



## Full wwPDB EM Validation Report ⓘ

Apr 9, 2026 – 01:16 AM UTC

PDB ID : 9OVT / pdb\_00009ovt  
EMDB ID : EMD-70912  
Title : Heteromeric GluA1/A2 in the inactive state, composite map of LBD-TMD  
Authors : Yen, L.Y.; Sobolevsky, A.I.; Newton, T.P.; Gangwar, S.P.  
Deposited on : 2025-05-31  
Resolution : 3.43 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](mailto: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>.

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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

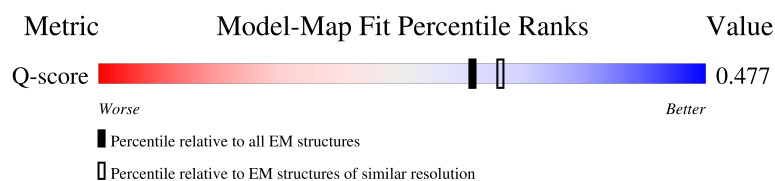
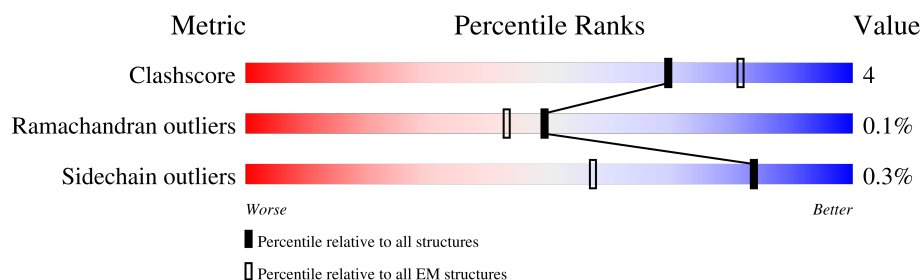
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.43 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	13927 ( 2.93 - 3.93 )

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  $\geq 3$ , 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	431	
1	C	431	
2	B	429	
2	D	429	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13011 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3252	2106	530	597	19		
1	C	414	Total	C	N	O	S	0	0
			3252	2106	530	597	19		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	740	GLY	ASN	conflict	UNP P19490
A	750	SER	ASN	conflict	UNP P19490
A	754	VAL	LEU	conflict	UNP P19490
A	760	SER	ASN	conflict	UNP P19490
C	740	GLY	ASN	conflict	UNP P19490
C	750	SER	ASN	conflict	UNP P19490
C	754	VAL	LEU	conflict	UNP P19490
C	760	SER	ASN	conflict	UNP P19490

- Molecule 2 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	410	Total	C	N	O	S	0	0
			3194	2068	520	585	21		
2	D	410	Total	C	N	O	S	0	0
			3194	2068	520	585	21		

There are 12 discrepancies between the modelled and reference sequences:

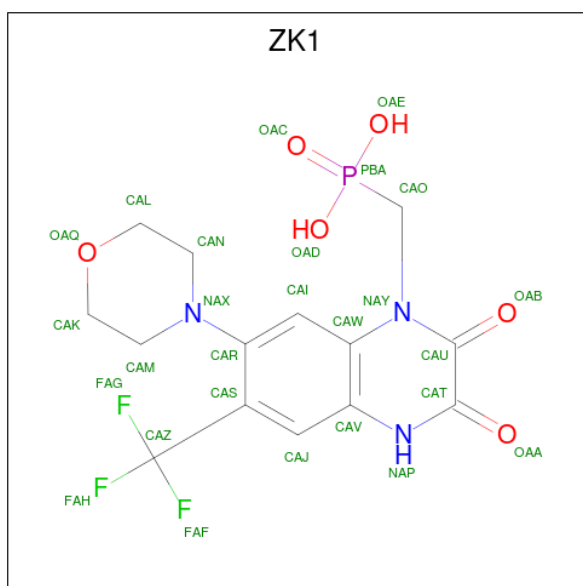
Chain	Residue	Modelled	Actual	Comment	Reference
B	392	GLN	ASN	conflict	UNP P19491
B	586	ARG	GLN	conflict	UNP P19491
B	744	THR	ASN	conflict	UNP P19491
B	745	PRO	ALA	conflict	UNP P19491
B	754	SER	ASN	conflict	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	758	VAL	LEU	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491
D	744	THR	ASN	conflict	UNP P19491
D	745	PRO	ALA	conflict	UNP P19491
D	754	SER	ASN	conflict	UNP P19491
D	758	VAL	LEU	conflict	UNP P19491

- Molecule 3 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (CCD ID: ZK1) (formula: C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Na 1	0
4	C	2	Total 2	Na 2	0

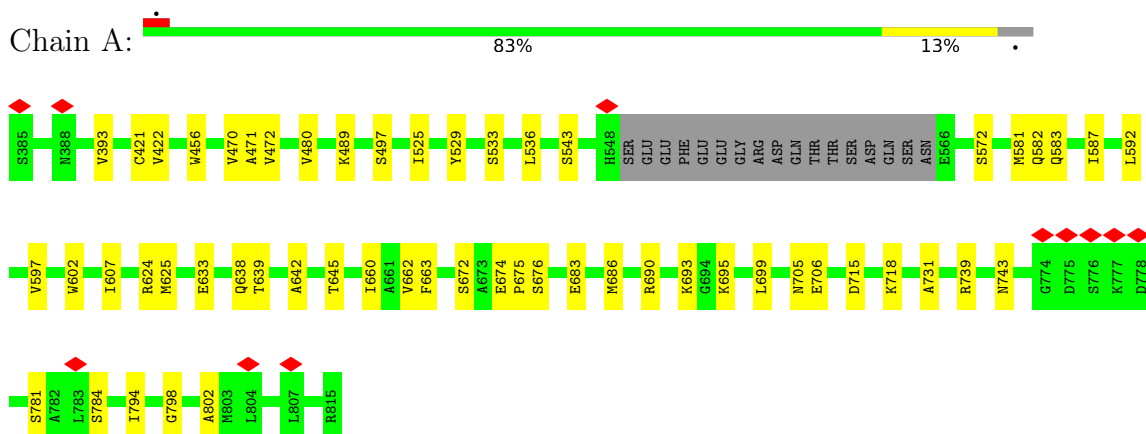
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total 2	O 2	0
5	B	1	Total 1	O 1	0
5	C	3	Total 3	O 3	0
5	D	2	Total 2	O 2	0

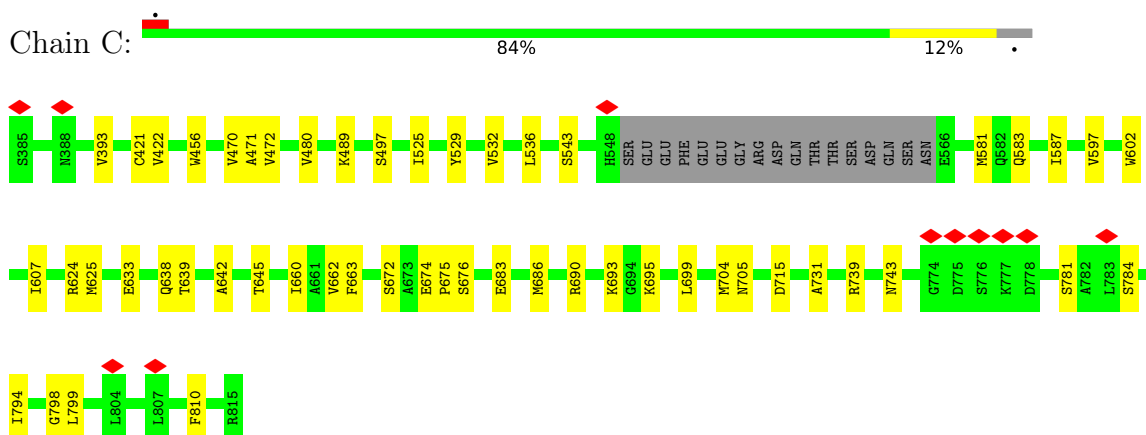
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

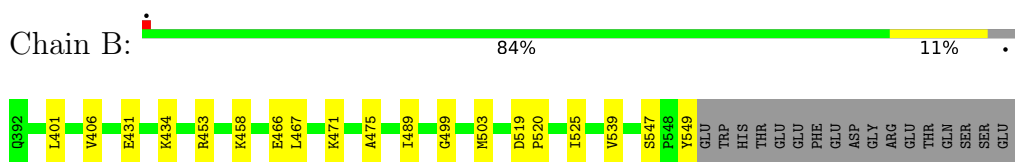
- Molecule 1: Glutamate receptor 1

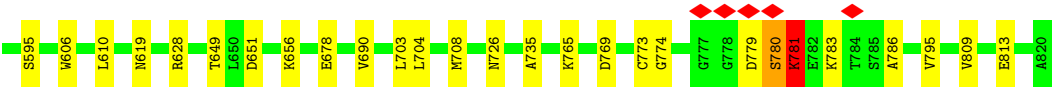


- Molecule 1: Glutamate receptor 1

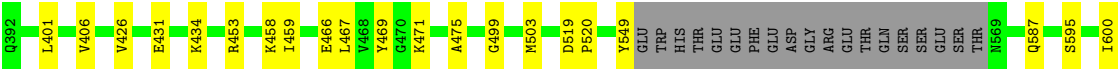
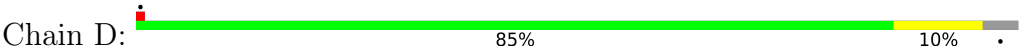


- Molecule 2: Glutamate receptor 2





● Molecule 2: Glutamate receptor 2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	216104	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 ( $e^-/\text{\AA}^2$ )	45.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	68.442	Depositor
Minimum map value	-40.900	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.956	Depositor
Recommended contour level	5	Depositor
Map size (Å)	370.04797, 370.04797, 370.04797	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8259999, 0.8259999, 0.8259999	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: ZK1, NA

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	0.26	0/3326	0.75	6/4491 (0.1%)
1	C	0.26	0/3326	0.75	6/4491 (0.1%)
2	B	0.28	1/3263 (0.0%)	0.70	0/4401
2	D	0.28	1/3263 (0.0%)	0.70	0/4401
All	All	0.27	2/13178 (0.0%)	0.73	12/17784 (0.1%)

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	3
1	C	0	3
2	B	0	4
2	D	0	4
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	519	ASP	C-N	6.17	1.41	1.34
2	B	519	ASP	C-N	6.06	1.40	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	422	VAL	N-CA-C	-7.23	105.59	111.81
1	A	422	VAL	N-CA-C	-7.20	105.62	111.81
1	C	638	GLN	CA-C-N	5.78	132.58	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	638	GLN	C-N-CA	5.78	132.58	121.54
1	A	638	GLN	CA-C-N	5.78	132.57	121.54
1	A	638	GLN	C-N-CA	5.78	132.57	121.54
1	C	676	SER	N-CA-C	5.44	117.31	110.24
1	A	676	SER	N-CA-C	5.42	117.29	110.24
1	A	672	SER	CA-C-N	5.40	131.85	121.54
1	A	672	SER	C-N-CA	5.40	131.85	121.54
1	C	672	SER	CA-C-N	5.38	131.81	121.54
1	C	672	SER	C-N-CA	5.38	131.81	121.54

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	674	GLU	Peptide
1	A	675	PRO	Peptide
1	A	693	LYS	Peptide
2	B	678	GLU	Peptide
2	B	780	SER	Peptide
2	B	781	LYS	Peptide
2	B	786	ALA	Peptide
1	C	674	GLU	Peptide
1	C	675	PRO	Peptide
1	C	693	LYS	Peptide
2	D	678	GLU	Peptide
2	D	780	SER	Peptide
2	D	781	LYS	Peptide
2	D	786	ALA	Peptide

## 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	3252	0	3268	29	0
1	C	3252	0	3268	30	0
2	B	3194	0	3238	29	0
2	D	3194	0	3238	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	13	0	0
3	B	27	0	13	0	0
3	C	27	0	13	1	0
3	D	27	0	13	1	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	2	0	0	1	0
5	B	1	0	0	0	0
5	C	3	0	0	1	0
5	D	2	0	0	0	0
All	All	13011	0	13064	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (95) 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:625:MET:HE1	1:C:625:MET:HE1	1.74	0.68
1:C:489:LYS:HG2	1:C:743:ASN:HD21	1.62	0.65
1:A:489:LYS:HG2	1:A:743:ASN:HD21	1.62	0.64
1:A:624:ARG:O	2:D:628:ARG:NH1	2.35	0.60
1:A:581:MET:O	1:A:583:GLN:NE2	2.38	0.57
1:C:581:MET:O	1:C:583:GLN:NE2	2.38	0.57
2:D:649:THR:HG22	2:D:703:LEU:HB2	1.87	0.56
2:B:649:THR:HG22	2:B:703:LEU:HB2	1.87	0.56
1:A:781:SER:HB3	1:A:784:SER:HB3	1.87	0.56
1:C:781:SER:HB3	1:C:784:SER:HB3	1.87	0.56
1:A:581:MET:HA	2:D:610:LEU:HD11	1.88	0.56
1:C:704:MET:HG3	3:C:1101:ZK1:HAK	1.88	0.56
1:A:393:VAL:HG22	1:A:470:VAL:HB	1.88	0.55
1:C:393:VAL:HG22	1:C:470:VAL:HB	1.88	0.55
2:B:628:ARG:NH1	1:C:624:ARG:O	2.40	0.55
2:B:781:LYS:HB2	2:B:783:LYS:HD2	1.89	0.54
1:C:690:ARG:NH1	1:C:715:ASP:OD1	2.41	0.54
1:A:690:ARG:NH1	1:A:715:ASP:OD1	2.41	0.54
2:B:499:GLY:HA3	2:B:726:ASN:HB3	1.91	0.53
2:D:781:LYS:HB2	2:D:783:LYS:HD2	1.89	0.53
2:D:499:GLY:HA3	2:D:726:ASN:HB3	1.91	0.53
2:B:431:GLU:OE1	2:B:434:LYS:NZ	2.42	0.52
2:D:453:ARG:HD3	2:D:458:LYS:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:431:GLU:OE1	2:D:434:LYS:NZ	2.42	0.52
2:B:453:ARG:HD3	2:B:458:LYS:HD3	1.91	0.52
1:C:607:ILE:HG21	2:D:795:VAL:HG21	1.92	0.51
1:C:739:ARG:NH1	5:C:1201:HOH:O	2.44	0.51
2:D:503:MET:HE1	2:D:690:VAL:HG23	1.92	0.51
1:A:739:ARG:NH1	5:A:1201:HOH:O	2.43	0.51
2:B:503:MET:HE1	2:B:690:VAL:HG23	1.92	0.51
1:A:642:ALA:N	1:A:695:LYS:O	2.43	0.51
1:C:642:ALA:N	1:C:695:LYS:O	2.44	0.50
2:D:651:ASP:HA	2:D:656:LYS:HE3	1.93	0.50
2:B:651:ASP:HA	2:B:656:LYS:HE3	1.93	0.50
1:A:645:THR:HG22	1:A:699:LEU:HB2	1.94	0.50
1:A:802:ALA:HB2	2:D:600:ILE:HB	1.94	0.49
1:C:645:THR:HG22	1:C:699:LEU:HB2	1.94	0.49
1:C:471:ALA:HB3	1:C:731:ALA:HB3	1.94	0.49
1:A:525:ILE:O	1:A:529:TYR:N	2.46	0.48
1:A:471:ALA:HB3	1:A:731:ALA:HB3	1.94	0.48
1:C:633:GLU:HG3	1:C:662:VAL:HG21	1.97	0.47
2:D:779:ASP:OD2	2:D:780:SER:OG	2.24	0.47
1:A:633:GLU:HG3	1:A:662:VAL:HG21	1.97	0.47
1:A:794:ILE:O	1:A:798:GLY:N	2.47	0.47
2:B:779:ASP:OD2	2:B:780:SER:OG	2.24	0.47
1:C:543:SER:OG	2:D:813:GLU:OE1	2.27	0.47
1:A:543:SER:OG	2:B:813:GLU:OE1	2.29	0.47
1:C:532:VAL:HG22	2:D:803:LEU:HD11	1.97	0.47
2:D:466:GLU:HG2	2:D:471:LYS:HE2	1.97	0.47
1:C:794:ILE:O	1:C:798:GLY:N	2.47	0.46
1:A:421:CYS:HB3	1:A:472:VAL:HG12	1.97	0.46
2:B:401:LEU:HA	2:B:406:VAL:HB	1.98	0.46
1:C:421:CYS:HB3	1:C:472:VAL:HG12	1.97	0.46
1:A:660:ILE:HB	1:A:663:PHE:HD2	1.82	0.45
1:A:456:TRP:HH2	1:A:480:VAL:HG12	1.81	0.45
2:B:466:GLU:HG2	2:B:471:LYS:HE2	1.97	0.45
2:B:539:VAL:HG11	1:C:799:LEU:HD22	1.97	0.45
2:B:547:SER:HB2	1:C:810:PHE:HB2	1.98	0.45
1:C:660:ILE:HB	1:C:663:PHE:HD2	1.81	0.45
2:D:467:LEU:HD11	2:D:475:ALA:HB2	1.99	0.45
1:C:456:TRP:HH2	1:C:480:VAL:HG12	1.81	0.45
1:A:607:ILE:HG21	2:B:795:VAL:HG21	1.98	0.45
2:B:610:LEU:HD11	1:C:581:MET:HA	1.98	0.45
1:A:683:GLU:HG3	1:A:686:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:773:CYS:SG	2:B:774:GLY:N	2.89	0.44
2:D:401:LEU:HA	2:D:406:VAL:HB	1.98	0.44
2:B:467:LEU:HD11	2:B:475:ALA:HB2	1.99	0.44
2:B:765:LYS:HA	2:B:769:ASP:HB2	1.99	0.44
2:D:765:LYS:HA	2:D:769:ASP:HB2	1.99	0.44
2:B:525:ILE:HD11	1:C:784:SER:HA	1.99	0.44
1:C:525:ILE:O	1:C:529:TYR:N	2.46	0.44
2:B:475:ALA:HB3	2:B:735:ALA:HB3	1.99	0.43
2:D:475:ALA:HB3	2:D:735:ALA:HB3	1.99	0.43
1:C:683:GLU:HG3	1:C:686:MET:HE2	1.99	0.43
1:A:533:SER:O	1:A:572:SER:OG	2.32	0.43
2:B:520:PRO:HB3	2:B:619:ASN:HB3	2.01	0.43
1:A:497:SER:OG	1:A:705:ASN:ND2	2.42	0.43
1:A:602:TRP:CG	2:B:587:GLN:HG3	2.54	0.43
2:B:549:TYR:HD1	2:B:595:SER:HB3	1.83	0.43
2:B:606:TRP:HB3	1:C:581:MET:HB3	2.00	0.42
2:D:549:TYR:HD1	2:D:595:SER:HB3	1.83	0.42
2:D:520:PRO:HB3	2:D:619:ASN:HB3	2.01	0.42
1:C:536:LEU:HB2	1:C:597:VAL:HG11	2.02	0.41
2:B:704:LEU:HD13	2:B:708:MET:HB3	2.02	0.41
1:C:602:TRP:CG	2:D:587:GLN:HG3	2.55	0.41
1:A:536:LEU:HB2	1:A:597:VAL:HG11	2.03	0.41
1:C:497:SER:OG	1:C:705:ASN:ND2	2.42	0.41
1:A:706:GLU:OE2	1:A:718:LYS:NZ	2.44	0.41
2:D:406:VAL:HG22	2:D:426:VAL:HG23	2.03	0.41
2:D:459:ILE:HG23	2:D:469:TYR:HE2	1.86	0.41
3:D:1101:ZK1:HAOA	3:D:1101:ZK1:HAI	1.76	0.40
1:A:582:GLN:HE21	2:B:586:ARG:HB3	1.86	0.40
1:A:592:LEU:HD12	2:B:809:VAL:HG11	2.04	0.40
2:B:489:ILE:HD12	2:B:735:ALA:HB1	2.03	0.40
2:D:704:LEU:HD13	2:D:708:MET:HB3	2.02	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	410/431 (95%)	375 (92%)	35 (8%)	0	100	100
1	C	410/431 (95%)	376 (92%)	34 (8%)	0	100	100
2	B	406/429 (95%)	369 (91%)	36 (9%)	1 (0%)	43	73
2	D	406/429 (95%)	368 (91%)	37 (9%)	1 (0%)	43	73
All	All	1632/1720 (95%)	1488 (91%)	142 (9%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	781	LYS
2	D	781	LYS

### 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	348/364 (96%)	346 (99%)	2 (1%)	78	80
1	C	348/364 (96%)	346 (99%)	2 (1%)	78	80
2	B	344/362 (95%)	344 (100%)	0	100	100
2	D	344/362 (95%)	344 (100%)	0	100	100
All	All	1384/1452 (95%)	1380 (100%)	4 (0%)	84	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	587	ILE
1	A	639	THR
1	C	587	ILE
1	C	639	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	ASN
1	A	571	ASN
1	A	582	GLN
1	A	743	ASN
2	B	747	ASN
1	C	409	ASN
1	C	571	ASN
1	C	743	ASN
2	D	747	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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	ZK1	B	1101	-	29,29,29	3.34	10 (34%)	45,45,45	1.62	9 (20%)
3	ZK1	D	1101	-	29,29,29	3.34	10 (34%)	45,45,45	1.64	9 (20%)
3	ZK1	A	1101	-	29,29,29	3.34	10 (34%)	45,45,45	1.87	13 (28%)
3	ZK1	C	1101	-	29,29,29	3.31	10 (34%)	45,45,45	1.80	11 (24%)

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	ZK1	B	1101	-	-	2/13/23/23	0/3/3/3
3	ZK1	D	1101	-	-	5/13/23/23	0/3/3/3
3	ZK1	A	1101	-	-	8/13/23/23	0/3/3/3
3	ZK1	C	1101	-	-	11/13/23/23	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1101	ZK1	CAU-CAT	-10.23	1.39	1.53
3	B	1101	ZK1	CAU-CAT	-10.17	1.39	1.53
3	A	1101	ZK1	CAU-CAT	-10.13	1.39	1.53
3	C	1101	ZK1	CAU-CAT	-10.06	1.39	1.53
3	B	1101	ZK1	OAA-CAT	8.91	1.40	1.23
3	A	1101	ZK1	OAA-CAT	8.81	1.40	1.23
3	D	1101	ZK1	OAA-CAT	8.80	1.40	1.23
3	C	1101	ZK1	OAA-CAT	8.53	1.39	1.23
3	A	1101	ZK1	OAB-CAU	8.52	1.40	1.23
3	D	1101	ZK1	OAB-CAU	8.51	1.40	1.23
3	B	1101	ZK1	OAB-CAU	8.46	1.40	1.23
3	C	1101	ZK1	OAB-CAU	8.45	1.40	1.23
3	B	1101	ZK1	CAW-NAY	-3.52	1.35	1.41
3	A	1101	ZK1	CAW-NAY	-3.40	1.35	1.41
3	C	1101	ZK1	CAV-NAP	-3.39	1.34	1.39
3	D	1101	ZK1	CAW-NAY	-3.37	1.35	1.41
3	C	1101	ZK1	CAW-NAY	-3.31	1.35	1.41
3	A	1101	ZK1	CAU-NAY	-3.07	1.32	1.38
3	C	1101	ZK1	CAU-NAY	-3.06	1.32	1.38
3	D	1101	ZK1	CAV-NAP	-3.05	1.34	1.39
3	B	1101	ZK1	CAV-NAP	-3.00	1.34	1.39
3	B	1101	ZK1	CAU-NAY	-3.00	1.32	1.38
3	A	1101	ZK1	CAV-NAP	-3.00	1.34	1.39
3	D	1101	ZK1	CAV-CAW	-2.98	1.37	1.40
3	D	1101	ZK1	CAU-NAY	-2.98	1.32	1.38
3	C	1101	ZK1	CAV-CAW	-2.94	1.37	1.40
3	A	1101	ZK1	CAV-CAW	-2.91	1.37	1.40
3	B	1101	ZK1	CAV-CAW	-2.89	1.37	1.40
3	C	1101	ZK1	CAT-NAP	-2.65	1.32	1.35
3	D	1101	ZK1	CAT-NAP	-2.39	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1101	ZK1	CAR-NAX	2.36	1.46	1.41
3	B	1101	ZK1	CAR-NAX	2.32	1.46	1.41
3	A	1101	ZK1	CAR-NAX	2.32	1.46	1.41
3	A	1101	ZK1	PBA-CAO	2.28	1.86	1.81
3	B	1101	ZK1	CAT-NAP	-2.27	1.32	1.35
3	C	1101	ZK1	PBA-CAO	2.25	1.86	1.81
3	A	1101	ZK1	CAT-NAP	-2.19	1.32	1.35
3	C	1101	ZK1	CAR-NAX	2.11	1.46	1.41
3	D	1101	ZK1	PBA-CAO	2.03	1.86	1.81
3	B	1101	ZK1	PBA-CAO	2.00	1.85	1.81

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	ZK1	CAI-CAR-NAX	-4.79	115.61	122.59
3	C	1101	ZK1	CAI-CAR-NAX	-4.72	115.72	122.59
3	C	1101	ZK1	CAN-NAX-CAM	4.65	122.03	111.57
3	A	1101	ZK1	CAS-CAR-NAX	4.51	125.09	119.92
3	D	1101	ZK1	CAI-CAR-NAX	-4.23	116.42	122.59
3	B	1101	ZK1	CAI-CAR-NAX	-4.18	116.50	122.59
3	C	1101	ZK1	CAS-CAR-NAX	4.06	124.57	119.92
3	B	1101	ZK1	CAN-NAX-CAM	3.93	120.41	111.57
3	D	1101	ZK1	CAN-NAX-CAM	3.88	120.29	111.57
3	A	1101	ZK1	CAN-NAX-CAM	3.86	120.24	111.57
3	D	1101	ZK1	CAS-CAR-NAX	3.83	124.31	119.92
3	B	1101	ZK1	CAS-CAR-NAX	3.73	124.20	119.92
3	D	1101	ZK1	CAV-NAP-CAT	-3.29	120.21	124.82
3	A	1101	ZK1	CAV-NAP-CAT	-3.28	120.22	124.82
3	B	1101	ZK1	CAV-NAP-CAT	-3.27	120.24	124.82
3	C	1101	ZK1	CAV-NAP-CAT	-3.24	120.28	124.82
3	A	1101	ZK1	CAL-OAQ-CAK	3.16	120.11	109.88
3	D	1101	ZK1	CAO-NAY-CAU	3.12	119.72	116.55
3	B	1101	ZK1	CAO-NAY-CAU	2.84	119.44	116.55
3	A	1101	ZK1	OAQ-CAL-CAN	2.72	117.63	111.77
3	A	1101	ZK1	CAO-NAY-CAU	2.65	119.24	116.55
3	C	1101	ZK1	CAZ-CAS-CAR	2.59	125.38	122.06
3	A	1101	ZK1	CAK-CAM-NAX	2.58	114.81	109.93
3	C	1101	ZK1	FAH-CAZ-CAS	-2.57	108.09	112.65
3	C	1101	ZK1	CAO-NAY-CAU	2.56	119.16	116.55
3	A	1101	ZK1	CAT-CAU-NAY	2.55	120.18	117.41
3	D	1101	ZK1	CAT-CAU-NAY	2.54	120.17	117.41
3	B	1101	ZK1	CAT-CAU-NAY	2.54	120.16	117.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	ZK1	CAU-CAT-NAP	2.49	120.00	117.46
3	C	1101	ZK1	CAW-NAY-CAU	-2.46	119.82	122.84
3	A	1101	ZK1	CAW-NAY-CAU	-2.40	119.89	122.84
3	D	1101	ZK1	CAW-NAY-CAU	-2.37	119.92	122.84
3	C	1101	ZK1	CAT-CAU-NAY	2.37	119.98	117.41
3	C	1101	ZK1	FAG-CAZ-CAS	-2.33	108.52	112.65
3	D	1101	ZK1	CAU-CAT-NAP	2.32	119.83	117.46
3	A	1101	ZK1	CAU-CAT-NAP	2.30	119.81	117.46
3	B	1101	ZK1	CAW-NAY-CAU	-2.26	120.06	122.84
3	A	1101	ZK1	FAH-CAZ-CAS	-2.22	108.70	112.65
3	B	1101	ZK1	CAU-CAT-NAP	2.22	119.72	117.46
3	D	1101	ZK1	FAH-CAZ-CAS	-2.09	108.95	112.65
3	A	1101	ZK1	OAQ-CAK-CAM	2.05	116.19	111.77
3	B	1101	ZK1	FAH-CAZ-CAS	-2.03	109.06	112.65

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1101	ZK1	CAR-CAS-CAZ-FAG
3	C	1101	ZK1	CAR-CAS-CAZ-FAH
3	C	1101	ZK1	CAR-CAS-CAZ-FAF
3	D	1101	ZK1	CAI-CAR-NAX-CAN
3	B	1101	ZK1	CAI-CAR-NAX-CAN
3	A	1101	ZK1	CAI-CAR-NAX-CAN
3	A	1101	ZK1	NAY-CAO-PBA-OAD
3	A	1101	ZK1	NAY-CAO-PBA-OAE
3	C	1101	ZK1	NAY-CAO-PBA-OAD
3	C	1101	ZK1	NAY-CAO-PBA-OAE
3	A	1101	ZK1	CAR-CAS-CAZ-FAG
3	A	1101	ZK1	CAR-CAS-CAZ-FAH
3	C	1101	ZK1	CAI-CAR-NAX-CAN
3	A	1101	ZK1	CAR-CAS-CAZ-FAF
3	C	1101	ZK1	CAJ-CAS-CAZ-FAF
3	C	1101	ZK1	CAJ-CAS-CAZ-FAG
3	C	1101	ZK1	CAJ-CAS-CAZ-FAH
3	A	1101	ZK1	NAY-CAO-PBA-OAC
3	C	1101	ZK1	NAY-CAO-PBA-OAC
3	D	1101	ZK1	NAY-CAO-PBA-OAC
3	D	1101	ZK1	NAY-CAO-PBA-OAD
3	D	1101	ZK1	NAY-CAO-PBA-OAE
3	B	1101	ZK1	CAS-CAR-NAX-CAN

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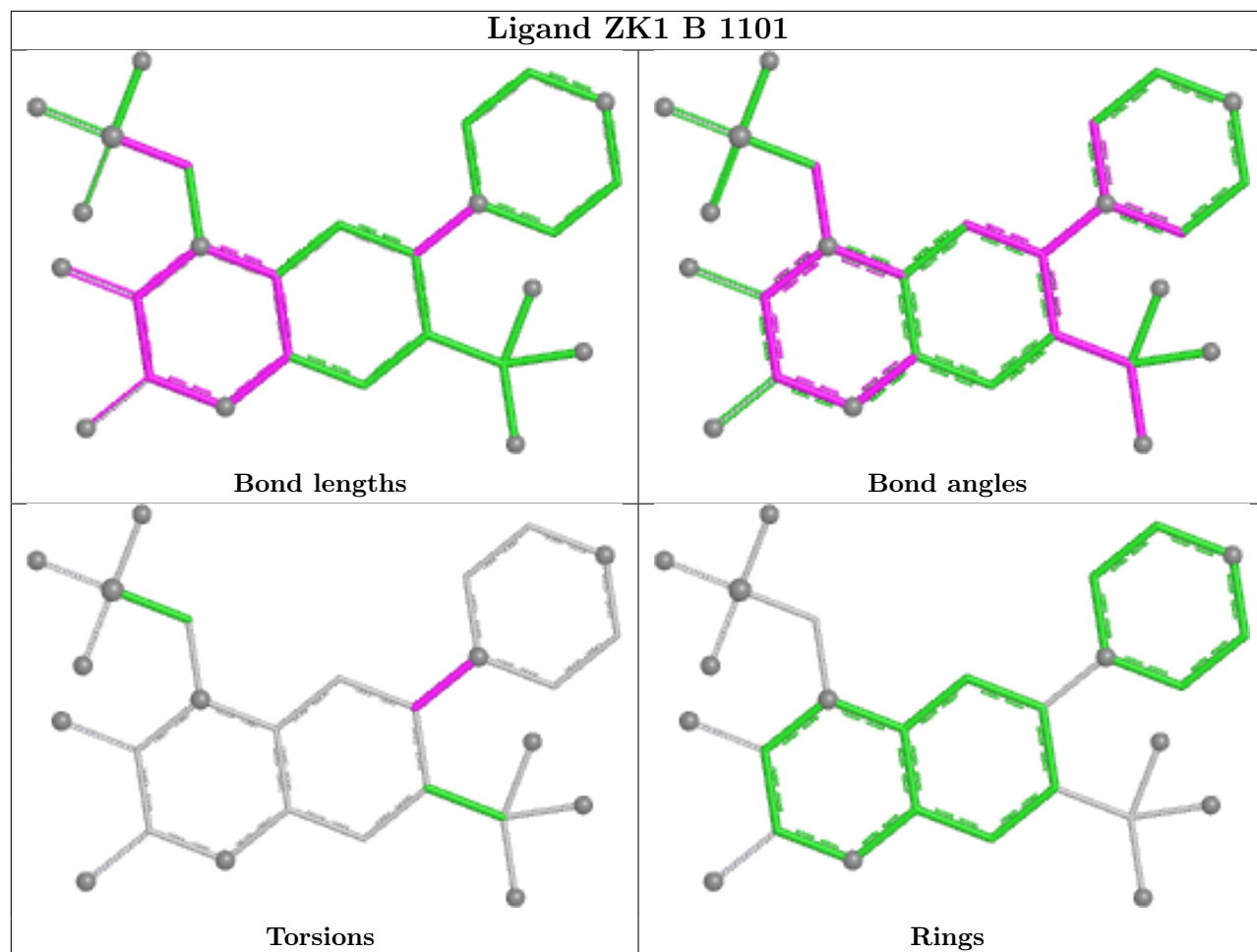
Mol	Chain	Res	Type	Atoms
3	D	1101	ZK1	CAS-CAR-NAX-CAN
3	A	1101	ZK1	CAS-CAR-NAX-CAN
3	C	1101	ZK1	CAI-CAR-NAX-CAM

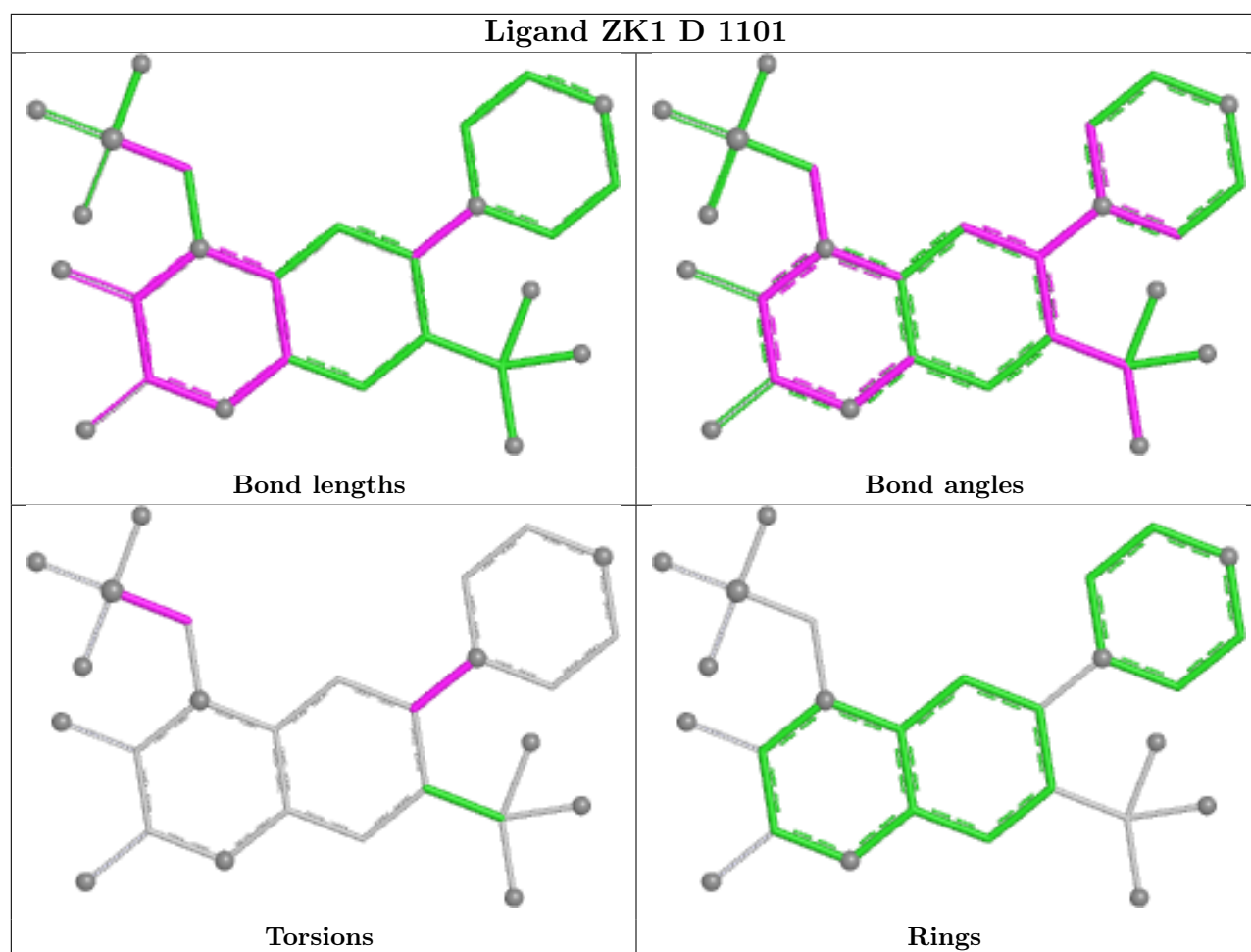
There are no ring outliers.

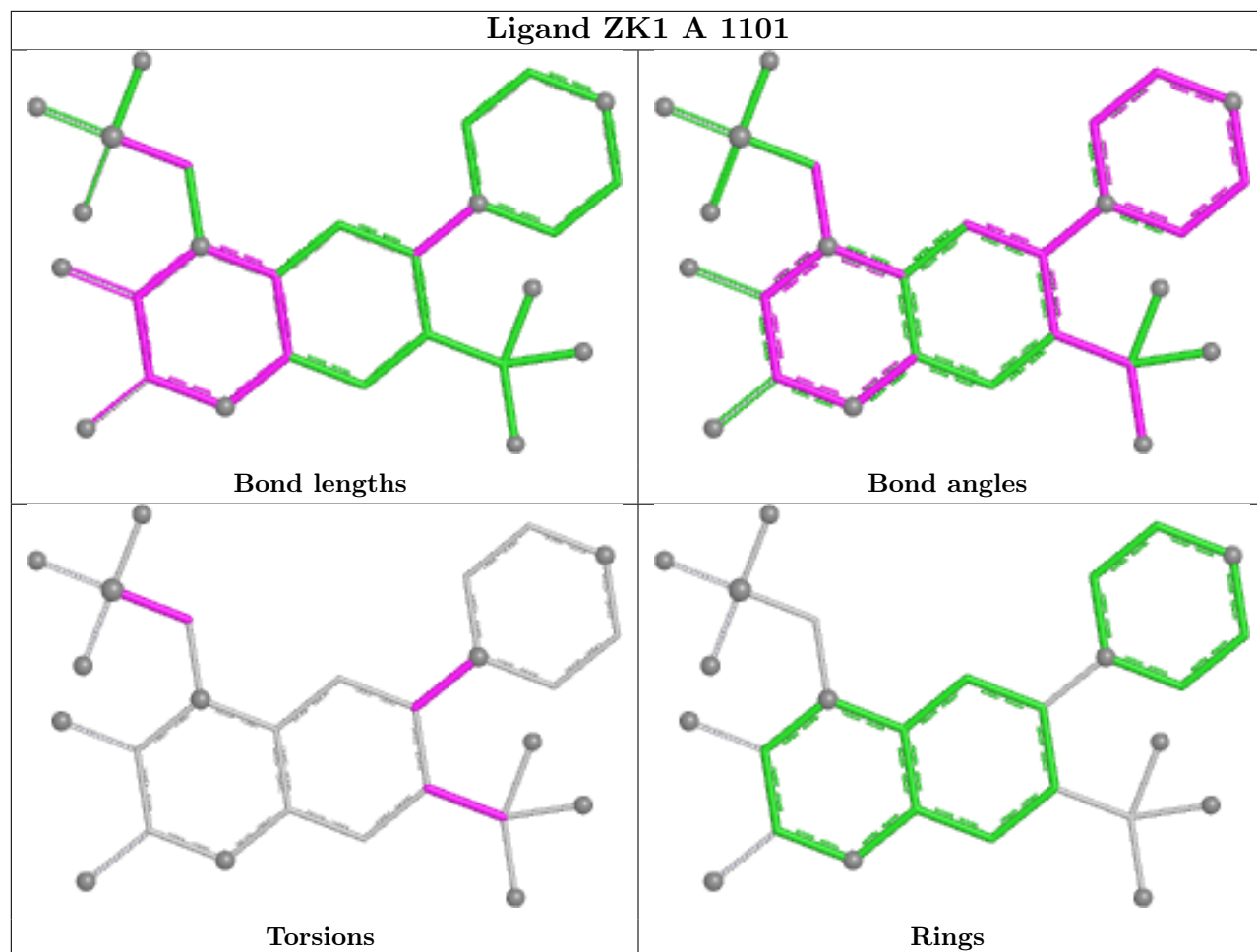
2 monomers are involved in 2 short contacts:

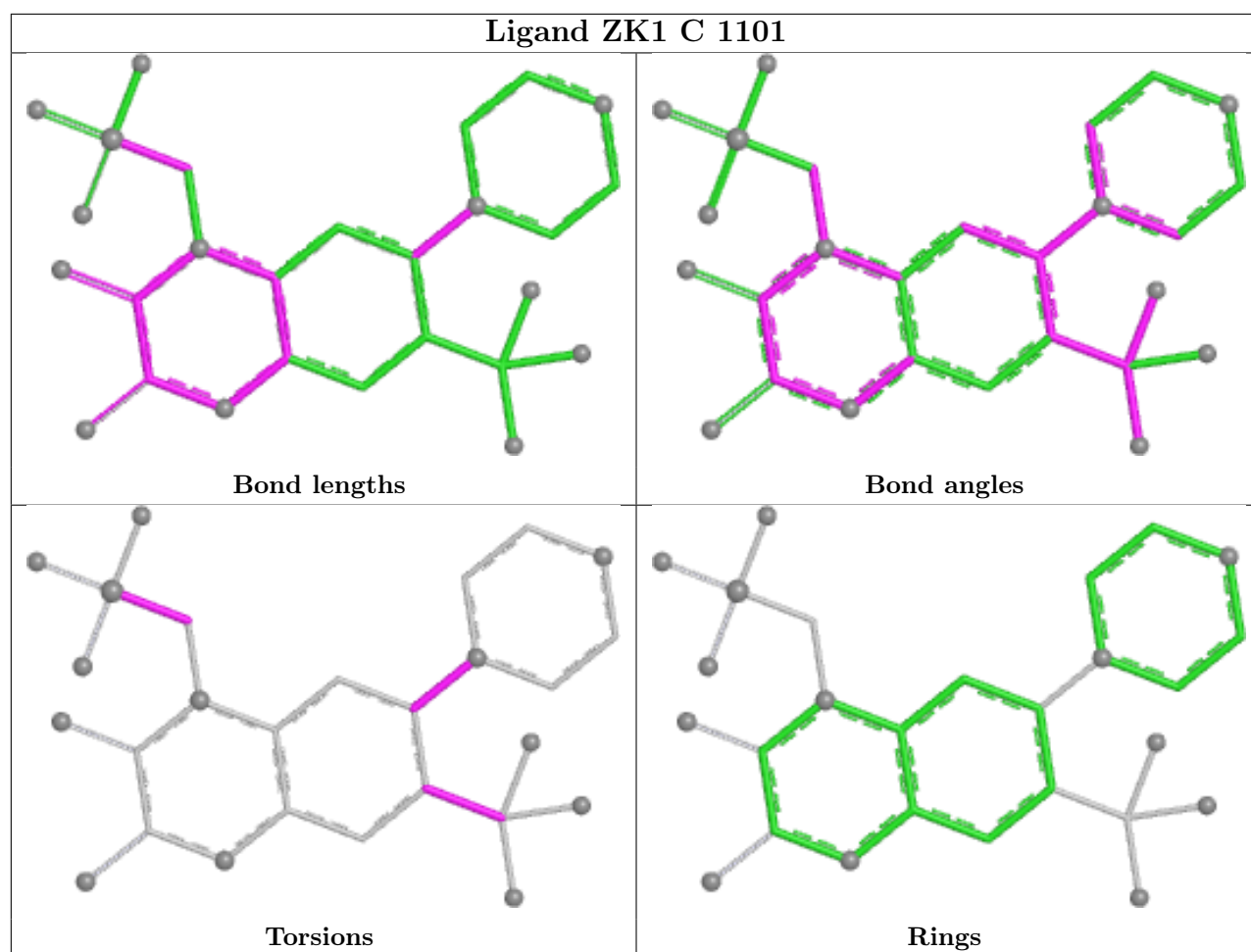
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1101	ZK1	1	0
3	C	1101	ZK1	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

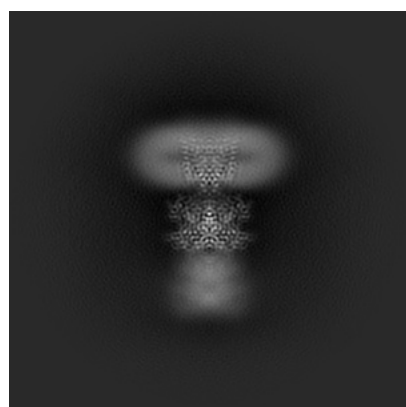
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70912. These allow visual inspection of the internal detail of the map and identification of artifacts.

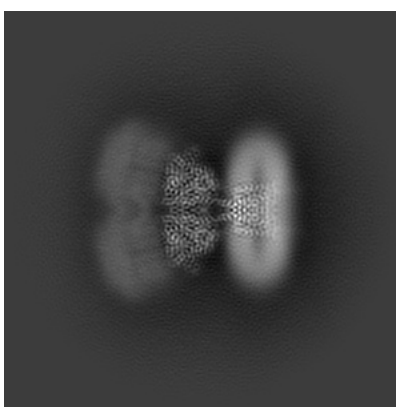
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

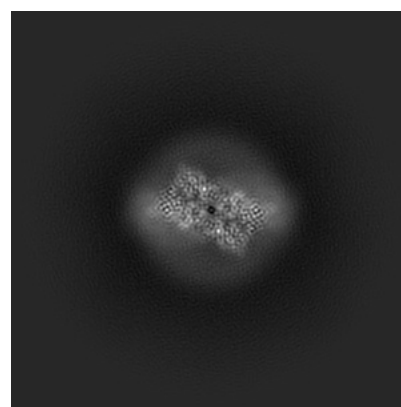
#### 6.1.1 Primary map



X



Y

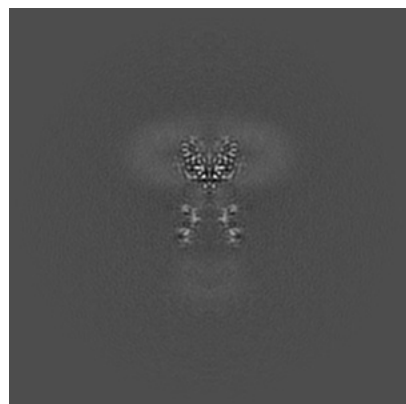


Z

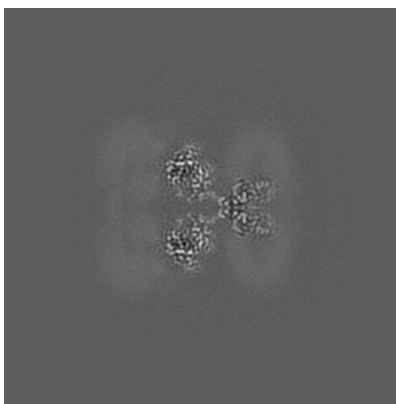
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

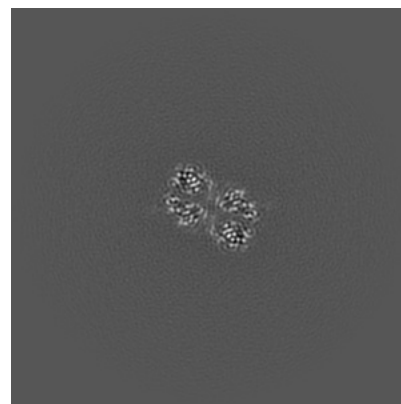
#### 6.2.1 Primary map



X Index: 224



Y Index: 224



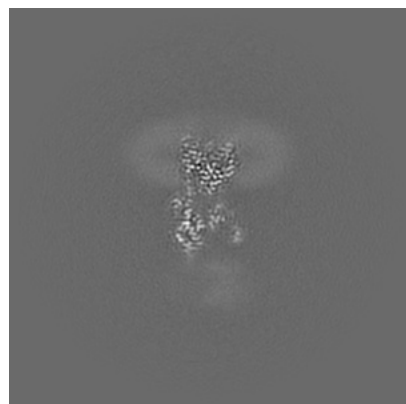
Z Index: 224



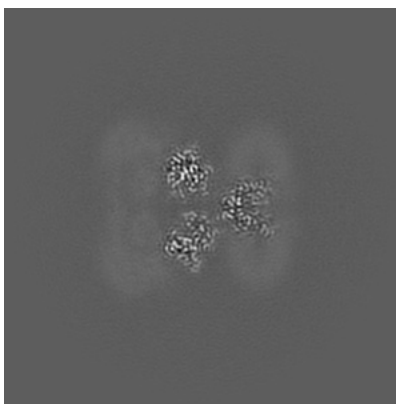
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

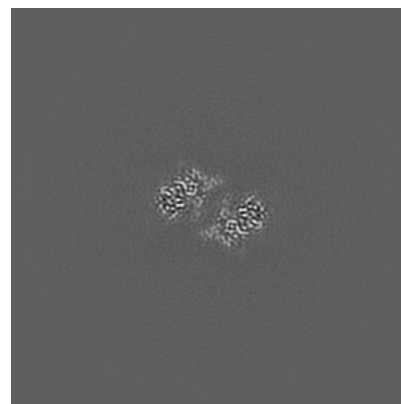
### 6.3.1 Primary map



X Index: 232



Y Index: 221

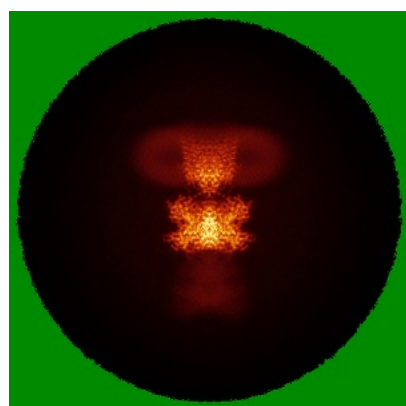


Z Index: 199

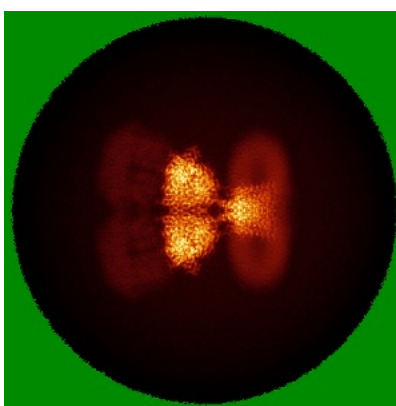
The images above show the largest variance slices of the map in three orthogonal directions.

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

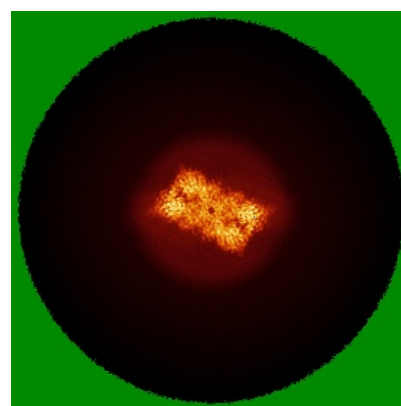
### 6.4.1 Primary map



X



Y

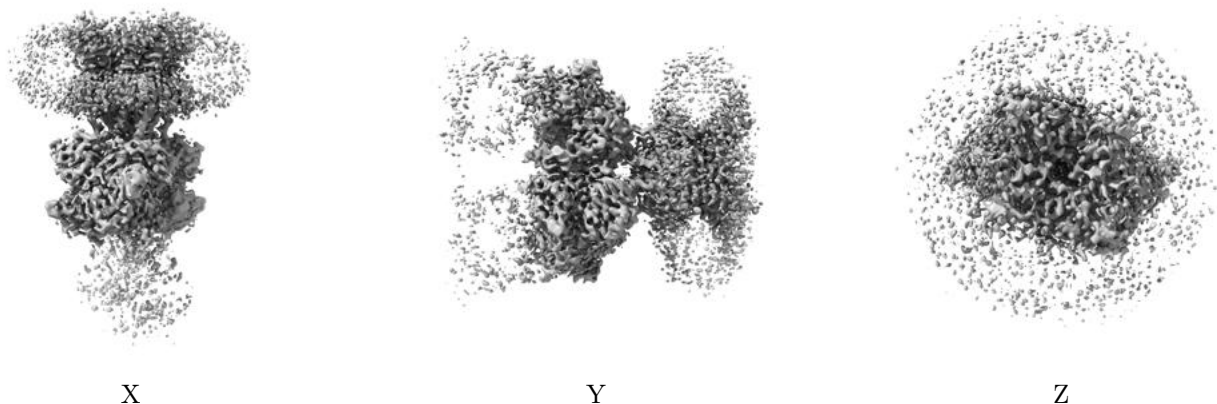


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

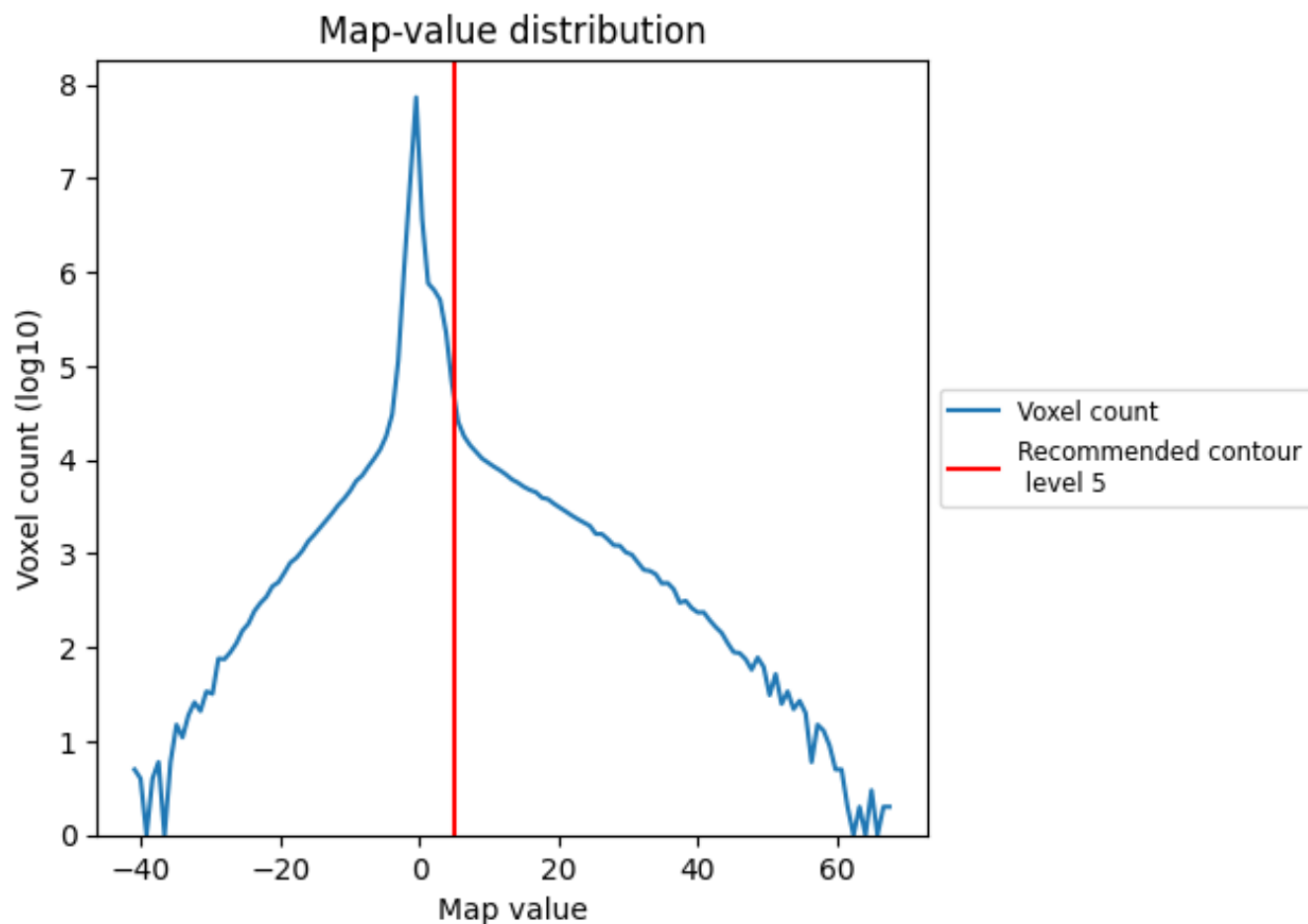
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

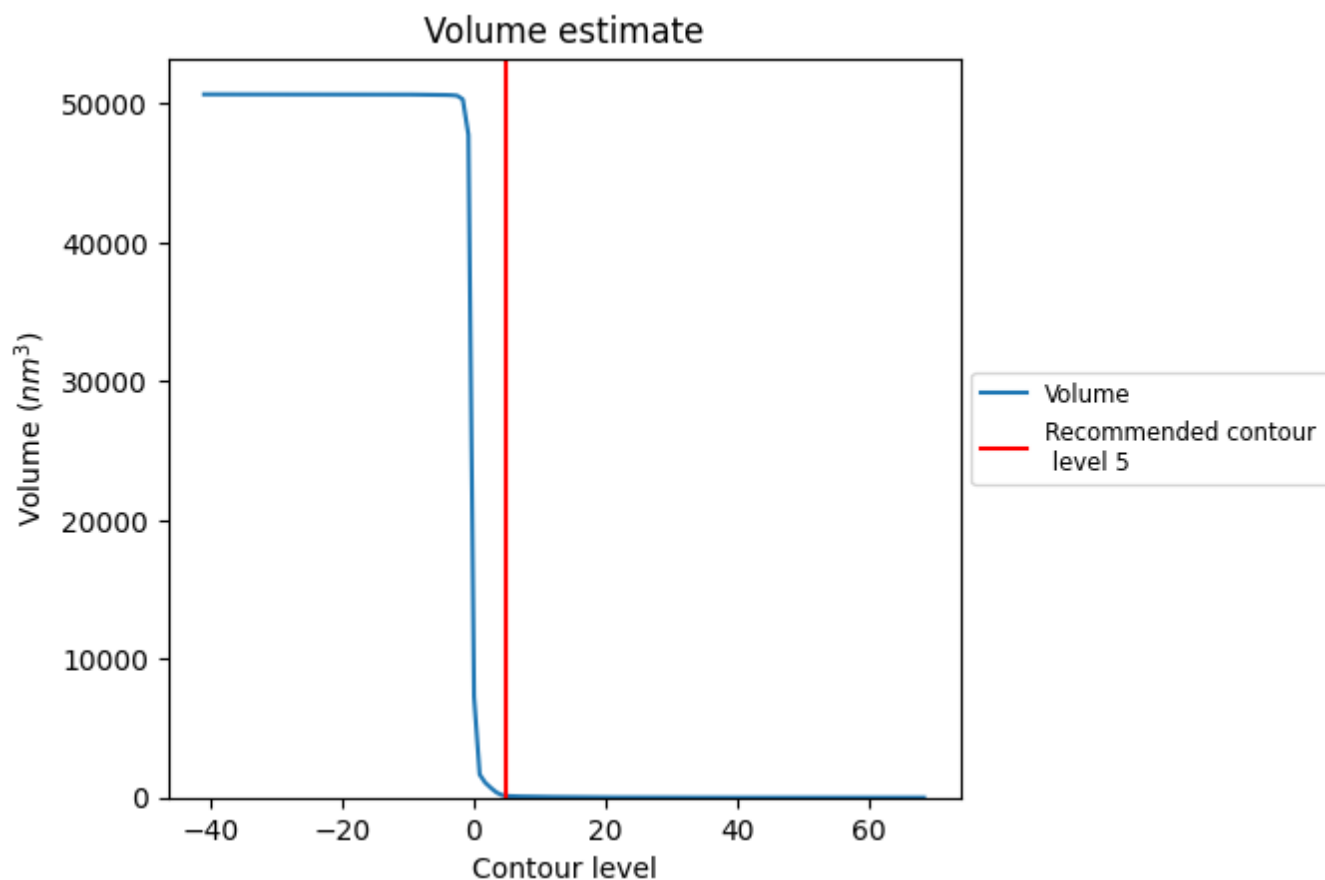
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

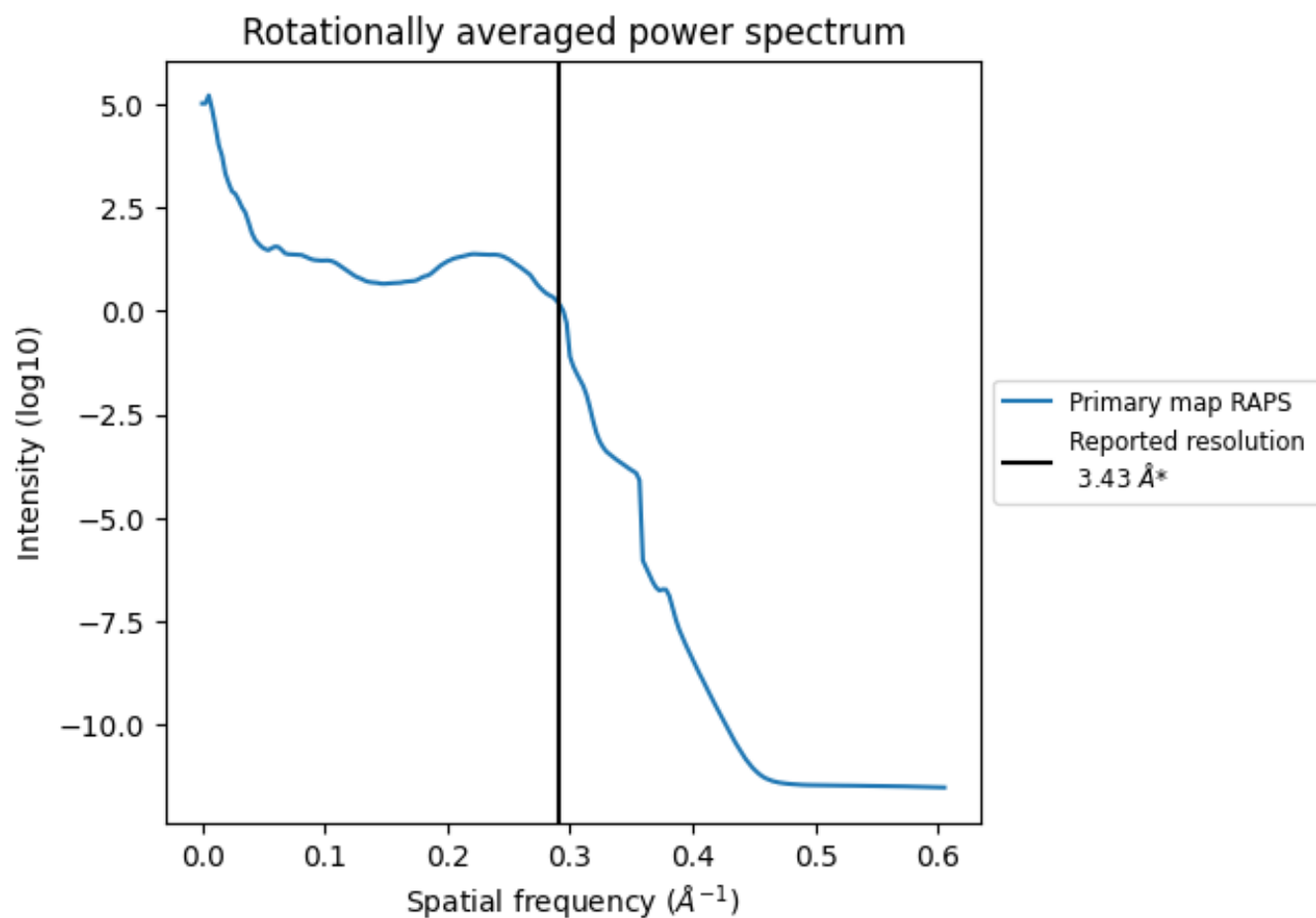
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm<sup>3</sup>; this corresponds to an approximate mass of 116 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 0.292 Å<sup>-1</sup>

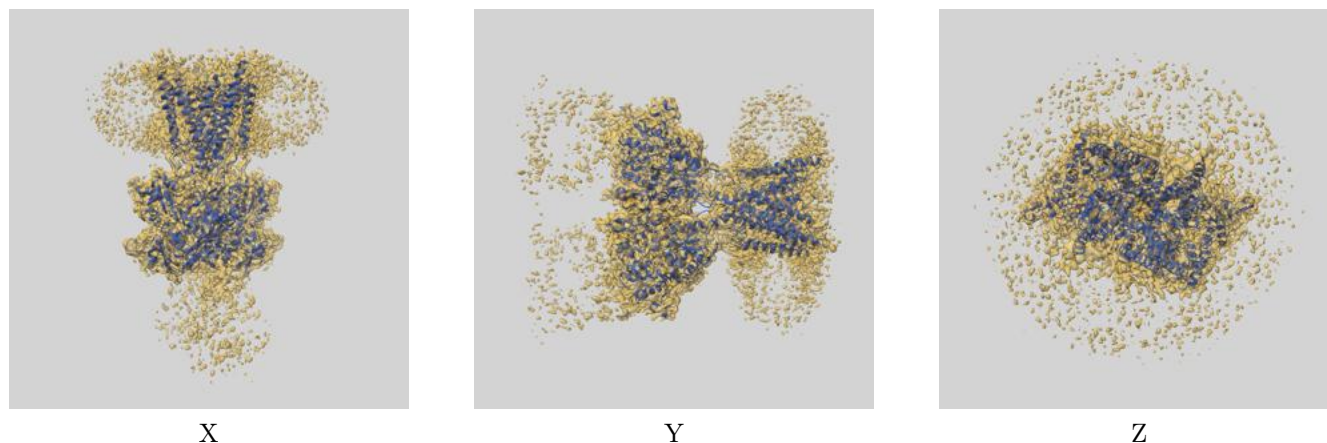
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

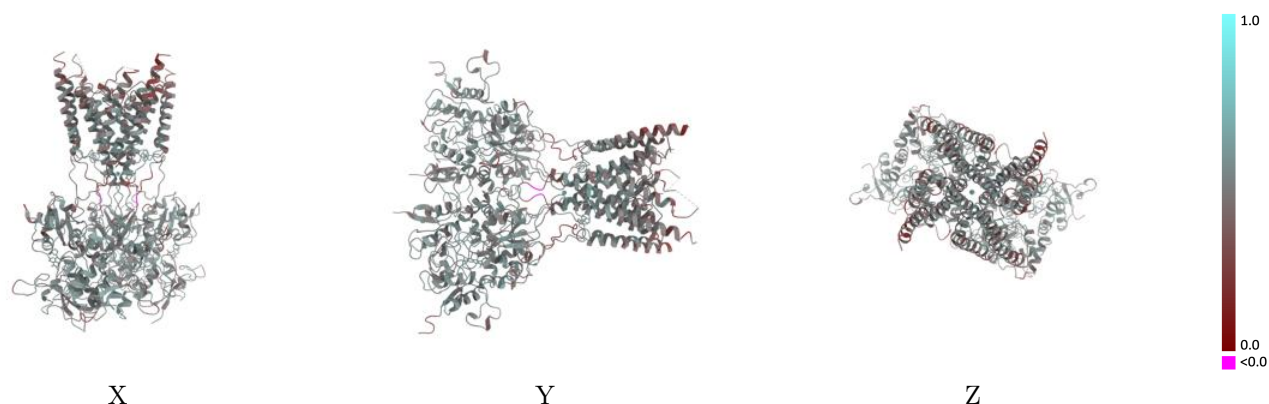
This section contains information regarding the fit between EMDB map EMD-70912 and PDB model 9OVT. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

### 9.1 Map-model overlay [i](#)



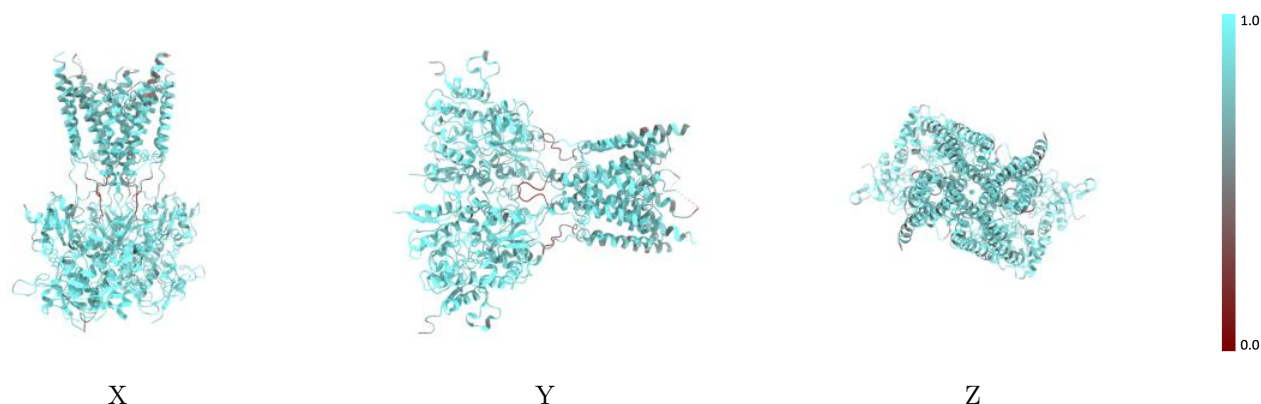
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

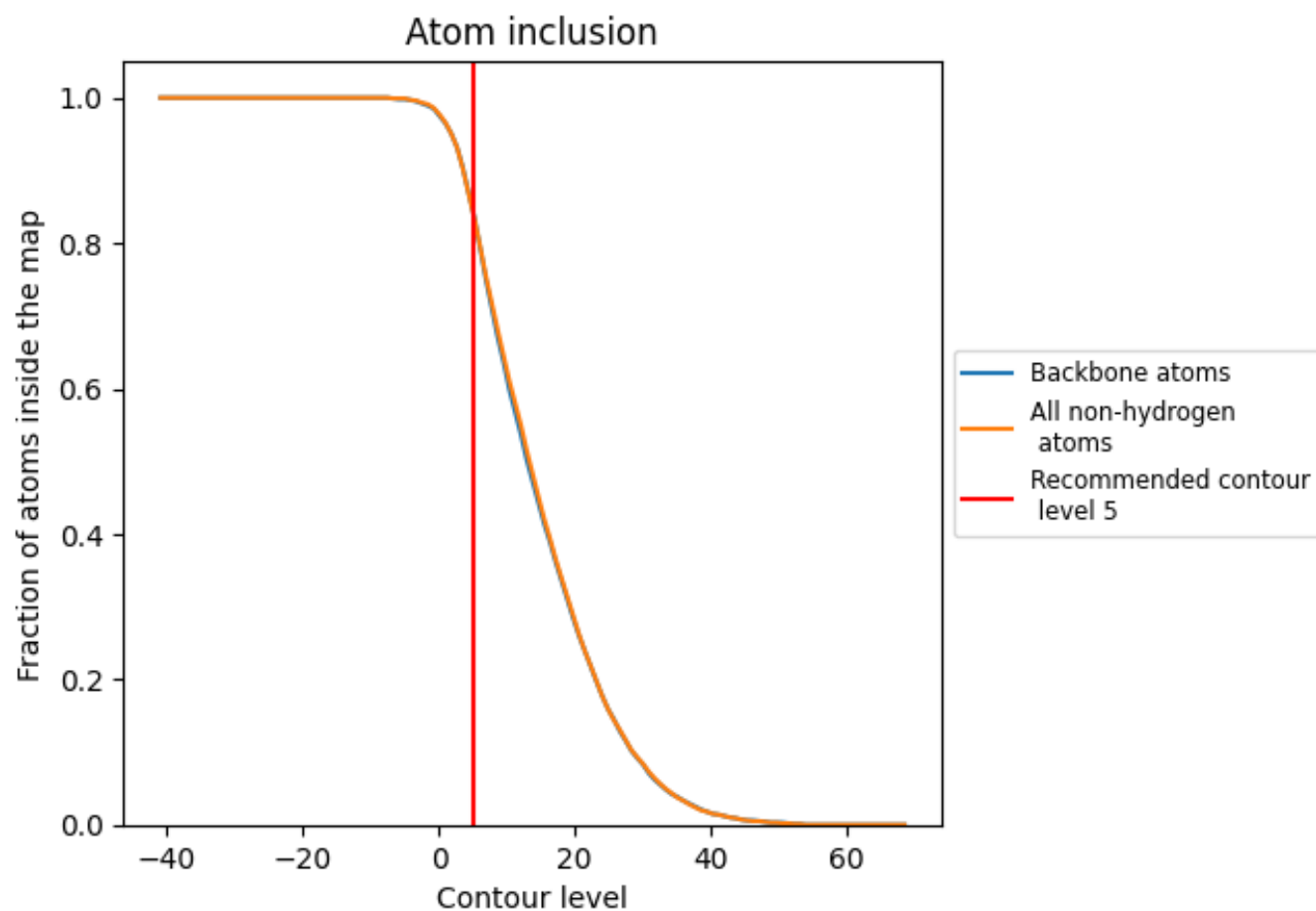
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (5).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8440	<div><div></div></div> 0.4770
A	<div><div></div></div> 0.8460	<div><div></div></div> 0.4790
B	<div><div></div></div> 0.8560	<div><div></div></div> 0.4770
C	<div><div></div></div> 0.8460	<div><div></div></div> 0.4790
D	<div><div></div></div> 0.8490	<div><div></div></div> 0.4740

