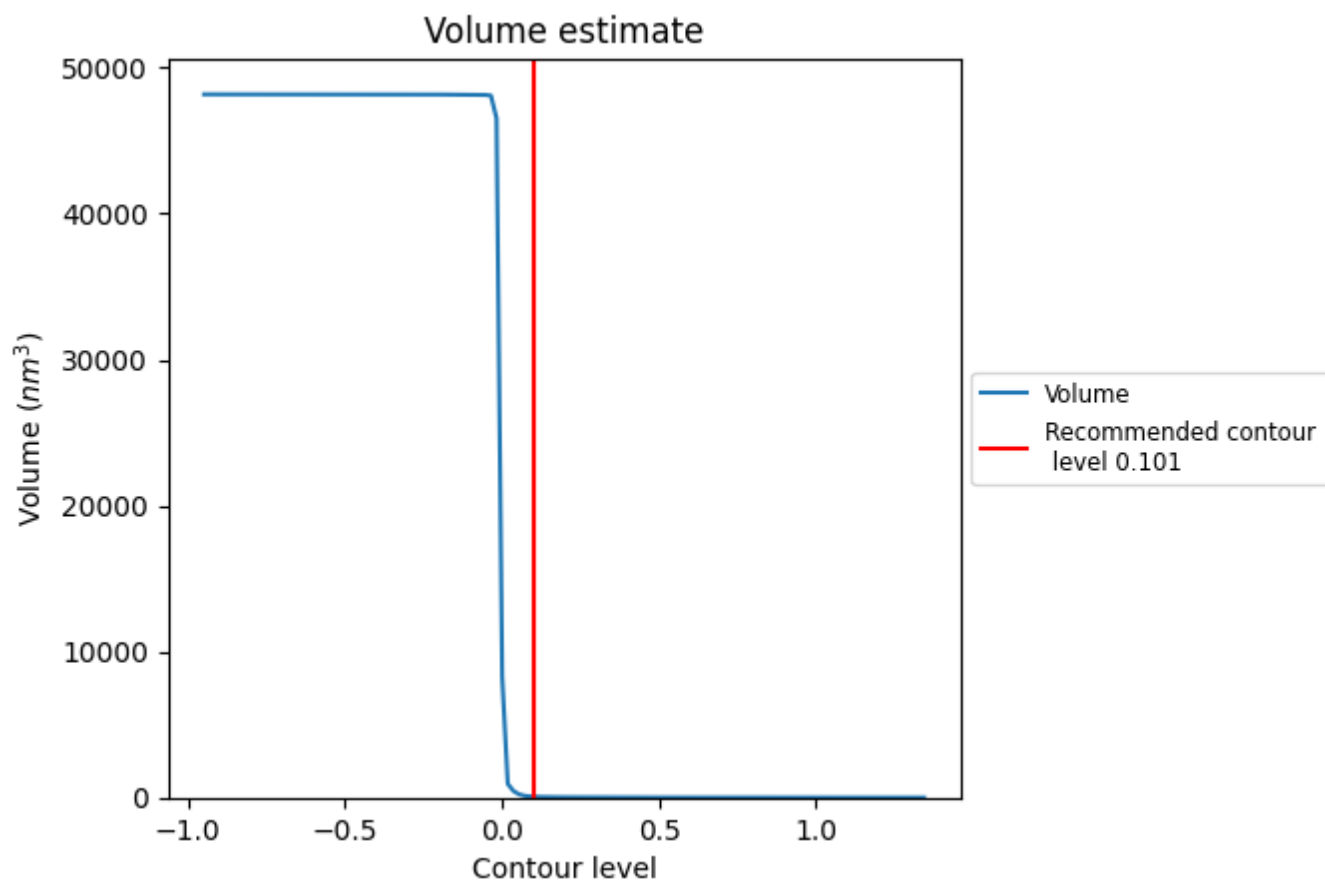
This section contains the results of statistical analysis of the map.

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.

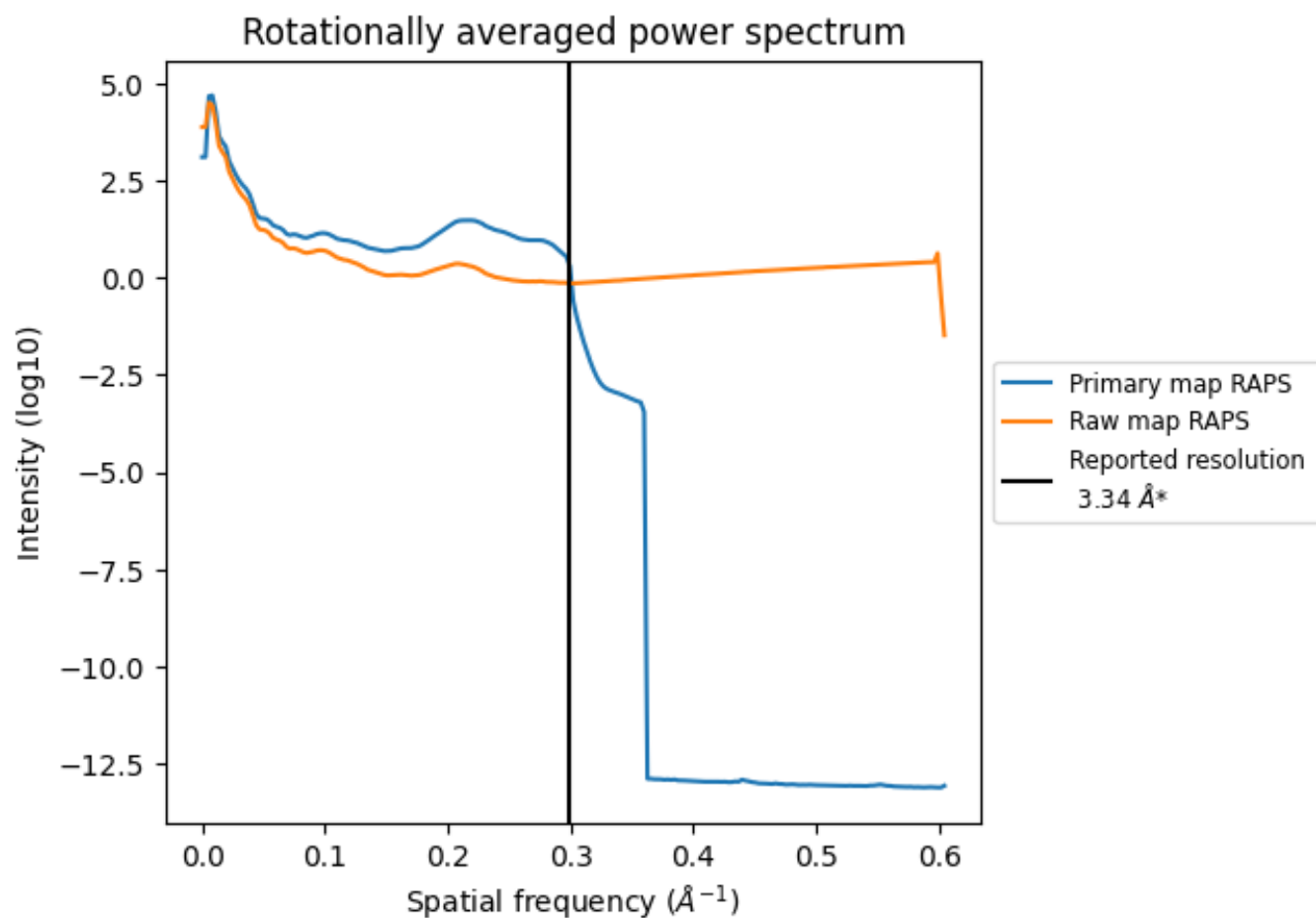
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm³; this corresponds to an approximate mass of 57 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 ⓘ

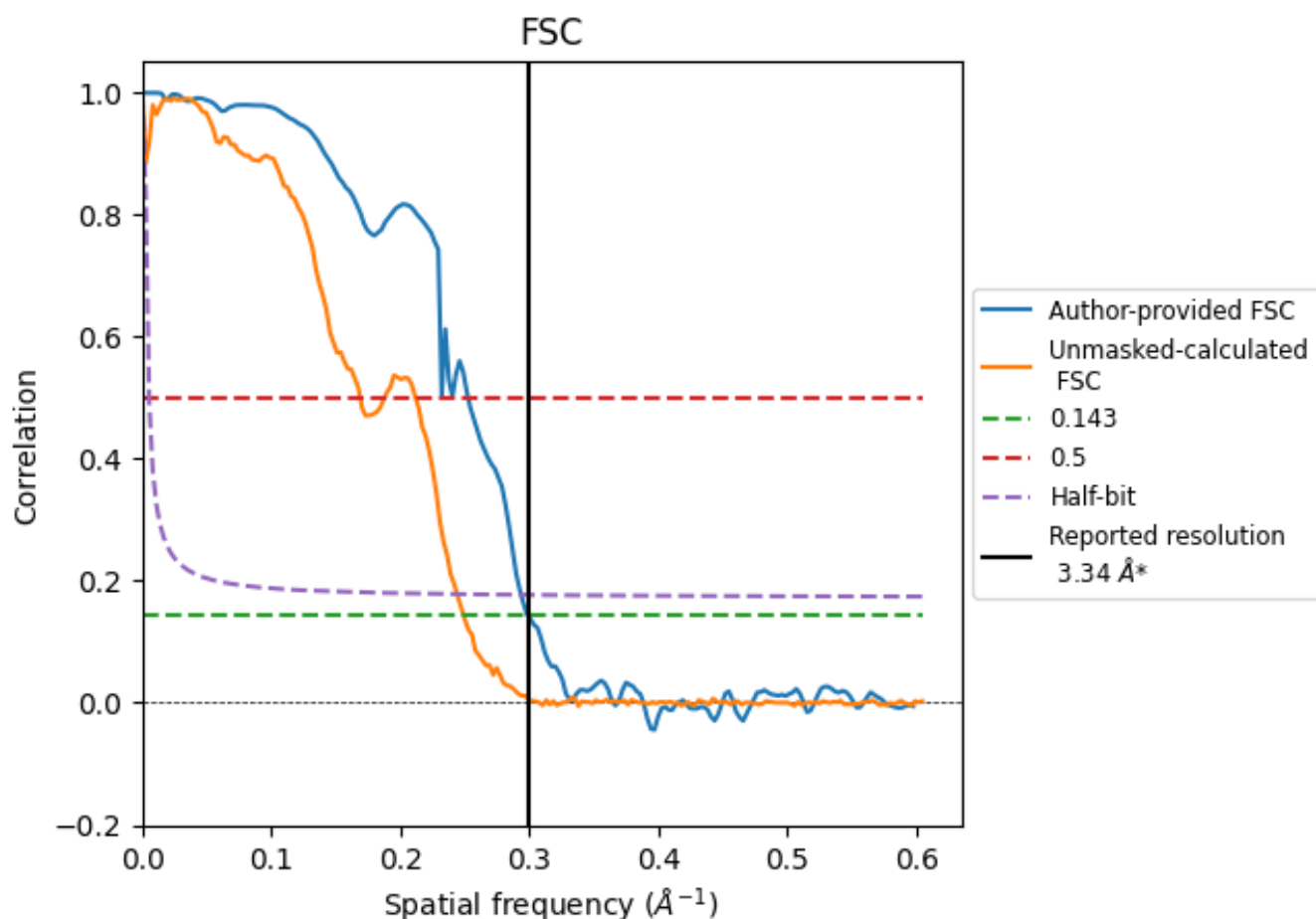


*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

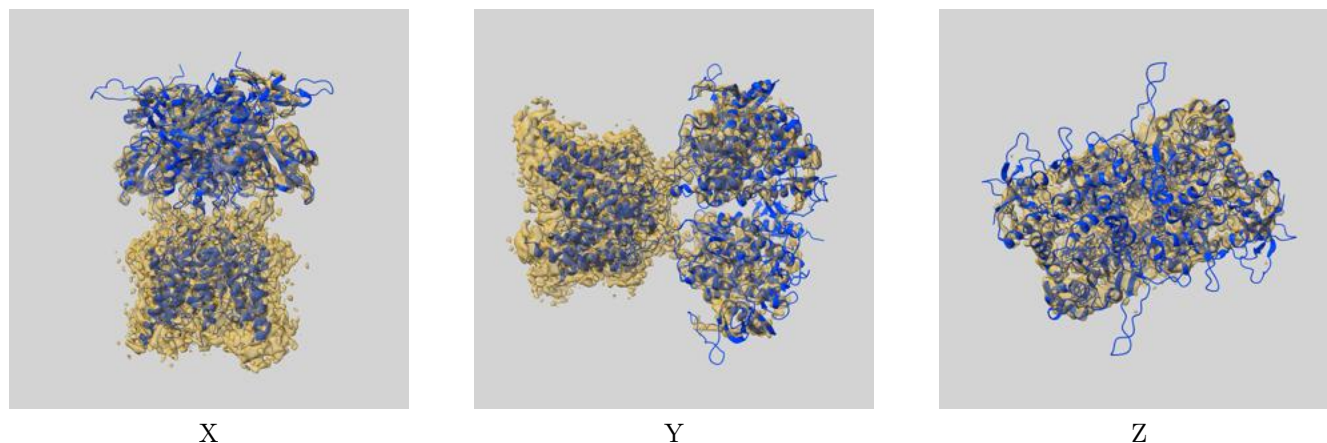
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	3.96	3.40
Unmasked-calculated*	4.01	5.92	4.10

*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 4.01 differs from the reported value 3.34 by more than 10 %

9 Map-model fit [i](#)

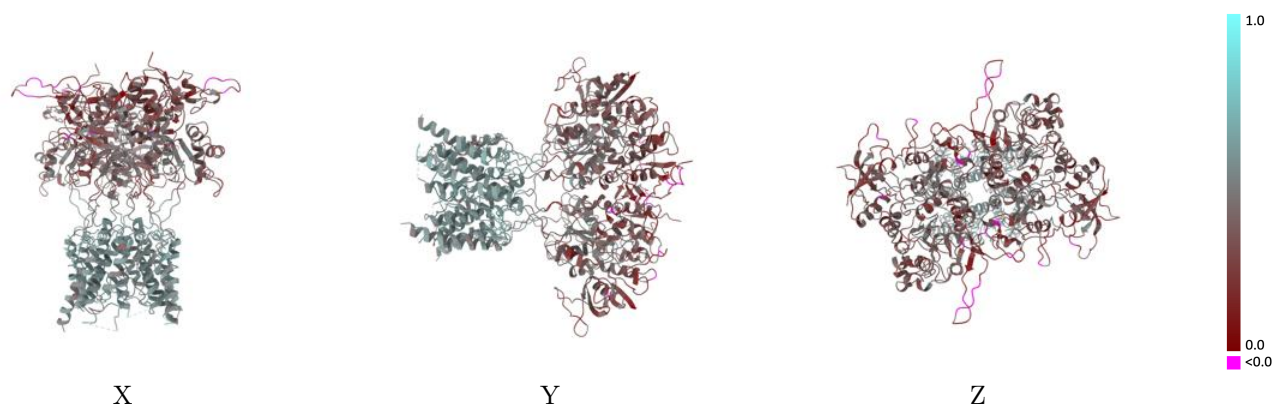
This section contains information regarding the fit between EMDB map EMD-70673 and PDB model 90OU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



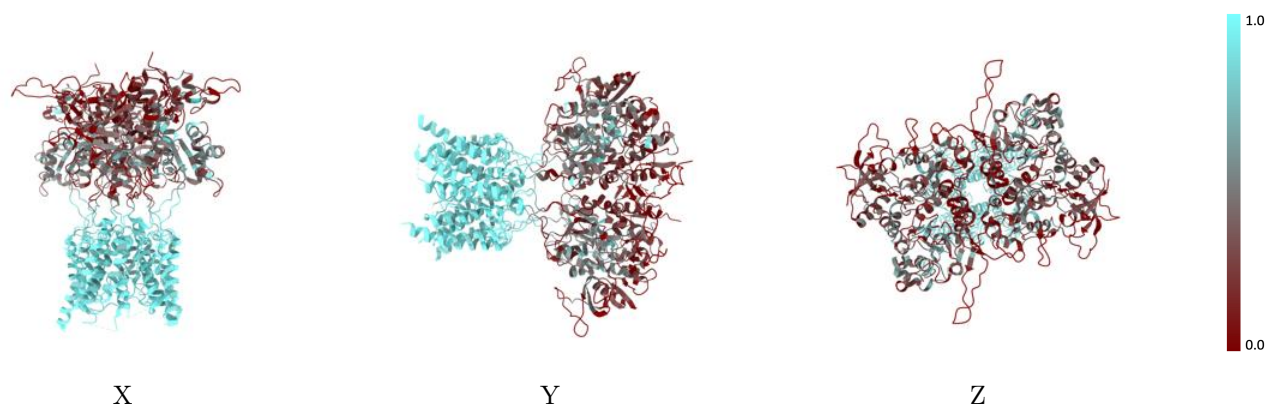
The images above show the 3D surface view of the map at the recommended contour level 0.101 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



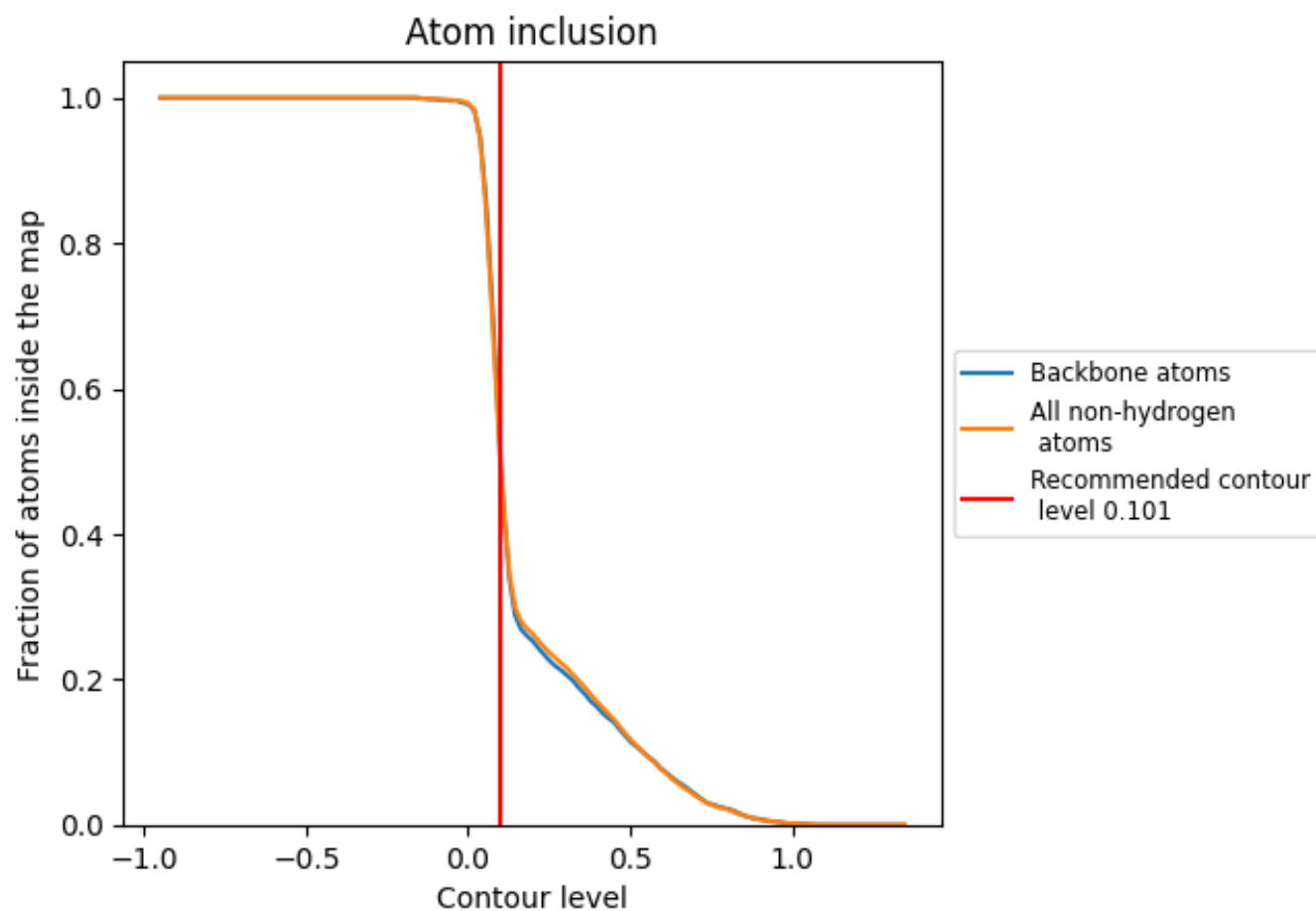
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.101).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 48% 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 (0.101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4840	0.4060
A	0.4720	0.4060
B	0.5030	0.4030
C	0.4740	0.4100
D	0.5010	0.4050

