



Full wwPDB EM Validation Report ⓘ

Sep 23, 2025 – 05:20 am BST

PDB ID : 9QPW / pdb_00009qpw
EMDB ID : EMD-53285
Title : GluA4, resting state, structure of TMD/LBD
Authors : Vega-Gutierrez, C.; Herguedas, B.
Deposited on : 2025-03-29
Resolution : 3.80 Å(reported)
Based on initial models : ., 3UA8

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.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

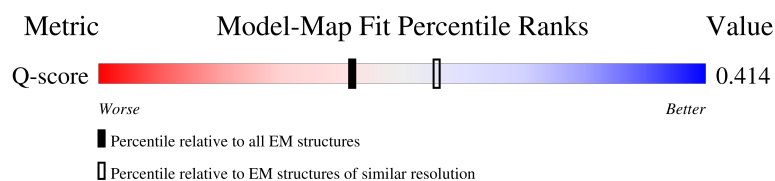
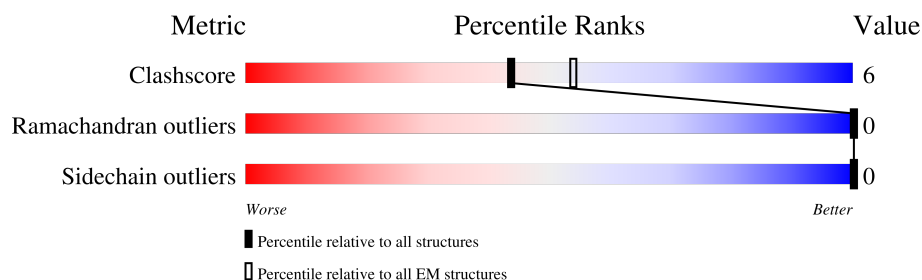
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	882	
1	B	882	
1	C	882	
1	D	882	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12030 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.

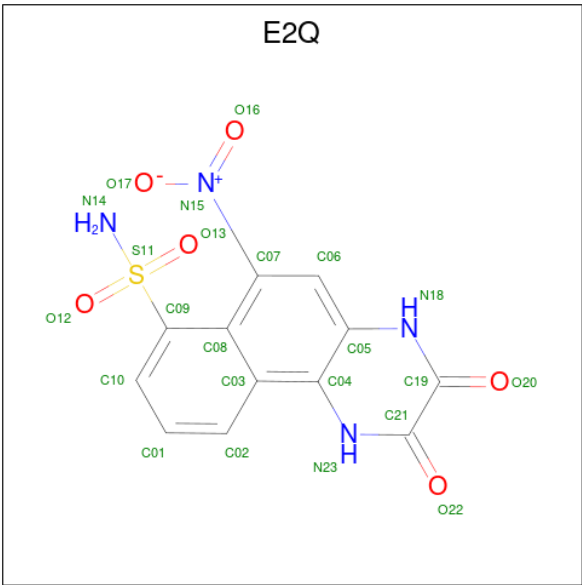
- Molecule 1 is a protein called Isoform 2 of Glutamate receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	388	Total	C	N	O	S	1	0
			3020	1970	482	549	19		
1	B	379	Total	C	N	O	S	0	0
			2949	1920	473	538	18		
1	D	379	Total	C	N	O	S	0	0
			2949	1920	473	538	18		
1	C	388	Total	C	N	O	S	1	0
			3020	1970	482	549	19		

There are 4 discrepancies between the modelled and reference sequences:

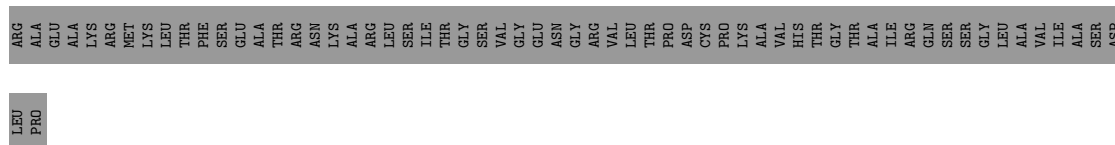
Chain	Residue	Modelled	Actual	Comment	Reference
A	734	ILE	THR	variant	UNP P19493
B	734	ILE	THR	variant	UNP P19493
D	734	ILE	THR	variant	UNP P19493
C	734	ILE	THR	variant	UNP P19493

- Molecule 2 is 6-nitro-2,3-bis(oxidanylidene)-1,4-dihydrobenzo[f]quinoxaline-7-sulfonamide (CCD ID: E2Q) (formula: C₁₂H₈N₄O₆S) (labeled as "Ligand of Interest" by depositor).

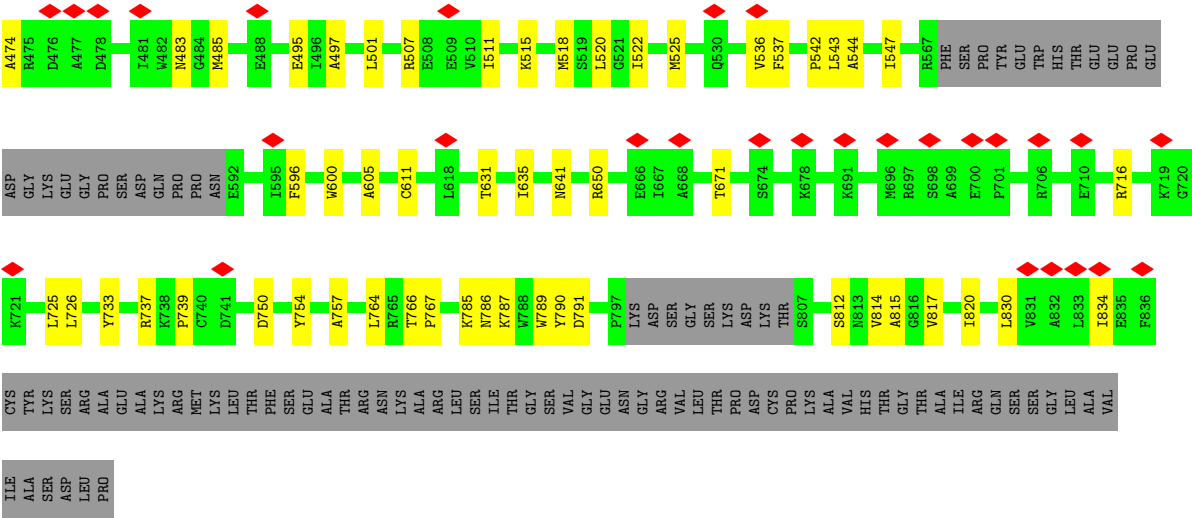


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			23	12	4	6	1	
2	B	1	Total	C	N	O	S	0
			23	12	4	6	1	
2	D	1	Total	C	N	O	S	0
			23	12	4	6	1	
2	C	1	Total	C	N	O	S	0
			23	12	4	6	1	

ASP	ILE	ASP	GLY	LEU	LEU	ALA	ASN	GLY
SER	PHE	ASP	PHE	ASP	LEU	LEU	ALA	ALA
ARG	GLN	ARG	ARG	GLN	SER	SER	PHE	PHE
VAL	VAL	ARG	VAL	GLN	LEU	LEU	CYS	PRO
GLY	ASP	GLY	ASP	GLU	LEU	LEU	GLN	SER
ASN	PHE	LYS	PHE	LYS	ASP	ASP	TYR	VAL
ALA	ALA	LYS	ASN	LYS	HIS	HIS	ASN	GLN
GLY	THR	PHE	THR	PHE	TYR	TYR	ARG	SER
ASP	THR	VAL	THR	VAL	GLU	GLU	GLY	GLY
CYS	MET	ILE	MET	ILE	TRP	TRP	VAL	LEU
LEU	VAL	ASP	VAL	ASP	ASN	CYS	PHE	LEU
ALA	THR	CYS	THR	CYS	ASN	ALA	ALA	PHE
ASN	LYS	GLU	LYS	GLU	PHE	PHE	ILE	ILE
PRO	PRO	LEU	PRO	ILE	VAL	GLY	PHE	ARG
ALA	MET	GLU	MET	GLU	PHE	PHE	ASN	ASN
ALA	ALA	LEU	LEU	LEU	LEU	LEU	LEU	THR
PRO	ARG	LEU	ARG	LEU	TYR	TYR	TYR	ASP
TRP	TRP	GLN	TRP	GLN	ASP	ASP	ASP	GLN
GLY	GLY	ASN	LYS	ASN	THR	THR	LYS	GLU
GLN	GLN	LYS	LYS	LEU	ASP	ASP	ARG	TYR
GLY	LEU	LEU	LEU	LEU	ASP	ASP	SER	THR
ILE	ILE	GLU	GLU	GLU	GLY	GLY	VAL	ALA
ASP	MET	GLN	GLN	GLN	TYR	TYR	HIS	PHE
GLU	ARG	ILE	ARG	ILE	SER	SER	THR	ARG
GLU	GLU	VAL	GLU	VAL	ILE	ILE	LEU	LEU
THR	TYR	VAL	VAL	VAL	GLN	GLN	SER	ALA
LEU	GLY	GLY	GLY	GLY	ALA	ALA	CYS	PHE
LYS	SER	LYS	LYS	LYS	ILE	ILE	VAL	LEU
GLN	GLU	HIS	HIS	HIS	MET	MET	ASN	ASN
VAL	THR	VAL	VAL	VAL	GLU	GLU	ALA	ASN
ARG	ARG	PRO	PRO	PRO	LYS	LYS	LEU	ASN
ILE	ILE	ILE	PRO	GLY	ALA	ALA	HIS	SER
GLN	LYS	TYR	LYS	TYR	GLY	GLY	ILE	PRO
GLY	TYR	THR	THR	THR	ASN	ASN	SER	ASN
THR	THR	SER	SER	TYR	GLY	GLY	ILE	ALA
ASN	ASN	ASN	ASN	ASN	HIS	HIS	PRO	ALA
VAL	THR	VAL	VAL	VAL	VAL	VAL	SER	PRO
GLN	TYR	LEU	TYR	LEU	SER	SER	PHE	PHE
ASP	ASP	GLY	GLY	GLY	ALA	ALA	PRO	ASN
HIS	HIS	LYS	LYS	LYS	CYS	CYS	GLU	VAL
TYR	TYR	VAL	VAL	VAL	GLU	GLU	VAL	HIS
GLY	VAL	VAL	VAL	ILE	GLU	GLU	SER	VAL
ARG	ARG	MET	MET	SER	ASN	ASN	GLN	ASN
ALA	ALA	LEU	LEU	LEU	PHE	PHE	ASN	ASN
THR	THR	GLU	GLU	GLU	ASN	ASN	VAL	ILE
MET	SER	ILE	ILE	ILE	SER	SER	GLN	THR
ASP	LEU	GLY	GLY	GLY	ARG	ARG	LEU	ALA
VAL	VAL	ARG	ARG	ARG	GLN	GLN	ARG	ASN
PHE	PHE	ALA	ALA	ALA	THR	THR	PRO	SER
GLU	GLU	ASN	ASN	ASN	LEU	LEU	SER	PHE
LEU	LEU	VAL	VAL	VAL	GLU	GLU	LEU	ALA
THR	THR	THR	THR	THR	GLY	GLY	ARG	VAL



LEU	ASP	ALA	LEU	ASP	ASN	GLY
ARG	ALA	LEU	PHE	ALA	ALA	PHE
ARG	CYS	SER	CYS	CYS	PRO	SER
GLN	SER	LEU	SER	GLN	SER	SER
GLY	ASP	LEU	TYR	TYR	VAL	VAL
LYS	LYS	ASP	HIS	SER	GLN	GLN
LYS	PHE	TYR	GLU	ARG	ILE	ILE
VAL	VAL	TRP	TRP	VAL	GLY	GLY
ILE	ASP	ASN	ASN	PHE	LEU	LEU
CYS	CYS	CYS	CYS	ALA	PHE	PHE
GLU	GLU	PHE	PHE	ILE	ILE	ILE
ILE	ILE	VAL	VAL	GLY	ARG	ARG
GLU	GLU	PHE	PHE	GLY	ASN	ASN
ARG	ARG	LEU	LEU	LEU	THR	THR
LEU	LEU	TYR	TYR	ASP	ASP	ASP
GLN	GLN	ASP	ASP	ASP	GLN	GLN
ASN	ASN	THR	THR	LYS	GLU	GLU
ILE	ILE	ASP	ASP	ARG	TYR	TYR
LEU	LEU	ARG	SER	SER	ALA	ALA
GLN	GLN	GLY	TYR	VAL	HIS	PHE
ILE	ILE	SER	ILE	THR	ARG	ARG
VAL	VAL	ILE	ILE	LEU	LEU	LEU
VAL	VAL	GLN	GLN	SER	ILE	ALA
GLY	GLY	ALA	ALA	PHE	PHE	PHE
LYS	LYS	ILE	MET	CYS	LEU	LEU
HIS	HIS	GLY	GLY	ILE	HIS	HIS
VAL	VAL	GLU	GLU	ALA	ASN	ASN
LYS	LYS	LYS	LYS	ALA	THR	THR
GLY	GLY	ALA	ALA	HIS	SER	SER
TYR	TYR	GLY	GLY	ILE	PRO	PRO
HIS	HIS	GLN	GLN	SER	ASN	ASN
TYR	TYR	ASN	ASN	LEU	ALA	ALA
ILE	ILE	GLY	GLY	ILE	SER	SER
ILE	ILE	TRP	TRP	THR	GLU	GLU
ALA	ALA	HIS	VAL	PRO	ALA	ALA
ASN	ASN	VAL	VAL	SER	PRO	PRO
LEU	LEU	SER	SER	PHE	PHE	PHE
GLY	GLY	ALA	ALA	PRO	ASN	ASN
PHE	PHE	ILE	ILE	THR	LEU	LEU
LYS	LYS	CYS	CYS	GLY	VAL	VAL
ASP	ASP	VAL	VAL	GLY	PRO	PRO
ILE	ILE	GLU	GLU	GLU	HIS	HIS
SER	SER	ASN	ASN	SER	VAL	VAL
LEU	LEU	PHE	PHE	GLN	ASP	ASP
GLU	GLU	ASN	ASN	GLN	ASN	ASN
VAL	VAL	ASP	ASP	VAL	ILE	ILE
PHE	PHE	VAL	VAL	LEU	GLU	GLU
ILE	ILE	SER	SER	GLN	THR	THR
HIS	HIS	TYR	TYR	LEU	ALA	ALA
GLY	GLY	ARG	ARG	ARG	ASN	ASN
ALA	ALA	LEU	LEU	SER	PHE	PHE
ASN	ASN	LEU	LEU	LEU	VAL	VAL
VAL	VAL	GLU	GLU	ARG	THR	THR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59714	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0171	Depositor
Map size (Å)	334.40002, 334.40002, 334.40002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8360001, 0.8360001, 0.8360001	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: E2Q

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	0.10	0/3091	0.31	0/4179
1	B	0.10	0/3013	0.31	0/4074
1	C	0.10	0/3091	0.31	0/4179
1	D	0.10	0/3013	0.31	0/4074
All	All	0.10	0/12208	0.31	0/16506

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	3020	0	3052	41	0
1	B	2949	0	2994	36	0
1	C	3020	0	3052	39	0
1	D	2949	0	2994	43	0
2	A	23	0	0	2	0
2	B	23	0	0	2	0
2	C	23	0	0	2	0
2	D	23	0	0	3	0
All	All	12030	0	12092	152	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 6.

All (152) 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:611:CYS:N	1:D:611:CYS:SG	2.55	0.78
1:C:485:MET:HE3	1:C:501:LEU:HD13	1.67	0.77
1:A:485:MET:HE3	1:A:501:LEU:HD13	1.67	0.75
1:D:806:THR:HG22	1:D:807:SER:H	1.55	0.71
2:D:1001:E2Q:N14	2:D:1001:E2Q:O17	2.23	0.70
2:B:1001:E2Q:O17	2:B:1001:E2Q:N14	2.23	0.70
1:B:806:THR:HG22	1:B:807:SER:H	1.55	0.70
1:B:520:LEU:HD12	1:B:727:GLU:HB3	1.75	0.68
1:B:611:CYS:SG	1:C:611:CYS:N	2.68	0.67
1:D:520:LEU:HD12	1:D:727:GLU:HB3	1.75	0.67
1:A:518:MET:HE2	1:A:785:LYS:HD2	1.80	0.63
1:C:518:MET:HE2	1:C:785:LYS:HD2	1.80	0.63
1:D:449:ASP:OD2	1:D:788:TRP:NE1	2.32	0.62
1:B:449:ASP:OD2	1:B:788:TRP:NE1	2.32	0.62
1:A:542:PRO:O	1:A:641:ASN:ND2	2.36	0.59
1:D:678:LYS:HE2	1:D:682:ARG:HH22	1.68	0.59
1:C:417:VAL:HG13	1:C:495:GLU:HB2	1.84	0.59
1:C:542:PRO:O	1:C:641:ASN:ND2	2.36	0.59
1:D:660:ASP:HA	1:D:663:LYS:HE2	1.85	0.58
1:A:417:VAL:HG13	1:A:495:GLU:HB2	1.84	0.58
1:B:660:ASP:HA	1:B:663:LYS:HE2	1.85	0.57
1:B:678:LYS:HE2	1:B:682:ARG:HH22	1.68	0.57
1:C:497:ALA:HB3	1:C:757:ALA:HB3	1.86	0.57
1:A:497:ALA:HB3	1:A:757:ALA:HB3	1.86	0.57
1:B:419:VAL:N	1:B:463:LYS:O	2.36	0.56
1:D:542:PRO:O	1:D:641:ASN:ND2	2.40	0.55
2:A:1001:E2Q:N14	2:A:1001:E2Q:N15	2.55	0.55
1:D:419:VAL:N	1:D:463:LYS:O	2.36	0.54
1:D:538:SER:OG	1:D:813:ASN:O	2.26	0.53
2:C:1001:E2Q:N15	2:C:1001:E2Q:N14	2.55	0.53
1:B:542:PRO:O	1:B:641:ASN:ND2	2.40	0.53
1:A:671:THR:HG22	1:A:725:LEU:HB2	1.91	0.53
1:A:787:LYS:HA	1:A:791:ASP:HB2	1.91	0.53
1:D:510:VAL:HG23	1:D:511:ILE:HG23	1.91	0.52
1:A:596:PHE:HD2	1:D:618:LEU:HD21	1.74	0.52
1:B:525:MET:HB3	1:B:724:PHE:HB3	1.92	0.52
1:C:416:THR:HA	1:C:461:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:787:LYS:HA	1:C:791:ASP:HB2	1.91	0.52
1:D:525:MET:HB3	1:D:724:PHE:HB3	1.92	0.52
1:C:671:THR:HG22	1:C:725:LEU:HB2	1.91	0.52
1:A:416:THR:HA	1:A:461:LYS:HG3	1.92	0.52
1:B:538:SER:OG	1:B:813:ASN:O	2.26	0.52
1:D:671:THR:HG22	1:D:725:LEU:HB2	1.92	0.52
1:C:520:LEU:HD13	1:C:754:TYR:CZ	2.45	0.51
1:A:520:LEU:HD13	1:A:754:TYR:CZ	2.45	0.51
1:B:618:LEU:HD21	1:C:596:PHE:HD2	1.75	0.51
1:B:671:THR:HG22	1:B:725:LEU:HB2	1.92	0.51
1:A:508:GLU:OE2	1:D:769:ASN:ND2	2.43	0.51
1:B:510:VAL:HG23	1:B:511:ILE:HG23	1.91	0.51
1:B:743:MET:HG2	1:B:744:LYS:H	1.76	0.51
1:B:429:MET:N	1:B:444:GLU:O	2.44	0.51
2:D:1001:E2Q:O17	2:D:1001:E2Q:S11	2.69	0.50
1:C:814:VAL:O	1:C:817:VAL:HG12	2.11	0.50
1:D:429:MET:N	1:D:444:GLU:O	2.44	0.50
2:B:1001:E2Q:O17	2:B:1001:E2Q:S11	2.70	0.50
1:D:743:MET:HG2	1:D:744:LYS:H	1.76	0.50
1:A:460:ILE:O	1:A:460:ILE:HG13	2.12	0.50
1:A:786:ASN:HA	1:A:790:TYR:HD2	1.77	0.49
1:B:806:THR:HG22	1:B:807:SER:N	2.27	0.49
1:C:460:ILE:HG13	1:C:460:ILE:O	2.12	0.49
1:C:733:TYR:OH	1:C:737:ARG:NH1	2.46	0.49
1:C:786:ASN:HA	1:C:790:TYR:HD2	1.78	0.49
1:A:733:TYR:OH	1:A:737:ARG:NH1	2.46	0.48
1:A:814:VAL:O	1:A:817:VAL:HG12	2.13	0.48
1:D:609:GLN:NE2	1:C:605:ALA:O	2.34	0.48
1:C:537:PHE:HE1	1:C:820:ILE:HD11	1.79	0.48
1:D:806:THR:HG22	1:D:807:SER:N	2.27	0.48
1:A:455:ALA:O	1:A:459:GLY:N	2.43	0.47
1:B:545:TYR:HA	1:B:548:TRP:HD1	1.79	0.47
1:B:648:VAL:HB	1:C:650:ARG:HH11	1.79	0.47
1:A:544:ALA:O	1:A:547:ILE:HG22	2.15	0.47
1:C:544:ALA:O	1:C:547:ILE:HG22	2.15	0.47
1:C:455:ALA:O	1:C:459:GLY:N	2.43	0.47
1:C:507:ARG:O	1:C:511:ILE:HG12	2.15	0.47
1:D:545:TYR:HA	1:D:548:TRP:HD1	1.79	0.46
1:C:469:ASP:OD1	1:C:469:ASP:N	2.49	0.46
2:A:1001:E2Q:N14	2:A:1001:E2Q:O16	2.48	0.46
2:C:1001:E2Q:N14	2:C:1001:E2Q:O16	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ARG:O	1:A:511:ILE:HG12	2.15	0.46
1:A:505:LEU:HD11	1:D:774:LYS:HA	1.98	0.45
1:B:511:ILE:HD12	1:B:757:ALA:HB1	1.98	0.45
1:B:455:ALA:O	1:B:459:GLY:N	2.49	0.45
1:B:776:SER:HB2	1:B:781:LEU:HD12	1.99	0.45
1:D:511:ILE:HD12	1:D:757:ALA:HB1	1.98	0.45
1:D:455:ALA:O	1:D:459:GLY:N	2.50	0.45
1:A:628:TRP:CG	1:B:609:GLN:HG3	2.52	0.45
1:A:650:ARG:HH11	1:D:648:VAL:HB	1.81	0.45
1:D:776:SER:HB2	1:D:781:LEU:HD12	1.99	0.44
1:A:543:LEU:HB3	1:A:547:ILE:HG21	1.99	0.44
1:B:527:LYS:HE2	1:B:716:ARG:HA	2.00	0.44
1:C:525:MET:HE3	1:C:726:LEU:HD21	2.00	0.44
1:C:785:LYS:O	1:C:789:TRP:HB2	2.18	0.44
1:A:766:THR:HB	1:A:767:PRO:HD3	2.00	0.44
1:A:596:PHE:CD2	1:D:618:LEU:HD21	2.53	0.44
1:D:646:LEU:HD22	1:D:809:LEU:HD21	1.99	0.44
1:A:525:MET:HE3	1:A:726:LEU:HD21	2.00	0.43
1:A:537:PHE:HE1	1:A:820:ILE:HD11	1.83	0.43
1:B:622:ILE:O	1:B:626:VAL:HG22	2.18	0.43
1:A:469:ASP:N	1:A:469:ASP:OD1	2.49	0.43
1:B:646:LEU:HD22	1:B:809:LEU:HD21	1.99	0.43
1:C:812:SER:HA	1:C:815:ALA:HB2	2.00	0.43
1:B:614:SER:OG	1:C:600:TRP:NE1	2.50	0.43
1:D:502:THR:O	1:D:507:ARG:NH1	2.50	0.43
1:A:536:VAL:HG23	1:A:537:PHE:CD2	2.53	0.43
1:B:543:LEU:O	1:B:548:TRP:NE1	2.47	0.43
1:D:504:THR:HG22	1:D:505:LEU:N	2.34	0.43
1:C:766:THR:HB	1:C:767:PRO:HD3	2.00	0.43
1:A:785:LYS:O	1:A:789:TRP:HB2	2.18	0.43
1:B:504:THR:HG22	1:B:505:LEU:N	2.34	0.43
1:D:622:ILE:O	1:D:626:VAL:HG22	2.18	0.43
1:C:543:LEU:HB3	1:C:547:ILE:HG21	1.99	0.43
1:C:474:ALA:N	1:C:483:ASN:OD1	2.40	0.43
1:A:511:ILE:HD12	1:A:757:ALA:HB1	2.01	0.42
1:B:517:PHE:CZ	1:B:754:TYR:HB3	2.54	0.42
1:D:527:LYS:HE2	1:D:716:ARG:HA	2.00	0.42
1:C:511:ILE:HD12	1:C:757:ALA:HB1	2.01	0.42
1:A:812:SER:HA	1:A:815:ALA:HB2	2.01	0.42
1:D:786:ASN:HA	1:D:790:TYR:HD2	1.84	0.42
1:C:536:VAL:HG23	1:C:537:PHE:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:LEU:HD21	1:C:596:PHE:CD2	2.52	0.42
1:B:786:ASN:HA	1:B:790:TYR:HD2	1.84	0.42
1:C:716:ARG:CZ	1:C:739:PRO:HD2	2.50	0.42
1:C:515:LYS:HD3	1:C:515:LYS:HA	1.83	0.42
1:A:631:THR:O	1:A:635:ILE:HG12	2.20	0.42
1:A:635:ILE:HD12	1:D:632:LEU:HD11	2.02	0.42
1:D:543:LEU:O	1:D:548:TRP:NE1	2.47	0.42
1:B:631:THR:O	1:B:635:ILE:HG12	2.20	0.42
1:D:517:PHE:CE1	1:D:518:MET:HG2	2.55	0.42
1:D:821:LEU:HG	1:D:825:LEU:HD23	2.02	0.42
1:D:631:THR:O	1:D:635:ILE:HG12	2.20	0.41
1:D:517:PHE:CZ	1:D:754:TYR:HB3	2.55	0.41
1:C:460:ILE:HD13	1:C:764:LEU:HD13	2.02	0.41
1:C:830:LEU:O	1:C:834:ILE:HG12	2.21	0.41
1:A:515:LYS:HD3	1:A:515:LYS:HA	1.83	0.41
1:B:517:PHE:CE1	1:B:518:MET:HG2	2.55	0.41
1:C:631:THR:O	1:C:635:ILE:HG12	2.20	0.41
1:A:460:ILE:HD13	1:A:764:LEU:HD13	2.02	0.41
1:A:505:LEU:HD21	1:D:774:LYS:HG3	2.02	0.41
1:A:716:ARG:CZ	1:A:739:PRO:HD2	2.50	0.41
1:D:512:ASP:OD1	1:D:760:LYS:NZ	2.42	0.41
1:D:427:TYR:HB3	1:D:447:CYS:SG	2.61	0.41
1:C:522:ILE:HG12	1:C:750:ASP:OD1	2.21	0.41
1:A:427:TYR:HA	1:A:446:TYR:HB3	2.03	0.40
1:D:682:ARG:HB2	1:D:693:TRP:CH2	2.56	0.40
1:D:743:MET:HE2	1:D:743:MET:HB3	1.95	0.40
1:C:427:TYR:HA	1:C:446:TYR:HB3	2.03	0.40
1:B:821:LEU:HG	1:B:825:LEU:HD23	2.02	0.40
1:D:655:ILE:HD12	1:D:661:LEU:HA	2.03	0.40
1:A:499:ALA:HB1	1:A:500:PRO:HD2	2.04	0.40
1:B:682:ARG:HB2	1:B:693:TRP:CH2	2.56	0.40
2:D:1001:E2Q:N14	2:D:1001:E2Q:N15	2.69	0.40
1:A:641:ASN:ND2	1:B:809:LEU:HG	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/882 (43%)	357 (93%)	26 (7%)	0	100	100
1	B	373/882 (42%)	363 (97%)	10 (3%)	0	100	100
1	C	383/882 (43%)	357 (93%)	26 (7%)	0	100	100
1	D	373/882 (42%)	363 (97%)	10 (3%)	0	100	100
All	All	1512/3528 (43%)	1440 (95%)	72 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	323/752 (43%)	323 (100%)	0	100	100
1	B	317/752 (42%)	317 (100%)	0	100	100
1	C	323/752 (43%)	323 (100%)	0	100	100
1	D	317/752 (42%)	317 (100%)	0	100	100
All	All	1280/3008 (43%)	1280 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	748	ASN
1	C	748	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	E2Q	D	1001	-	24,25,25	1.17	2 (8%)	32,39,39	1.56	4 (12%)
2	E2Q	A	1001	-	24,25,25	0.75	1 (4%)	32,39,39	1.22	4 (12%)
2	E2Q	B	1001	-	24,25,25	1.16	2 (8%)	32,39,39	1.55	4 (12%)
2	E2Q	C	1001	-	24,25,25	0.75	1 (4%)	32,39,39	1.22	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	E2Q	D	1001	-	-	6/8/10/10	0/3/3/3
2	E2Q	A	1001	-	-	4/8/10/10	0/3/3/3
2	E2Q	B	1001	-	-	6/8/10/10	0/3/3/3
2	E2Q	C	1001	-	-	4/8/10/10	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	E2Q	C09-C08	4.07	1.49	1.43
2	B	1001	E2Q	C09-C08	4.05	1.49	1.43
2	D	1001	E2Q	C07-C08	2.75	1.47	1.43
2	B	1001	E2Q	C07-C08	2.74	1.47	1.43
2	C	1001	E2Q	C09-C08	2.42	1.47	1.43
2	A	1001	E2Q	C09-C08	2.41	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	E2Q	C08-C09-S11	4.29	127.14	121.67
2	B	1001	E2Q	C08-C09-S11	4.26	127.10	121.67
2	D	1001	E2Q	C10-C09-S11	-3.77	112.35	117.53
2	B	1001	E2Q	C10-C09-S11	-3.75	112.36	117.53
2	B	1001	E2Q	C02-C03-C04	-3.50	118.48	124.78
2	D	1001	E2Q	C02-C03-C04	-3.49	118.49	124.78
2	A	1001	E2Q	C08-C09-S11	3.40	126.00	121.67
2	C	1001	E2Q	C08-C09-S11	3.40	126.00	121.67
2	D	1001	E2Q	C05-C06-C07	2.95	123.80	118.55
2	B	1001	E2Q	C05-C06-C07	2.93	123.77	118.55
2	A	1001	E2Q	C10-C09-S11	-2.73	113.78	117.53
2	C	1001	E2Q	C10-C09-S11	-2.72	113.79	117.53
2	A	1001	E2Q	C02-C03-C04	-2.69	119.94	124.78
2	C	1001	E2Q	C02-C03-C04	-2.68	119.95	124.78
2	A	1001	E2Q	C05-C06-C07	2.25	122.55	118.55
2	C	1001	E2Q	C05-C06-C07	2.24	122.54	118.55

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	E2Q	C06-C07-N15-O16
2	A	1001	E2Q	C08-C07-N15-O16

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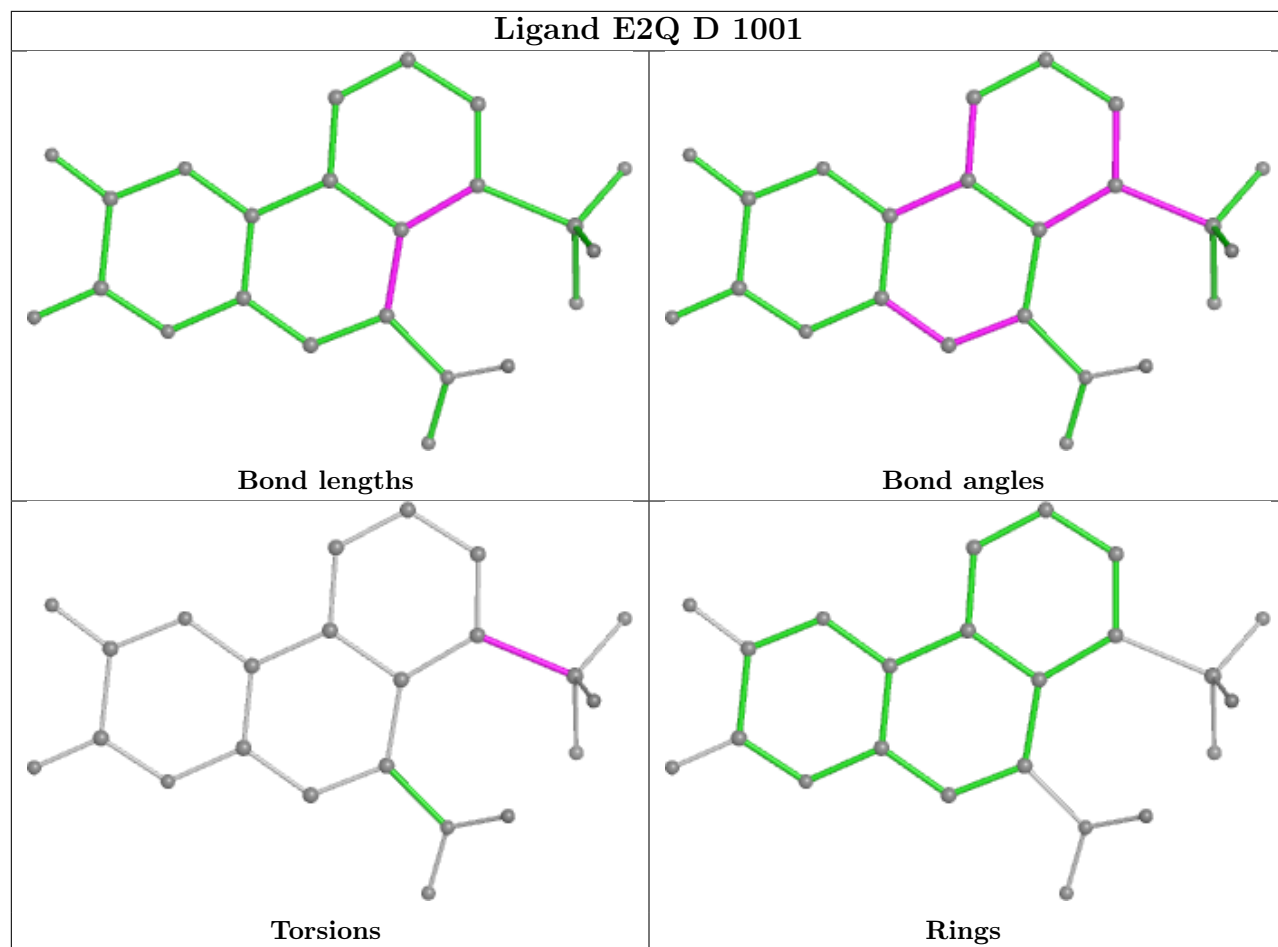
Mol	Chain	Res	Type	Atoms
2	C	1001	E2Q	C06-C07-N15-O16
2	C	1001	E2Q	C08-C07-N15-O16
2	B	1001	E2Q	C08-C09-S11-O12
2	B	1001	E2Q	C08-C09-S11-O13
2	D	1001	E2Q	C08-C09-S11-O12
2	D	1001	E2Q	C08-C09-S11-O13
2	B	1001	E2Q	C10-C09-S11-N14
2	D	1001	E2Q	C10-C09-S11-N14
2	B	1001	E2Q	C10-C09-S11-O12
2	D	1001	E2Q	C10-C09-S11-O12
2	B	1001	E2Q	C08-C09-S11-N14
2	D	1001	E2Q	C08-C09-S11-N14
2	B	1001	E2Q	C10-C09-S11-O13
2	D	1001	E2Q	C10-C09-S11-O13
2	A	1001	E2Q	C08-C09-S11-O12
2	C	1001	E2Q	C08-C09-S11-O12
2	A	1001	E2Q	C10-C09-S11-O12
2	C	1001	E2Q	C10-C09-S11-O12

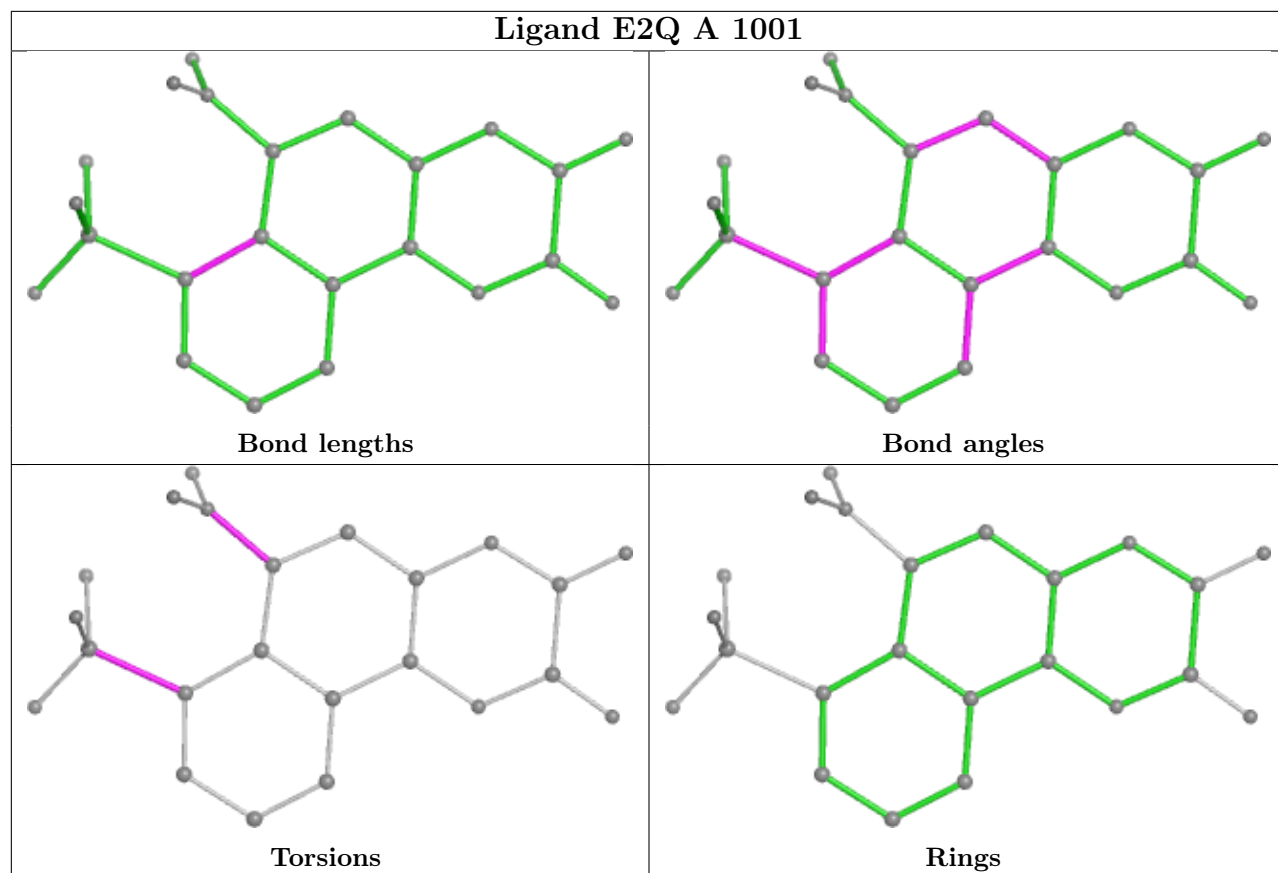
There are no ring outliers.

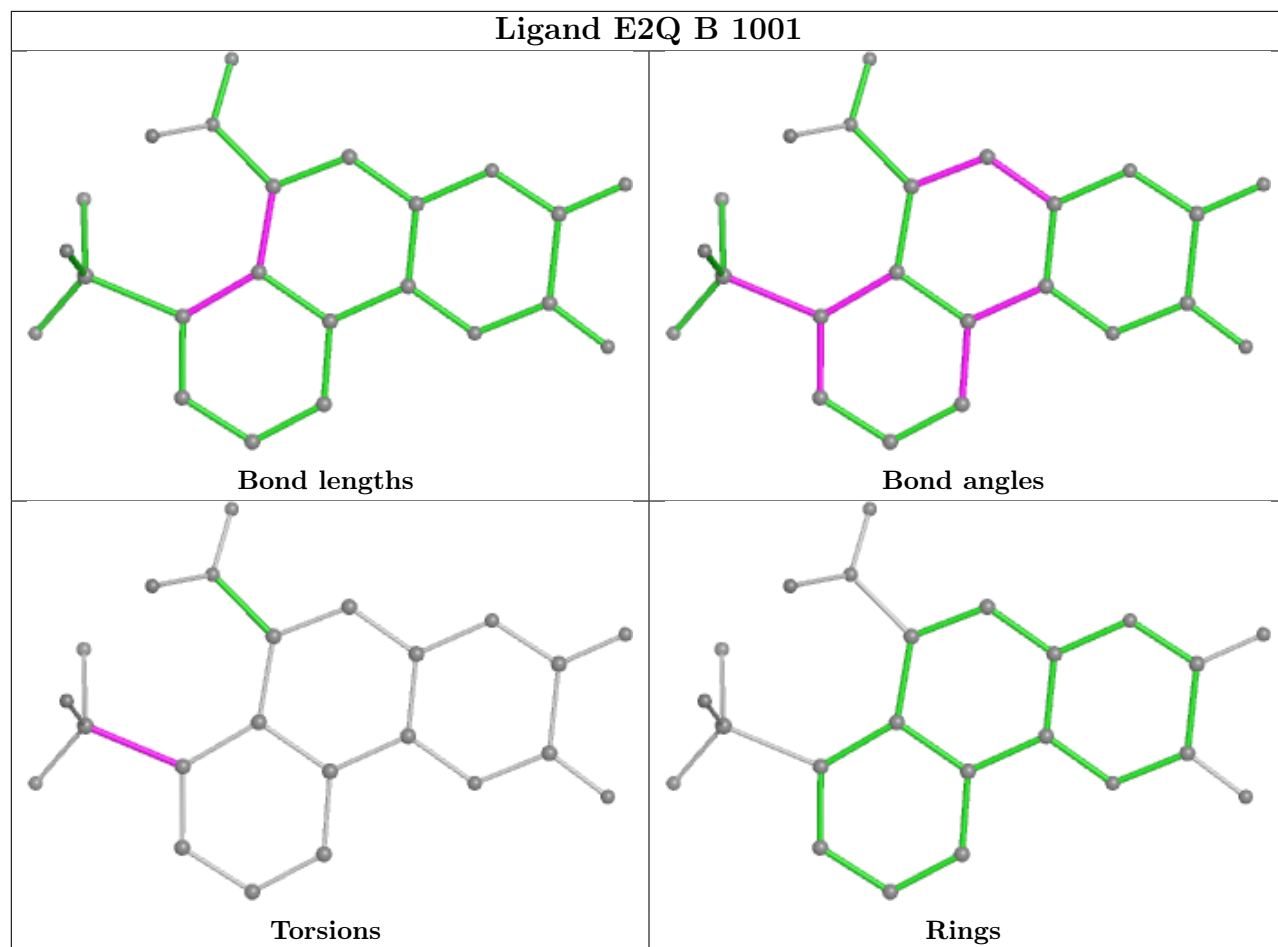
4 monomers are involved in 9 short contacts:

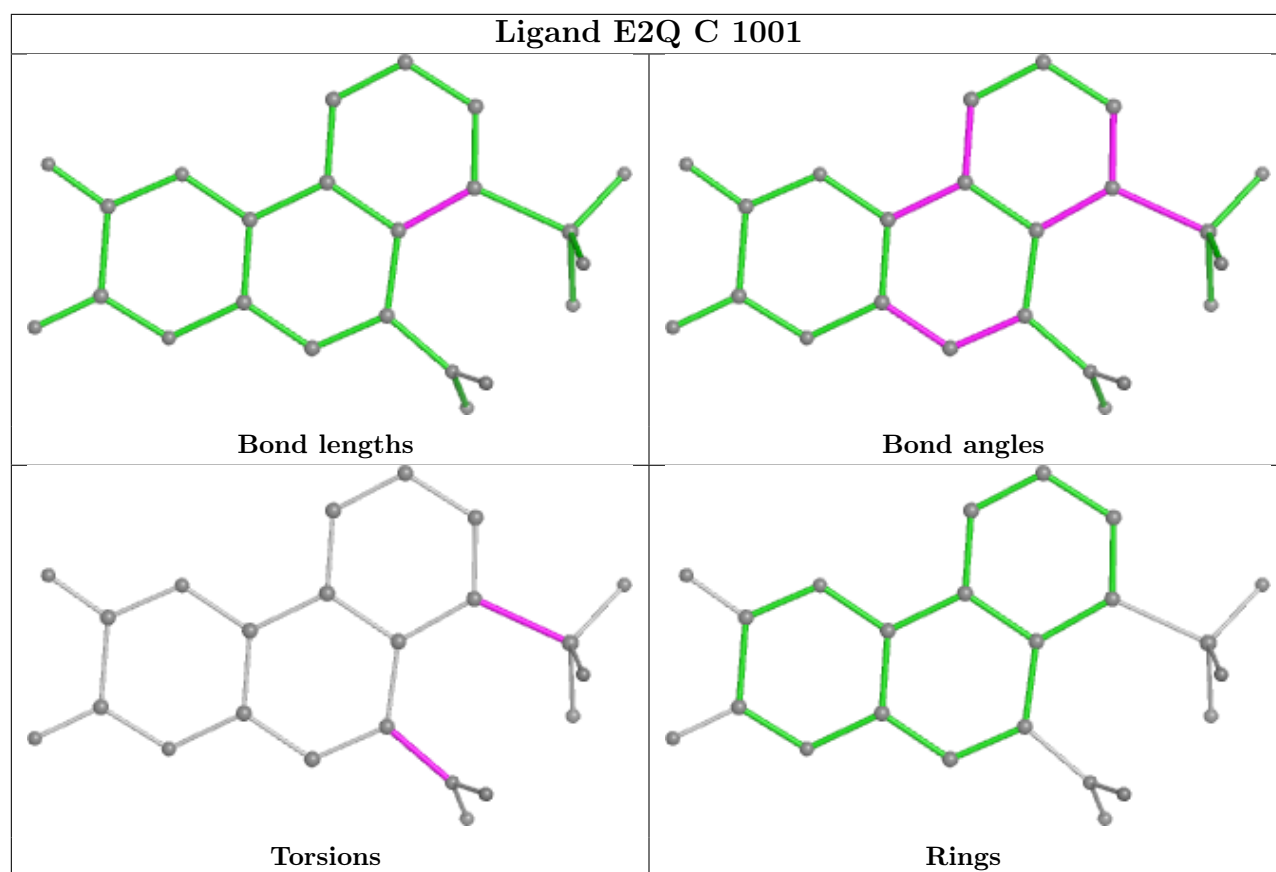
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	E2Q	3	0
2	A	1001	E2Q	2	0
2	B	1001	E2Q	2	0
2	C	1001	E2Q	2	0

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.









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.

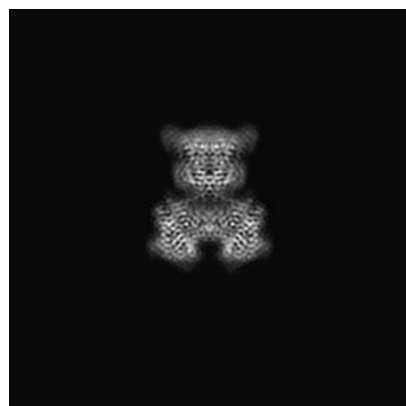
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53285. These allow visual inspection of the internal detail of the map and identification of artifacts.

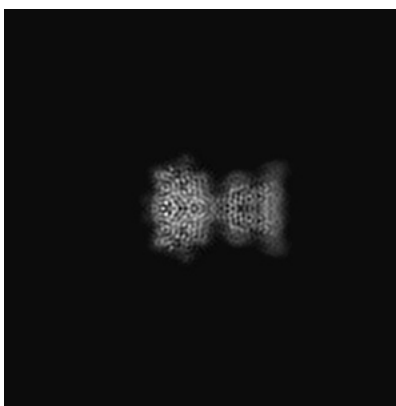
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

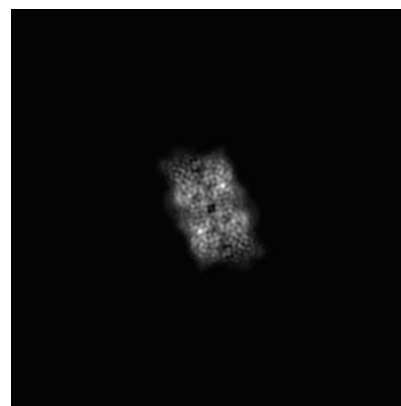
6.1.1 Primary map



X

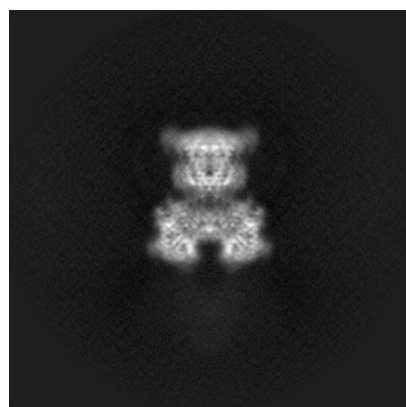


Y

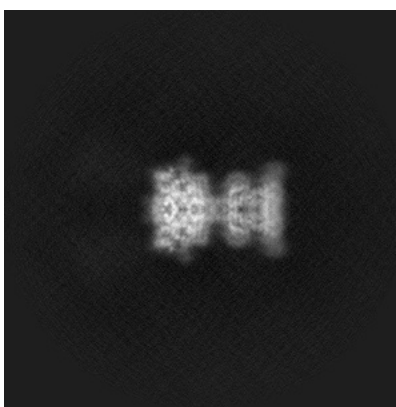


Z

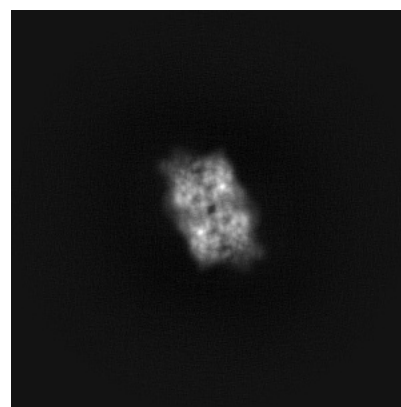
6.1.2 Raw map



X



Y

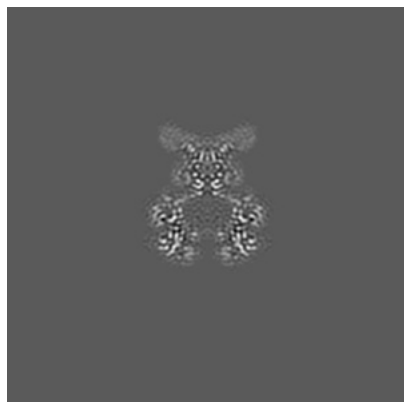


Z

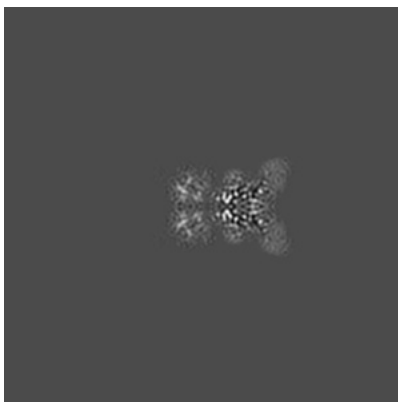
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

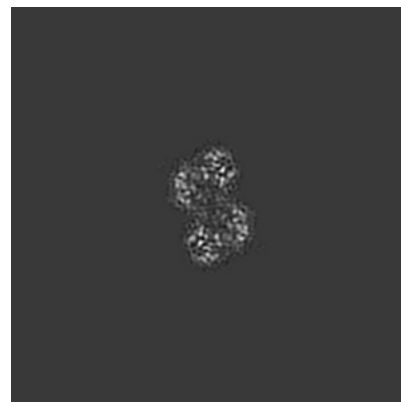
6.2.1 Primary map



X Index: 200

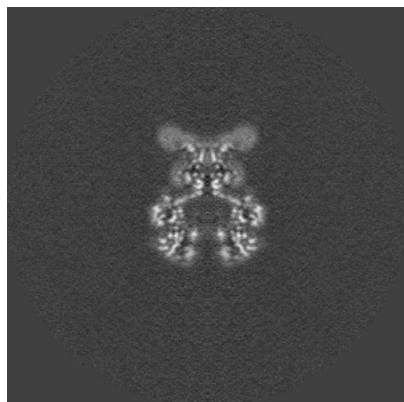


Y Index: 200

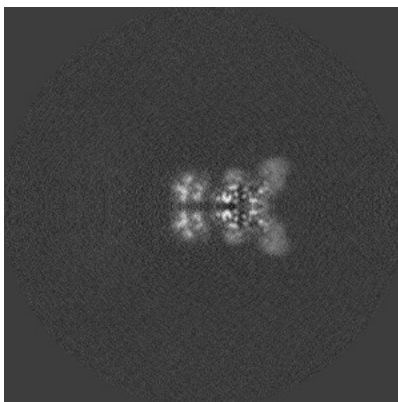


Z Index: 200

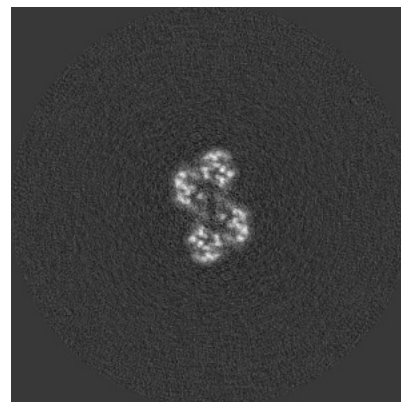
6.2.2 Raw map



X Index: 200



Y Index: 200

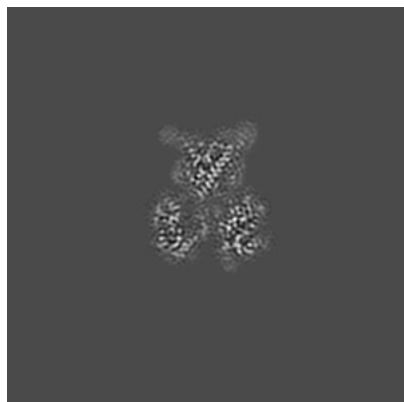


Z Index: 200

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

6.3 Largest variance slices [i](#)

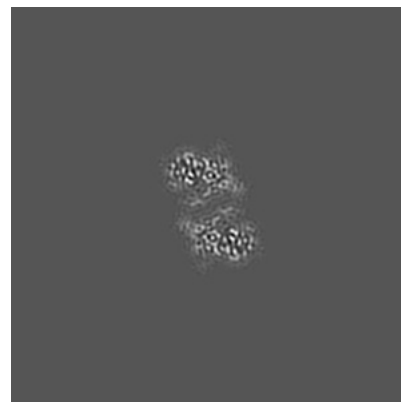
6.3.1 Primary map



X Index: 206

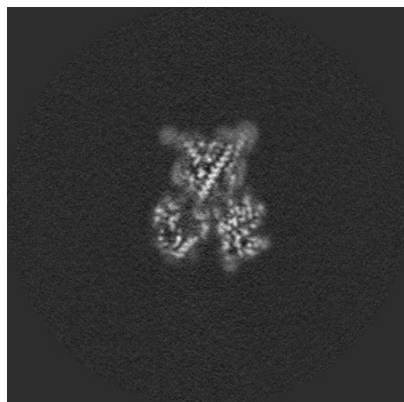


Y Index: 231

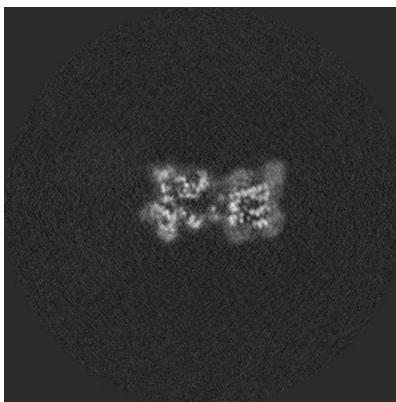


Z Index: 169

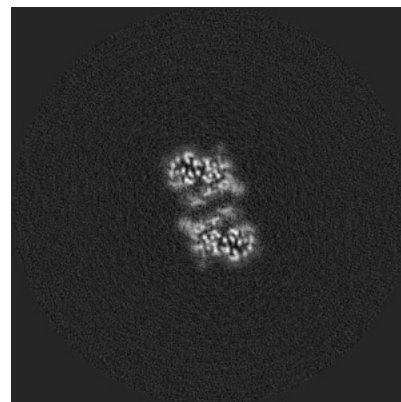
6.3.2 Raw map



X Index: 207



Y Index: 181

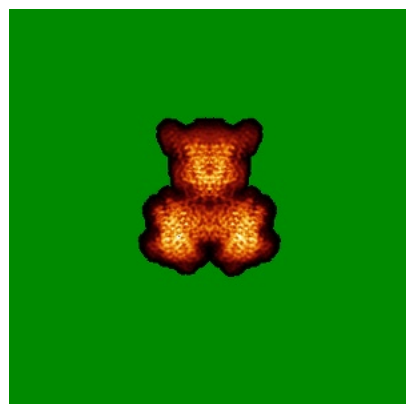


Z Index: 169

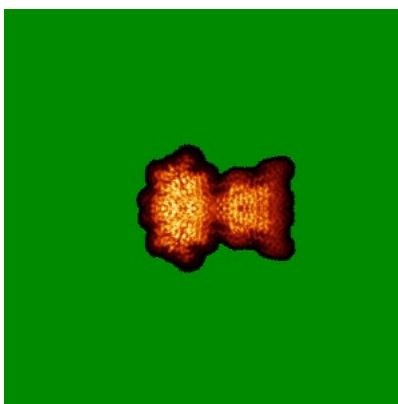
The images above show the largest variance slices of the map in three orthogonal directions.

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

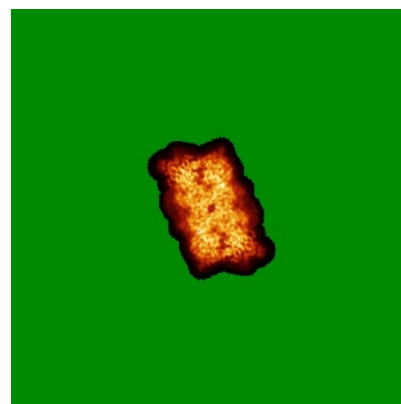
6.4.1 Primary map



X

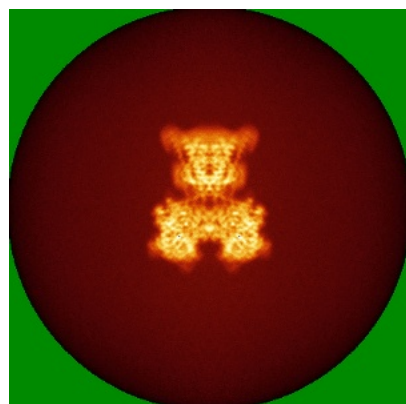


Y

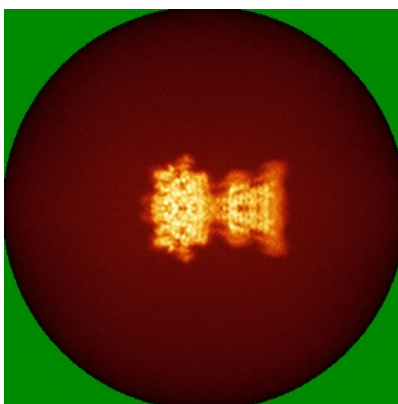


Z

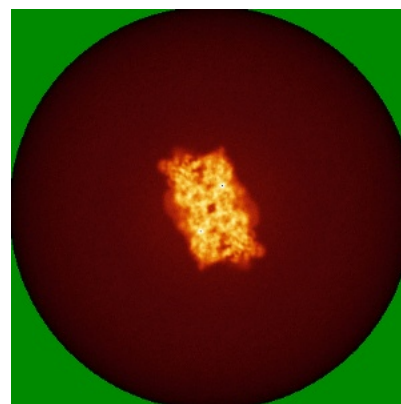
6.4.2 Raw map



X



Y

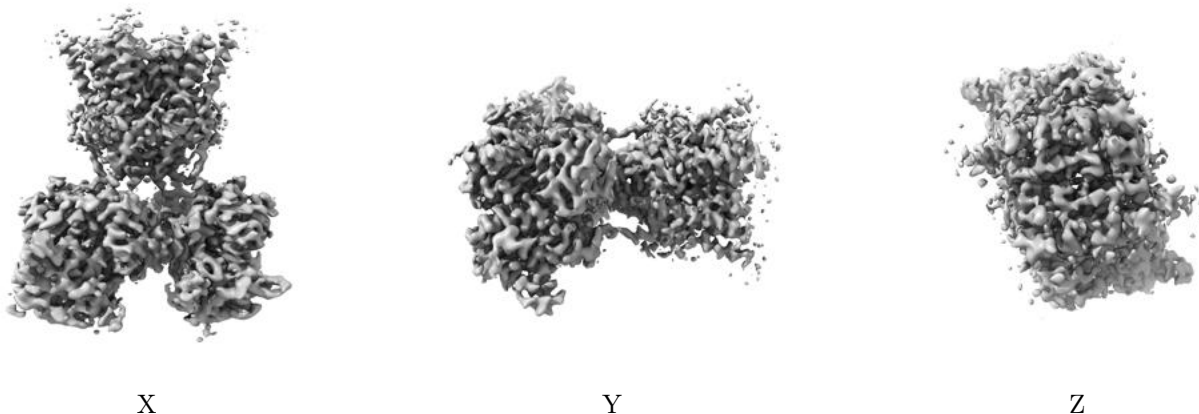


Z

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.

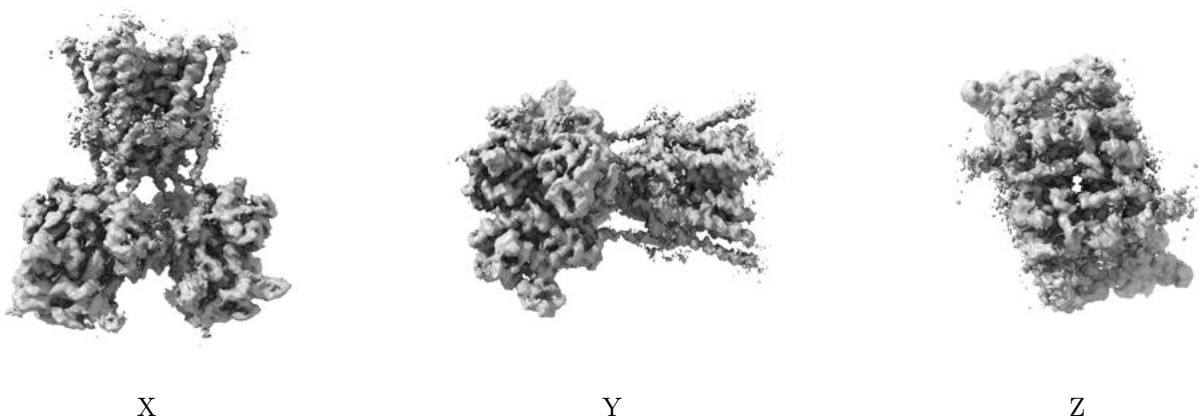
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0171. 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.

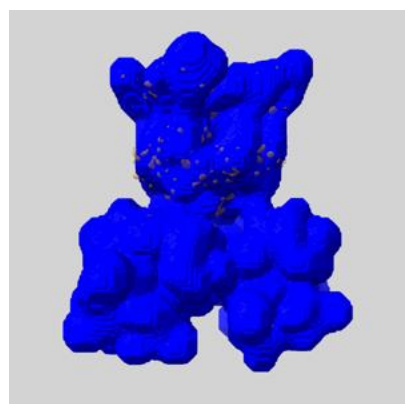
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

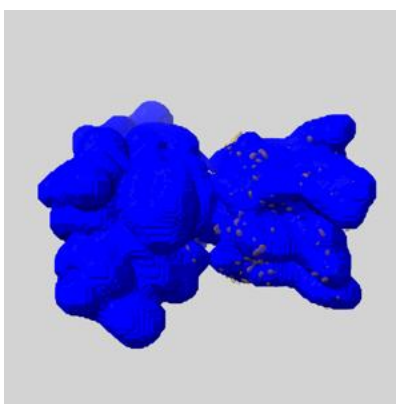
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

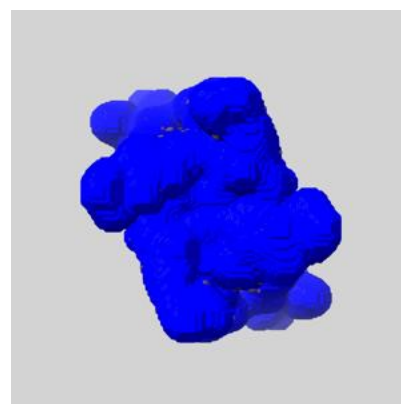
6.6.1 emd_53285_msk_1.map [i](#)



X



Y

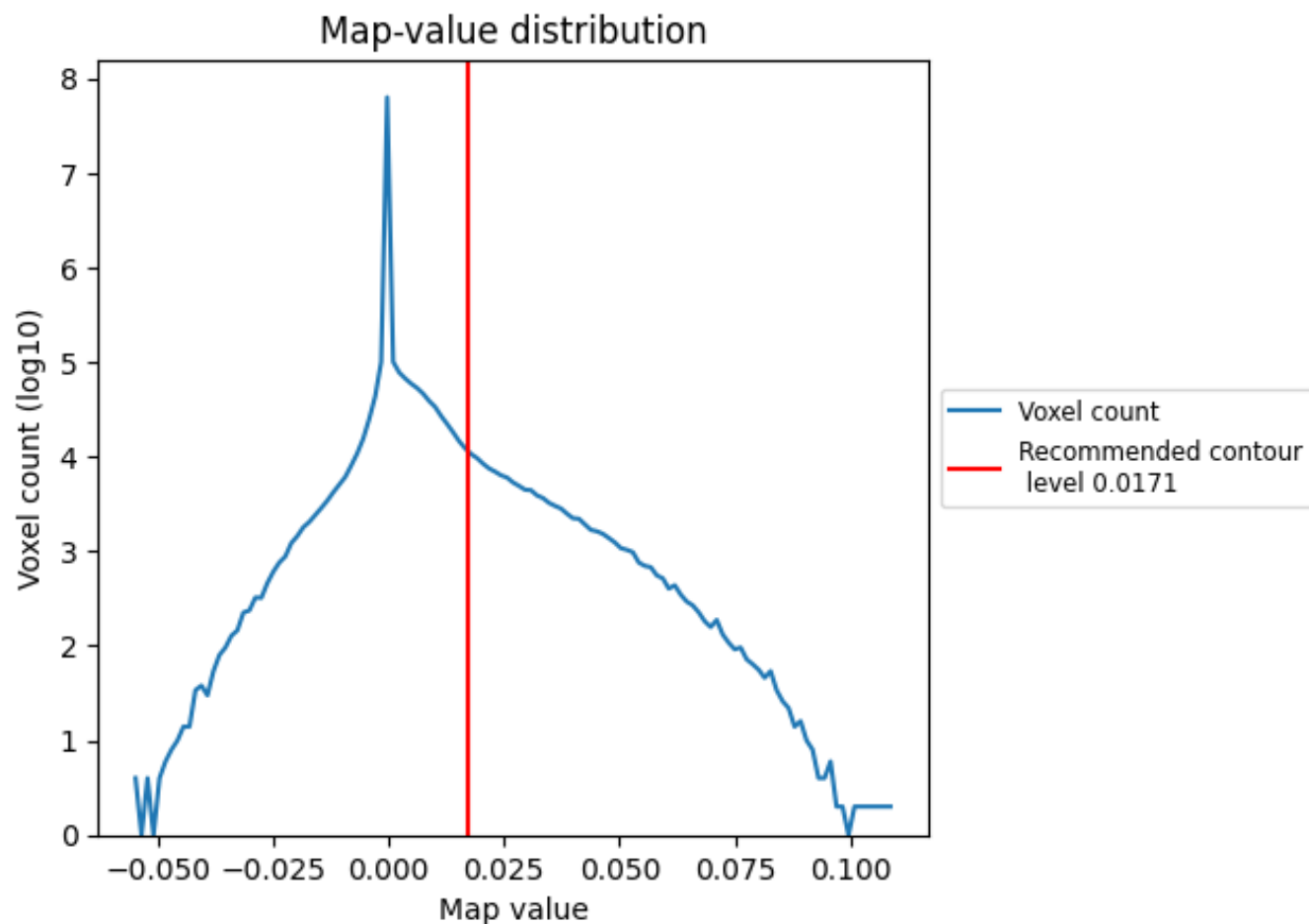


Z

7 Map analysis [i](#)

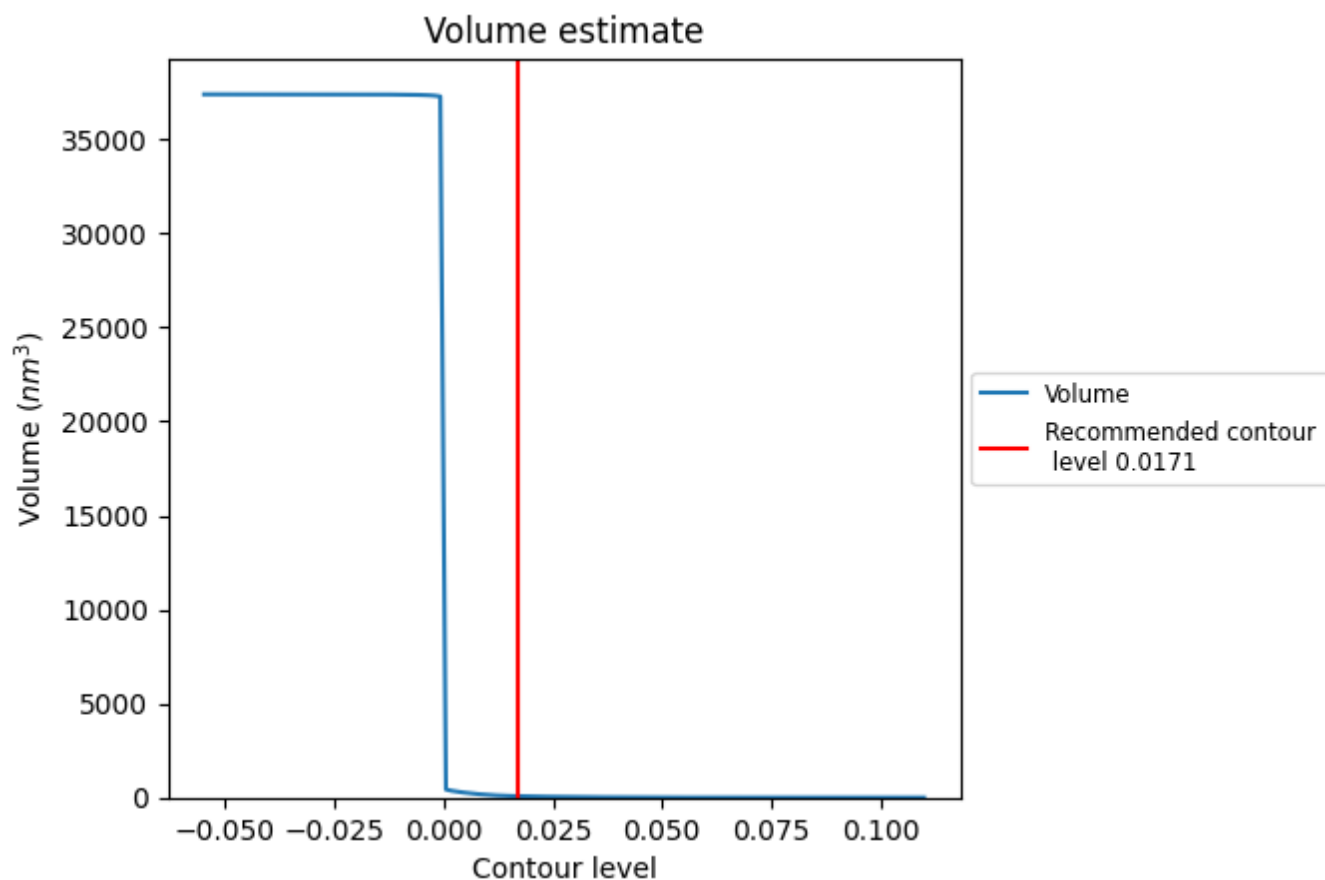
This section contains the results of statistical analysis of the map.

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.

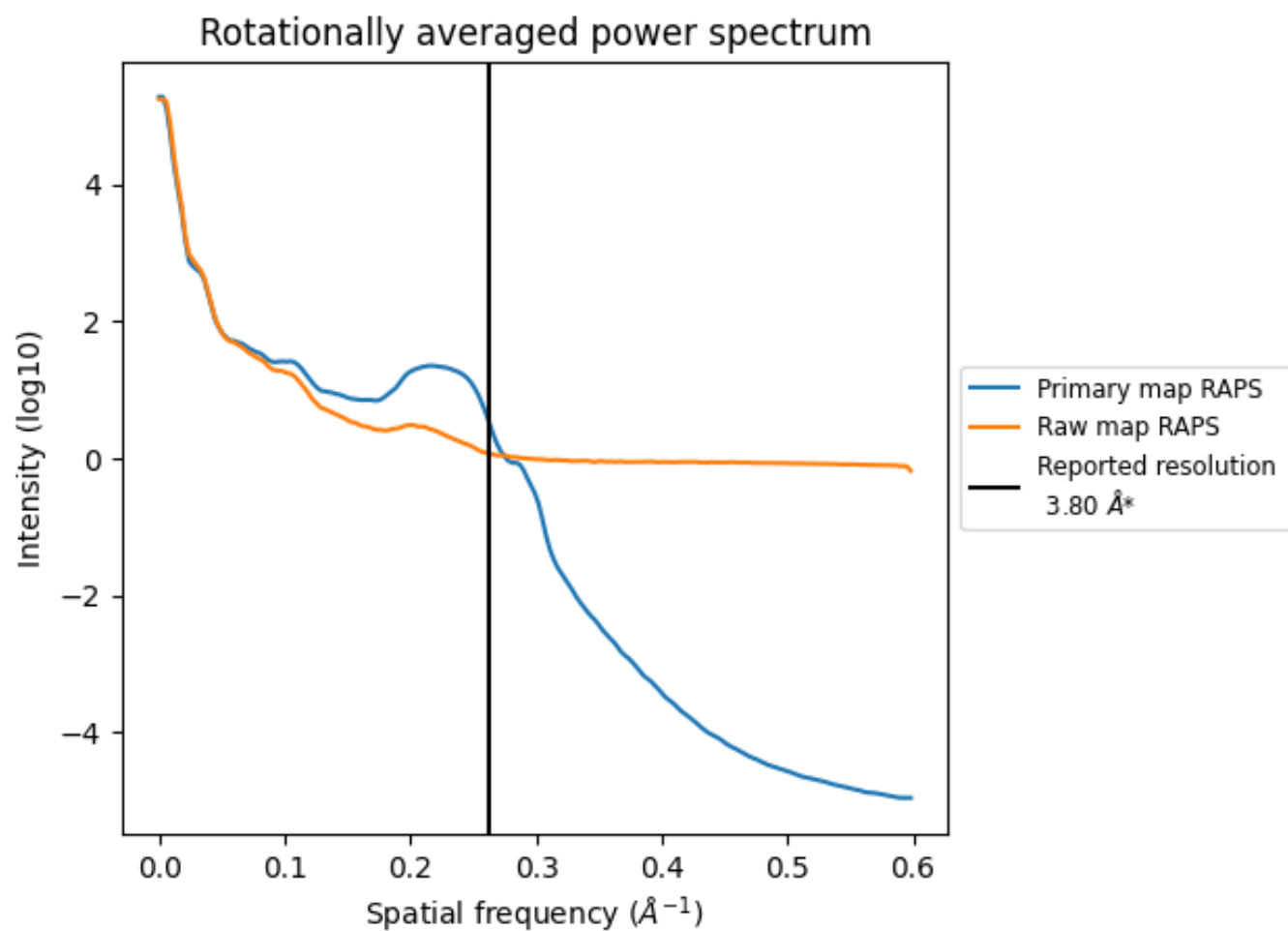
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm^3 ; this corresponds to an approximate mass of 66 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 ⓘ

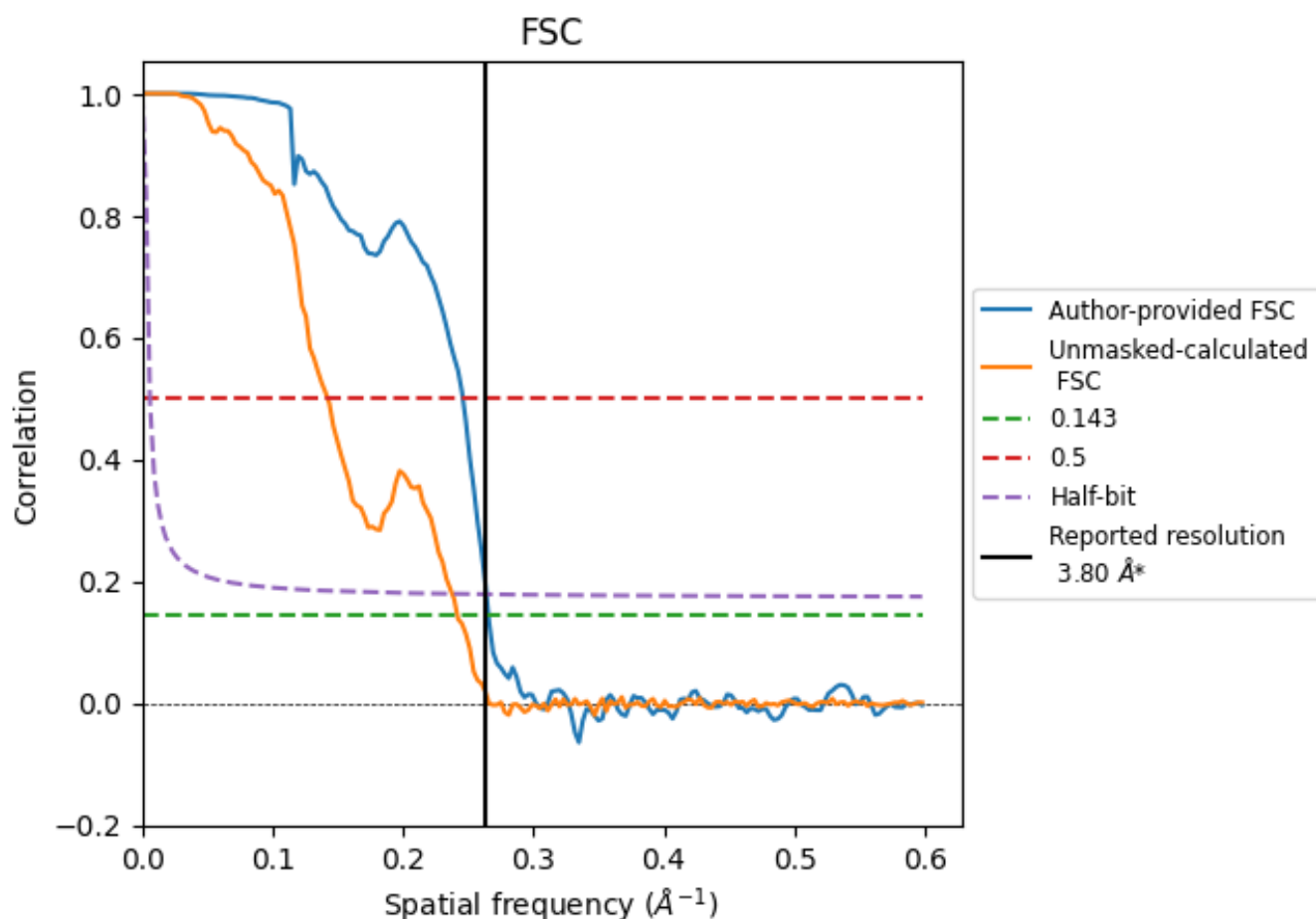


*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

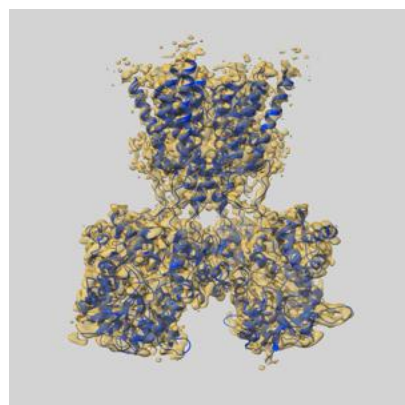
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.07	3.79
Unmasked-calculated*	4.14	7.04	4.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

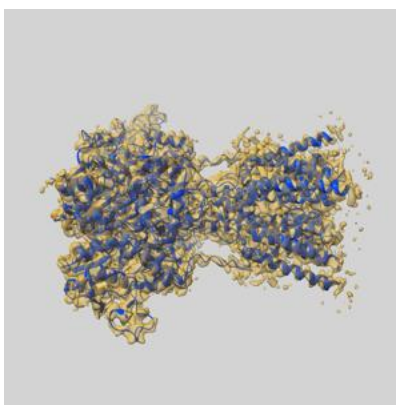
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53285 and PDB model 9QPW. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

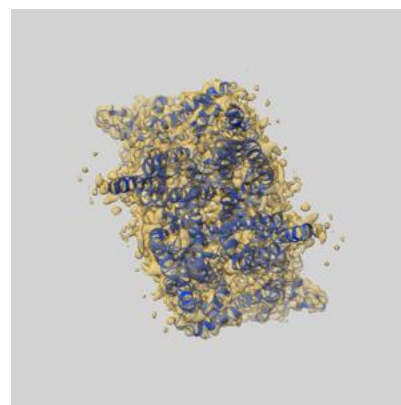
9.1 Map-model overlay [i](#)



X



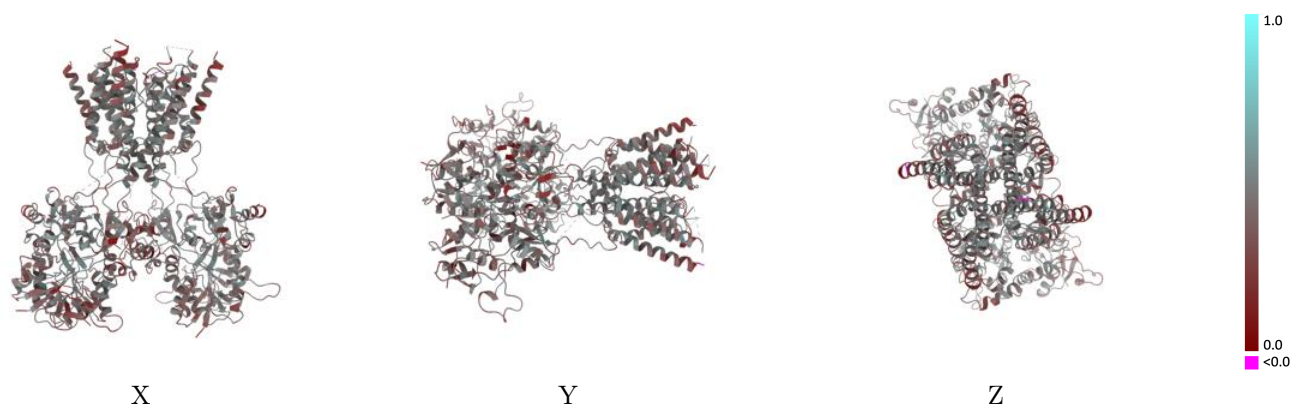
Y



Z

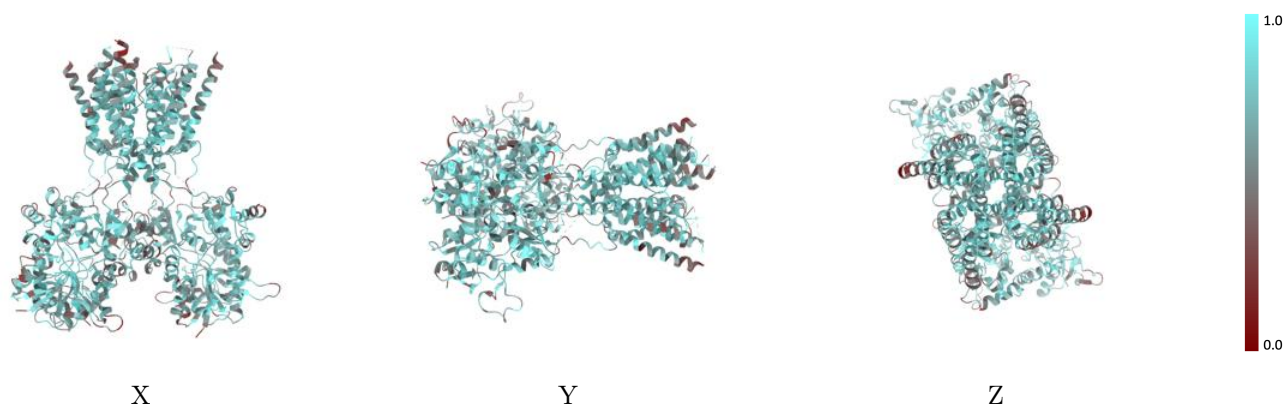
The images above show the 3D surface view of the map at the recommended contour level 0.0171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



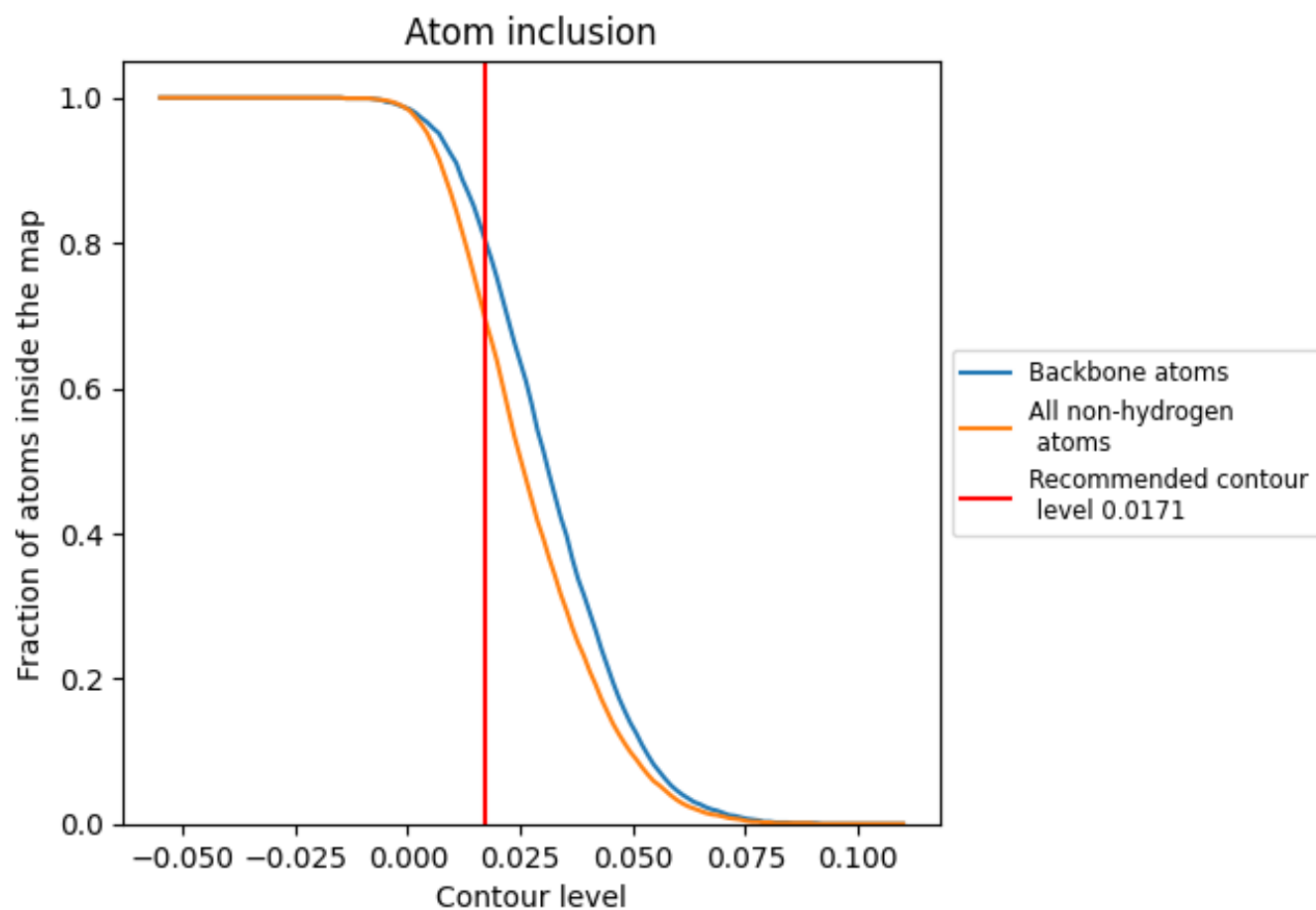
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0171).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 70% 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 (0.0171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6980	<div></div> 0.4140
A	<div></div> 0.6980	<div></div> 0.4090
B	<div></div> 0.7020	<div></div> 0.4250
C	<div></div> 0.6890	<div></div> 0.3980
D	<div></div> 0.7030	<div></div> 0.4250

