



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:34 PM UTC

PDB ID : 9RMS / pdb_00009rms
EMDB ID : EMD-54065
Title : GluA4 in complex with TARP-2, Resting II state, structure of TMD/LBD domains
Authors : Vega-Gutierrez, C.; Herguedas, B.
Deposited on : 2025-06-18
Resolution : 3.80 Å (reported)
Based on initial models : 4U2R, 9QDN, 4O3B

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:

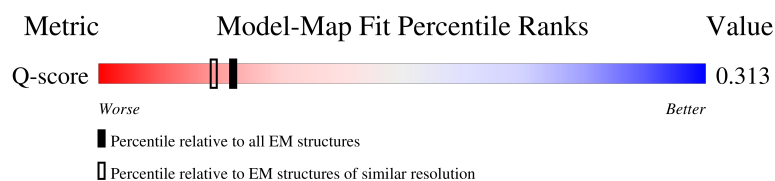
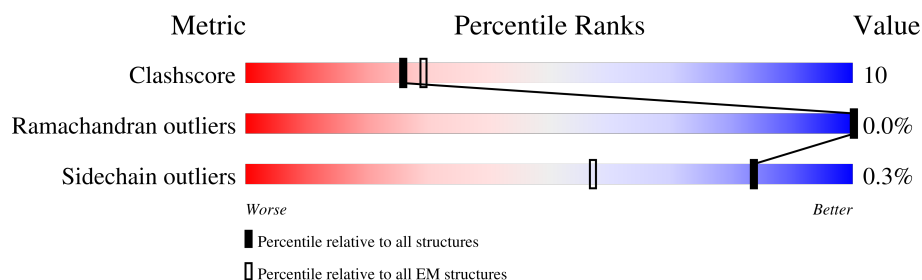
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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.



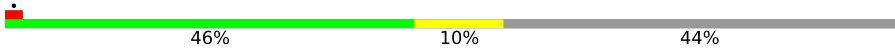
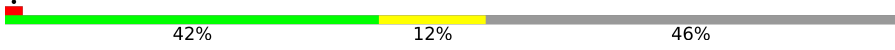
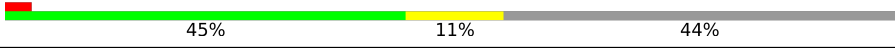
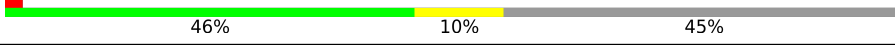
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	

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Mol	Chain	Length	Quality of chain
2	E	323	
2	F	323	
2	G	323	
2	H	323	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	E2Q	C	1001	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18061 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	401	Total	C	N	O	S	0	0
			3127	2037	504	566	20		
1	B	399	Total	C	N	O	S	0	0
			3095	2013	501	561	20		
1	C	403	Total	C	N	O	S	0	0
			3132	2041	504	567	20		
1	D	406	Total	C	N	O	S	0	0
			3163	2060	506	577	20		

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
C	734	ILE	THR	variant	UNP P19493
D	734	ILE	THR	variant	UNP P19493

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	181	Total	C	N	O	S	0	0
			1379	907	226	235	11		
2	F	175	Total	C	N	O	S	0	0
			1332	877	215	229	11		
2	G	180	Total	C	N	O	S	0	0
			1370	901	224	234	11		
2	H	179	Total	C	N	O	S	0	0
			1371	902	224	234	11		

There are 4 discrepancies between the modelled and reference sequences:

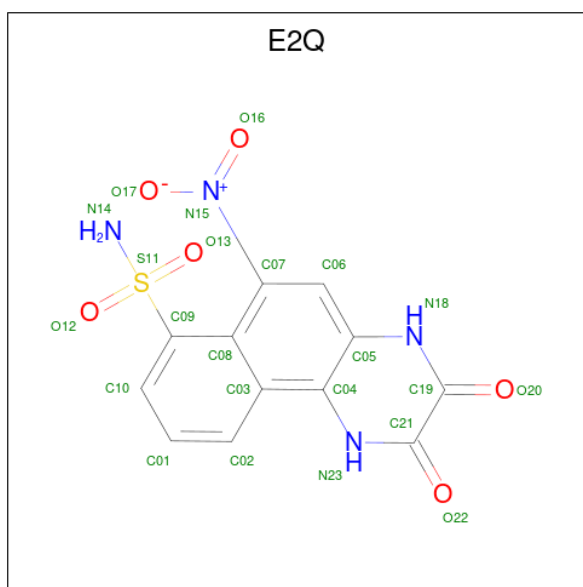
Chain	Residue	Modelled	Actual	Comment	Reference
E	14	ILE	THR	engineered mutation	UNP Q71RJ2

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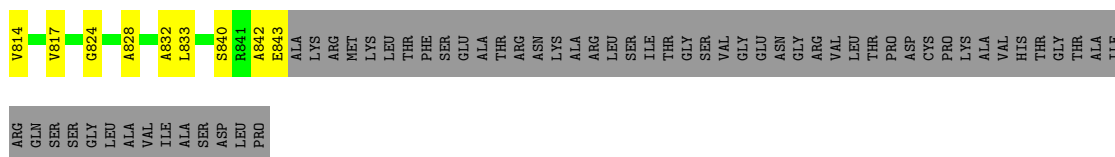
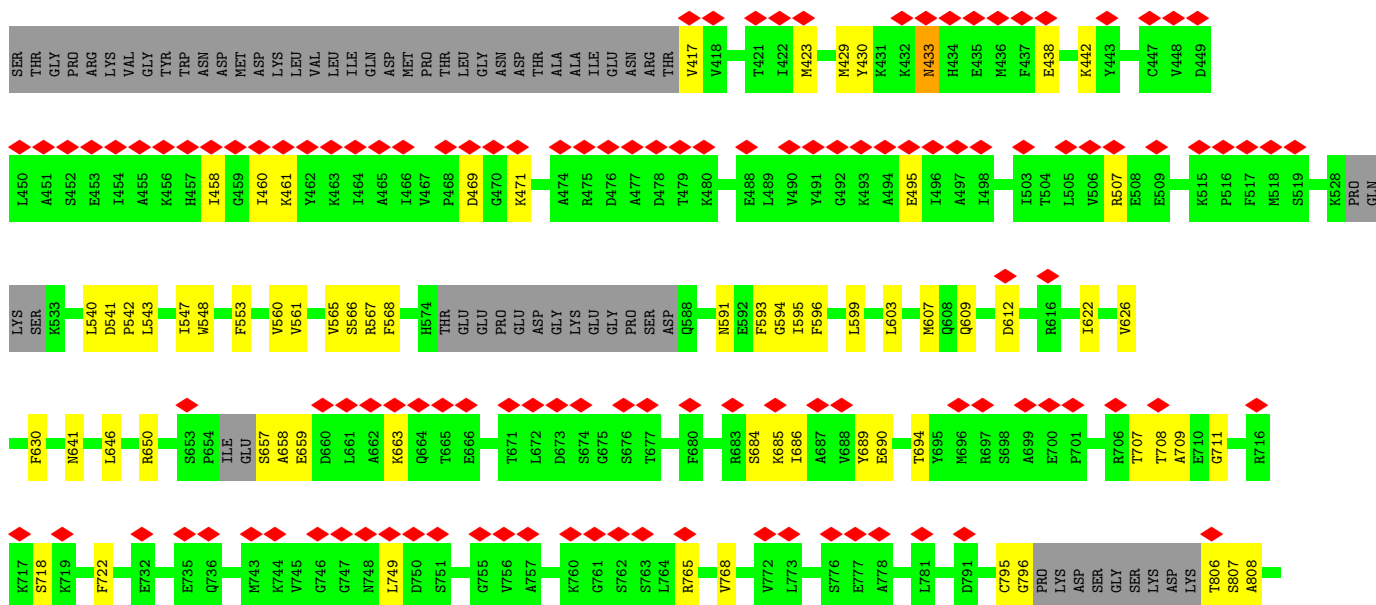
Chain	Residue	Modelled	Actual	Comment	Reference
F	14	ILE	THR	engineered mutation	UNP Q71RJ2
G	14	ILE	THR	engineered mutation	UNP Q71RJ2
H	14	ILE	THR	engineered mutation	UNP Q71RJ2

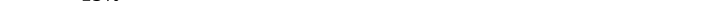
- Molecule 3 is 6-nitro-2,3-bis(oxidanylidene)-1,4-dihydrobenzo[f]quinoxaline-7-sulfonamide (CCD ID: E2Q) (formula: C₁₂H₈N₄O₆S) (labeled as "Ligand of Interest" by depositor).

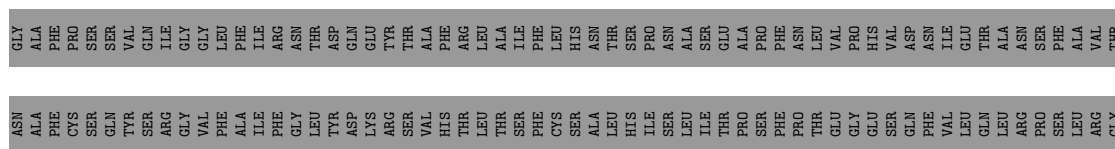


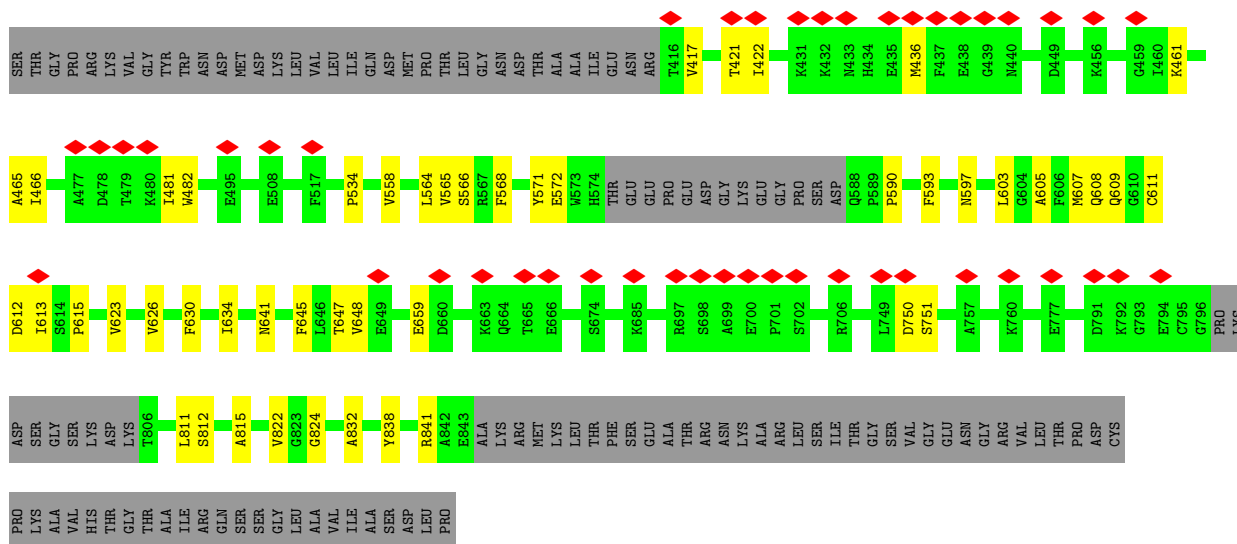
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			23	12	4	6	1	
3	B	1	Total	C	N	O	S	0
			23	12	4	6	1	
3	C	1	Total	C	N	O	S	0
			23	12	4	6	1	
3	D	1	Total	C	N	O	S	0
			23	12	4	6	1	

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

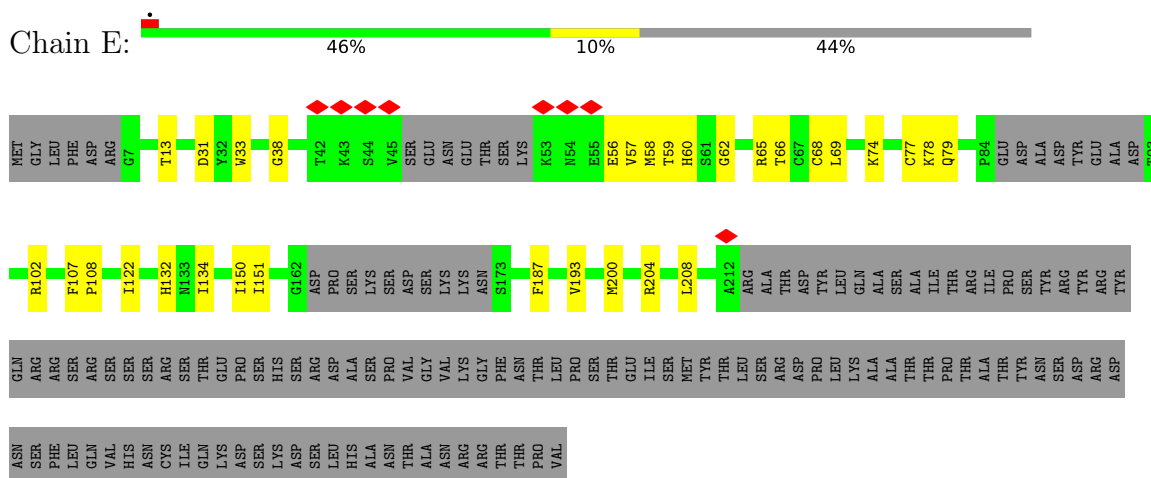


Chain C:  13% 38% 7% 42%

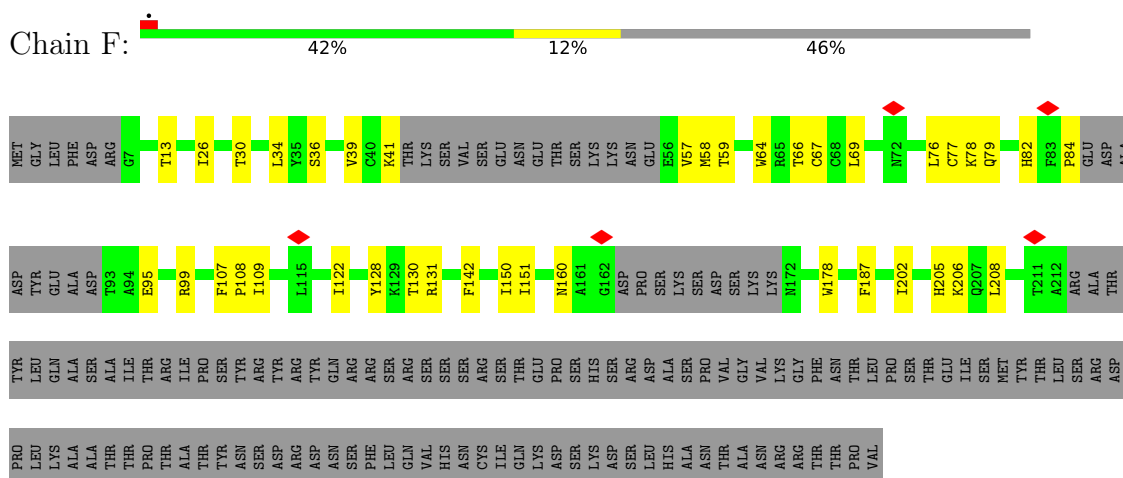




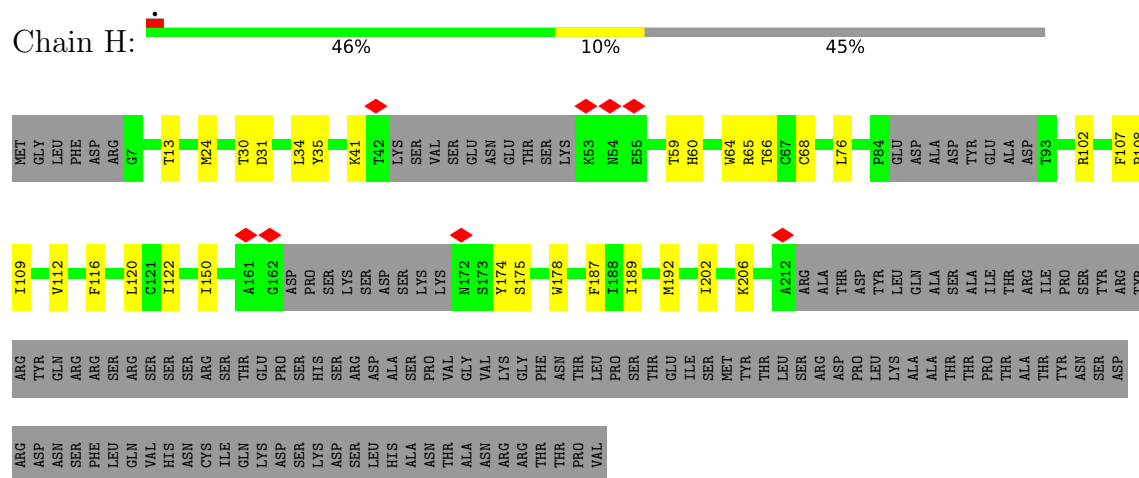
- Molecule 2: Voltage-dependent calcium channel gamma-2 subunit



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- Molecule 2: Voltage-dependent calcium channel gamma-2 subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35082	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	0.637	Depositor
Minimum map value	-0.318	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	320.5152, 320.5152, 320.5152	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6462, 0.6462, 0.6462	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	0.25	0/3201	0.37	0/4328
1	B	0.59	0/3164	0.73	2/4276 (0.0%)
1	C	0.60	2/3202 (0.1%)	0.77	10/4326 (0.2%)
1	D	0.23	0/3237	0.33	0/4379
2	E	0.06	0/1410	0.17	0/1906
2	F	0.14	0/1361	0.24	0/1840
2	G	0.08	0/1401	0.19	0/1896
2	H	0.09	0/1402	0.18	0/1895
All	All	0.38	2/18378 (0.0%)	0.50	12/24846 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	H	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	759	PRO	CA-C	8.45	1.60	1.52
1	C	759	PRO	N-CA	5.61	1.53	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	760	LYS	CA-C-N	-9.64	103.23	121.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	760	LYS	C-N-CA	-9.64	103.23	121.93
1	C	758	THR	CA-C-N	8.97	132.45	120.79
1	C	758	THR	C-N-CA	8.97	132.45	120.79
1	C	759	PRO	N-CA-C	6.72	121.90	110.74
1	B	707	THR	CA-C-N	-6.49	111.08	120.29
1	B	707	THR	C-N-CA	-6.49	111.08	120.29
1	C	759	PRO	CA-C-N	6.38	133.72	121.54
1	C	759	PRO	C-N-CA	6.38	133.72	121.54
1	C	758	THR	CA-CB-OG1	-5.77	100.95	109.60
1	C	765	ARG	N-CA-CB	-5.58	101.64	110.28
1	C	759	PRO	CA-N-CD	-5.38	104.47	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	475	ARG	Sidechain
2	H	102	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3127	0	3128	60	0
1	B	3095	0	3099	89	0
1	C	3132	0	3151	107	0
1	D	3163	0	3170	48	0
2	E	1379	0	1359	21	0
2	F	1332	0	1324	34	0
2	G	1370	0	1349	27	0
2	H	1371	0	1360	24	0
3	A	23	0	0	3	0
3	B	23	0	0	5	0
3	C	23	0	0	15	0
3	D	23	0	0	2	0
All	All	18061	0	17940	366	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 10.

All (366) 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:C:714:ARG:HB3	1:C:724:PHE:CZ	1.70	1.27
1:C:718:SER:CB	1:C:722:PHE:HD2	1.52	1.21
1:C:433:ASN:ND2	1:C:437:PHE:CE2	2.15	1.15
1:C:714:ARG:HB3	1:C:724:PHE:HZ	0.98	1.14
1:C:689:TYR:HE1	1:C:749:LEU:HD23	1.09	1.11
1:C:718:SER:HB3	1:C:722:PHE:HD2	1.13	1.09
1:C:689:TYR:CE1	1:C:749:LEU:HD23	1.89	1.08
1:B:718:SER:CB	1:B:722:PHE:HD2	1.67	1.07
1:C:715:VAL:N	1:C:724:PHE:CE2	2.25	1.05
1:C:433:ASN:ND2	1:C:437:PHE:HE2	1.51	1.05
1:C:718:SER:CB	1:C:722:PHE:CD2	2.41	1.04
1:C:715:VAL:N	1:C:724:PHE:HE2	1.56	1.03
1:C:715:VAL:CA	1:C:724:PHE:HE2	1.65	1.02
1:C:714:ARG:CB	1:C:724:PHE:HZ	1.74	1.01
1:C:516:PRO:HD2	1:D:436:MET:HE2	1.39	1.01
1:C:417:VAL:CG2	1:C:460:ILE:HG21	1.92	1.00
1:B:718:SER:HB3	1:B:722:PHE:HD2	1.26	0.99
1:C:718:SER:HB3	1:C:722:PHE:CD2	1.96	0.98
1:A:609:GLN:HE22	1:D:608:GLN:HA	1.26	0.98
1:C:433:ASN:CG	1:C:437:PHE:HE2	1.70	0.97
1:B:689:TYR:HE1	1:B:749:LEU:HD13	1.28	0.97
2:F:67:CYS:HA	2:F:77:CYS:HA	1.48	0.95
1:C:672:LEU:HD11	3:C:1001:E2Q:O13	1.69	0.92
1:B:417:VAL:HA	1:B:495:GLU:OE1	1.71	0.91
1:B:417:VAL:CG2	1:B:460:ILE:HG21	2.02	0.90
1:C:689:TYR:HE1	1:C:749:LEU:CD2	1.83	0.90
1:C:718:SER:OG	1:C:722:PHE:CD2	2.24	0.89
1:B:718:SER:CB	1:B:722:PHE:CD2	2.56	0.88
1:C:433:ASN:ND2	1:C:437:PHE:CZ	2.42	0.87
1:C:685:LYS:HA	1:C:690:GLU:OE2	1.75	0.87
1:B:507:ARG:NH2	3:B:1001:E2Q:O22	2.08	0.86
1:B:718:SER:HB3	1:B:722:PHE:CD2	2.08	0.86
1:C:417:VAL:HG23	1:C:460:ILE:HG21	1.57	0.86
1:C:417:VAL:HG21	1:C:460:ILE:HG21	1.59	0.83
1:C:711:GLY:O	1:C:724:PHE:CZ	2.32	0.83
1:C:765:ARG:HA	1:C:768:VAL:CG2	2.10	0.82
1:B:417:VAL:HG21	1:B:460:ILE:HG21	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:SER:HB3	1:A:591:ASN:HD21	1.46	0.80
1:B:689:TYR:CE1	1:B:749:LEU:HD13	2.17	0.79
1:C:765:ARG:HA	1:C:768:VAL:HG22	1.65	0.79
1:A:609:GLN:NE2	1:D:608:GLN:HA	1.98	0.78
1:B:567:ARG:HE	1:B:594:GLY:HA2	1.48	0.77
1:C:754:TYR:CE1	3:C:1001:E2Q:O20	2.38	0.76
1:B:567:ARG:HE	1:B:594:GLY:CA	1.98	0.76
2:G:83:PHE:CD2	2:G:99:ARG:NH1	2.53	0.76
1:B:567:ARG:NE	1:B:594:GLY:HA2	2.01	0.76
1:C:500:PRO:O	3:C:1001:E2Q:C19	2.33	0.76
1:A:632:LEU:HD22	1:B:607:MET:HE1	1.66	0.75
1:A:628:TRP:CD2	1:B:609:GLN:HG3	2.21	0.75
1:B:567:ARG:HE	1:B:593:PHE:C	1.94	0.75
1:B:685:LYS:HA	1:B:690:GLU:OE2	1.86	0.75
1:C:715:VAL:CA	1:C:724:PHE:CE2	2.58	0.73
1:C:454:ILE:HG22	1:C:458:ILE:HD12	1.69	0.73
1:C:454:ILE:CG2	1:C:458:ILE:HD12	2.18	0.73
1:C:711:GLY:O	1:C:724:PHE:CE2	2.41	0.73
1:C:433:ASN:CG	1:C:437:PHE:CE2	2.59	0.72
1:C:628:TRP:CD2	1:D:609:GLN:HG3	2.25	0.72
2:G:40:CYS:HA	2:G:78:LYS:HE3	1.72	0.71
1:B:417:VAL:HG23	1:B:460:ILE:HG21	1.73	0.71
1:B:566:SER:HB3	1:B:591:ASN:HD21	1.56	0.71
1:A:648:VAL:HG21	1:B:650:ARG:HD3	1.72	0.70
1:B:438:GLU:HA	1:B:442:LYS:HE3	1.74	0.70
1:C:423:MET:HE1	1:C:430:TYR:N	2.05	0.70
1:C:764:LEU:O	1:C:768:VAL:HG13	1.91	0.69
1:C:424:GLU:OE2	3:C:1001:E2Q:O16	2.09	0.69
1:B:718:SER:OG	1:B:722:PHE:CD2	2.46	0.69
2:F:58:MET:O	2:F:69:LEU:HB3	1.93	0.68
1:C:765:ARG:C	1:C:768:VAL:HG22	2.18	0.68
1:C:754:TYR:CD1	3:C:1001:E2Q:O20	2.47	0.68
1:C:417:VAL:HG23	1:C:460:ILE:CG2	2.24	0.67
1:C:672:LEU:CD1	3:C:1001:E2Q:O13	2.43	0.66
1:B:458:ILE:HD11	1:B:768:VAL:HA	1.75	0.66
1:C:423:MET:HE1	1:C:429:MET:C	2.20	0.66
1:D:647:THR:HG22	1:D:648:VAL:H	1.62	0.65
1:C:765:ARG:O	1:C:768:VAL:HG22	1.96	0.65
1:B:567:ARG:HE	1:B:594:GLY:N	1.95	0.65
3:A:1001:E2Q:O13	3:A:1001:E2Q:O17	2.15	0.65
1:C:685:LYS:CA	1:C:690:GLU:OE2	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:67:CYS:CA	2:F:77:CYS:HA	2.25	0.64
2:F:95:GLU:O	2:F:99:ARG:HG2	1.98	0.63
1:A:546:GLU:OE2	2:H:174:TYR:OH	2.09	0.63
1:A:573:TRP:CE3	1:A:589:PRO:HA	2.35	0.62
1:C:715:VAL:N	1:C:724:PHE:CZ	2.67	0.62
1:B:694:THR:HB	1:C:796:GLY:HA2	1.82	0.62
2:F:34:LEU:CD2	2:F:36:SER:HB3	2.29	0.62
1:A:651:MET:HA	1:D:648:VAL:HG21	1.81	0.61
1:B:568:PHE:CE1	1:C:832:ALA:HB1	2.35	0.61
1:C:765:ARG:CA	1:C:768:VAL:HG22	2.31	0.61
2:H:34:LEU:HD11	2:H:174:TYR:HB2	1.83	0.60
3:A:1001:E2Q:O17	3:A:1001:E2Q:S11	2.60	0.60
2:G:60:HIS:ND1	2:G:69:LEU:HB3	2.16	0.60
1:A:611:CYS:N	1:D:611:CYS:SG	2.74	0.59
1:D:647:THR:HG22	1:D:648:VAL:N	2.17	0.59
1:B:567:ARG:NE	1:B:594:GLY:CA	2.63	0.59
1:D:811:LEU:O	1:D:815:ALA:HB2	2.03	0.59
1:C:658:ALA:HB1	1:C:688:VAL:HG11	1.84	0.59
2:E:200:MET:O	2:E:204:ARG:HG2	2.03	0.58
2:F:41:LYS:HG2	2:F:76:LEU:HD23	1.86	0.58
1:C:765:ARG:HA	1:C:768:VAL:HG21	1.83	0.58
1:A:628:TRP:CG	1:B:609:GLN:HG3	2.38	0.58
3:B:1001:E2Q:N15	3:B:1001:E2Q:O13	2.36	0.58
2:E:102:ARG:O	2:E:102:ARG:NH1	2.36	0.57
1:C:458:ILE:HD11	1:C:768:VAL:HA	1.85	0.57
2:F:66:THR:HG23	2:F:66:THR:O	2.04	0.57
1:D:564:LEU:O	1:D:568:PHE:HB3	2.03	0.57
1:C:714:ARG:HB3	1:C:724:PHE:CE1	2.34	0.57
2:F:64:TRP:CH2	2:F:109:ILE:HD11	2.40	0.57
1:B:417:VAL:HG23	1:B:460:ILE:CG2	2.35	0.56
1:B:568:PHE:HE1	1:C:832:ALA:HB1	1.71	0.56
2:E:78:LYS:HG2	2:E:79:GLN:H	1.70	0.56
2:F:122:ILE:HD11	2:F:142:PHE:HE2	1.70	0.56
1:B:423:MET:HE1	1:B:429:MET:C	2.31	0.56
1:A:716:ARG:NE	1:A:741:ASP:OD1	2.39	0.56
1:C:689:TYR:CE1	1:C:749:LEU:HB3	2.41	0.56
2:E:66:THR:HG23	2:E:66:THR:O	2.06	0.55
1:A:522:ILE:N	1:A:750:ASP:OD1	2.39	0.55
1:C:433:ASN:HD21	1:C:437:PHE:HZ	1.54	0.55
1:B:708:THR:O	1:B:709:ALA:C	2.48	0.55
2:H:59:THR:HA	2:H:68:CYS:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:ASP:OD1	1:B:469:ASP:O	2.25	0.55
1:C:689:TYR:HE1	1:C:749:LEU:CG	2.19	0.55
2:F:128:TYR:HD1	2:F:131:ARG:HH21	1.55	0.55
2:H:30:THR:HG21	2:H:178:TRP:CH2	2.42	0.55
1:C:606:PHE:HA	1:C:631:THR:CG2	2.37	0.55
1:D:572:GLU:O	1:D:590:PRO:HG3	2.07	0.55
2:F:130:THR:OG1	2:F:131:ARG:NH1	2.40	0.54
1:C:454:ILE:HG23	1:C:458:ILE:CD1	2.36	0.54
2:H:30:THR:HG21	2:H:178:TRP:HH2	1.72	0.54
1:A:824:GLY:HA3	1:D:626:VAL:HG11	1.90	0.54
1:A:573:TRP:CZ3	1:A:589:PRO:HA	2.44	0.53
1:B:567:ARG:NE	1:B:593:PHE:O	2.41	0.53
2:E:33:TRP:HB2	2:E:62:GLY:HA2	1.89	0.53
2:H:66:THR:O	2:H:66:THR:HG23	2.08	0.53
1:B:708:THR:CB	3:B:1001:E2Q:O12	2.56	0.53
2:F:202:ILE:O	2:F:206:LYS:HG3	2.09	0.53
2:G:40:CYS:O	2:G:78:LYS:HB2	2.09	0.53
1:A:532:SER:O	1:A:533:LYS:C	2.52	0.53
1:A:564:LEU:O	1:A:568:PHE:HB3	2.08	0.53
1:A:648:VAL:HG11	1:B:650:ARG:HH11	1.74	0.53
1:C:502:THR:N	3:C:1001:E2Q:O20	2.41	0.53
1:C:765:ARG:O	1:C:768:VAL:CG2	2.57	0.53
1:C:460:ILE:HG22	1:C:461:LYS:O	2.09	0.53
1:C:628:TRP:CG	1:D:609:GLN:HG3	2.44	0.53
1:C:454:ILE:CG2	1:C:458:ILE:CD1	2.86	0.52
2:F:58:MET:HG2	2:F:69:LEU:HD23	1.91	0.52
1:C:423:MET:HE1	1:C:429:MET:CA	2.39	0.52
1:D:481:ILE:HG22	1:D:482:TRP:N	2.24	0.52
1:C:685:LYS:C	1:C:690:GLU:OE2	2.51	0.52
2:E:31:ASP:HA	2:E:62:GLY:HA3	1.90	0.52
2:E:132:HIS:CD2	2:E:208:LEU:HD11	2.45	0.52
2:F:64:TRP:CZ2	2:F:109:ILE:HD11	2.45	0.52
1:B:565:VAL:HA	1:B:568:PHE:CD1	2.45	0.52
1:D:648:VAL:O	1:D:648:VAL:HG22	2.10	0.51
1:A:568:PHE:CE1	1:B:832:ALA:HB1	2.44	0.51
1:C:657:SER:C	1:C:659:GLU:H	2.18	0.51
1:C:689:TYR:CE1	1:C:749:LEU:CD2	2.71	0.51
2:F:150:ILE:HD11	2:F:187:PHE:CE1	2.45	0.51
1:C:754:TYR:CE1	3:C:1001:E2Q:C19	2.93	0.51
2:E:107:PHE:HB2	2:E:108:PRO:HD3	1.92	0.51
1:A:630:PHE:HA	1:B:817:VAL:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LEU:CD2	1:B:607:MET:HE1	2.40	0.51
1:B:641:ASN:HA	1:C:646:LEU:HD13	1.92	0.51
1:A:542:PRO:O	1:A:641:ASN:ND2	2.42	0.51
1:D:565:VAL:HG23	1:D:566:SER:N	2.25	0.50
1:A:809:LEU:HD13	1:D:641:ASN:HB2	1.94	0.50
2:E:66:THR:O	2:E:77:CYS:HA	2.11	0.50
2:G:83:PHE:CE2	2:G:99:ARG:NH1	2.79	0.50
1:D:822:VAL:HG11	2:F:151:ILE:HD11	1.93	0.50
2:H:24:MET:HG3	2:H:112:VAL:HG23	1.94	0.50
1:B:708:THR:HB	3:B:1001:E2Q:O12	2.11	0.50
1:A:837:CYS:O	1:A:841:ARG:HG2	2.11	0.49
1:A:825:LEU:HD21	1:D:558:VAL:HG22	1.94	0.49
2:G:107:PHE:HB2	2:G:108:PRO:HD3	1.94	0.49
1:A:568:PHE:CZ	1:B:832:ALA:HB1	2.47	0.49
1:C:655:ILE:HB	1:C:660:ASP:OD2	2.12	0.49
1:C:711:GLY:HA2	1:C:724:PHE:CE1	2.47	0.49
2:F:78:LYS:HG2	2:F:79:GLN:N	2.27	0.49
2:H:41:LYS:HD3	2:H:76:LEU:CD2	2.42	0.49
1:B:417:VAL:CA	1:B:495:GLU:OE1	2.54	0.49
1:D:421:THR:HG22	1:D:422:ILE:H	1.77	0.49
2:G:60:HIS:CE1	2:G:69:LEU:HB3	2.47	0.49
1:A:650:ARG:NH1	1:D:645:PHE:HA	2.28	0.49
1:B:460:ILE:HG22	1:B:461:LYS:O	2.13	0.49
1:D:838:TYR:O	1:D:841:ARG:HG2	2.13	0.49
1:A:811:LEU:O	1:A:815:ALA:HB2	2.12	0.49
1:A:632:LEU:HD22	1:B:607:MET:CE	2.40	0.48
1:D:421:THR:HG22	1:D:422:ILE:N	2.28	0.48
1:D:572:GLU:HB3	1:D:590:PRO:HG2	1.96	0.48
1:C:754:TYR:HE1	3:C:1001:E2Q:C19	2.26	0.48
3:D:1001:E2Q:S11	3:D:1001:E2Q:O17	2.71	0.48
1:C:658:ALA:HB1	1:C:688:VAL:CG1	2.44	0.48
2:G:34:LEU:HD11	2:G:174:TYR:HB2	1.96	0.48
1:B:458:ILE:HG22	1:B:458:ILE:O	2.14	0.48
1:D:565:VAL:HG23	1:D:566:SER:H	1.78	0.48
2:G:10:MET:CE	2:G:200:MET:HE1	2.43	0.48
3:A:1001:E2Q:O17	3:A:1001:E2Q:N14	2.47	0.48
1:D:612:ASP:CG	1:D:613:ILE:H	2.22	0.48
2:H:107:PHE:HB2	2:H:108:PRO:HD3	1.95	0.48
1:C:715:VAL:HA	1:C:724:PHE:HE2	1.71	0.47
1:D:565:VAL:HA	1:D:568:PHE:CD1	2.49	0.47
1:D:593:PHE:HZ	1:D:615:PRO:HD3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:ARG:NH1	3:B:1001:E2Q:O20	2.47	0.47
1:A:650:ARG:HH12	1:D:645:PHE:HA	1.80	0.47
2:G:65:ARG:HG3	2:G:65:ARG:HH11	1.79	0.47
1:A:657:SER:OG	1:A:658:ALA:N	2.47	0.47
1:B:603:LEU:O	1:B:607:MET:HG2	2.14	0.47
1:C:829:MET:O	1:C:833:LEU:HG	2.14	0.47
1:B:607:MET:HB2	1:B:609:GLN:HG2	1.96	0.47
2:F:39:VAL:HG12	2:F:41:LYS:H	1.78	0.47
1:A:567:ARG:HH21	1:A:592:GLU:HA	1.80	0.47
1:B:565:VAL:HG23	1:B:566:SER:N	2.29	0.47
1:B:814:VAL:HG12	1:B:817:VAL:HG12	1.97	0.47
1:A:572:GLU:HG3	1:A:590:PRO:HB3	1.97	0.47
1:C:711:GLY:O	1:C:724:PHE:CE1	2.66	0.47
2:E:59:THR:HG23	2:E:68:CYS:HA	1.96	0.47
2:E:150:ILE:HD11	2:E:187:PHE:CE1	2.50	0.47
2:F:107:PHE:HB2	2:F:108:PRO:HD3	1.96	0.47
2:E:107:PHE:CZ	2:E:151:ILE:HG21	2.50	0.47
1:B:541:ASP:N	1:B:542:PRO:CD	2.78	0.47
1:C:619:SER:HB3	1:D:832:ALA:HB2	1.97	0.47
2:G:26:ILE:O	2:G:30:THR:HG23	2.14	0.47
2:H:174:TYR:CG	2:H:174:TYR:O	2.67	0.47
1:A:473:GLY:O	1:A:474:ALA:HB2	2.15	0.46
1:A:832:ALA:HB1	1:D:568:PHE:HE1	1.81	0.46
2:H:59:THR:CB	2:H:68:CYS:HA	2.45	0.46
1:C:502:THR:HG1	3:C:1001:E2Q:C19	2.27	0.46
1:B:540:LEU:HD22	1:B:548:TRP:CE2	2.51	0.46
1:B:469:ASP:OD2	1:B:471:LYS:HD2	2.15	0.46
1:B:622:ILE:O	1:B:626:VAL:HG22	2.15	0.46
1:B:565:VAL:HG23	1:B:566:SER:H	1.81	0.46
2:F:95:GLU:O	2:F:99:ARG:CG	2.64	0.46
2:H:13:THR:HG22	2:H:122:ILE:CD1	2.46	0.46
2:G:69:LEU:HD23	2:G:69:LEU:H	1.81	0.46
2:G:79:GLN:HG3	2:G:80:ILE:H	1.79	0.46
2:H:41:LYS:HD3	2:H:76:LEU:HD21	1.97	0.46
1:D:630:PHE:CZ	1:D:634:ILE:HG13	2.51	0.45
1:A:609:GLN:NE2	1:D:605:ALA:O	2.49	0.45
1:B:595:ILE:HG23	1:B:596:PHE:N	2.32	0.45
2:E:60:HIS:ND1	2:E:69:LEU:HG	2.31	0.45
2:F:34:LEU:HD21	2:F:36:SER:HB3	1.97	0.45
2:F:122:ILE:HD11	2:F:142:PHE:CE2	2.51	0.45
2:F:205:HIS:HA	2:F:208:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:10:MET:HE2	2:G:200:MET:HE1	1.98	0.45
2:G:200:MET:O	2:G:204:ARG:HG2	2.16	0.45
1:B:423:MET:HE1	1:B:430:TYR:N	2.31	0.45
3:D:1001:E2Q:N15	3:D:1001:E2Q:O13	2.49	0.45
2:F:41:LYS:HE3	2:F:76:LEU:HD22	1.99	0.45
1:D:534:PRO:HG3	1:D:812:SER:OG	2.17	0.45
1:A:571:TYR:CE2	1:B:840:SER:HA	2.52	0.45
1:C:423:MET:CE	1:C:429:MET:HA	2.47	0.45
1:A:607:MET:O	1:A:608:GLN:HB2	2.17	0.45
1:A:609:GLN:OE1	1:D:608:GLN:HG2	2.16	0.45
1:A:623:VAL:HG23	1:B:828:ALA:CB	2.46	0.45
1:B:460:ILE:HG22	1:B:461:LYS:N	2.32	0.45
2:F:58:MET:CG	2:F:69:LEU:HD23	2.46	0.45
2:H:202:ILE:HG22	2:H:206:LYS:HE2	1.98	0.45
1:A:648:VAL:HG11	1:B:650:ARG:NH1	2.31	0.45
1:B:595:ILE:O	1:B:599:LEU:HD23	2.16	0.45
2:E:68:CYS:O	2:E:74:LYS:HA	2.16	0.45
2:H:60:HIS:O	2:H:60:HIS:ND1	2.50	0.45
1:C:500:PRO:O	3:C:1001:E2Q:N18	2.50	0.44
1:C:502:THR:OG1	3:C:1001:E2Q:C19	2.65	0.44
1:C:611:CYS:SG	1:C:611:CYS:O	2.75	0.44
2:F:66:THR:HG23	2:F:78:LYS:HB3	1.98	0.44
1:A:626:VAL:HG11	1:B:824:GLY:HA3	1.99	0.44
1:C:689:TYR:CE1	1:C:749:LEU:CG	3.00	0.44
1:A:641:ASN:HA	1:B:646:LEU:HD13	2.00	0.44
2:G:59:THR:HG22	2:G:68:CYS:HA	1.98	0.44
1:A:766:THR:HB	1:A:767:PRO:HD3	2.00	0.44
1:A:614:SER:OG	1:B:612:ASP:HB2	2.17	0.44
1:C:714:ARG:HH21	1:C:722:PHE:HE1	1.64	0.44
1:B:708:THR:O	1:B:711:GLY:N	2.51	0.44
1:C:454:ILE:HG23	1:C:458:ILE:HD11	1.99	0.44
1:C:672:LEU:HD11	3:C:1001:E2Q:S11	2.57	0.44
2:E:132:HIS:NE2	2:E:208:LEU:HD11	2.32	0.44
2:H:64:TRP:CZ2	2:H:109:ILE:HD11	2.52	0.44
1:B:795:CYS:O	1:B:796:GLY:C	2.60	0.44
1:A:572:GLU:HG3	1:A:590:PRO:CB	2.47	0.44
1:D:597:ASN:HB3	1:D:613:ILE:HD13	2.00	0.44
1:C:759:PRO:O	1:C:762:SER:HB2	2.18	0.43
1:C:834:ILE:HG13	1:C:835:GLU:N	2.33	0.43
2:F:13:THR:HG22	2:F:122:ILE:HD13	2.00	0.43
1:B:641:ASN:CA	1:C:646:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:ILE:HD11	2:H:187:PHE:CE1	2.54	0.43
1:D:647:THR:O	1:D:648:VAL:C	2.61	0.43
3:C:1001:E2Q:N15	3:C:1001:E2Q:O12	2.51	0.43
1:D:659:GLU:OE1	1:D:659:GLU:N	2.48	0.43
2:H:41:LYS:HB2	2:H:76:LEU:CD2	2.48	0.43
2:H:189:ILE:HD13	2:H:192:MET:HE2	1.99	0.43
1:A:840:SER:HB2	1:D:571:TYR:HE2	1.84	0.43
1:C:541:ASP:N	1:C:542:PRO:CD	2.81	0.43
1:A:429:MET:N	1:A:444:GLU:O	2.47	0.43
1:A:571:TYR:HE2	1:B:840:SER:HA	1.83	0.43
1:C:626:VAL:HG11	1:D:824:GLY:HA3	2.01	0.43
2:E:57:VAL:HG22	2:E:58:MET:N	2.33	0.43
1:C:423:MET:CE	1:C:430:TYR:N	2.80	0.43
2:E:38:GLY:O	2:E:56:GLU:HA	2.19	0.43
1:B:547:ILE:HD11	1:C:810:SER:C	2.44	0.43
1:C:606:PHE:HA	1:C:631:THR:HG21	2.01	0.43
1:C:754:TYR:CE1	3:C:1001:E2Q:N18	2.87	0.43
1:B:433:ASN:OD1	1:B:433:ASN:N	2.53	0.42
1:B:561:VAL:O	1:B:565:VAL:HG22	2.19	0.42
1:B:842:ALA:O	1:B:843:GLU:C	2.62	0.42
2:G:79:GLN:HG3	2:G:80:ILE:N	2.33	0.42
1:B:553:PHE:CZ	2:G:184:ALA:HB1	2.54	0.42
1:B:806:THR:HG23	1:B:808:ALA:H	1.83	0.42
1:C:538:SER:OG	1:C:813:ASN:O	2.37	0.42
2:F:30:THR:HG21	2:F:178:TRP:CH2	2.55	0.42
1:C:423:MET:HE1	1:C:429:MET:HA	2.01	0.42
2:E:13:THR:HG23	2:E:193:VAL:HG13	2.01	0.42
2:F:128:TYR:HD1	2:F:131:ARG:NH2	2.17	0.42
2:G:137:SER:O	2:G:141:PHE:HD2	2.03	0.42
2:H:35:TYR:N	2:H:175:SER:O	2.47	0.42
2:H:41:LYS:HB2	2:H:76:LEU:HD21	2.00	0.42
1:B:626:VAL:HG11	1:C:824:GLY:HA3	2.02	0.42
1:C:758:THR:HA	1:C:759:PRO:HD3	1.82	0.42
2:E:65:ARG:HB3	2:E:77:CYS:HB3	2.02	0.42
2:F:26:ILE:O	2:F:30:THR:HG23	2.19	0.42
1:A:541:ASP:N	1:A:542:PRO:CD	2.82	0.42
1:D:465:ALA:O	1:D:466:ILE:C	2.63	0.42
1:D:603:LEU:O	1:D:607:MET:HG2	2.20	0.42
2:F:57:VAL:O	2:F:59:THR:HG23	2.20	0.42
2:G:58:MET:O	2:G:69:LEU:HD23	2.20	0.42
1:B:460:ILE:CG2	1:B:461:LYS:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:ILE:O	1:C:626:VAL:HG22	2.20	0.42
2:F:34:LEU:HD23	2:F:36:SER:HB3	2.01	0.42
1:D:481:ILE:CG2	1:D:482:TRP:N	2.82	0.41
2:G:93:THR:HG22	2:G:93:THR:O	2.20	0.41
1:A:495:GLU:O	1:A:496:ILE:HG13	2.20	0.41
1:B:659:GLU:HG2	1:B:663:LYS:HE3	2.01	0.41
1:D:417:VAL:N	1:D:461:LYS:O	2.48	0.41
1:D:647:THR:CG2	1:D:648:VAL:H	2.31	0.41
1:B:657:SER:C	1:B:659:GLU:N	2.79	0.41
1:A:568:PHE:CE2	1:B:833:LEU:HD23	2.55	0.41
1:A:572:GLU:CG	1:A:590:PRO:HG3	2.50	0.41
1:C:558:VAL:HG21	1:C:627:TRP:CE3	2.55	0.41
2:G:122:ILE:HD11	2:G:142:PHE:HE2	1.85	0.41
2:G:142:PHE:CD2	2:G:193:VAL:HG12	2.55	0.41
1:A:572:GLU:HG3	1:A:572:GLU:O	2.20	0.41
1:B:684:SER:O	1:B:690:GLU:OE2	2.38	0.41
1:C:460:ILE:HG22	1:C:461:LYS:N	2.36	0.41
2:H:13:THR:HG22	2:H:122:ILE:HD11	2.03	0.41
1:A:421:THR:HG22	1:A:422:ILE:N	2.36	0.41
1:A:711:GLY:HA3	1:A:724:PHE:CE1	2.56	0.41
2:H:116:PHE:CZ	2:H:120:LEU:HD11	2.55	0.41
1:A:828:ALA:CB	1:D:623:VAL:HG23	2.51	0.41
2:E:13:THR:HG22	2:E:122:ILE:CD1	2.51	0.41
2:E:134:ILE:O	2:E:134:ILE:HG22	2.20	0.41
1:A:623:VAL:HG23	1:B:828:ALA:HB1	2.02	0.41
1:B:543:LEU:HD12	1:B:548:TRP:CZ2	2.55	0.41
1:B:686:ILE:HB	1:B:689:TYR:HD2	1.85	0.41
1:A:495:GLU:C	1:A:496:ILE:HG13	2.46	0.41
1:B:560:VAL:HG13	2:G:195:VAL:CG1	2.50	0.41
2:G:57:VAL:HG22	2:G:58:MET:N	2.36	0.40
2:G:136:LEU:HB2	2:G:201:PHE:CG	2.56	0.40
1:A:611:CYS:O	1:D:611:CYS:HB2	2.22	0.40
1:C:607:MET:O	1:C:608:GLN:HB2	2.21	0.40
1:D:750:ASP:OD1	1:D:751:SER:N	2.50	0.40
2:F:67:CYS:CB	2:F:77:CYS:HA	2.51	0.40
1:C:564:LEU:HD23	1:C:564:LEU:C	2.46	0.40
2:H:31:ASP:OD2	2:H:65:ARG:NH2	2.55	0.40
1:C:830:LEU:O	1:C:834:ILE:HG12	2.22	0.40
1:B:630:PHE:HD2	1:C:817:VAL:HG22	1.87	0.40
1:B:806:THR:HG23	1:B:807:SER:N	2.35	0.40
2:F:82:HIS:O	2:F:84:PRO:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:150:ILE:HD11	2:G:187:PHE:CE1	2.56	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	395/882 (45%)	367 (93%)	28 (7%)	0	100	100
1	B	389/882 (44%)	374 (96%)	14 (4%)	1 (0%)	36	67
1	C	393/882 (45%)	382 (97%)	11 (3%)	0	100	100
1	D	400/882 (45%)	384 (96%)	16 (4%)	0	100	100
2	E	173/323 (54%)	161 (93%)	12 (7%)	0	100	100
2	F	167/323 (52%)	155 (93%)	12 (7%)	0	100	100
2	G	172/323 (53%)	165 (96%)	7 (4%)	0	100	100
2	H	171/323 (53%)	159 (93%)	12 (7%)	0	100	100
All	All	2260/4820 (47%)	2147 (95%)	112 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	658	ALA

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/752 (44%)	330 (100%)	0	100	100
1	B	327/752 (44%)	325 (99%)	2 (1%)	78	79
1	C	333/752 (44%)	331 (99%)	2 (1%)	78	79
1	D	337/752 (45%)	337 (100%)	0	100	100
2	E	139/275 (50%)	139 (100%)	0	100	100
2	F	136/275 (50%)	135 (99%)	1 (1%)	76	77
2	G	139/275 (50%)	139 (100%)	0	100	100
2	H	140/275 (51%)	140 (100%)	0	100	100
All	All	1881/4108 (46%)	1876 (100%)	5 (0%)	84	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	433	ASN
1	B	765	ARG
1	C	708	THR
1	C	758	THR
2	F	160	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	813	ASN
1	C	591	ASN
1	D	434	HIS
1	D	641	ASN
2	E	9	GLN
2	E	160	ASN
2	H	160	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	E2Q	B	1001	-	25,25,25	0.82	0	32,39,39	1.26	4 (12%)
3	E2Q	C	1001	-	25,25,25	0.70	0	32,39,39	1.24	4 (12%)
3	E2Q	D	1001	-	25,25,25	0.64	0	32,39,39	1.00	2 (6%)
3	E2Q	A	1001	-	25,25,25	1.05	3 (12%)	32,39,39	1.47	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	E2Q	B	1001	-	-	2/8/10/10	0/3/3/3
3	E2Q	C	1001	-	-	2/8/10/10	0/3/3/3
3	E2Q	D	1001	-	-	5/8/10/10	0/3/3/3
3	E2Q	A	1001	-	-	0/8/10/10	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	E2Q	C09-C08	2.52	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	E2Q	C07-C08	2.46	1.47	1.43
3	A	1001	E2Q	O17-N15	-2.12	1.21	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	E2Q	C08-C09-S11	4.10	126.83	121.74
3	A	1001	E2Q	C10-C09-S11	-3.59	112.63	117.53
3	B	1001	E2Q	C08-C09-S11	3.50	126.09	121.74
3	C	1001	E2Q	C08-C09-S11	2.89	125.33	121.74
3	B	1001	E2Q	C10-C09-S11	-2.83	113.67	117.53
3	C	1001	E2Q	C02-C03-C04	-2.80	119.65	124.70
3	A	1001	E2Q	C02-C03-C04	-2.78	119.70	124.70
3	A	1001	E2Q	C05-C06-C07	2.46	123.01	118.46
3	C	1001	E2Q	C10-C09-S11	-2.35	114.33	117.53
3	D	1001	E2Q	C02-C03-C04	-2.32	120.51	124.70
3	C	1001	E2Q	O12-S11-C09	2.28	110.56	107.26
3	B	1001	E2Q	C02-C03-C04	-2.22	120.71	124.70
3	D	1001	E2Q	C08-C09-S11	2.18	124.45	121.74
3	A	1001	E2Q	C19-C21-N23	2.07	118.26	116.82
3	B	1001	E2Q	C05-C06-C07	2.05	122.25	118.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 25 short contacts:

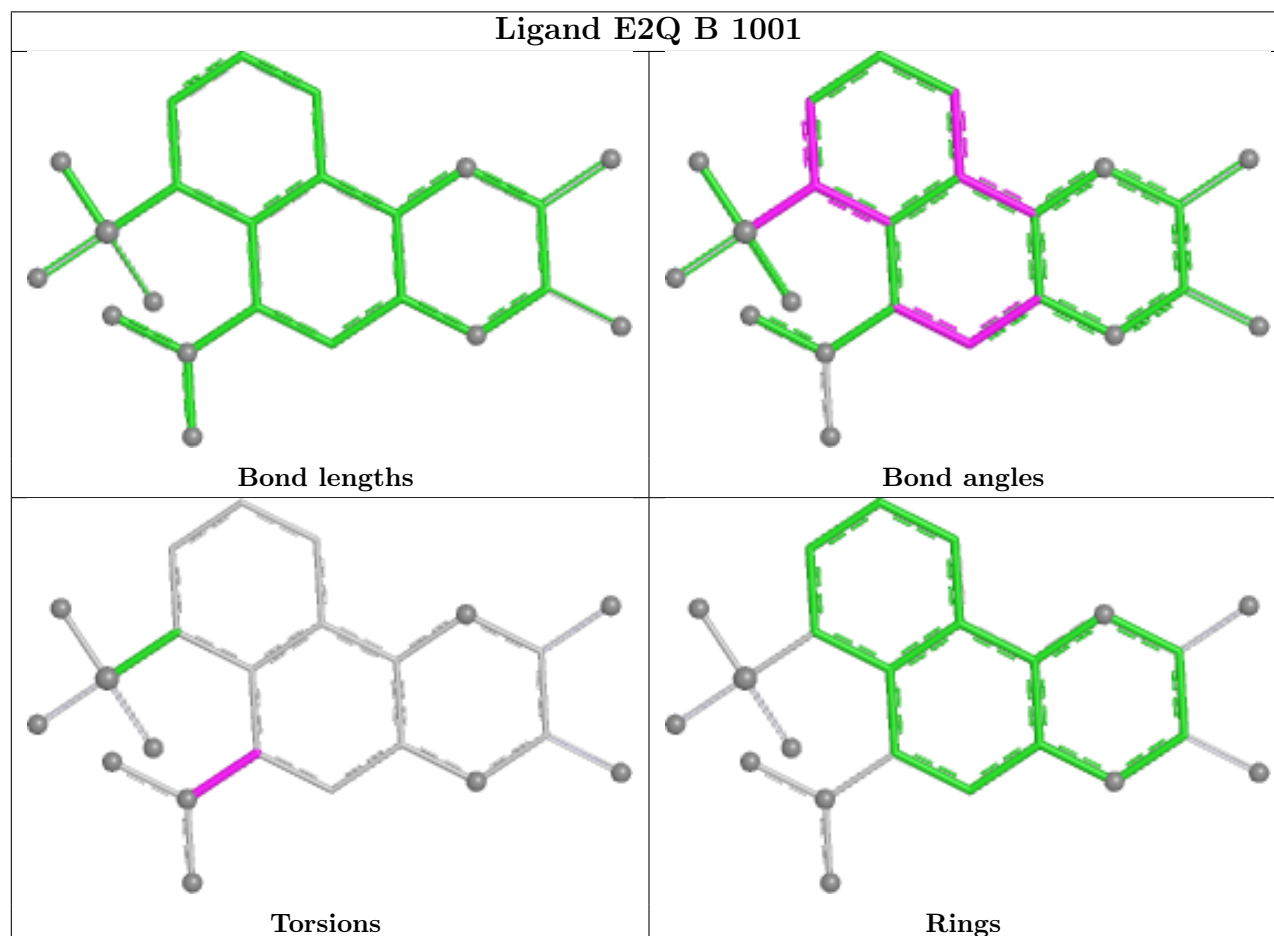
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	E2Q	5	0

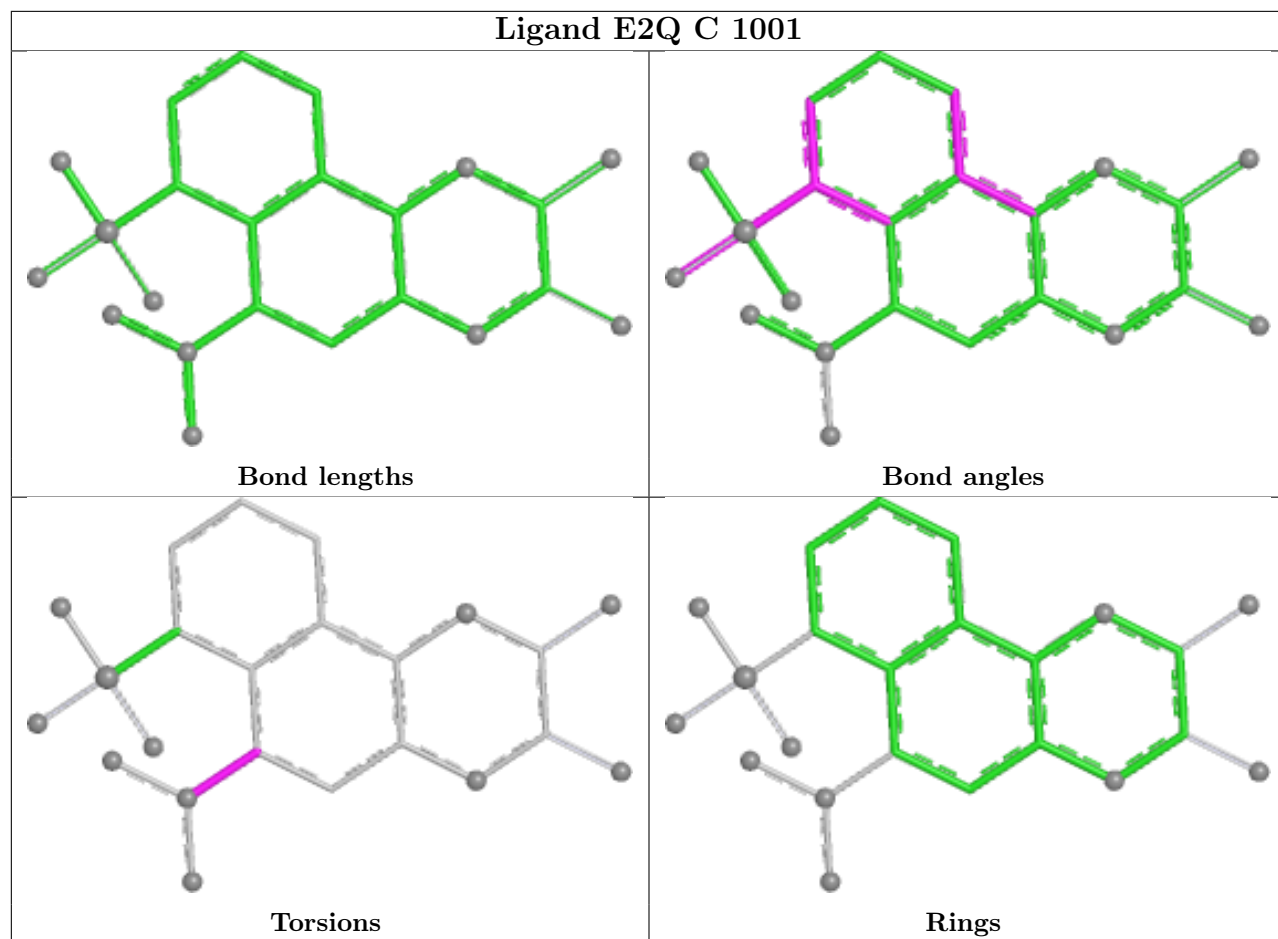
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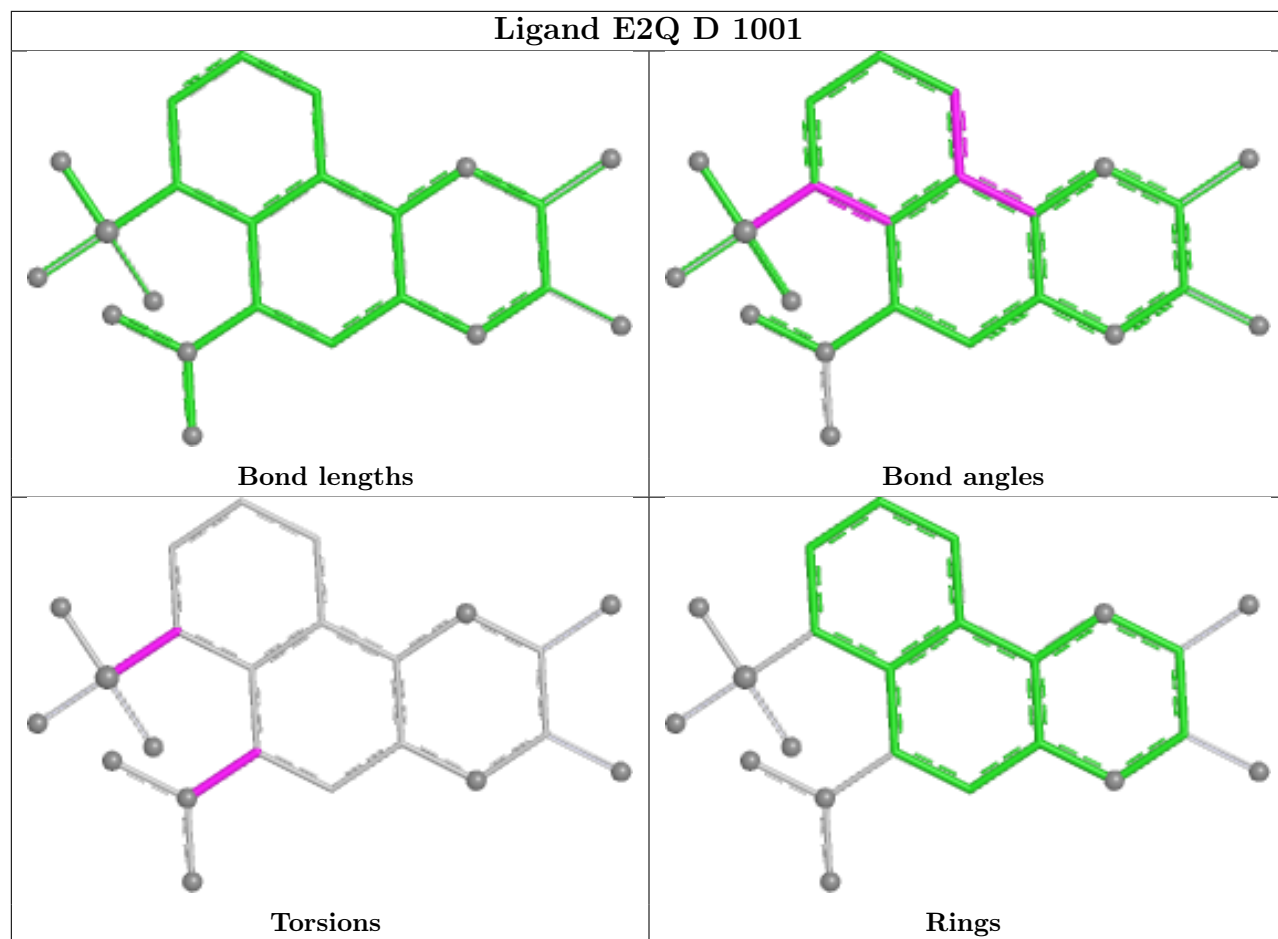
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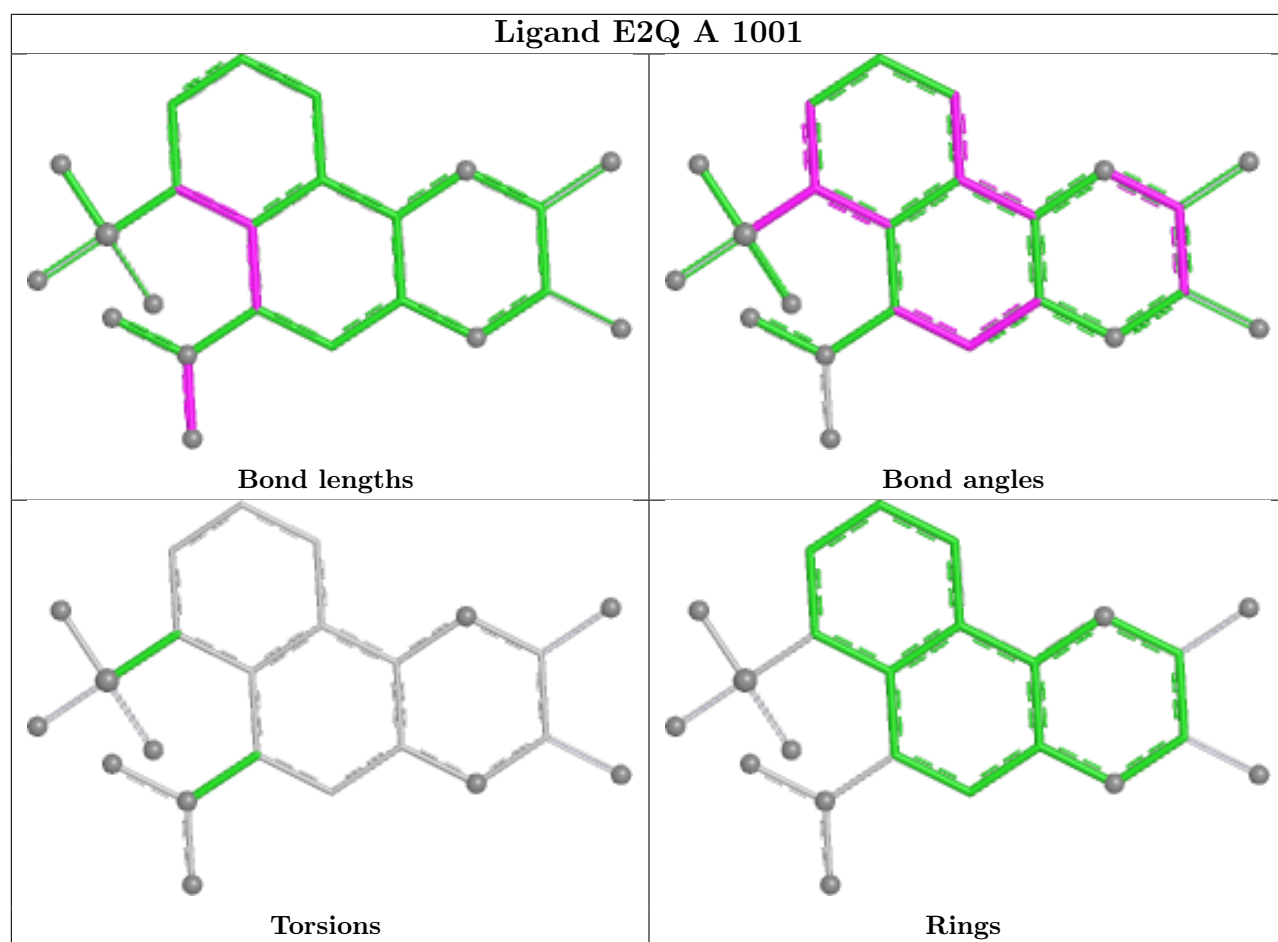
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	E2Q	15	0
3	D	1001	E2Q	2	0
3	A	1001	E2Q	3	0

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.

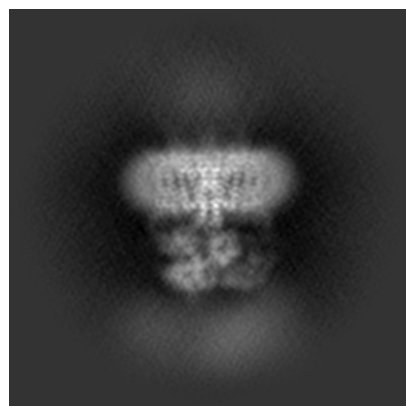
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54065. These allow visual inspection of the internal detail of the map and identification of artifacts.

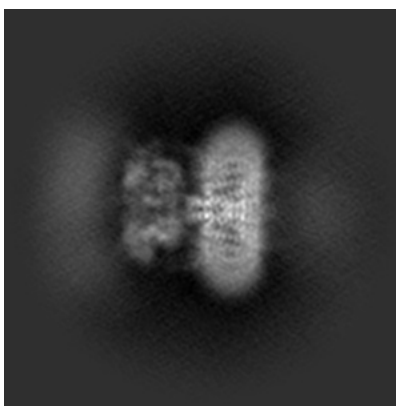
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

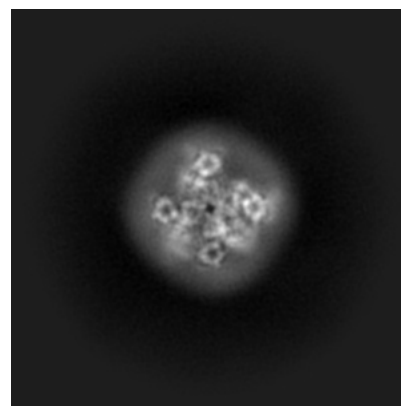
6.1.1 Primary map



X

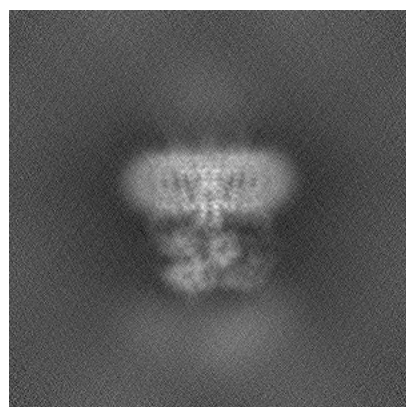


Y

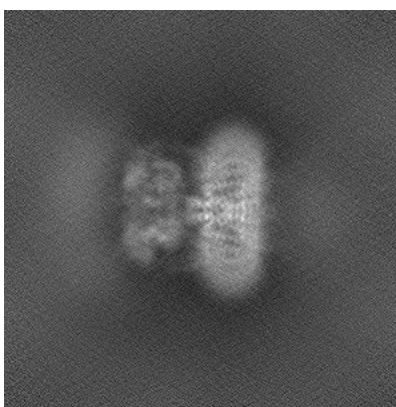


Z

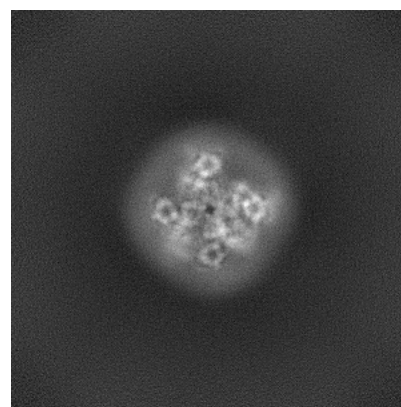
6.1.2 Raw map



X



Y

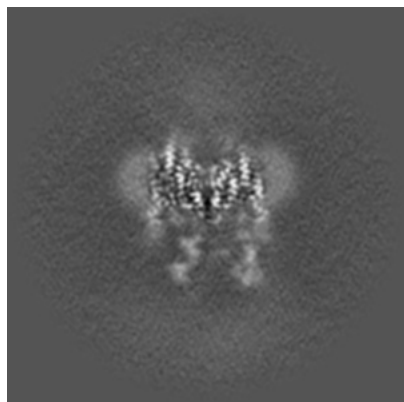


Z

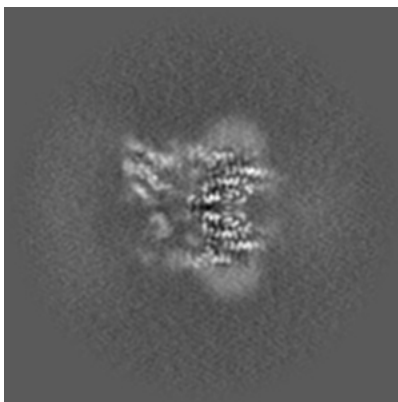
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

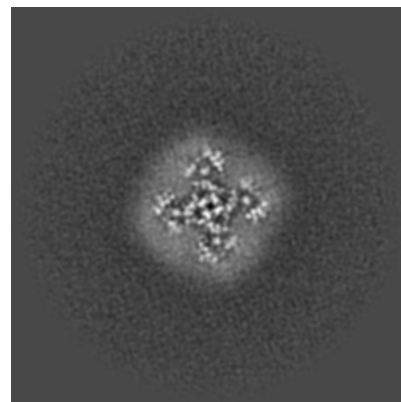
6.2.1 Primary map



X Index: 248

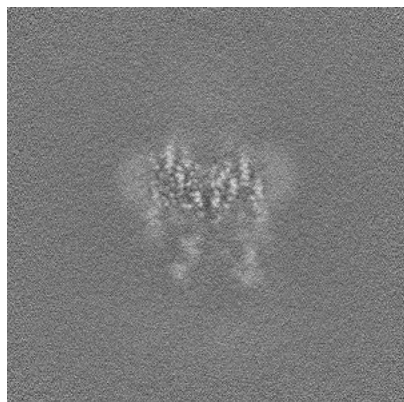


Y Index: 248

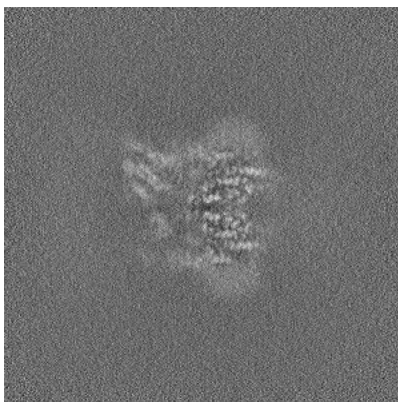


Z Index: 248

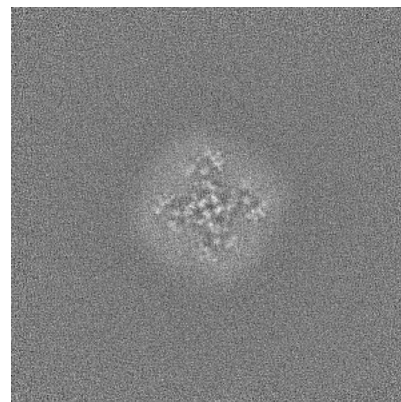
6.2.2 Raw map



X Index: 248



Y Index: 248

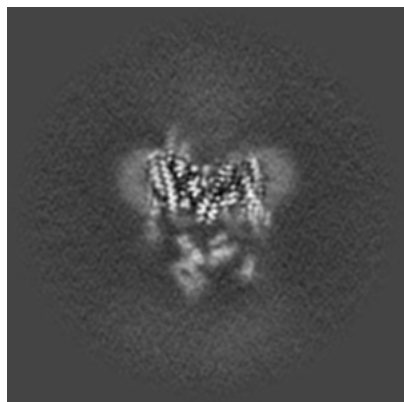


Z Index: 248

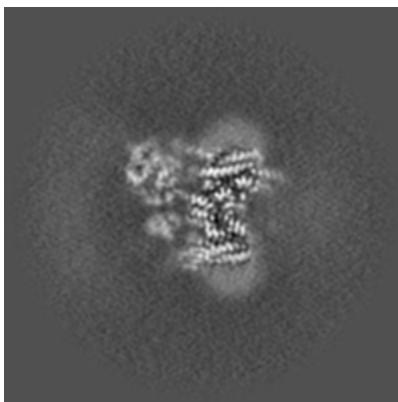
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

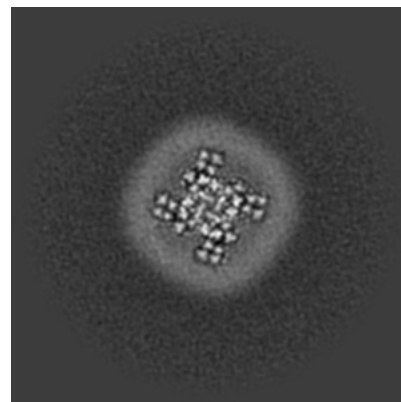
6.3.1 Primary map



X Index: 255

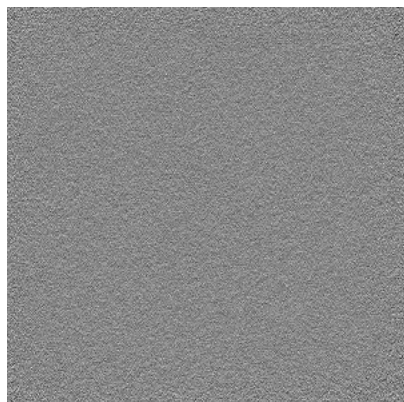


Y Index: 255

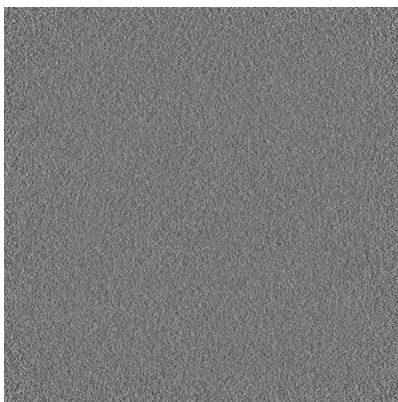


Z Index: 296

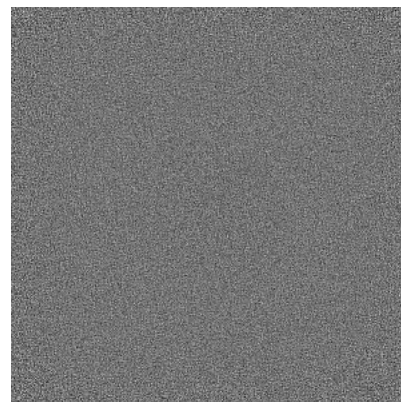
6.3.2 Raw map



X Index: 0



Y Index: 0

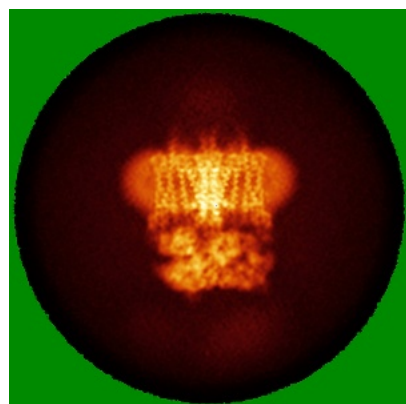


Z Index: 0

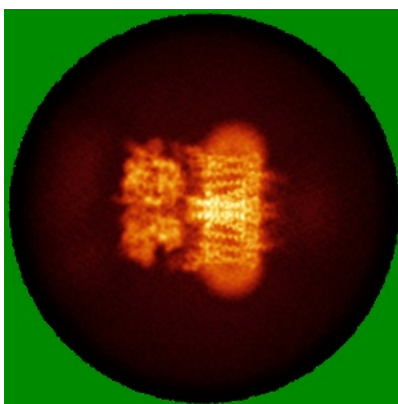
The images above show the largest variance slices of the map in three orthogonal directions.

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

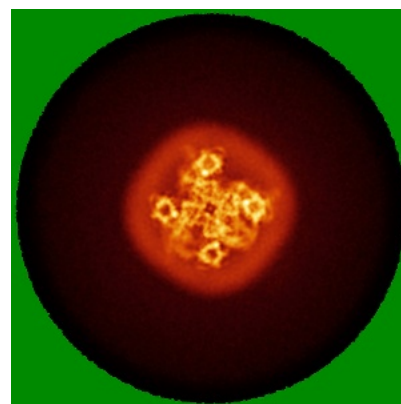
6.4.1 Primary map



X

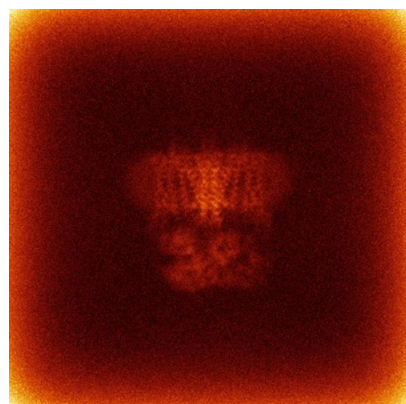


Y

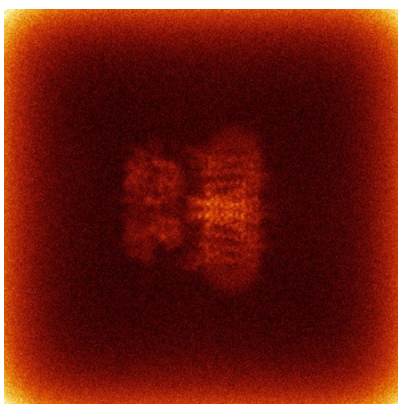


Z

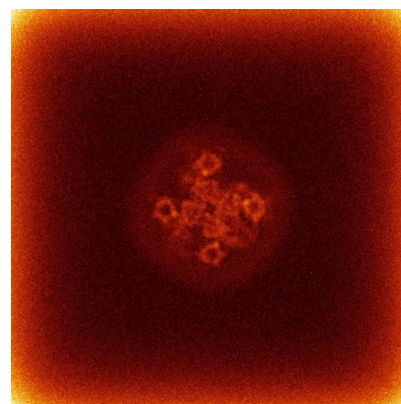
6.4.2 Raw map



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.

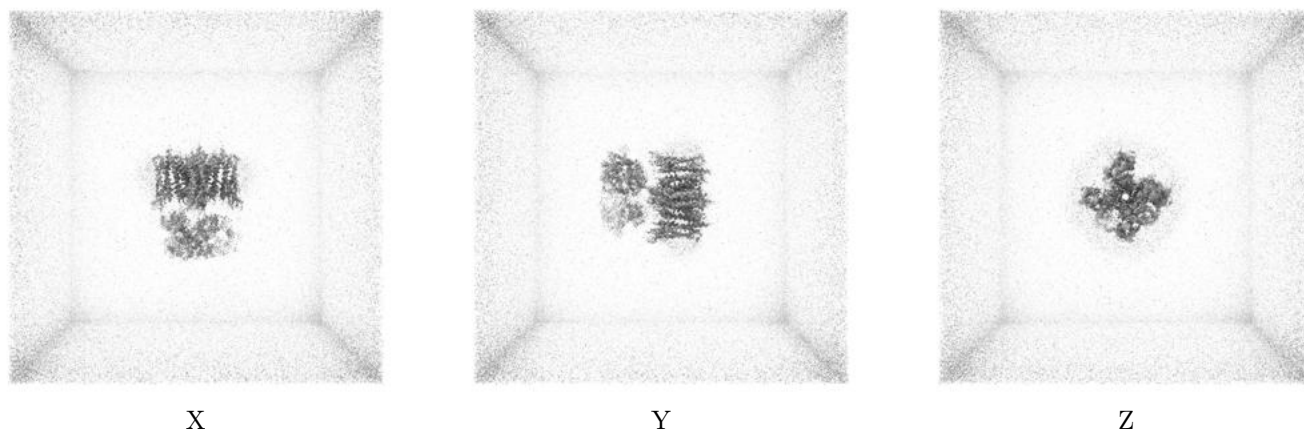
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

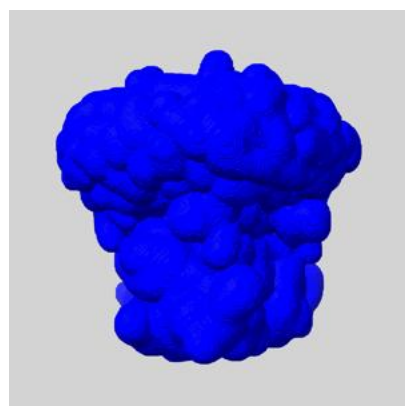
6.6 Mask visualisation [i](#)

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

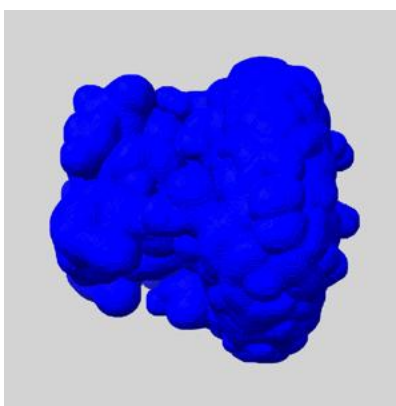
A mask typically either:

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

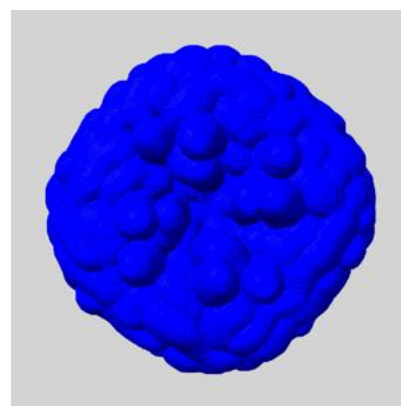
6.6.1 emd_54065_msk_1.map [i](#)



X



Y

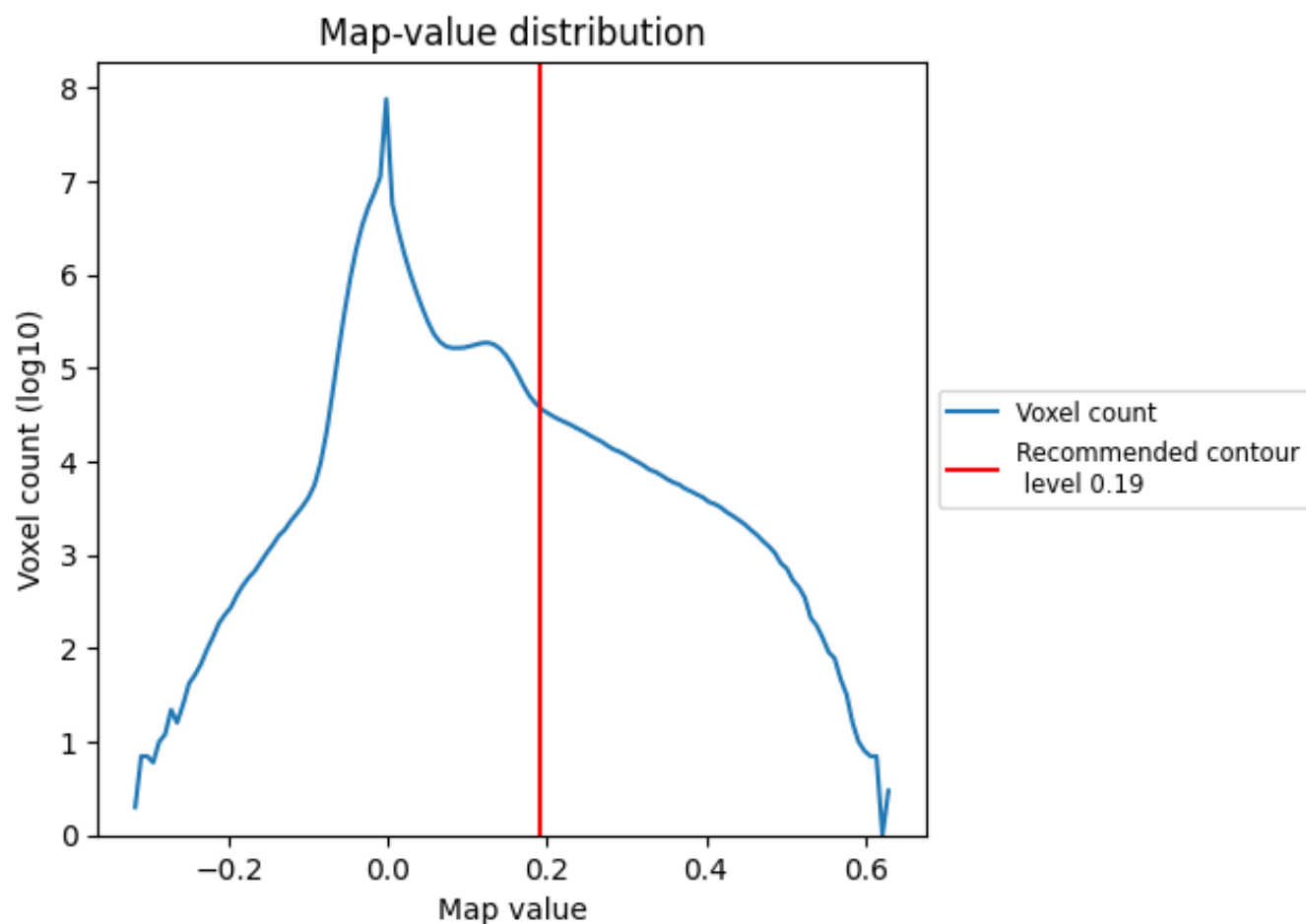


Z

7 Map analysis [i](#)

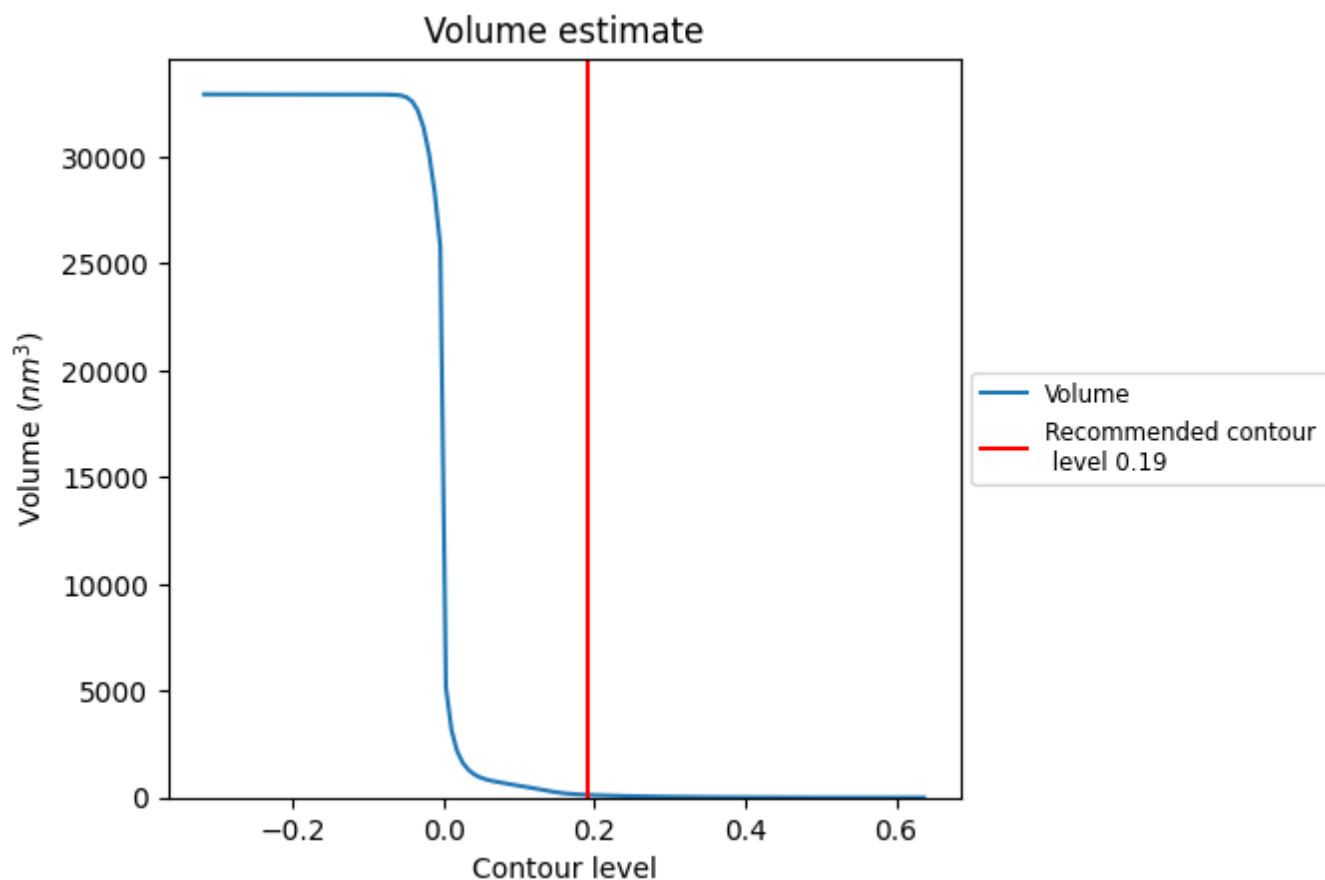
This section contains the results of statistical analysis of the map.

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.

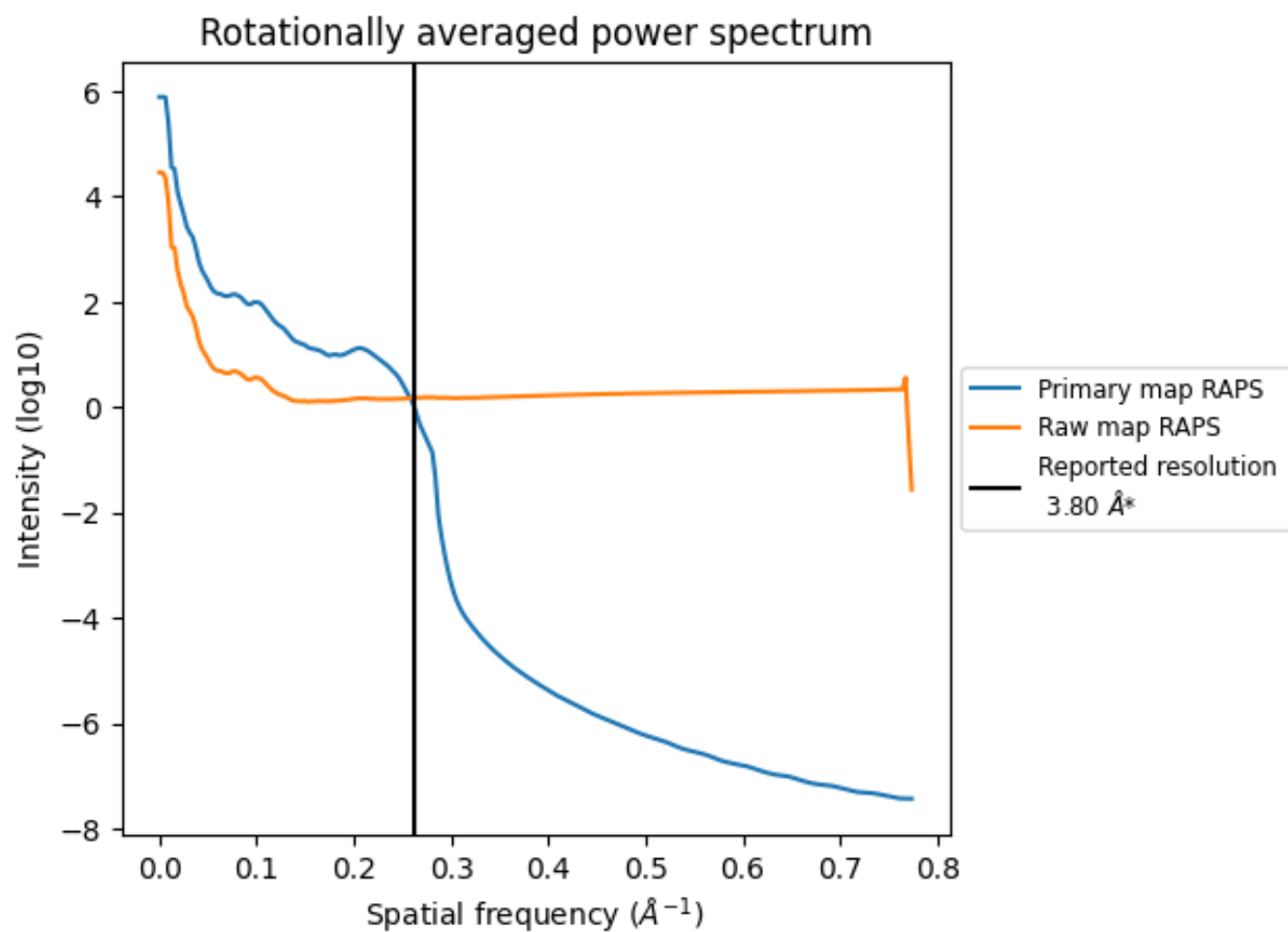
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 126 nm³; this corresponds to an approximate mass of 113 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 ⓘ

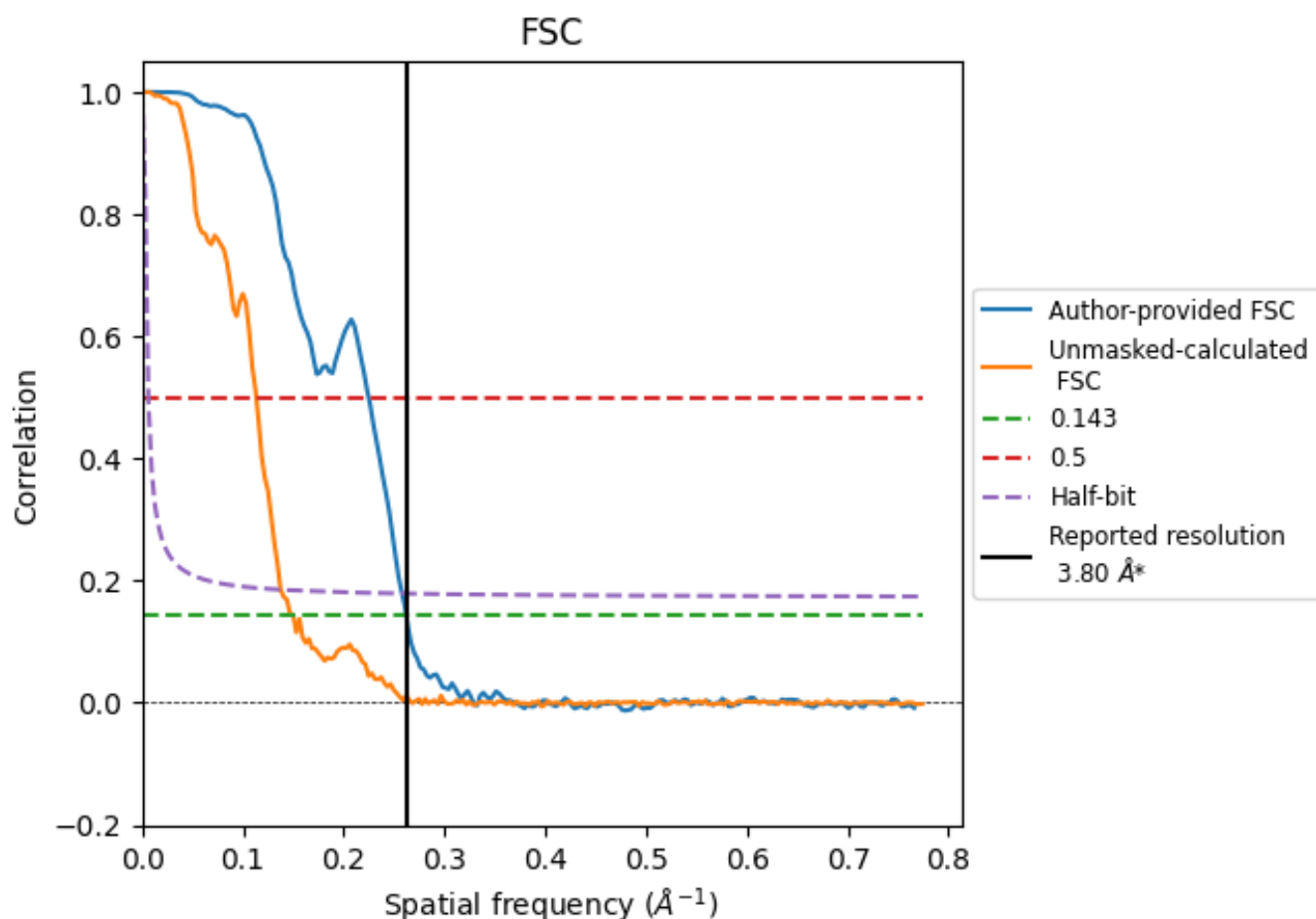


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

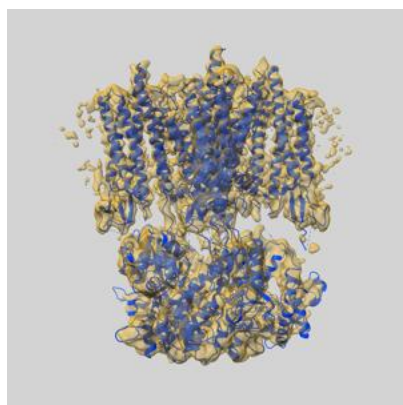
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.45	3.88
Unmasked-calculated*	6.68	8.83	7.28

*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 6.68 differs from the reported value 3.8 by more than 10 %

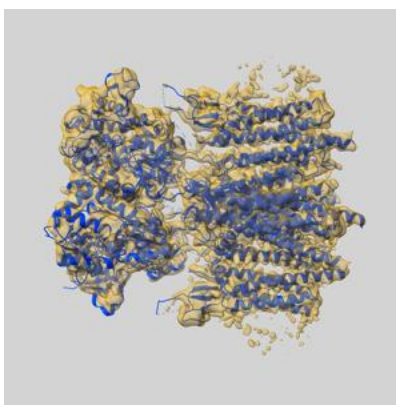
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54065 and PDB model 9RMS. Per-residue inclusion information can be found in section [3](#) on page [6](#).

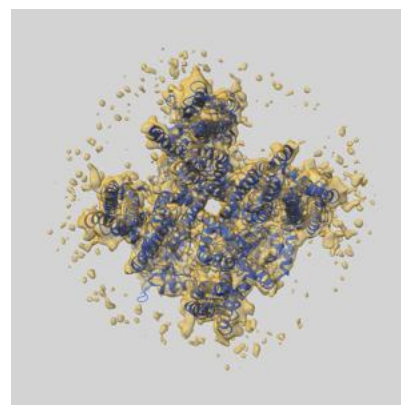
9.1 Map-model overlay [i](#)



X



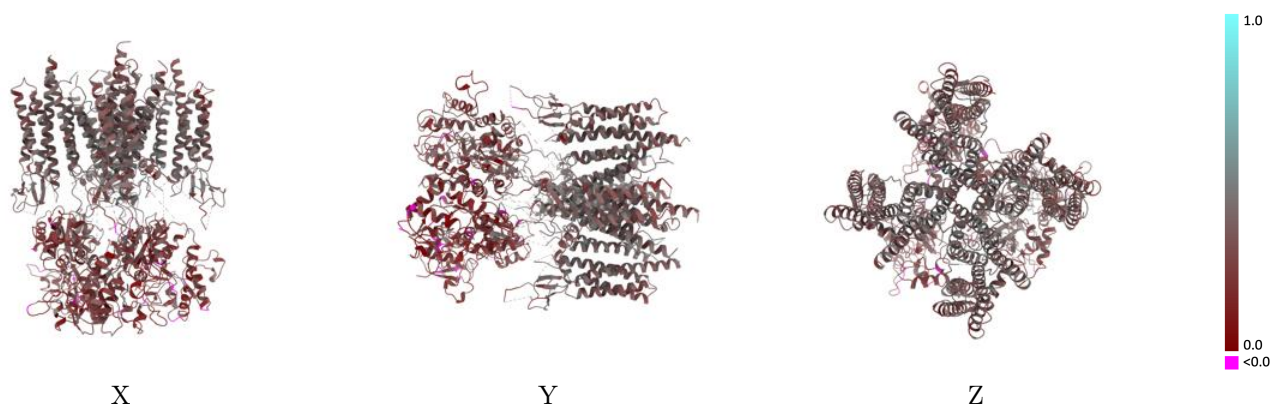
Y



Z

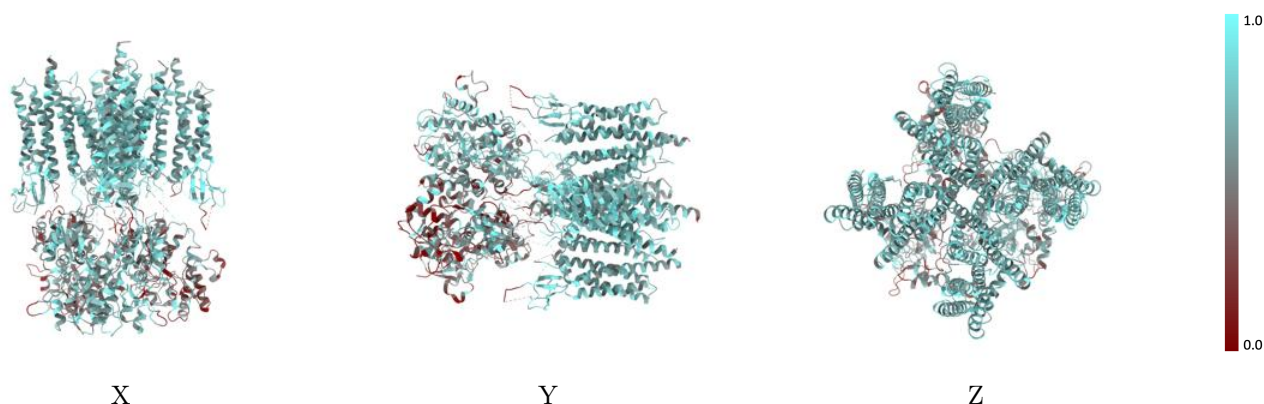
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



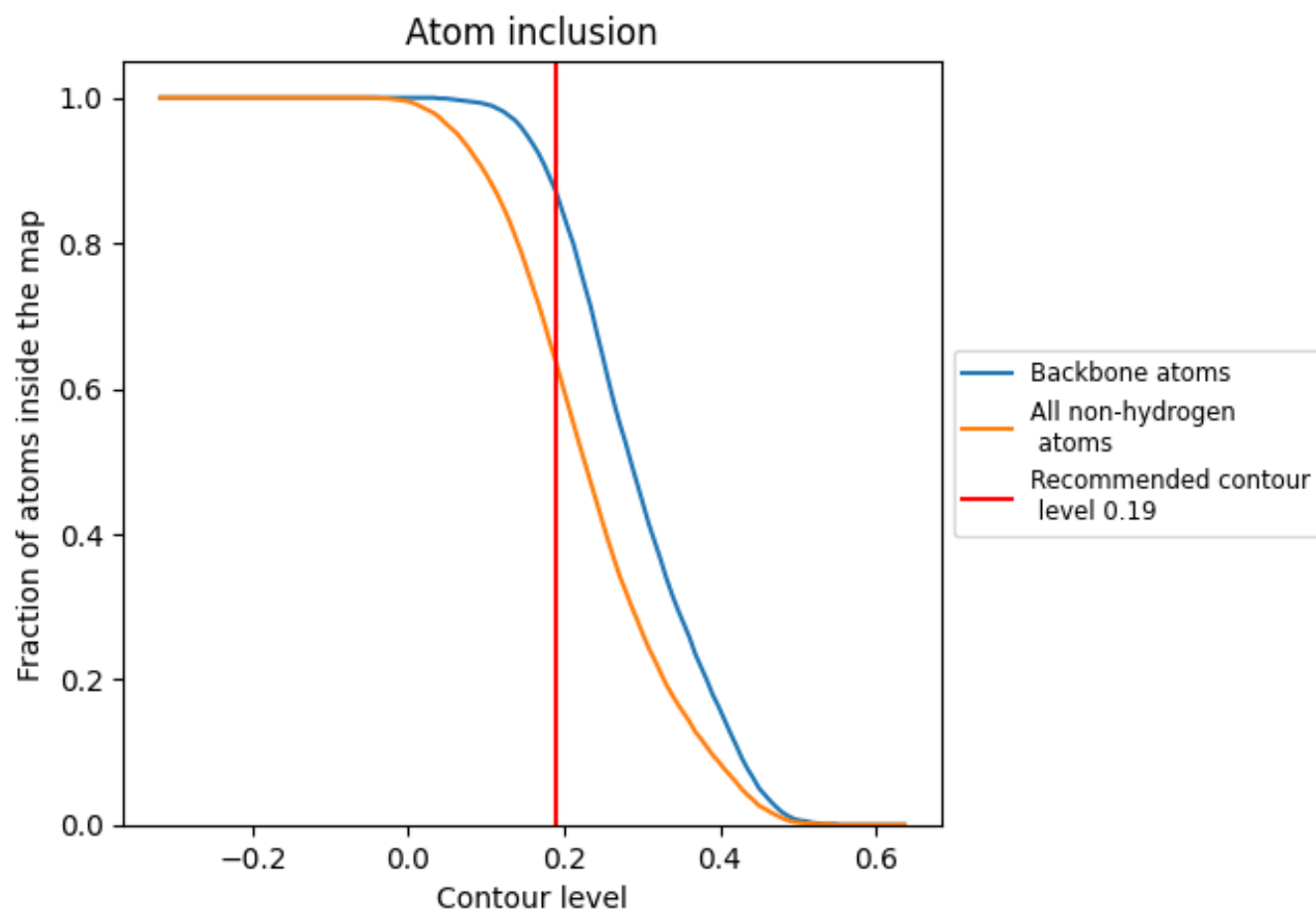
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 64% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6350	0.3130
A	0.6720	0.3150
B	0.5440	0.2710
C	0.5600	0.2710
D	0.6460	0.3130
E	0.7070	0.3530
F	0.7070	0.3660
G	0.6910	0.3590
H	0.7130	0.3610

1.0

0.0

<0.0