



Full wwPDB EM Validation Report ⓘ

Oct 23, 2025 – 03:07 PM EDT

PDB ID : 9OOT / pdb_00009oot
EMDB ID : EMD-70672
Title : Pre-active state of Gly/Glu/Pregnenolone Sulfate bound hGluN1a-2B NM-DAR
Authors : Hyunook, K.; Hiro, F.
Deposited on : 2025-05-16
Resolution : 3.13 Å(reported)
Based on initial model : 7saa

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 : 2022.3.0, CSD as543be (2022)
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

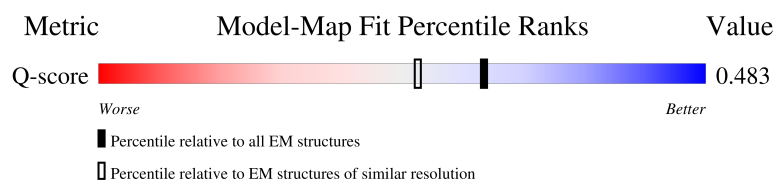
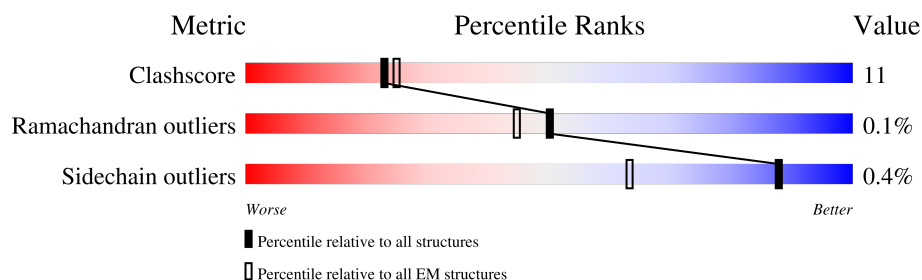
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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	14478 (2.63 - 3.63)

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	830	<div> <div>6%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
1	C	830	<div> <div>7%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
2	B	861	<div> <div>8%</div> <div>66%</div> <div>24%</div> <div>10%</div> </div>
2	D	861	<div> <div>8%</div> <div>67%</div> <div>22%</div> <div>10%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24825 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	800	Total	C	N	O	S	0	0
			6200	3962	1064	1139	35		
1	C	800	Total	C	N	O	S	0	0
			6196	3958	1063	1140	35		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	CYS	engineered mutation	UNP Q05586
A	844	ASN	ARG	engineered mutation	UNP Q05586
A	845	GLY	ARG	engineered mutation	UNP Q05586
A	846	ALA	LYS	engineered mutation	UNP Q05586
C	22	SER	CYS	engineered mutation	UNP Q05586
C	844	ASN	ARG	engineered mutation	UNP Q05586
C	845	GLY	ARG	engineered mutation	UNP Q05586
C	846	ALA	LYS	engineered mutation	UNP Q05586

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	775	Total	C	N	O	S	0	0
			6039	3898	971	1132	38		
2	D	775	Total	C	N	O	S	0	0
			6044	3902	970	1134	38		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	TRP	-	expression tag	UNP Q13224
B	-7	SER	-	expression tag	UNP Q13224
B	-6	HIS	-	expression tag	UNP Q13224
B	-5	PRO	-	expression tag	UNP Q13224
B	-4	GLN	-	expression tag	UNP Q13224

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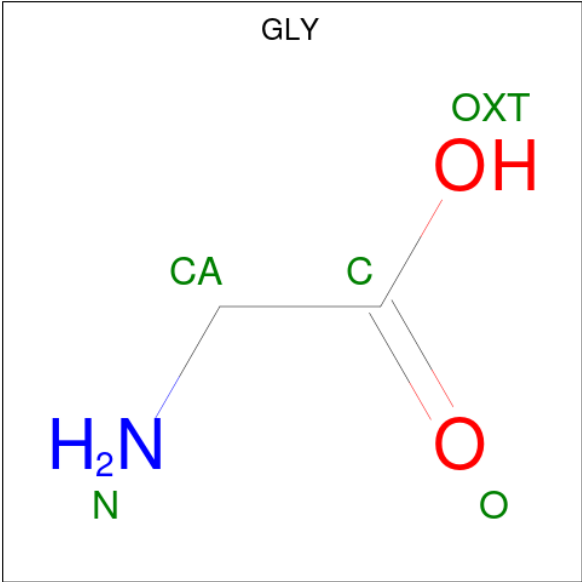
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	PHE	-	expression tag	UNP Q13224
B	-2	GLU	-	expression tag	UNP Q13224
B	-1	LYS	-	expression tag	UNP Q13224
B	0	GLY	-	expression tag	UNP Q13224
B	1	GLY	-	expression tag	UNP Q13224
B	2	GLY	-	expression tag	UNP Q13224
B	3	SER	-	expression tag	UNP Q13224
B	4	GLY	-	expression tag	UNP Q13224
B	5	GLY	-	expression tag	UNP Q13224
B	6	GLY	-	expression tag	UNP Q13224
B	7	SER	-	expression tag	UNP Q13224
B	8	GLY	-	expression tag	UNP Q13224
B	9	GLY	-	expression tag	UNP Q13224
B	10	SER	-	expression tag	UNP Q13224
B	11	ALA	-	expression tag	UNP Q13224
B	12	TRP	-	expression tag	UNP Q13224
B	13	SER	-	expression tag	UNP Q13224
B	14	HIS	-	expression tag	UNP Q13224
B	15	PRO	-	expression tag	UNP Q13224
B	16	GLN	-	expression tag	UNP Q13224
B	17	PHE	-	expression tag	UNP Q13224
B	18	GLU	-	expression tag	UNP Q13224
B	19	LYS	-	expression tag	UNP Q13224
B	20	GLY	-	expression tag	UNP Q13224
B	21	ALA	-	expression tag	UNP Q13224
B	22	LEU	-	expression tag	UNP Q13224
B	23	VAL	-	expression tag	UNP Q13224
B	24	PRO	-	expression tag	UNP Q13224
B	25	ARG	-	expression tag	UNP Q13224
B	26	GLY	-	expression tag	UNP Q13224
B	588	SER	CYS	engineered mutation	UNP Q13224
B	838	SER	CYS	engineered mutation	UNP Q13224
B	849	SER	CYS	engineered mutation	UNP Q13224
D	-8	TRP	-	expression tag	UNP Q13224
D	-7	SER	-	expression tag	UNP Q13224
D	-6	HIS	-	expression tag	UNP Q13224
D	-5	PRO	-	expression tag	UNP Q13224
D	-4	GLN	-	expression tag	UNP Q13224
D	-3	PHE	-	expression tag	UNP Q13224
D	-2	GLU	-	expression tag	UNP Q13224
D	-1	LYS	-	expression tag	UNP Q13224
D	0	GLY	-	expression tag	UNP Q13224

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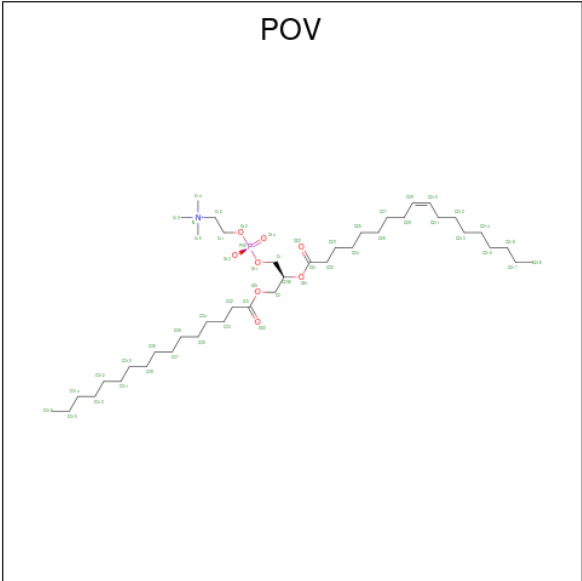
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP Q13224
D	2	GLY	-	expression tag	UNP Q13224
D	3	SER	-	expression tag	UNP Q13224
D	4	GLY	-	expression tag	UNP Q13224
D	5	GLY	-	expression tag	UNP Q13224
D	6	GLY	-	expression tag	UNP Q13224
D	7	SER	-	expression tag	UNP Q13224
D	8	GLY	-	expression tag	UNP Q13224
D	9	GLY	-	expression tag	UNP Q13224
D	10	SER	-	expression tag	UNP Q13224
D	11	ALA	-	expression tag	UNP Q13224
D	12	TRP	-	expression tag	UNP Q13224
D	13	SER	-	expression tag	UNP Q13224
D	14	HIS	-	expression tag	UNP Q13224
D	15	PRO	-	expression tag	UNP Q13224
D	16	GLN	-	expression tag	UNP Q13224
D	17	PHE	-	expression tag	UNP Q13224
D	18	GLU	-	expression tag	UNP Q13224
D	19	LYS	-	expression tag	UNP Q13224
D	20	GLY	-	expression tag	UNP Q13224
D	21	ALA	-	expression tag	UNP Q13224
D	22	LEU	-	expression tag	UNP Q13224
D	23	VAL	-	expression tag	UNP Q13224
D	24	PRO	-	expression tag	UNP Q13224
D	25	ARG	-	expression tag	UNP Q13224
D	26	GLY	-	expression tag	UNP Q13224
D	588	SER	CYS	engineered mutation	UNP Q13224
D	838	SER	CYS	engineered mutation	UNP Q13224
D	849	SER	CYS	engineered mutation	UNP Q13224

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



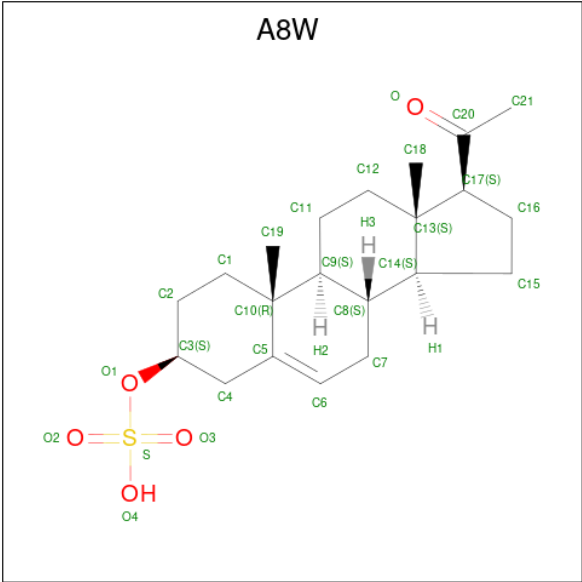
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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

- GLU
-
- Chemical structure of L-glutamic acid (GLU) is shown. The structure includes the amino group (NH₂), the carboxyl group (COOH), and the side chain (CH₂CH₂COOH). The atoms are labeled with their element symbols and names: C for carbon, O for oxygen, H for hydrogen, N for nitrogen, and the side chain atoms CB, CG, CD. The carboxyl groups are labeled with HO and OH. The amino group is labeled with NH₂. The side chain is labeled with CA(S).

- Molecule 6 is Pregnenolone sulfate (CCD ID: A8W) (formula: $C_{21}H_{32}O_5S$) (labeled as "Ligand of Interest" by depositor).

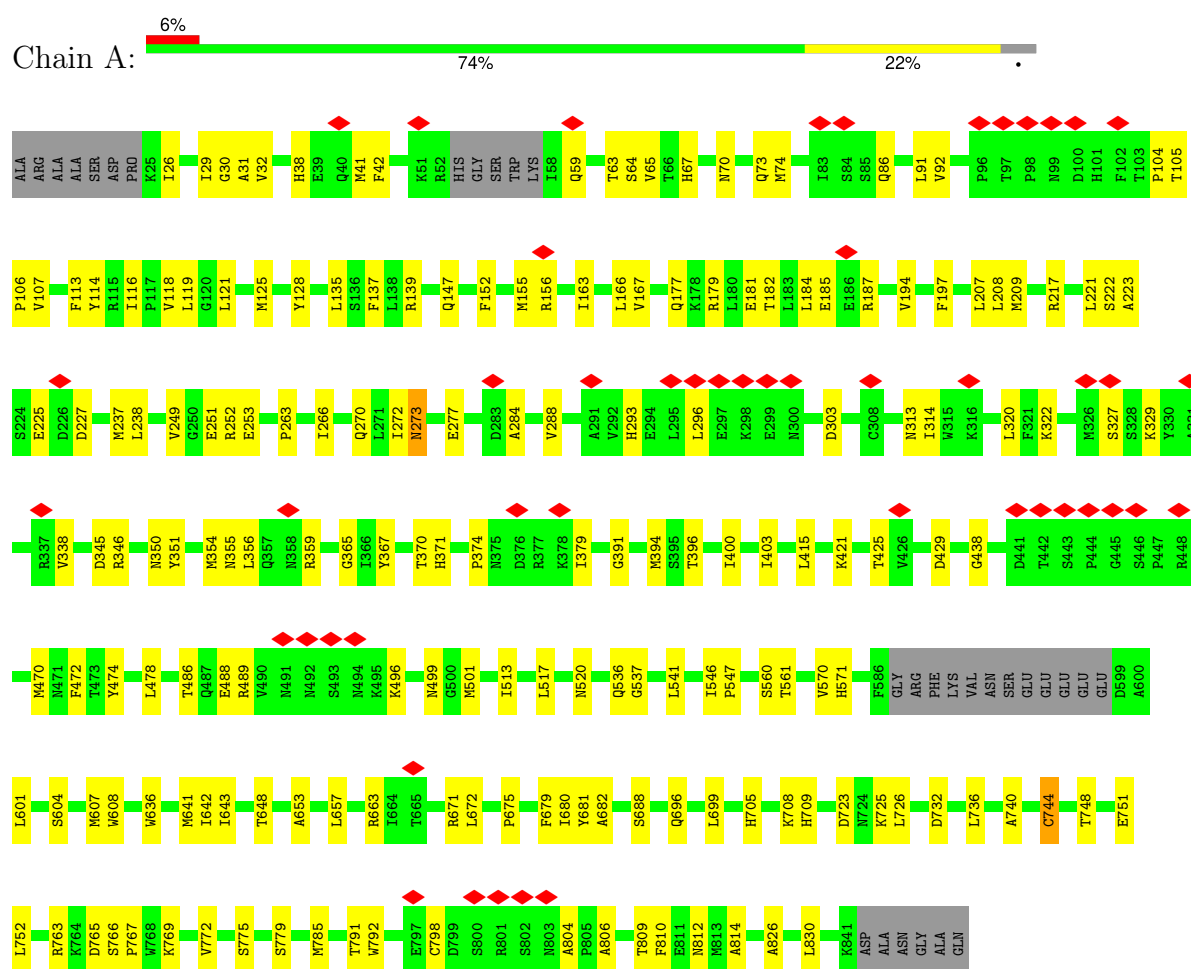


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	O	S	0
			27	21	5	1	
6	B	1	Total	C	O	S	0
			27	21	5	1	
6	D	1	Total	C	O	S	0
			27	21	5	1	
6	D	1	Total	C	O	S	0
			27	21	5	1	

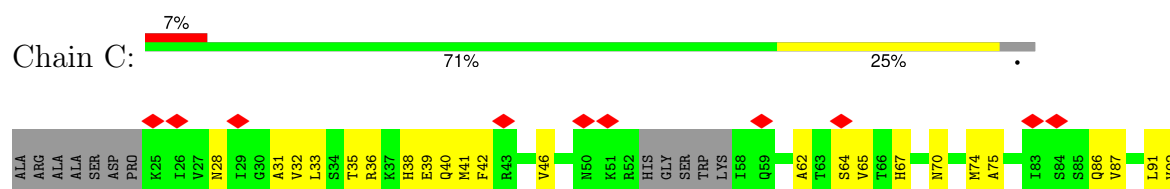
3 Residue-property plots [i](#)

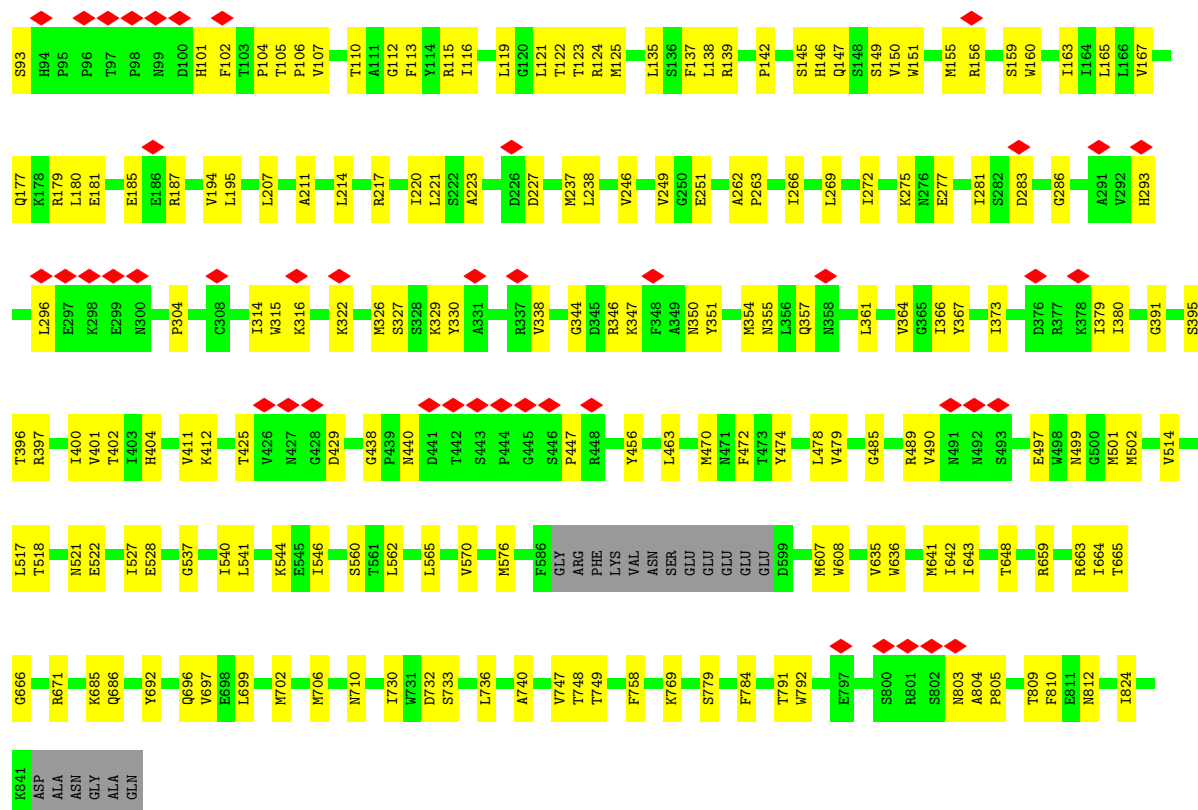
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 ionotropic, NMDA 1

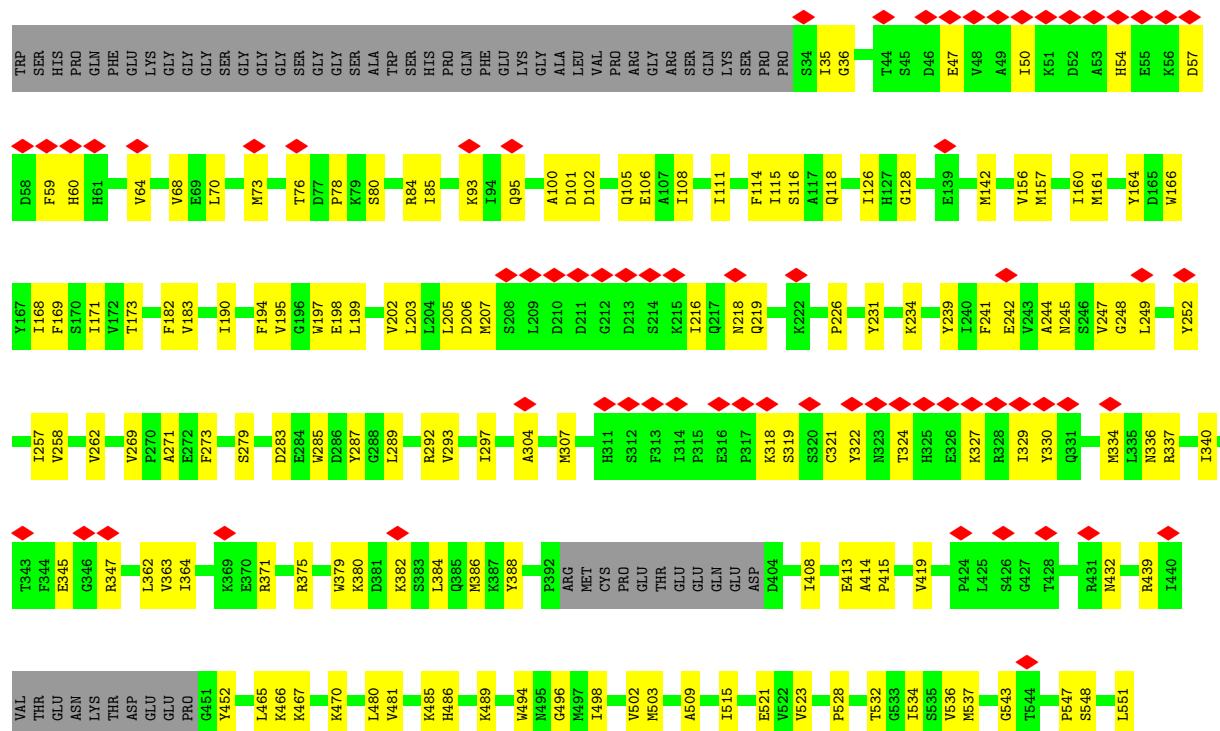


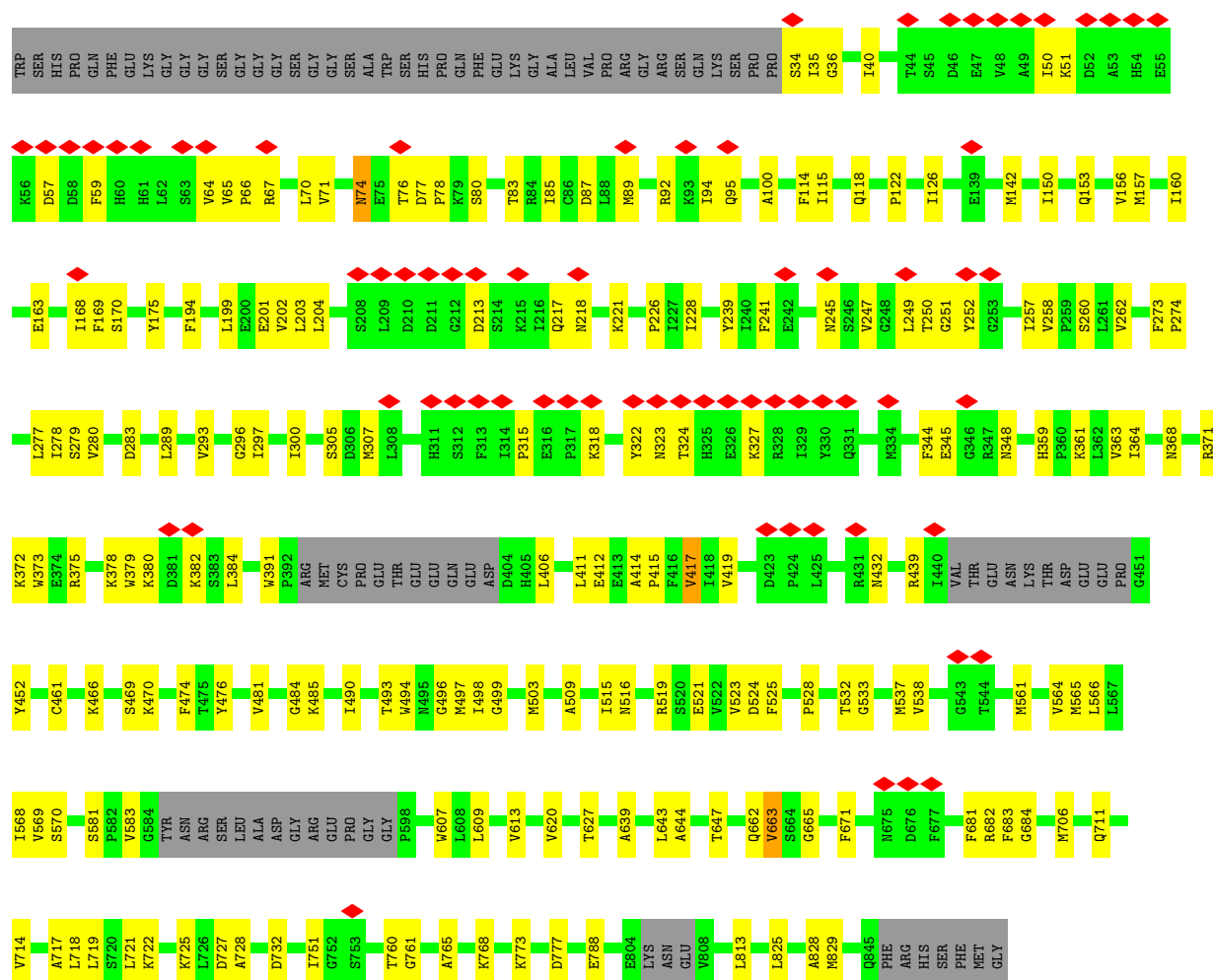
- Molecule 1: Glutamate receptor ionotropic, NMDA 1





• Molecule 2: Glutamate receptor ionotropic, NMDA 2B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	109420	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 ($e^-/\text{\AA}^2$)	56.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.508	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.048	Depositor
Map size (Å)	330.80002, 330.80002, 330.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POV, A8W

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	0.21	0/6340	0.30	0/8611
1	C	0.21	0/6336	0.30	0/8607
2	B	0.21	0/6175	0.30	0/8375
2	D	0.20	0/6181	0.30	0/8383
All	All	0.21	0/25032	0.30	0/33976

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	6200	0	6088	133	0
1	C	6196	0	6078	150	0
2	B	6039	0	5934	134	0
2	D	6044	0	5932	140	0
3	A	5	0	2	1	0
3	C	5	0	2	1	0
4	A	104	0	164	11	0
4	C	104	0	164	9	0
5	B	10	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	10	0	5	1	0
6	B	54	0	0	0	0
6	D	54	0	0	0	0
All	All	24825	0	24374	541	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 11.

All (541) 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:32:VAL:HG13	1:C:65:VAL:HG13	1.69	0.75
1:C:665:THR:HG22	1:C:666:GLY:H	1.49	0.75
2:B:203:LEU:HD11	2:B:219:GLN:HG2	1.67	0.74
2:B:318:LYS:HD2	2:B:327:LYS:HG2	1.70	0.74
2:D:361:LYS:HG2	2:D:380:LYS:HD3	1.69	0.73
2:B:364:ILE:HD11	2:B:384:LEU:HD11	1.71	0.72
2:D:168:ILE:HG21	2:D:226:PRO:HD2	1.72	0.72
1:A:91:LEU:HD23	1:A:121:LEU:HD21	1.72	0.71
1:A:92:VAL:HG11	1:A:104:PRO:HB3	1.73	0.71
2:B:47:GLU:HB3	2:B:70:LEU:HD21	1.72	0.71
1:A:470:MET:HE1	1:A:772:VAL:HG22	1.70	0.71
2:B:548:SER:HB2	2:B:551:LEU:HD12	1.71	0.70
1:C:351:TYR:H	1:C:367:TYR:HB3	1.57	0.70
1:C:497:GLU:N	1:C:497:GLU:OE1	2.24	0.70
1:C:32:VAL:HG11	1:C:74:MET:HE1	1.73	0.69
2:B:419:VAL:HG21	2:B:480:LEU:HD21	1.72	0.69
1:C:36:ARG:HH21	1:C:40:GLN:HG3	1.57	0.69
1:C:125:MET:O	1:C:139:ARG:NH2	2.26	0.69
2:B:173:THR:HG22	2:B:231:TYR:HB3	1.74	0.69
1:A:147:GLN:HE22	1:A:251:GLU:H	1.41	0.67
1:C:327:SER:O	1:C:329:LYS:NZ	2.28	0.67
2:B:414:ALA:HB3	2:B:415:PRO:HD3	1.77	0.67
1:C:316:LYS:H	1:C:316:LYS:HD2	1.60	0.66
1:A:125:MET:O	1:A:139:ARG:NH2	2.27	0.66
2:D:273:PHE:O	2:D:371:ARG:NH2	2.29	0.66
2:B:273:PHE:O	2:B:371:ARG:NH2	2.28	0.66
2:D:318:LYS:HD2	2:D:327:LYS:HG2	1.78	0.65
1:A:791:THR:HG1	1:A:792:TRP:CD1	2.14	0.65
1:C:663:ARG:O	1:C:671:ARG:NH2	2.30	0.65
1:A:732:ASP:OD2	3:A:1000:GLY:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:732:ASP:OD2	5:D:1000:GLU:N	2.30	0.65
2:D:324:THR:HA	2:D:327:LYS:HD2	1.79	0.64
1:A:663:ARG:HH22	1:A:679:PHE:HB3	1.63	0.64
1:A:513:ILE:HG21	1:A:517:LEU:HD22	1.80	0.64
2:B:168:ILE:HG21	2:B:226:PRO:HG2	1.80	0.64
1:C:155:MET:HE1	1:C:163:ILE:HG21	1.79	0.63
1:C:364:VAL:HG11	1:C:379:ILE:HG13	1.79	0.63
1:C:499:ASN:ND2	1:C:686:GLN:OE1	2.32	0.63
1:A:32:VAL:HG11	1:A:74:MET:HE1	1.79	0.63
2:B:626:THR:HB	4:C:1001:POV:H15B	1.82	0.62
4:C:1002:POV:H25	4:C:1002:POV:H31A	1.82	0.62
2:B:732:ASP:OD2	5:B:1000:GLU:N	2.32	0.62
2:D:175:TYR:HE1	2:D:204:LEU:HD21	1.64	0.62
1:C:147:GLN:HE22	1:C:251:GLU:H	1.47	0.62
2:D:532:THR:HG22	2:D:533:GLY:H	1.65	0.62
1:C:740:ALA:HB2	1:C:748:THR:HG23	1.82	0.62
2:D:67:ARG:HH12	2:D:92:ARG:HB3	1.65	0.62
2:D:684:GLY:N	2:D:728:ALA:O	2.32	0.62
2:D:307:MET:HE1	2:D:315:PRO:HD3	1.82	0.61
2:B:786:ASP:HA	1:C:696:GLN:HE22	1.65	0.61
1:A:675:PRO:HB3	1:A:705:HIS:ND1	2.16	0.61
2:D:788:GLU:OE2	2:D:788:GLU:N	2.34	0.60
2:B:665:GLY:HA2	2:B:751:ILE:HD12	1.82	0.60
4:C:1001:POV:H314	4:C:1002:POV:H28	1.82	0.60
1:A:223:ALA:HB1	1:A:227:ASP:HB2	1.84	0.60
2:B:50:ILE:HG23	2:B:293:VAL:HG11	1.84	0.59
2:B:36:GLY:H	2:B:95:GLN:HG3	1.68	0.59
2:B:247:VAL:HG12	2:B:249:LEU:H	1.66	0.59
2:D:115:ILE:HD12	2:D:115:ILE:H	1.67	0.59
1:C:463:LEU:HB2	1:C:514:VAL:HG11	1.84	0.59
2:B:105:GLN:HE21	2:B:108:ILE:HG12	1.67	0.59
2:B:269:VAL:HG12	2:B:271:ALA:H	1.67	0.59
2:D:414:ALA:HB3	2:D:415:PRO:HD3	1.83	0.59
1:C:101:HIS:CD2	1:C:125:MET:HG3	2.38	0.59
2:B:156:VAL:HG21	2:B:362:LEU:HD12	1.85	0.58
2:D:283:ASP:OD2	2:D:378:LYS:NZ	2.32	0.58
1:C:150:VAL:HG11	1:C:269:LEU:HD11	1.84	0.58
1:A:765:ASP:O	1:A:769:LYS:NZ	2.34	0.58
1:A:263:PRO:HG2	1:A:266:ILE:HD11	1.85	0.58
1:A:70:ASN:ND2	2:B:321:CYS:O	2.36	0.58
1:C:28:ASN:HB3	1:C:87:VAL:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ASN:HD21	1:C:379:ILE:HG23	1.68	0.58
1:C:101:HIS:HD2	1:C:125:MET:HG3	1.67	0.58
1:C:576:MET:HE2	2:D:829:MET:HB3	1.84	0.58
2:D:76:THR:OG1	2:D:80:SER:OG	2.21	0.58
2:D:175:TYR:CE1	2:D:204:LEU:HD21	2.38	0.58
2:B:485:LYS:HD3	2:B:688:ASN:HB2	1.84	0.58
1:C:528:GLU:OE1	1:C:769:LYS:HD3	2.02	0.58
1:C:46:VAL:HG21	1:C:62:ALA:HB2	1.86	0.57
1:A:167:VAL:HG11	1:A:177:GLN:HB2	1.85	0.57
1:C:663:ARG:HE	1:C:749:THR:HG21	1.70	0.57
1:C:36:ARG:O	1:C:36:ARG:NE	2.37	0.57
2:D:163:GLU:HG3	2:D:384:LEU:HD23	1.87	0.57
1:C:663:ARG:HG2	1:C:749:THR:HG21	1.87	0.57
2:D:169:PHE:HB3	2:D:199:LEU:HA	1.87	0.57
1:C:732:ASP:OD2	3:C:1000:GLY:N	2.38	0.57
2:B:467:LYS:HA	2:B:470:LYS:HE2	1.86	0.57
2:D:274:PRO:HD2	2:D:277:LEU:HD13	1.85	0.57
2:D:51:LYS:HG2	2:D:70:LEU:HD13	1.86	0.56
2:D:322:TYR:O	2:D:327:LYS:NZ	2.35	0.56
1:A:488:GLU:OE1	1:A:499:ASN:ND2	2.38	0.56
2:B:486:HIS:CD2	5:B:1000:GLU:HB2	2.41	0.56
2:D:379:TRP:HZ2	2:D:382:LYS:HD3	1.70	0.56
1:A:32:VAL:HG22	1:A:65:VAL:HB	1.87	0.56
2:D:515:ILE:HD12	2:D:528:PRO:HG3	1.88	0.56
2:B:537:MET:HB3	2:B:721:LEU:HD21	1.88	0.56
2:D:538:VAL:HG22	2:D:727:ASP:O	2.06	0.56
2:B:536:VAL:HB	2:B:751:ILE:HD11	1.87	0.56
1:C:138:LEU:HD23	1:C:344:GLY:HA2	1.88	0.56
2:B:142:MET:SD	2:B:336:ASN:ND2	2.79	0.56
1:A:327:SER:OG	1:A:329:LYS:NZ	2.40	0.55
2:B:169:PHE:HB2	2:B:199:LEU:HA	1.86	0.55
4:A:1001:POV:H314	4:A:1002:POV:H28	1.87	0.55
2:B:293:VAL:O	2:B:297:ILE:HG12	2.07	0.55
1:C:156:ARG:HB3	1:C:187:ARG:HH12	1.72	0.55
1:C:163:ILE:HD12	1:C:220:ILE:HD12	1.89	0.55
4:A:1002:POV:H25	4:A:1002:POV:H39A	1.88	0.55
2:B:561:MET:HE3	2:B:565:MET:HE2	1.89	0.55
1:C:112:GLY:O	1:C:115:ARG:NH1	2.40	0.55
2:B:78:PRO:HB3	2:B:111:ILE:HD13	1.87	0.55
2:B:114:PHE:O	2:B:118:GLN:N	2.29	0.55
1:C:135:LEU:HD12	1:C:135:LEU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:TRP:HZ2	2:B:382:LYS:HD3	1.73	0.54
1:C:146:HIS:O	1:C:149:SER:OG	2.23	0.54
2:B:242:GLU:HA	2:B:245:ASN:HB2	1.90	0.54
1:C:167:VAL:HG11	1:C:177:GLN:HB2	1.89	0.54
1:A:38:HIS:CE1	1:A:277:GLU:HB2	2.43	0.54
2:B:205:LEU:HD13	2:B:216:ILE:HD11	1.88	0.54
2:D:153:GLN:NE2	2:D:260:SER:OG	2.40	0.54
1:C:86:GLN:NE2	1:C:304:PRO:O	2.40	0.54
1:C:546:ILE:HD12	1:C:546:ILE:H	1.73	0.54
2:D:258:VAL:O	2:D:279:SER:HA	2.08	0.54
2:D:760:THR:OG1	2:D:761:GLY:N	2.41	0.54
1:A:113:PHE:HE1	2:B:105:GLN:HE22	1.55	0.54
2:D:64:VAL:HG12	2:D:305:SER:HB3	1.89	0.54
2:B:683:PHE:HB3	2:B:728:ALA:HB3	1.90	0.54
2:D:247:VAL:HG12	2:D:249:LEU:H	1.72	0.54
2:D:565:MET:O	2:D:569:VAL:HG12	2.08	0.54
1:A:209:MET:HE3	1:A:209:MET:HA	1.90	0.53
1:A:682:ALA:HB3	1:A:726:LEU:HD21	1.90	0.53
1:A:135:LEU:H	1:A:135:LEU:HD12	1.73	0.53
2:B:515:ILE:HD12	2:B:528:PRO:HG3	1.89	0.53
1:A:42:PHE:HD2	1:A:64:SER:HB3	1.74	0.53
2:B:408:ILE:HD12	2:B:465:LEU:HD21	1.89	0.53
1:A:119:LEU:HD13	1:A:284:ALA:HB1	1.90	0.53
1:A:740:ALA:HB2	1:A:748:THR:HG23	1.91	0.53
1:C:113:PHE:CD2	2:D:78:PRO:HD3	2.44	0.53
2:B:318:LYS:HE3	2:B:330:TYR:HE2	1.73	0.53
2:D:566:LEU:O	2:D:570:SER:OG	2.27	0.53
2:B:218:ASN:OD1	2:D:252:TYR:OH	2.26	0.53
1:C:147:GLN:HE21	1:C:251:GLU:HG3	1.73	0.53
2:D:293:VAL:O	2:D:297:ILE:HG12	2.09	0.53
2:D:50:ILE:HG12	2:D:293:VAL:HG21	1.91	0.52
2:D:682:ARG:NH1	2:D:725:LYS:O	2.42	0.52
1:A:327:SER:O	1:A:329:LYS:NZ	2.37	0.52
1:A:763:ARG:O	1:A:766:SER:OG	2.25	0.52
2:B:35:ILE:HD12	2:B:64:VAL:HB	1.90	0.52
2:D:671:PHE:HA	2:D:683:PHE:CZ	2.44	0.52
2:D:439:ARG:HH11	2:D:452:TYR:HB2	1.74	0.52
1:A:30:GLY:HA3	1:A:63:THR:H	1.74	0.52
1:C:150:VAL:HG22	1:C:367:TYR:CD2	2.45	0.52
1:A:70:ASN:HD21	2:B:324:THR:HG23	1.75	0.52
1:A:152:PHE:HZ	1:A:187:ARG:HG3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:THR:HG22	2:D:644:ALA:HB1	1.92	0.52
1:C:560:SER:HB2	4:C:1002:POV:H22A	1.91	0.52
1:A:156:ARG:HH22	1:A:371:HIS:CD2	2.27	0.52
1:A:561:THR:HG22	2:B:815:ILE:HD11	1.92	0.52
2:B:695:ILE:HD13	2:B:706:MET:HE1	1.92	0.52
2:D:368:ASN:ND2	2:D:372:LYS:O	2.43	0.52
2:D:114:PHE:O	2:D:118:GLN:N	2.36	0.52
1:A:370:THR:O	1:A:371:HIS:ND1	2.43	0.51
2:B:202:VAL:HG12	2:B:202:VAL:O	2.09	0.51
1:C:36:ARG:CZ	1:C:39:GLU:HB2	2.39	0.51
1:A:425:THR:OG1	1:A:429:ASP:O	2.26	0.51
2:B:521:GLU:O	2:B:768:LYS:NZ	2.38	0.51
1:C:194:VAL:HG12	1:C:194:VAL:O	2.10	0.51
2:D:521:GLU:O	2:D:768:LYS:NZ	2.38	0.51
2:B:85:ILE:HG21	2:B:115:ILE:HG21	1.91	0.51
2:B:742:ARG:HA	2:B:800:ILE:HD12	1.91	0.51
2:B:553:PRO:HB3	2:B:649:ASN:HB3	1.92	0.51
2:D:516:ASN:HB2	2:D:519:ARG:HD2	1.92	0.51
1:C:283:ASP:HB3	1:C:338:VAL:HG21	1.92	0.51
2:D:278:ILE:HD11	2:D:391:TRP:HH2	1.76	0.51
2:B:101:ASP:HB3	2:B:128:GLY:HA3	1.92	0.51
2:D:277:LEU:HD23	2:D:373:TRP:HH2	1.76	0.51
1:A:365:GLY:HA2	1:A:374:PRO:HA	1.93	0.51
4:A:1001:POV:H31H	4:A:1002:POV:H31B	1.94	0.51
2:D:77:ASP:OD1	2:D:80:SER:N	2.34	0.51
1:A:547:PRO:HB2	1:A:806:ALA:HB2	1.92	0.50
2:B:247:VAL:HA	2:D:247:VAL:HA	1.93	0.50
1:C:262:ALA:HB1	1:C:266:ILE:HG13	1.93	0.50
2:D:569:VAL:HG13	2:D:609:LEU:HD13	1.93	0.50
2:D:773:LYS:NZ	2:D:777:ASP:OD2	2.39	0.50
1:A:217:ARG:HB2	1:A:391:GLY:HA2	1.92	0.50
1:A:766:SER:O	1:A:769:LYS:NZ	2.40	0.50
2:B:198:GLU:N	2:B:198:GLU:OE1	2.44	0.50
1:A:38:HIS:HE1	1:A:277:GLU:HB2	1.77	0.50
2:B:269:VAL:HG11	2:B:371:ARG:HE	1.77	0.50
1:C:316:LYS:HD2	1:C:316:LYS:N	2.24	0.50
2:B:561:MET:HG2	1:C:810:PHE:CE1	2.47	0.50
2:D:95:GLN:O	2:D:122:PRO:HD2	2.12	0.50
2:D:100:ALA:HB2	2:D:126:ILE:HD11	1.93	0.50
1:A:680:ILE:HB	1:A:726:LEU:HD12	1.94	0.49
2:B:322:TYR:O	2:B:327:LYS:NZ	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLN:NE2	1:C:251:GLU:H	2.10	0.49
1:C:211:ALA:HA	1:C:214:LEU:HD12	1.94	0.49
1:C:440:ASN:HD22	1:C:447:PRO:HB2	1.77	0.49
1:C:641:MET:HE2	1:C:642:ILE:HG13	1.93	0.49
2:D:202:VAL:HG12	2:D:202:VAL:O	2.12	0.49
2:B:485:LYS:O	2:B:496:GLY:HA3	2.12	0.49
2:B:644:ALA:HB1	1:C:648:THR:HG22	1.93	0.49
1:A:263:PRO:O	1:A:266:ILE:HG12	2.12	0.49
4:C:1001:POV:H27	4:C:1001:POV:H35A	1.93	0.49
2:D:50:ILE:HD11	2:D:289:LEU:HG	1.94	0.49
1:C:809:THR:OG1	1:C:812:ASN:ND2	2.45	0.49
2:D:411:LEU:HD11	2:D:485:LYS:HA	1.94	0.49
1:A:31:ALA:HB1	1:A:91:LEU:O	2.13	0.49
2:D:361:LYS:HB3	2:D:378:LYS:NZ	2.27	0.49
2:D:523:VAL:HG11	2:D:765:ALA:HB1	1.93	0.49
1:A:137:PHE:H	1:A:322:LYS:NZ	2.10	0.49
2:B:287:TYR:OH	2:B:347:ARG:NH2	2.46	0.49
2:D:711:GLN:HG2	2:D:717:ALA:HB2	1.94	0.49
1:C:42:PHE:HD2	1:C:64:SER:HB3	1.78	0.49
1:C:396:THR:O	1:C:472:PHE:HB2	2.13	0.49
2:D:157:MET:SD	2:D:257:ILE:HG22	2.52	0.49
1:A:222:SER:O	1:A:222:SER:OG	2.29	0.49
2:B:36:GLY:O	2:B:95:GLN:N	2.46	0.49
1:C:165:LEU:HD21	1:C:180:LEU:HD23	1.95	0.49
1:C:702:MET:O	1:C:706:MET:HG3	2.13	0.48
2:D:250:THR:OG1	2:D:251:GLY:N	2.45	0.48
2:D:683:PHE:HB2	2:D:706:MET:HG2	1.93	0.48
2:D:213:ASP:OD1	2:D:239:TYR:OH	2.31	0.48
1:A:679:PHE:HE2	1:A:681:TYR:CZ	2.31	0.48
2:B:498:ILE:O	2:B:502:VAL:HG23	2.13	0.48
1:C:121:LEU:HD13	1:C:281:ILE:HG12	1.95	0.48
2:D:36:GLY:HA3	2:D:94:ILE:HA	1.94	0.48
1:A:225:GLU:HG3	1:A:252:ARG:O	2.14	0.48
2:D:156:VAL:HG11	2:D:280:VAL:HG11	1.95	0.48
2:D:218:ASN:HA	2:D:221:LYS:HE2	1.95	0.48
1:A:139:ARG:NH1	1:A:345:ASP:OD1	2.46	0.48
1:A:830:LEU:HB3	2:D:627:THR:HG22	1.95	0.48
2:B:536:VAL:HA	2:B:729:PHE:O	2.13	0.48
1:C:485:GLY:HA3	1:C:502:MET:HB2	1.95	0.48
2:D:241:PHE:O	2:D:245:ASN:N	2.44	0.48
2:B:466:LYS:O	2:B:470:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:TRP:O	1:C:155:MET:HG2	2.14	0.48
1:C:366:ILE:HG22	1:C:373:ILE:HB	1.96	0.48
2:D:36:GLY:O	2:D:95:GLN:N	2.45	0.48
2:D:85:ILE:HG21	2:D:115:ILE:HG21	1.94	0.48
2:D:439:ARG:HD3	2:D:452:TYR:HD2	1.78	0.48
1:C:425:THR:OG1	1:C:429:ASP:O	2.32	0.48
1:C:544:LYS:HG2	1:C:747:VAL:HB	1.96	0.48
1:A:394:MET:HE3	1:A:767:PRO:HB2	1.96	0.48
1:C:91:LEU:HD22	1:C:119:LEU:HB2	1.94	0.48
1:C:124:ARG:NH1	1:C:142:PRO:O	2.46	0.48
2:D:80:SER:HA	2:D:83:THR:HG22	1.94	0.48
2:B:101:ASP:OD1	2:B:102:ASP:N	2.46	0.47
2:B:190:ILE:HD12	2:B:197:TRP:CG	2.49	0.47
2:D:77:ASP:O	2:D:80:SER:OG	2.29	0.47
2:D:714:VAL:O	2:D:718:LEU:HD23	2.15	0.47
2:B:100:ALA:HB2	2:B:126:ILE:HD11	1.96	0.47
1:C:277:GLU:O	1:C:281:ILE:HG13	2.14	0.47
1:C:489:ARG:HA	1:C:489:ARG:HD2	1.71	0.47
1:A:560:SER:HB2	4:A:1002:POV:H22A	1.96	0.47
2:B:574:VAL:HG21	2:B:602:ILE:HA	1.96	0.47
1:C:145:SER:OG	1:C:179:ARG:NH2	2.43	0.47
1:C:105:THR:OG1	1:C:106:PRO:HD3	2.14	0.47
2:D:485:LYS:O	2:D:496:GLY:HA3	2.13	0.47
1:A:396:THR:O	1:A:472:PHE:HB2	2.15	0.47
1:A:679:PHE:HD1	1:A:679:PHE:H	1.62	0.47
2:B:564:VAL:O	2:B:568:ILE:HG13	2.14	0.47
1:C:33:LEU:HD22	1:C:93:SER:HB3	1.97	0.47
1:A:705:HIS:HD2	1:A:709:HIS:HD2	1.62	0.47
1:A:31:ALA:O	1:A:64:SER:HA	2.15	0.47
1:A:105:THR:OG1	1:A:106:PRO:HD3	2.14	0.47
2:B:481:VAL:HG21	2:B:496:GLY:HA2	1.96	0.47
2:B:502:VAL:HG12	2:B:503:MET:HE2	1.97	0.47
2:B:684:GLY:HA2	2:B:706:MET:HG2	1.96	0.47
2:D:83:THR:O	2:D:87:ASP:HB3	2.15	0.47
2:D:76:THR:OG1	2:D:77:ASP:N	2.47	0.47
2:B:336:ASN:O	2:B:340:ILE:HG12	2.16	0.47
1:A:177:GLN:O	1:A:181:GLU:HG2	2.14	0.46
1:A:486:THR:O	1:A:499:ASN:ND2	2.48	0.46
2:B:439:ARG:HG3	2:B:452:TYR:CD1	2.50	0.46
1:C:160:TRP:CH2	1:C:246:VAL:HG11	2.50	0.46
1:A:293:HIS:HA	1:A:296:LEU:HG	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:ILE:HD13	1:C:730:ILE:HG12	1.97	0.46
2:B:244:ALA:O	2:B:248:GLY:N	2.45	0.46
2:B:283:ASP:OD1	2:B:363:VAL:HG13	2.16	0.46
1:C:32:VAL:O	1:C:67:HIS:NE2	2.45	0.46
2:B:168:ILE:HG12	2:B:226:PRO:HD2	1.98	0.46
1:C:412:LYS:NZ	1:C:456:TYR:OH	2.34	0.46
1:A:541:LEU:HD12	1:A:541:LEU:HA	1.82	0.46
2:B:258:VAL:O	2:B:279:SER:HA	2.16	0.46
1:A:338:VAL:HG13	1:A:346:ARG:HD3	1.98	0.46
1:A:775:SER:O	1:A:779:SER:OG	2.30	0.46
2:B:252:TYR:OH	2:D:218:ASN:OD1	2.27	0.46
2:B:760:THR:OG1	2:B:761:GLY:N	2.45	0.46
1:C:156:ARG:HB3	1:C:187:ARG:NH1	2.31	0.46
2:D:283:ASP:OD1	2:D:363:VAL:HG13	2.16	0.46
1:A:197:PHE:HE2	1:A:227:ASP:HB3	1.81	0.46
2:D:34:SER:HA	2:D:65:VAL:HB	1.98	0.46
2:D:74:ASN:OD1	2:D:74:ASN:N	2.49	0.46
1:A:249:VAL:HG13	1:A:253:GLU:HB2	1.97	0.46
1:A:672:LEU:HB3	1:A:679:PHE:CE2	2.50	0.46
2:B:523:VAL:HG21	2:B:765:ALA:HB1	1.97	0.46
2:B:573:ALA:HA	2:B:577:PHE:HB2	1.98	0.46
1:C:137:PHE:H	1:C:322:LYS:NZ	2.12	0.46
1:C:223:ALA:HB1	1:C:227:ASP:HB2	1.98	0.46
1:C:237:MET:HE2	1:C:238:LEU:HD22	1.98	0.46
2:D:417:VAL:HG13	2:D:461:CYS:HB2	1.97	0.46
4:A:1001:POV:H31C	4:A:1002:POV:H21B	1.97	0.45
1:C:565:LEU:HD23	1:C:565:LEU:HA	1.71	0.45
1:C:779:SER:HB2	1:C:784:PHE:HB3	1.97	0.45
2:B:164:TYR:OH	2:B:386:MET:HG2	2.17	0.45
1:C:499:ASN:OD1	1:C:499:ASN:N	2.49	0.45
1:A:29:ILE:HD11	1:A:288:VAL:HG11	1.98	0.45
1:A:826:ALA:HB2	4:A:1001:POV:H21E	1.97	0.45
1:A:570:VAL:HG22	1:A:636:TRP:CZ2	2.52	0.45
1:A:744:CYS:HB3	1:A:798:CYS:HB2	1.43	0.45
2:B:76:THR:OG1	2:B:80:SER:OG	2.30	0.45
2:B:543:GLY:HA3	2:B:660:VAL:H	1.81	0.45
1:C:522:GLU:H	1:C:522:GLU:CD	2.24	0.45
2:D:217:GLN:HE22	2:D:247:VAL:HG23	1.82	0.45
1:A:329:LYS:H	1:A:329:LYS:HG2	1.63	0.45
1:A:571:HIS:CE1	1:A:607:MET:HE1	2.51	0.45
1:A:643:ILE:HG22	4:A:1002:POV:H21J	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:HIS:CD2	1:A:709:HIS:HD2	2.35	0.45
2:B:345:GLU:OE2	2:B:347:ARG:NH1	2.50	0.45
1:C:354:MET:HB3	1:C:361:LEU:HD22	1.99	0.45
1:A:438:GLY:HA3	1:A:478:LEU:HD12	1.99	0.45
2:B:160:ILE:HG22	2:B:384:LEU:HD21	1.99	0.45
2:D:494:TRP:CE3	2:D:498:ILE:HD13	2.52	0.45
1:A:179:ARG:O	1:A:182:THR:OG1	2.25	0.45
2:D:150:ILE:HD12	2:D:150:ILE:HA	1.84	0.45
2:D:469:SER:HA	2:D:474:PHE:CE1	2.52	0.45
2:D:296:GLY:O	2:D:300:ILE:HG13	2.17	0.45
2:D:665:GLY:HA2	2:D:751:ILE:HG21	1.98	0.45
2:B:161:MET:HB3	2:B:166:TRP:HB2	1.99	0.45
1:C:804:ALA:N	1:C:805:PRO:HD3	2.31	0.45
2:D:662:GLN:O	2:D:663:VAL:HG12	2.16	0.45
1:A:501:MET:HE3	1:A:513:ILE:HG23	1.99	0.44
1:A:779:SER:HB2	1:A:785:MET:HE2	1.98	0.44
2:B:116:SER:HB2	2:B:142:MET:H	1.82	0.44
1:A:607:MET:HE3	1:A:607:MET:HB3	1.75	0.44
1:C:293:HIS:HA	1:C:296:LEU:HG	1.99	0.44
1:C:489:ARG:HG2	2:D:194:PHE:CD2	2.53	0.44
1:A:32:VAL:HG12	1:A:67:HIS:HD2	1.82	0.44
1:A:147:GLN:NE2	1:A:251:GLU:HG3	2.32	0.44
1:A:156:ARG:HG3	1:A:187:ARG:NH1	2.32	0.44
1:A:197:PHE:HB3	1:A:207:LEU:HD13	2.00	0.44
1:A:653:ALA:O	1:A:657:LEU:HG	2.17	0.44
1:C:181:GLU:O	1:C:185:GLU:HG2	2.17	0.44
4:C:1002:POV:H313	4:C:1002:POV:H310	1.82	0.44
2:D:170:SER:OG	2:D:228:ILE:HA	2.18	0.44
1:A:671:ARG:HA	2:B:800:ILE:HG23	2.00	0.44
1:C:147:GLN:NE2	1:C:251:GLU:HG3	2.32	0.44
2:D:481:VAL:HG12	2:D:484:GLY:H	1.83	0.44
1:A:489:ARG:HD2	1:A:489:ARG:HA	1.81	0.44
2:B:157:MET:HG2	2:B:257:ILE:HG22	1.98	0.44
2:D:67:ARG:NH1	2:D:92:ARG:HB3	2.32	0.44
2:D:581:SER:OG	2:D:583:VAL:O	2.31	0.44
1:A:70:ASN:HB3	1:A:73:GLN:HB2	2.00	0.44
1:A:86:GLN:NE2	1:A:303:ASP:HB2	2.31	0.44
2:B:547:PRO:HA	2:B:817:ASN:HA	2.00	0.44
1:C:570:VAL:HG22	1:C:636:TRP:CZ2	2.52	0.44
1:C:696:GLN:HG3	1:C:699:LEU:HD12	2.00	0.44
1:A:541:LEU:HD22	1:A:736:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:MET:HE2	1:A:642:ILE:HG13	2.00	0.44
2:B:241:PHE:O	2:B:245:ASN:N	2.48	0.44
2:D:85:ILE:O	2:D:89:MET:N	2.45	0.44
2:D:523:VAL:CG1	2:D:765:ALA:HB1	2.47	0.44
1:A:30:GLY:HA3	1:A:63:THR:HG22	2.00	0.44
2:B:384:LEU:HD12	2:B:384:LEU:HA	1.78	0.44
1:C:124:ARG:HG2	1:C:142:PRO:O	2.18	0.44
1:C:138:LEU:HD21	1:C:326:MET:HG3	2.00	0.44
2:D:375:ARG:H	2:D:375:ARG:HG3	1.67	0.44
1:A:107:VAL:HG23	1:A:118:VAL:HG11	2.00	0.44
1:C:347:LYS:HB3	1:C:347:LYS:HE3	1.74	0.44
1:C:537:GLY:O	1:C:733:SER:N	2.46	0.44
1:C:791:THR:HG1	1:C:792:TRP:CD1	2.35	0.44
4:A:1001:POV:H31G	4:A:1001:POV:H31D	1.85	0.43
1:C:115:ARG:HG2	1:C:314:ILE:HG12	1.99	0.43
1:C:275:LYS:HE2	1:C:275:LYS:HB3	1.91	0.43
1:C:122:THR:HG21	1:C:277:GLU:HG2	1.99	0.43
1:C:663:ARG:HG3	1:C:664:ILE:H	1.83	0.43
1:A:125:MET:HB2	1:A:128:TYR:HE2	1.83	0.43
1:A:272:ILE:HG13	1:A:350:ASN:HB2	2.01	0.43
1:A:601:LEU:HD12	1:A:601:LEU:HA	1.86	0.43
1:C:541:LEU:HD22	1:C:736:LEU:HD22	2.00	0.43
1:A:313:ASN:OD1	1:A:314:ILE:N	2.51	0.43
1:A:810:PHE:CE1	2:D:561:MET:HG2	2.53	0.43
2:B:643:LEU:O	2:B:647:THR:HG23	2.18	0.43
1:C:41:MET:HE1	1:C:281:ILE:HB	1.99	0.43
1:C:217:ARG:HB2	1:C:391:GLY:HA2	1.99	0.43
2:D:35:ILE:HD12	2:D:64:VAL:HB	2.00	0.43
2:D:278:ILE:HD11	2:D:391:TRP:CH2	2.54	0.43
2:B:329:ILE:H	2:B:329:ILE:HG13	1.59	0.43
1:C:659:ARG:NH2	1:C:803:ASN:O	2.51	0.43
1:C:692:TYR:O	1:C:696:GLN:HG2	2.18	0.43
1:A:31:ALA:H	1:A:42:PHE:HE2	1.65	0.43
2:B:171:ILE:HG21	2:B:183:VAL:HG22	2.00	0.43
1:C:75:ALA:HB1	1:C:110:THR:HG21	2.01	0.43
1:C:104:PRO:HA	1:C:107:VAL:HG22	2.01	0.43
1:C:404:HIS:ND1	1:C:411:VAL:HG22	2.33	0.43
1:A:272:ILE:H	1:A:272:ILE:HG12	1.63	0.43
2:B:106:GLU:N	2:B:106:GLU:OE1	2.52	0.43
1:C:105:THR:HB	2:D:114:PHE:CZ	2.53	0.43
1:C:195:LEU:HB3	1:C:207:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLY:HA3	1:C:330:TYR:HE2	1.84	0.43
1:A:496:LYS:HE2	2:B:194:PHE:CE1	2.54	0.43
1:A:520:ASN:HD21	1:A:688:SER:HB2	1.83	0.43
2:B:57:ASP:HB3	2:B:59:PHE:CE2	2.54	0.43
2:B:834:ILE:O	2:B:837:ILE:HG13	2.19	0.43
1:C:562:LEU:HD12	2:D:813:LEU:O	2.19	0.43
1:C:697:VAL:HG13	2:D:432:ASN:HB2	1.99	0.43
2:D:122:PRO:HA	2:D:142:MET:HB3	2.01	0.43
2:D:411:LEU:HB2	2:D:497:MET:HE2	2.00	0.43
2:B:534:ILE:HG12	2:B:691:THR:HG22	2.00	0.43
2:B:747:LYS:HG2	2:B:748:LEU:HD23	2.01	0.43
1:C:35:THR:OG1	1:C:38:HIS:HB2	2.19	0.43
1:C:272:ILE:HG13	1:C:350:ASN:ND2	2.34	0.43
1:C:665:THR:HG22	1:C:666:GLY:N	2.27	0.43
1:A:751:GLU:O	1:A:752:LEU:HG	2.19	0.43
2:B:157:MET:HE1	2:B:182:PHE:CZ	2.54	0.43
2:B:509:ALA:HB3	2:B:765:ALA:HB3	2.01	0.43
2:B:783:LEU:HD12	2:B:789:MET:HE2	1.99	0.43
1:C:70:ASN:ND2	2:D:323:ASN:H	2.17	0.43
2:D:57:ASP:HB3	2:D:59:PHE:CE2	2.54	0.43
2:D:499:GLY:O	2:D:503:MET:HG2	2.18	0.43
1:A:114:TYR:HB2	1:A:116:ILE:HG13	2.01	0.42
1:A:696:GLN:HG3	1:A:699:LEU:HD12	2.00	0.42
2:B:164:TYR:OH	2:B:388:TYR:O	2.28	0.42
2:B:334:MET:HG3	2:B:337:ARG:HH22	1.84	0.42
2:B:380:LYS:HA	2:B:380:LYS:HD2	1.69	0.42
2:B:778:LEU:O	1:C:521:ASN:ND2	2.52	0.42
1:C:489:ARG:HG2	2:D:194:PHE:HD2	1.82	0.42
2:D:613:VAL:HA	2:D:639:ALA:HB1	2.01	0.42
2:B:50:ILE:HD11	2:B:289:LEU:HG	2.01	0.42
2:D:643:LEU:O	2:D:647:THR:HG23	2.19	0.42
2:D:825:LEU:O	2:D:829:MET:HG3	2.19	0.42
1:A:166:LEU:HB3	1:A:221:LEU:HD12	2.01	0.42
1:A:400:ILE:HD12	1:A:474:TYR:HB2	2.01	0.42
2:D:537:MET:HB3	2:D:721:LEU:HD21	2.01	0.42
1:A:237:MET:HE2	1:A:238:LEU:HD22	2.01	0.42
2:B:73:MET:HG3	2:B:84:ARG:HH21	1.83	0.42
2:B:439:ARG:HG3	2:B:452:TYR:HD1	1.84	0.42
2:B:489:LYS:HD3	2:B:494:TRP:CE2	2.55	0.42
2:B:722:LYS:HG2	2:B:747:LYS:HE2	2.02	0.42
1:C:438:GLY:HA3	1:C:478:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:VAL:HG23	2:D:66:PRO:HD3	2.00	0.42
1:A:403:ILE:HB	1:A:501:MET:SD	2.60	0.42
1:A:809:THR:H	1:A:812:ASN:HD22	1.66	0.42
2:B:285:TRP:HB2	2:B:375:ARG:HH11	1.85	0.42
2:B:785:GLY:O	1:C:696:GLN:NE2	2.53	0.42
1:C:35:THR:O	1:C:38:HIS:N	2.53	0.42
2:D:114:PHE:N	2:D:114:PHE:CD1	2.87	0.42
2:D:607:TRP:CD1	2:D:620:VAL:HG12	2.54	0.42
1:A:356:LEU:HD11	1:A:359:ARG:HA	2.01	0.42
1:A:604:SER:HB2	4:A:1001:POV:H11A	2.02	0.42
1:C:346:ARG:HD2	1:C:346:ARG:HA	1.82	0.42
1:C:402:THR:HG22	1:C:514:VAL:O	2.19	0.42
2:D:344:PHE:CE2	2:D:345:GLU:HG3	2.54	0.42
2:D:564:VAL:O	2:D:568:ILE:HG13	2.20	0.42
1:A:155:MET:SD	1:A:163:ILE:HG21	2.60	0.42
1:A:249:VAL:CG1	1:A:253:GLU:HB2	2.50	0.42
2:B:54:HIS:HB3	2:B:68:VAL:HG21	2.02	0.42
2:B:825:LEU:O	2:B:829:MET:HG3	2.19	0.42
2:D:168:ILE:CG2	2:D:226:PRO:HD2	2.47	0.42
2:D:201:GLU:HG2	2:D:203:LEU:HG	2.02	0.42
2:D:719:LEU:HA	2:D:722:LYS:HG3	2.01	0.42
1:A:355:ASN:ND2	1:A:379:ILE:HG23	2.34	0.42
1:C:31:ALA:O	1:C:64:SER:HA	2.19	0.42
2:D:40:ILE:HG23	2:D:71:VAL:HG13	2.01	0.42
1:A:197:PHE:HZ	1:A:223:ALA:HB2	1.85	0.42
1:A:608:TRP:HE1	4:A:1001:POV:H13B	1.85	0.42
2:B:714:VAL:O	2:B:718:LEU:HD23	2.20	0.42
1:C:101:HIS:HE1	1:C:102:PHE:CE1	2.37	0.42
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.88	0.42
1:C:263:PRO:HD2	1:C:266:ILE:HD11	2.02	0.42
2:D:412:GLU:OE1	2:D:419:VAL:HG12	2.20	0.42
1:A:273:ASN:OD1	1:A:273:ASN:N	2.53	0.41
4:A:1002:POV:H35A	4:A:1002:POV:H22	2.01	0.41
2:B:552:GLU:HB3	2:B:653:PHE:CE2	2.55	0.41
1:C:357:GLN:HE21	1:C:380:ILE:H	1.67	0.41
4:C:1002:POV:H31E	4:C:1002:POV:H27A	2.02	0.41
2:D:114:PHE:N	2:D:114:PHE:HD1	2.18	0.41
2:D:751:ILE:HD13	2:D:751:ILE:HA	1.88	0.41
1:C:155:MET:O	1:C:159:SER:N	2.53	0.41
1:C:518:THR:HG22	1:C:758:PHE:HE1	1.85	0.41
2:D:160:ILE:HD11	2:D:364:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:VAL:O	2:D:202:VAL:CG1	2.68	0.41
2:D:380:LYS:HA	2:D:380:LYS:HD2	1.71	0.41
1:C:517:LEU:HD23	1:C:517:LEU:HA	1.93	0.41
2:D:258:VAL:CG1	2:D:262:VAL:HB	2.50	0.41
2:D:519:ARG:HB2	2:D:525:PHE:HE2	1.85	0.41
2:D:681:PHE:HB3	2:D:683:PHE:CE1	2.55	0.41
1:A:26:ILE:HD13	1:A:59:GLN:HB3	2.03	0.41
1:A:547:PRO:HG3	1:A:804:ALA:HB1	2.03	0.41
1:A:723:ASP:HB3	1:A:725:LYS:HG2	2.01	0.41
1:C:221:LEU:HB3	1:C:249:VAL:HG22	2.02	0.41
1:C:400:ILE:HD12	1:C:474:TYR:HB2	2.01	0.41
1:C:685:LYS:HG3	1:C:710:ASN:HB3	2.02	0.41
2:D:466:LYS:O	2:D:470:LYS:HG2	2.20	0.41
2:B:304:ALA:O	2:B:307:MET:HG3	2.21	0.41
1:C:395:SER:O	1:C:397:ARG:N	2.52	0.41
1:C:502:MET:HE1	1:C:527:ILE:HG23	2.03	0.41
1:A:181:GLU:O	1:A:185:GLU:HG2	2.20	0.41
1:A:421:LYS:HE3	1:A:421:LYS:HB3	1.82	0.41
1:A:536:GLN:OE1	1:A:732:ASP:HB3	2.21	0.41
1:A:537:GLY:HA3	1:A:752:LEU:HD22	2.01	0.41
2:B:432:ASN:OD1	2:B:466:LYS:NZ	2.54	0.41
2:B:572:VAL:HG11	1:C:824:ILE:HG23	2.01	0.41
2:B:721:LEU:HA	2:B:726:LEU:O	2.21	0.41
2:B:206:ASP:O	2:B:207:MET:HE2	2.21	0.41
2:D:406:LEU:O	2:D:476:TYR:HA	2.21	0.41
2:D:490:ILE:O	2:D:493:THR:OG1	2.30	0.41
1:A:270:GLN:HG3	1:A:354:MET:HG3	2.03	0.41
1:A:351:TYR:HB2	1:A:367:TYR:HB3	2.02	0.41
1:C:116:ILE:HG12	1:C:315:TRP:CZ3	2.55	0.41
2:D:509:ALA:HB3	2:D:765:ALA:HB3	2.03	0.41
1:A:708:LYS:HE3	1:A:708:LYS:HB2	1.78	0.41
1:A:810:PHE:O	1:A:814:ALA:N	2.54	0.41
1:C:401:VAL:CG2	1:C:479:VAL:HG22	2.51	0.41
1:C:528:GLU:CD	1:C:769:LYS:HD3	2.46	0.41
1:C:635:VAL:HG11	2:D:828:ALA:HB2	2.01	0.41
1:C:643:ILE:HG22	4:C:1002:POV:H21J	2.02	0.41
1:A:155:MET:HE1	1:A:184:LEU:HD21	2.03	0.41
2:B:93:LYS:HG2	2:B:319:SER:HB3	2.02	0.41
2:B:239:TYR:O	2:B:242:GLU:HG2	2.21	0.41
2:B:532:THR:HG21	2:B:762:TYR:CE1	2.56	0.41
1:C:92:VAL:HG11	1:C:104:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:MET:HE3	1:C:607:MET:HB3	1.84	0.41
1:C:608:TRP:HE1	4:C:1001:POV:H13B	1.85	0.41
2:D:348:ASN:HB3	2:D:359:HIS:CD2	2.56	0.41
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.90	0.40
1:A:663:ARG:HH22	1:A:679:PHE:CB	2.30	0.40
2:B:695:ILE:HG22	2:B:703:HIS:HB2	2.02	0.40
1:C:123:THR:O	1:C:139:ARG:HD3	2.21	0.40
2:D:153:GLN:O	2:D:157:MET:HG3	2.21	0.40
2:B:413:GLU:HG3	2:B:414:ALA:H	1.87	0.40
1:C:357:GLN:HG2	1:C:380:ILE:HB	2.02	0.40
2:B:287:TYR:HD2	2:B:292:ARG:HG2	1.86	0.40
2:B:307:MET:HE2	2:B:307:MET:HB2	2.01	0.40
1:C:42:PHE:CD2	1:C:64:SER:HB3	2.55	0.40
1:C:269:LEU:HD23	1:C:269:LEU:HA	1.82	0.40
2:B:234:LYS:HG3	2:B:262:VAL:O	2.22	0.40
2:B:679:PRO:HA	2:B:680:PRO:HD3	1.98	0.40
2:D:202:VAL:O	2:D:203:LEU:C	2.64	0.40
2:D:524:ASP:HB2	2:D:768:LYS:HA	2.02	0.40
1:C:470:MET:HE3	1:C:470:MET:HB2	1.85	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	794/830 (96%)	747 (94%)	46 (6%)	1 (0%)	48	77
1	C	794/830 (96%)	744 (94%)	49 (6%)	1 (0%)	48	77
2	B	765/861 (89%)	711 (93%)	54 (7%)	0	100	100
2	D	765/861 (89%)	711 (93%)	53 (7%)	1 (0%)	48	77
All	All	3118/3382 (92%)	2913 (93%)	202 (6%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	663	VAL
1	A	546	ILE
1	C	490	VAL

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	659/712 (93%)	654 (99%)	5 (1%)	79	88
1	C	659/712 (93%)	658 (100%)	1 (0%)	92	96
2	B	658/744 (88%)	655 (100%)	3 (0%)	86	92
2	D	658/744 (88%)	656 (100%)	2 (0%)	91	95
All	All	2634/2912 (90%)	2623 (100%)	11 (0%)	88	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	194	VAL
1	A	273	ASN
1	A	320	LEU
1	A	744	CYS
2	B	60	HIS
2	B	195	VAL
2	B	841	LEU
1	C	501	MET
2	D	74	ASN
2	D	417	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN

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Mol	Chain	Res	Type
1	A	38	HIS
1	A	61	ASN
1	A	86	GLN
1	A	147	GLN
1	A	203	ASN
1	A	270	GLN
1	A	355	ASN
1	A	404	HIS
1	A	440	ASN
1	A	453	GLN
1	A	499	ASN
1	A	520	ASN
1	A	709	HIS
1	A	812	ASN
2	B	105	GLN
2	B	118	GLN
2	B	127	HIS
2	B	153	GLN
2	B	224	GLN
2	B	245	ASN
2	B	359	HIS
2	B	486	HIS
2	B	703	HIS
2	B	767	GLN
2	B	782	GLN
1	C	38	HIS
1	C	61	ASN
1	C	70	ASN
1	C	94	HIS
1	C	101	HIS
1	C	146	HIS
1	C	147	GLN
1	C	171	HIS
1	C	177	GLN
1	C	196	GLN
1	C	293	HIS
1	C	355	ASN
1	C	440	ASN
1	C	453	GLN
1	C	509	GLN
1	C	520	ASN
1	C	571	HIS

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Mol	Chain	Res	Type
1	C	696	GLN
1	C	705	HIS
1	C	812	ASN
2	D	118	GLN
2	D	127	HIS
2	D	153	GLN
2	D	311	HIS
2	D	348	ASN
2	D	359	HIS

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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GLU	B	1000	-	8,9,9	1.09	1 (12%)	8,11,11	1.21	1 (12%)
6	A8W	D	1002	-	30,30,30	0.36	0	45,49,49	0.73	2 (4%)
5	GLU	D	1000	-	8,9,9	1.13	1 (12%)	8,11,11	1.23	1 (12%)
6	A8W	B	1001	-	30,30,30	0.36	0	45,49,49	0.73	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	A	1001	-	51,51,51	0.51	0	57,59,59	0.48	0
4	POV	C	1002	-	51,51,51	0.50	0	57,59,59	0.47	0
6	A8W	D	1001	-	30,30,30	0.36	0	45,49,49	0.73	1 (2%)
6	A8W	B	1002	-	30,30,30	0.35	0	45,49,49	0.73	2 (4%)
4	POV	A	1002	-	51,51,51	0.50	0	57,59,59	0.47	0
3	GLY	C	1000	-	4,4,4	1.24	1 (25%)	3,4,4	1.67	1 (33%)
4	POV	C	1001	-	51,51,51	0.51	0	57,59,59	0.49	0
3	GLY	A	1000	-	4,4,4	1.23	1 (25%)	3,4,4	1.62	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLU	B	1000	-	-	2/9/9/9	-
6	A8W	D	1002	-	-	6/9/67/67	0/4/4/4
5	GLU	D	1000	-	-	3/9/9/9	-
6	A8W	B	1001	-	-	4/9/67/67	0/4/4/4
4	POV	A	1001	-	-	13/55/55/55	-
4	POV	C	1002	-	-	15/55/55/55	-
6	A8W	D	1001	-	-	4/9/67/67	0/4/4/4
6	A8W	B	1002	-	-	6/9/67/67	0/4/4/4
4	POV	A	1002	-	-	20/55/55/55	-
3	GLY	C	1000	-	-	0/2/2/2	-
4	POV	C	1001	-	-	19/55/55/55	-
3	GLY	A	1000	-	-	0/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1000	GLY	OXT-C	-2.37	1.23	1.30
3	A	1000	GLY	OXT-C	-2.35	1.23	1.30
5	D	1000	GLU	OXT-C	-2.33	1.23	1.30
5	B	1000	GLU	OXT-C	-2.27	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1000	GLU	OXT-C-O	-2.75	117.85	124.08
5	B	1000	GLU	OXT-C-O	-2.61	118.15	124.08
3	C	1000	GLY	OXT-C-O	-2.23	117.59	123.33
6	D	1001	A8W	C13-C17-C20	2.21	118.02	114.95
3	A	1000	GLY	OXT-C-O	-2.15	117.81	123.33
6	B	1002	A8W	C13-C17-C20	2.13	117.92	114.95
6	D	1002	A8W	C13-C17-C20	2.13	117.91	114.95
6	B	1001	A8W	C13-C17-C20	2.12	117.90	114.95
6	D	1002	A8W	C17-C13-C14	-2.10	97.52	99.72
6	B	1002	A8W	C17-C13-C14	-2.04	97.59	99.72

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	POV	C1-O11-P-O13
4	A	1002	POV	C2-C1-O11-P
4	A	1002	POV	O12-C11-C12-N
4	C	1002	POV	C1-O11-P-O12
4	C	1002	POV	C11-O12-P-O14
4	C	1002	POV	O12-C11-C12-N
5	D	1000	GLU	C-CA-CB-CG
4	A	1002	POV	O21-C2-C3-O31
4	A	1002	POV	C25-C26-C27-C28
4	C	1001	POV	C311-C310-C39-C38
4	A	1001	POV	C21-C22-C23-C24
4	C	1002	POV	C25-C26-C27-C28
6	D	1001	A8W	C13-C17-C20-C21
4	C	1002	POV	C2-C1-O11-P
6	B	1002	A8W	C2-C3-O1-S
6	B	1002	A8W	C4-C3-O1-S
6	D	1002	A8W	C2-C3-O1-S
6	D	1002	A8W	C4-C3-O1-S
4	C	1001	POV	C312-C313-C314-C315
4	C	1002	POV	C23-C24-C25-C26
4	C	1001	POV	C21-C22-C23-C24
4	A	1001	POV	C25-C26-C27-C28
4	C	1001	POV	C22-C23-C24-C25
4	C	1001	POV	C25-C26-C27-C28
4	A	1002	POV	C23-C24-C25-C26
4	A	1001	POV	C36-C37-C38-C39
6	B	1001	A8W	C13-C17-C20-O
6	B	1001	A8W	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
6	B	1002	A8W	C13-C17-C20-C21
6	D	1001	A8W	C13-C17-C20-O
6	D	1002	A8W	C13-C17-C20-O
6	D	1002	A8W	C13-C17-C20-C21
4	A	1002	POV	O11-C1-C2-C3
4	A	1002	POV	C214-C215-C216-C217
4	C	1002	POV	C214-C215-C216-C217
4	A	1001	POV	C22-C23-C24-C25
6	B	1001	A8W	C16-C17-C20-C21
6	D	1001	A8W	C16-C17-C20-C21
4	A	1001	POV	C313-C314-C315-C316
4	C	1001	POV	C212-C213-C214-C215
4	C	1002	POV	O11-C1-C2-C3
4	C	1002	POV	C310-C311-C312-C313
4	A	1001	POV	C210-C211-C212-C213
4	C	1002	POV	O21-C2-C3-O31
4	C	1001	POV	C211-C212-C213-C214
4	A	1002	POV	C215-C216-C217-C218
4	C	1001	POV	C36-C37-C38-C39
6	B	1002	A8W	C16-C17-C20-C21
4	A	1002	POV	O11-C1-C2-O21
4	C	1002	POV	O11-C1-C2-O21
4	A	1002	POV	C1-C2-C3-O31
4	C	1001	POV	C32-C31-O31-C3
4	A	1002	POV	C12-C11-O12-P
4	A	1001	POV	C33-C34-C35-C36
4	A	1002	POV	C39-C310-C311-C312
6	B	1002	A8W	C13-C17-C20-O
4	C	1001	POV	C39-C310-C311-C312
4	C	1001	POV	O32-C31-O31-C3
4	C	1001	POV	C313-C314-C315-C316
4	A	1001	POV	C311-C310-C39-C38
4	A	1001	POV	C11-O12-P-O14
4	A	1002	POV	C1-O11-P-O12
4	A	1002	POV	C1-O11-P-O14
4	C	1001	POV	C11-O12-P-O14
6	B	1001	A8W	C16-C17-C20-O
6	D	1002	A8W	C16-C17-C20-C21
4	C	1001	POV	C33-C34-C35-C36
4	A	1001	POV	C2-C1-O11-P
4	C	1001	POV	C2-C1-O11-P
4	A	1001	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
4	C	1002	POV	C215-C216-C217-C218
6	B	1002	A8W	C16-C17-C20-O
6	D	1001	A8W	C16-C17-C20-O
6	D	1002	A8W	C16-C17-C20-O
4	C	1001	POV	C32-C33-C34-C35
4	C	1002	POV	C1-C2-C3-O31
4	A	1001	POV	C37-C38-C39-C310
5	D	1000	GLU	CA-CB-CG-CD
4	A	1002	POV	C311-C310-C39-C38
4	A	1002	POV	C34-C35-C36-C37
4	A	1002	POV	C310-C311-C312-C313
4	C	1002	POV	C31-C32-C33-C34
5	B	1000	GLU	OE1-CD-CG-CB
5	B	1000	GLU	OE2-CD-CG-CB
4	A	1002	POV	C312-C313-C314-C315
4	C	1001	POV	C311-C312-C313-C314
4	A	1001	POV	C211-C212-C213-C214
4	C	1001	POV	C210-C211-C212-C213
5	D	1000	GLU	N-CA-CB-CG
4	C	1002	POV	C27-C28-C29-C210
4	A	1002	POV	C35-C36-C37-C38
4	C	1001	POV	C214-C215-C216-C217

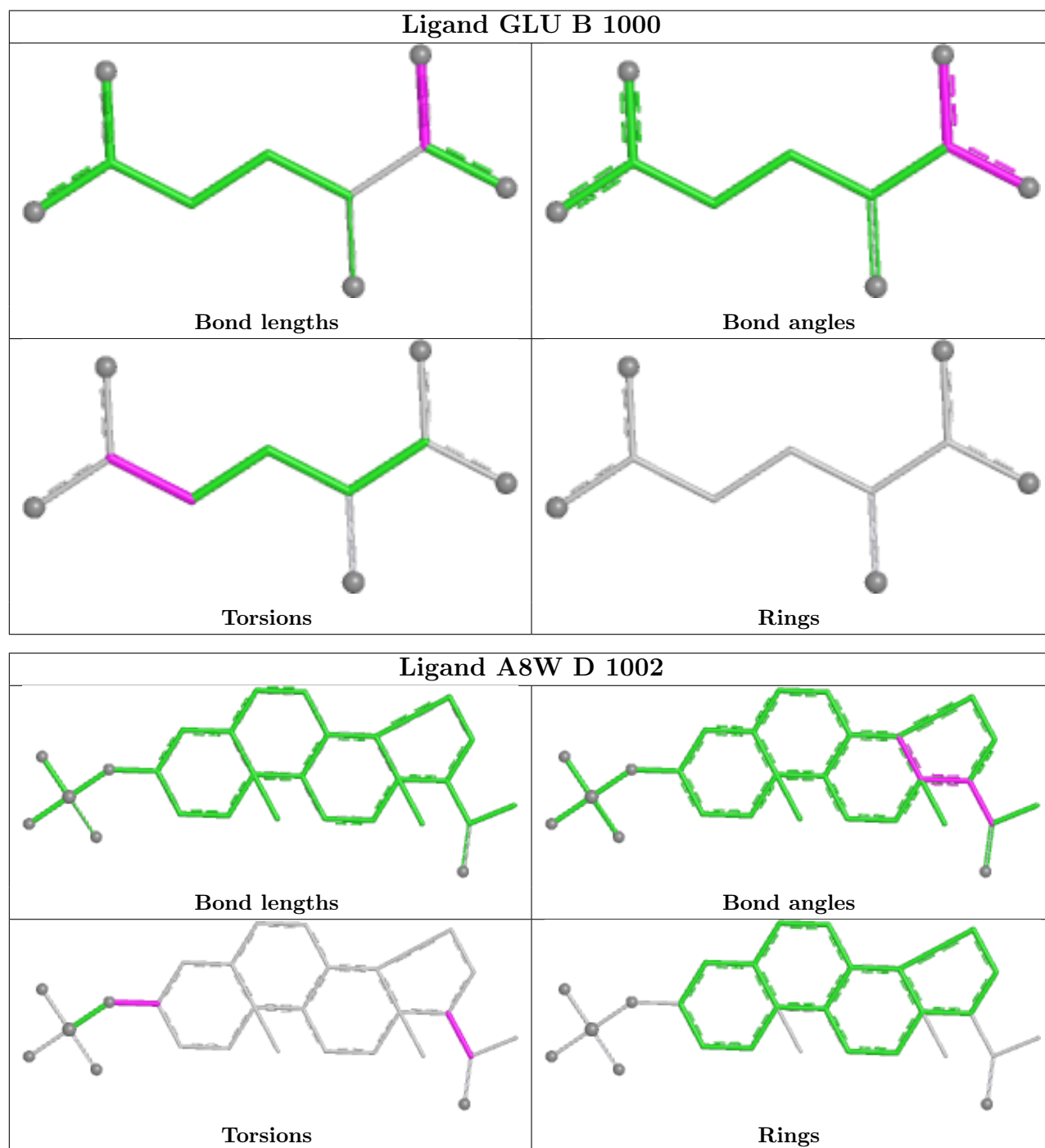
There are no ring outliers.

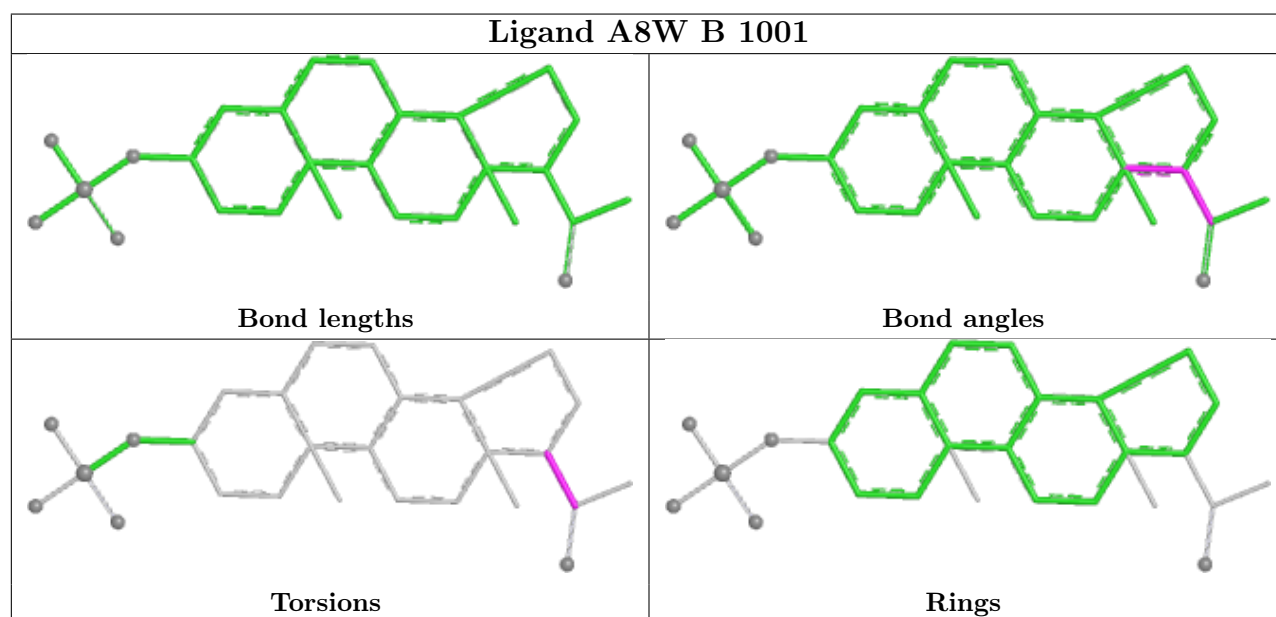
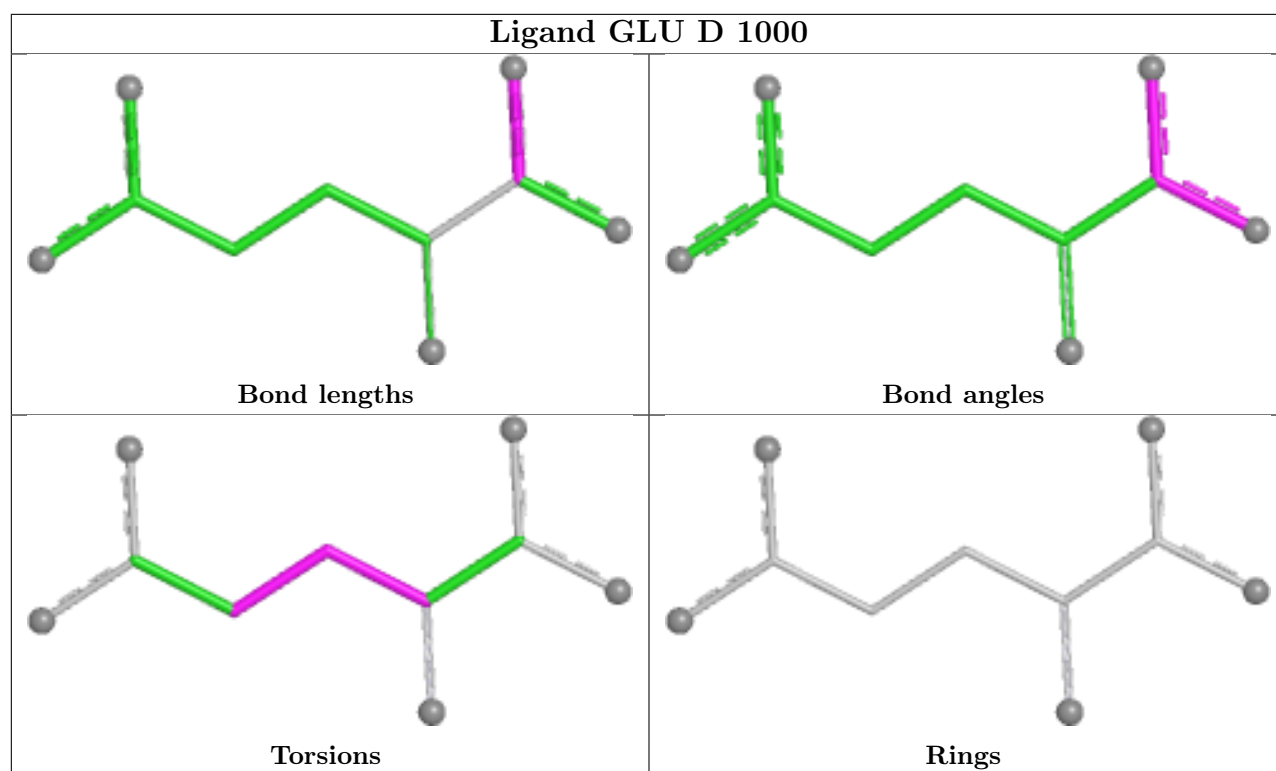
8 monomers are involved in 25 short contacts:

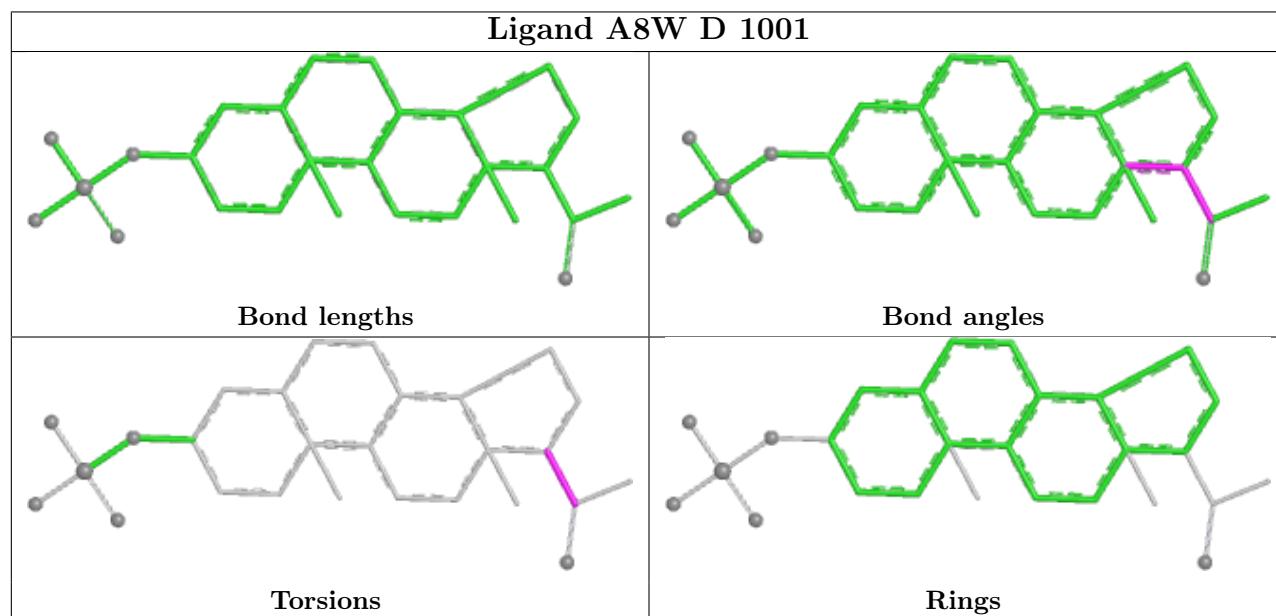
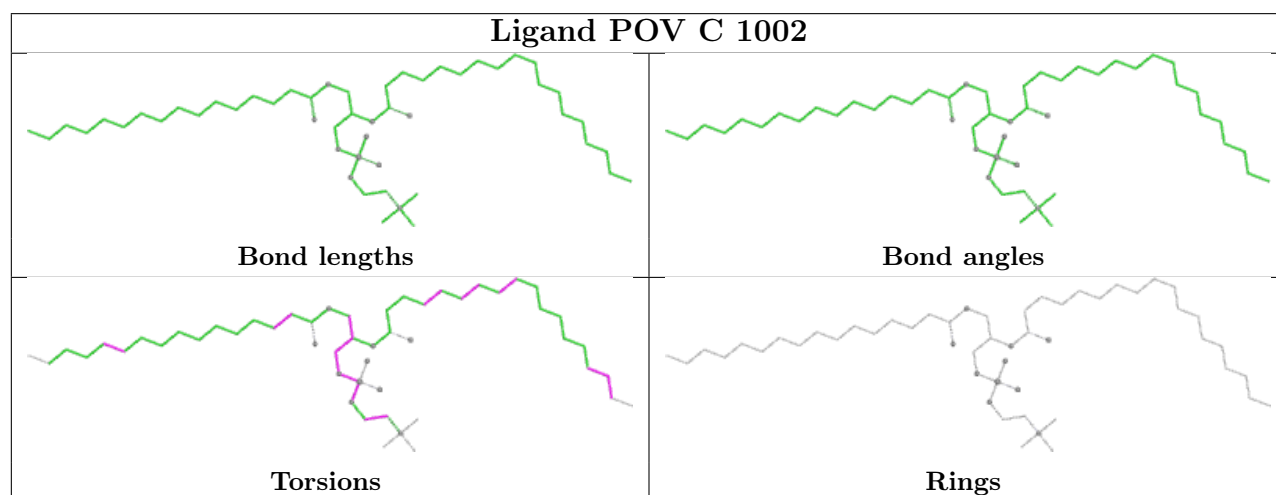
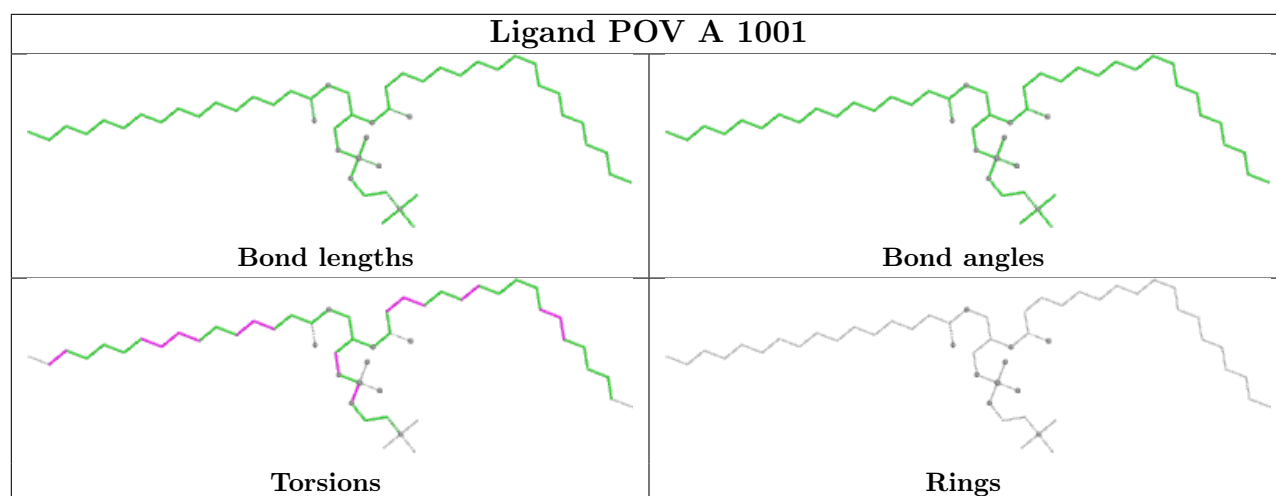
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1000	GLU	2	0
5	D	1000	GLU	1	0
4	A	1001	POV	7	0
4	C	1002	POV	6	0
4	A	1002	POV	7	0
3	C	1000	GLY	1	0
4	C	1001	POV	4	0
3	A	1000	GLY	1	0

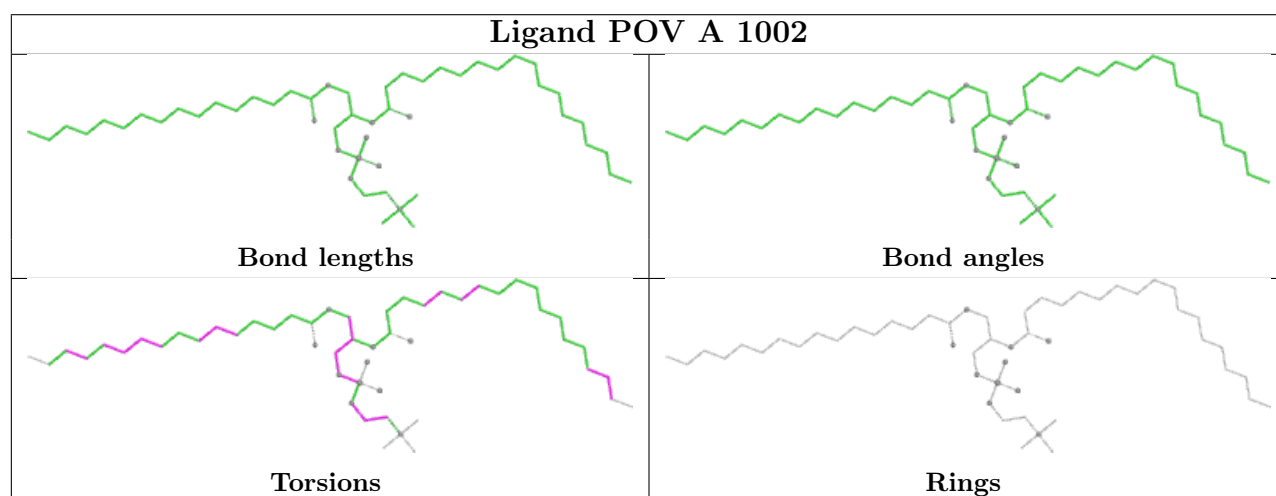
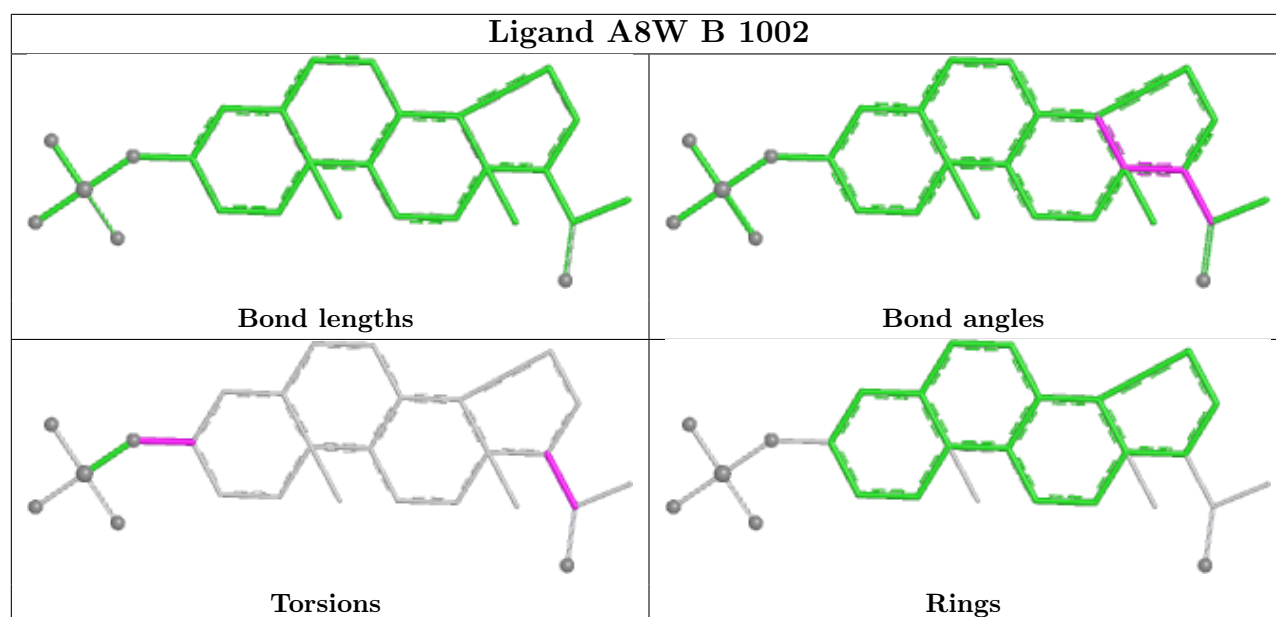
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

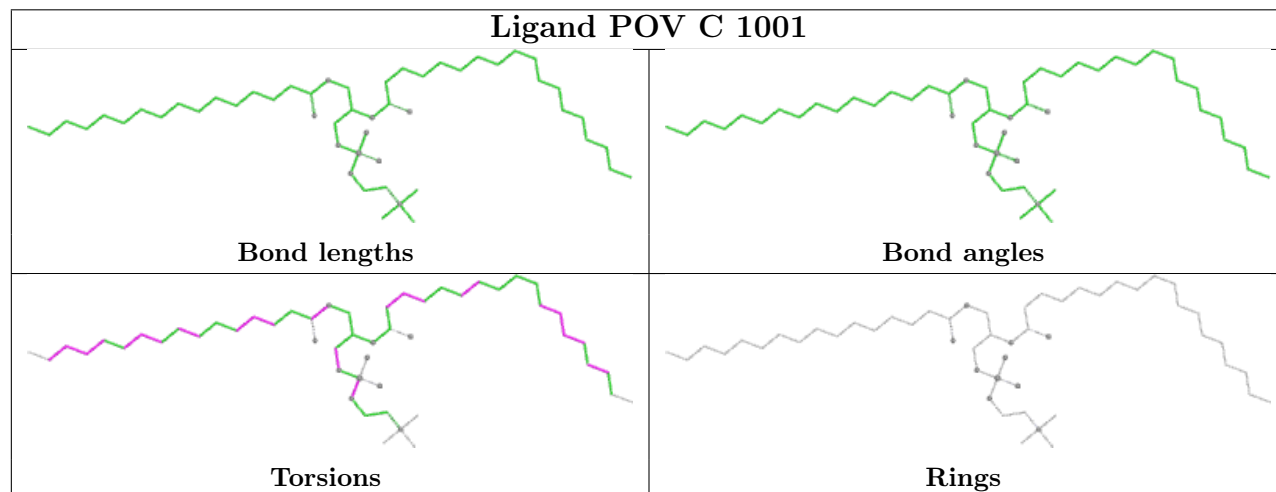
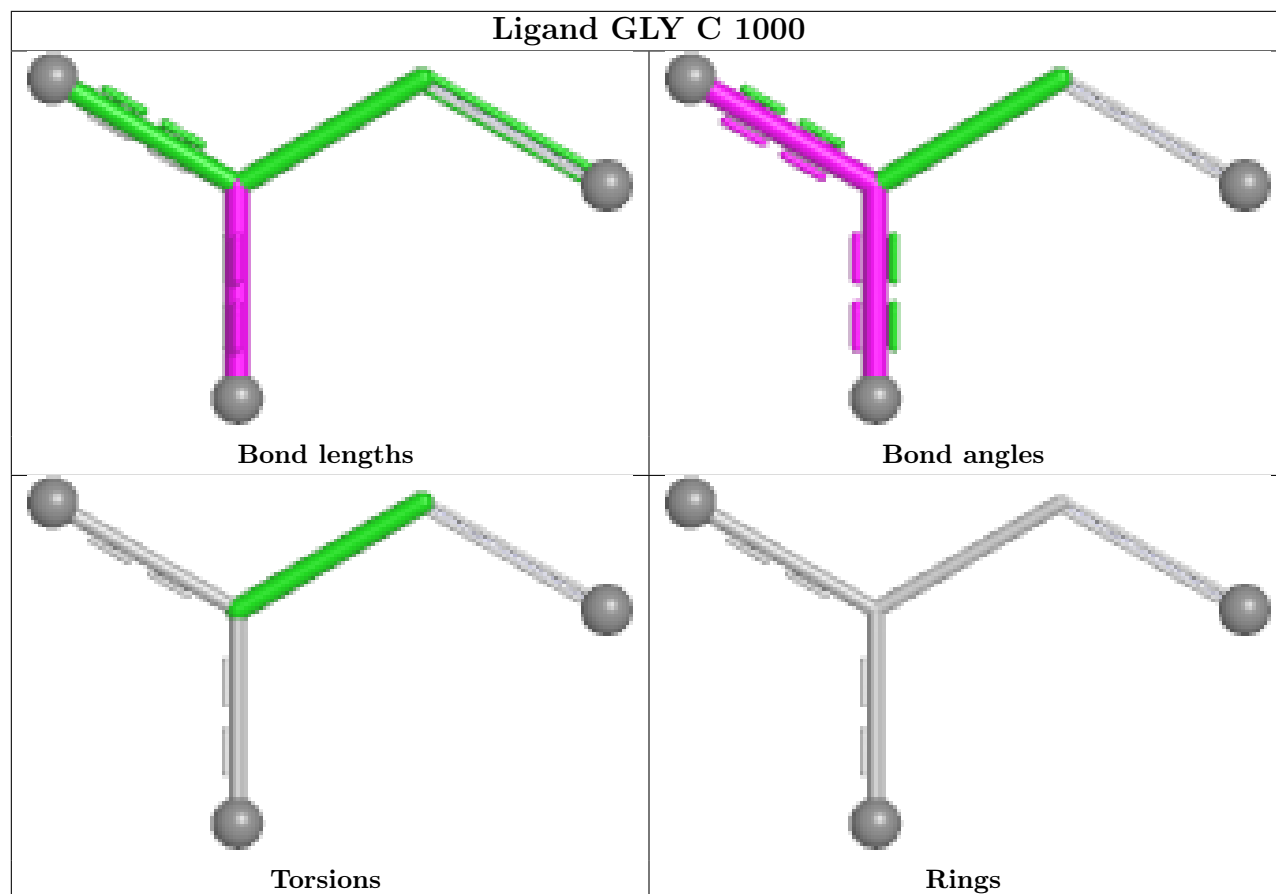
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

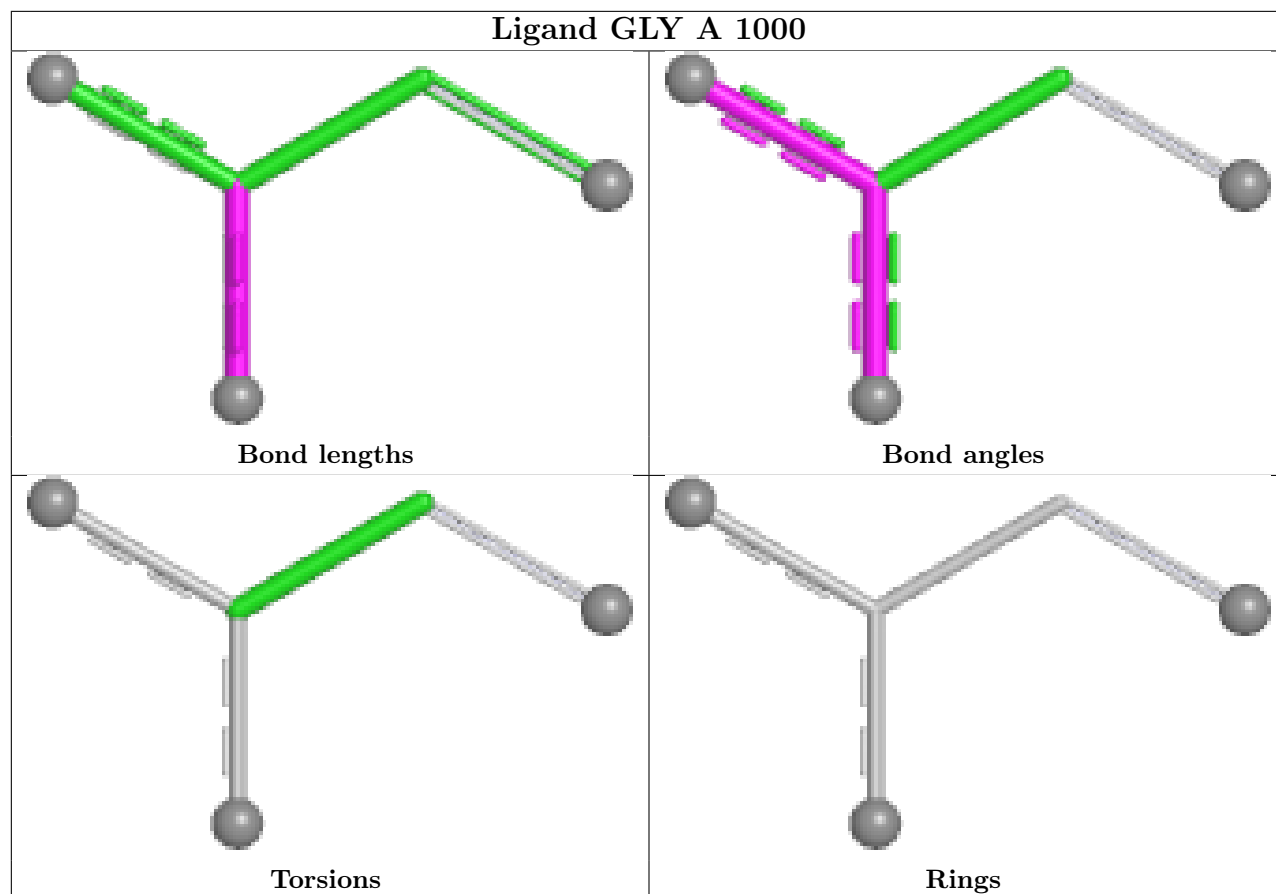












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

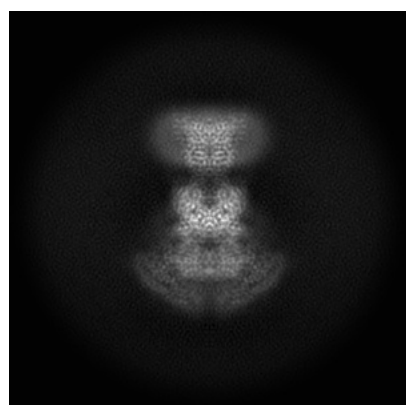
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70672. These allow visual inspection of the internal detail of the map and identification of artifacts.

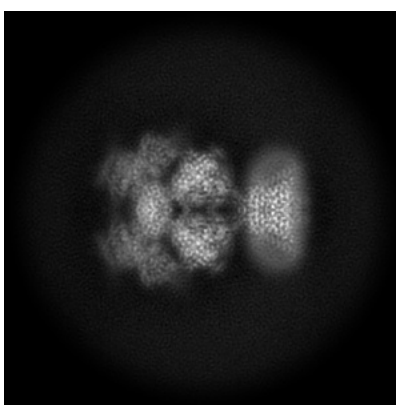
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

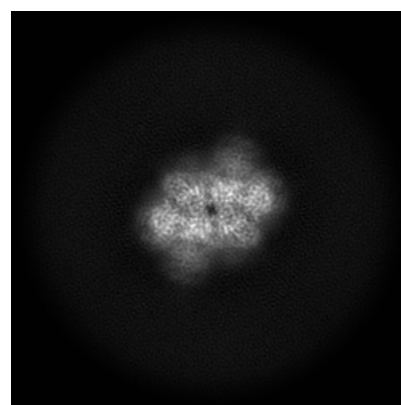
6.1.1 Primary map



X



Y

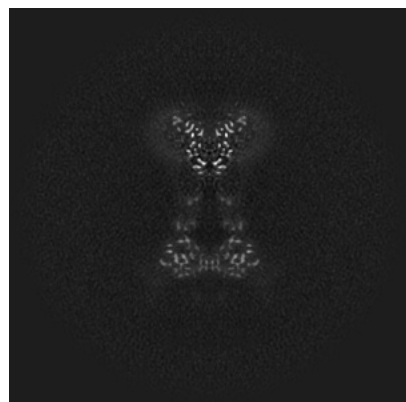


Z

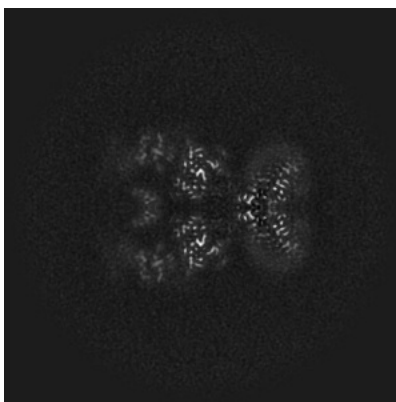
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

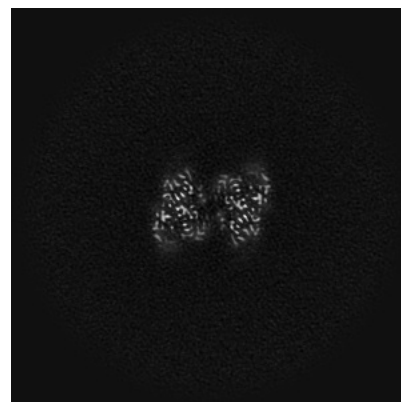
6.2.1 Primary map



X Index: 200



Y Index: 200

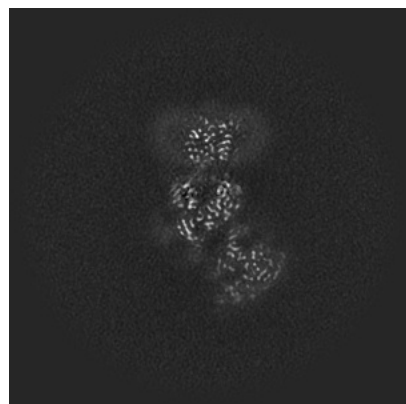


Z Index: 200

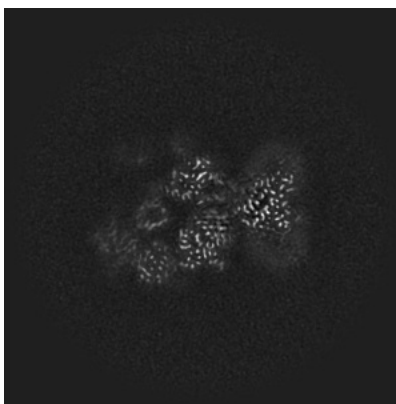
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

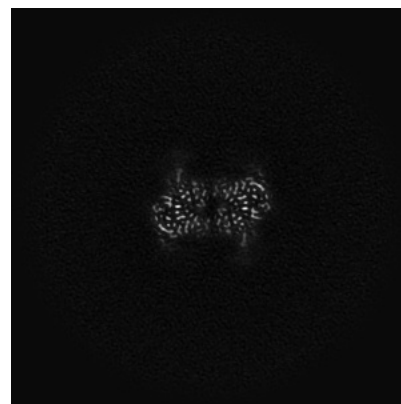
6.3.1 Primary map



X Index: 220



Y Index: 190

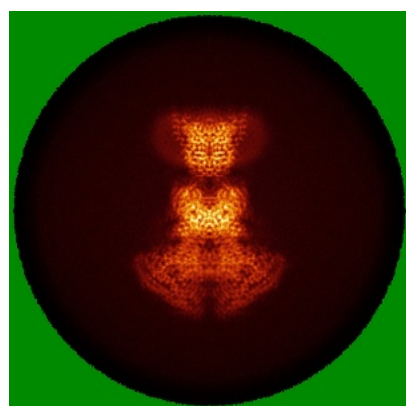


Z Index: 193

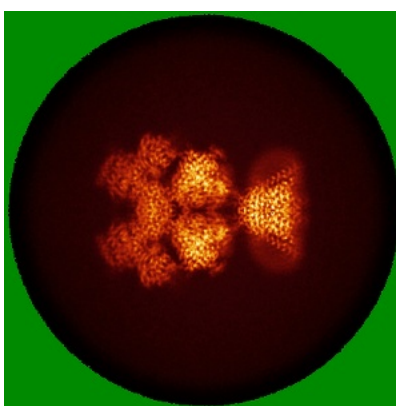
The images above show the largest variance slices of the map in three orthogonal directions.

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

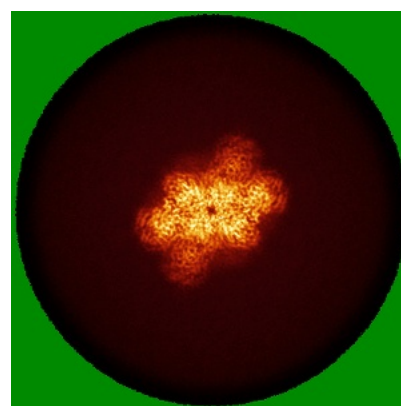
6.4.1 Primary map



X



Y

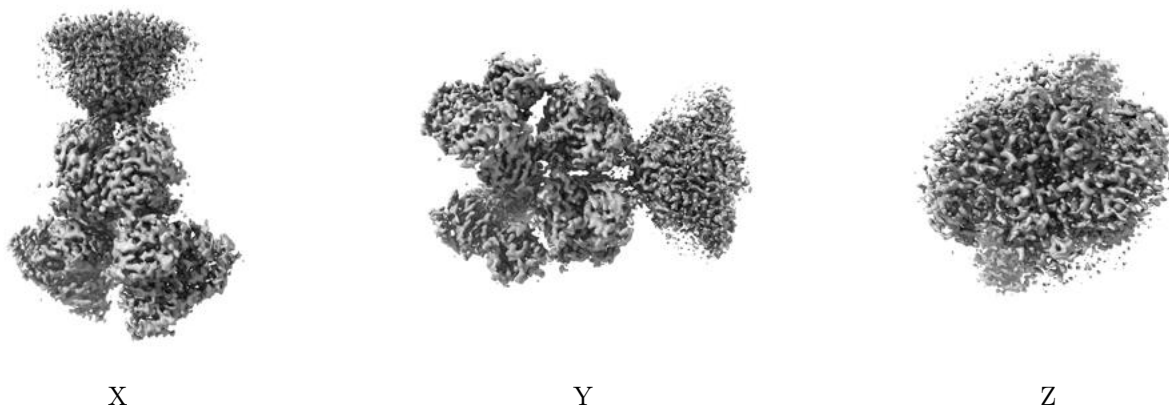


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.048. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

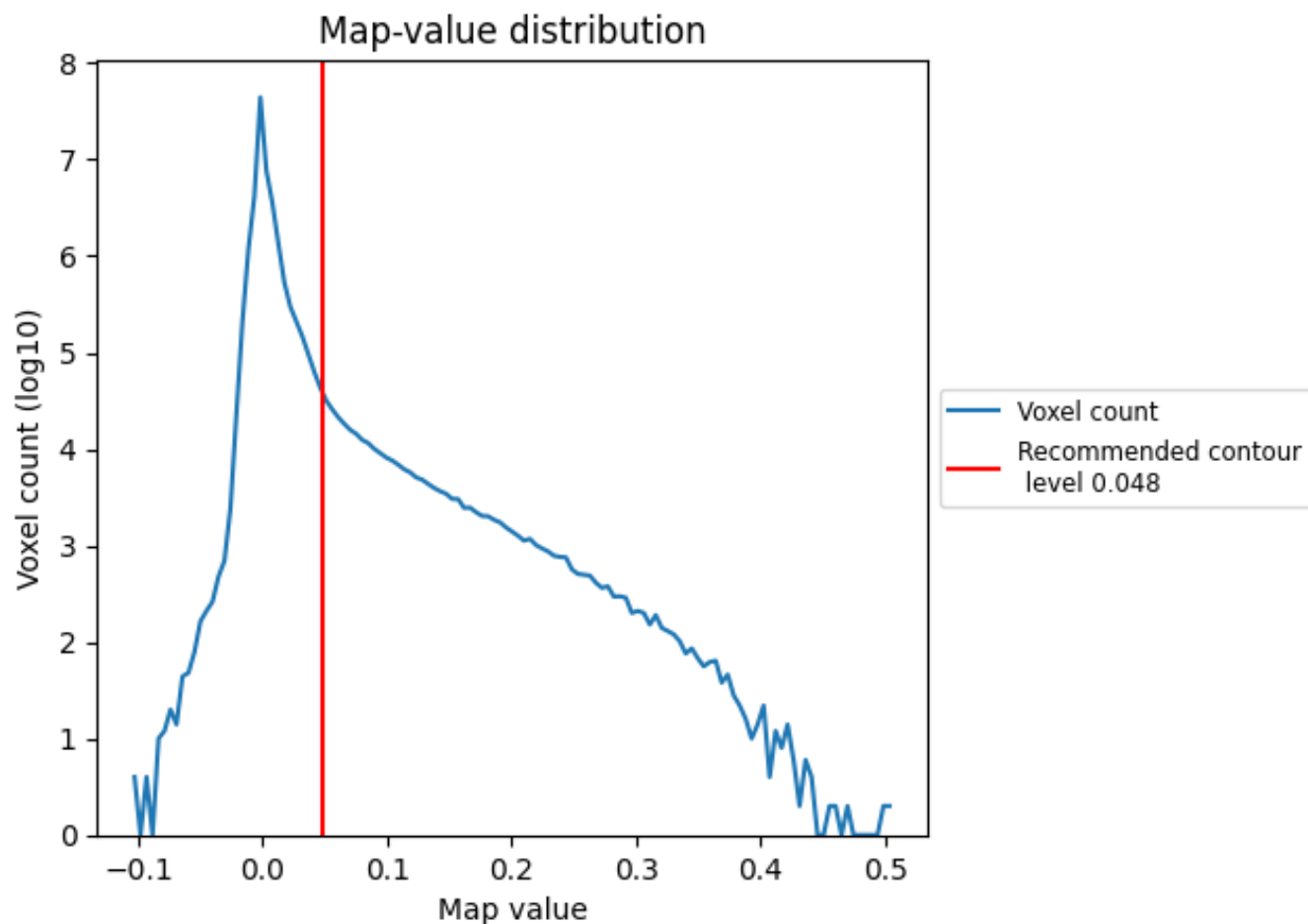
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

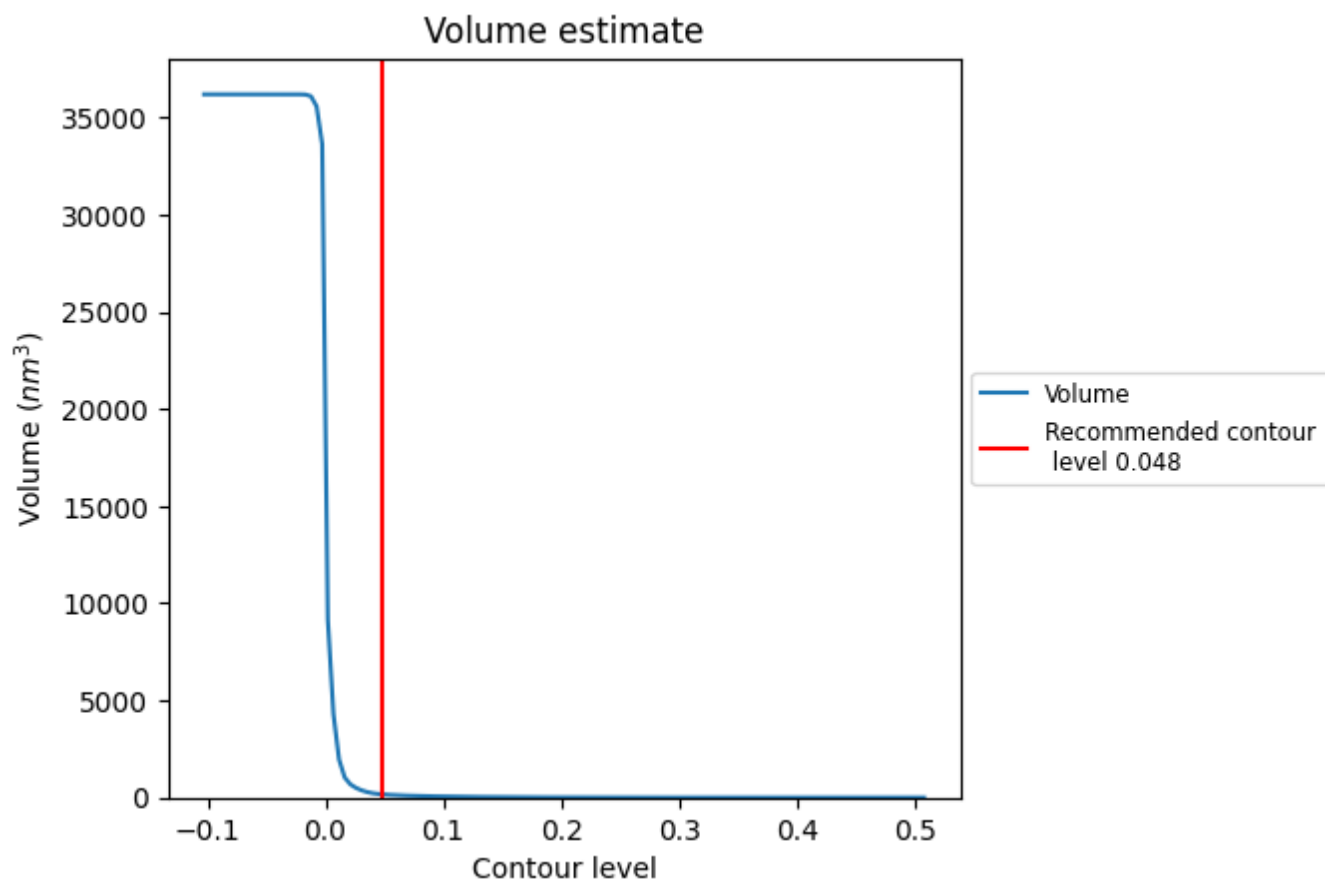
This section contains the results of statistical analysis of the map.

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.

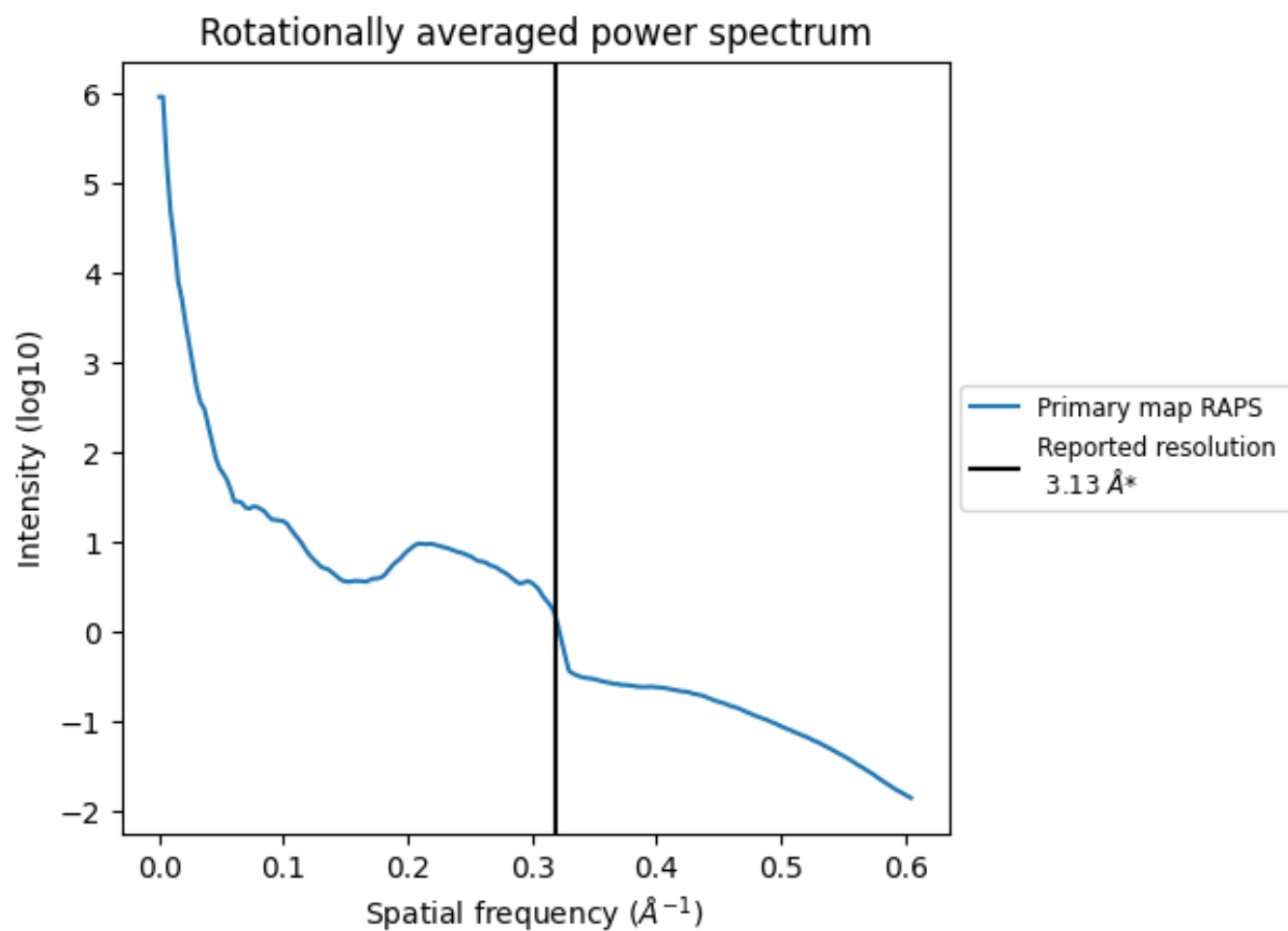
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 151 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 0.319 Å⁻¹

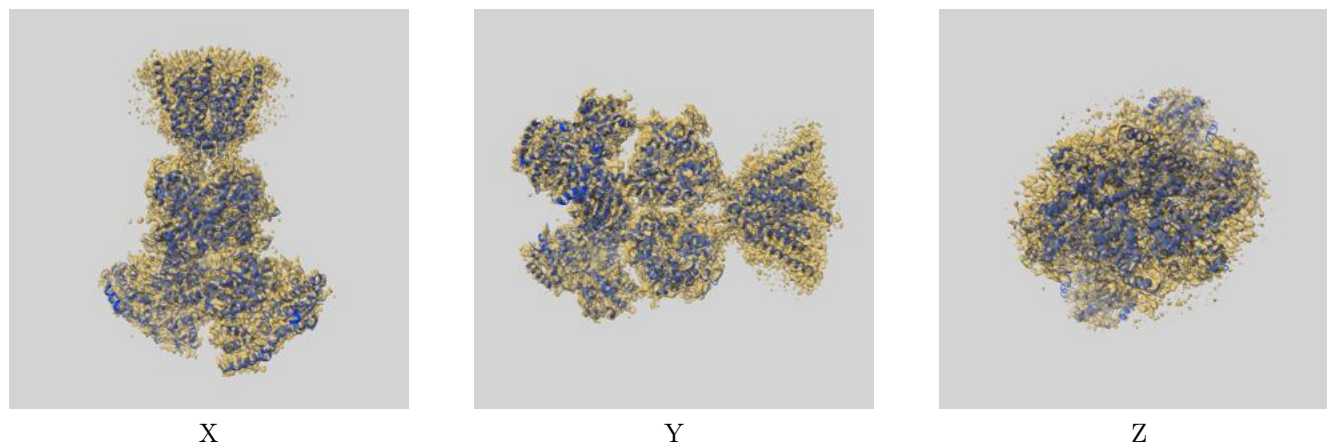
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

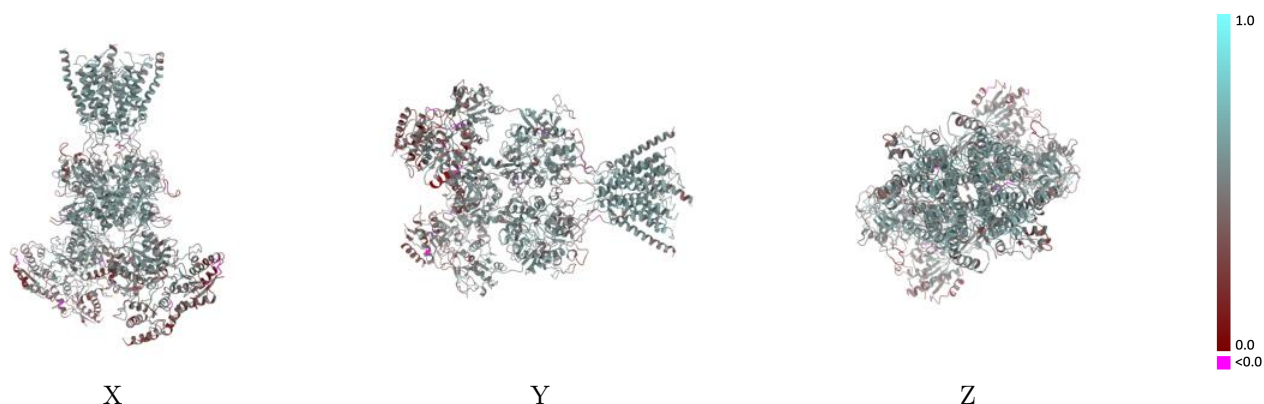
This section contains information regarding the fit between EMDB map EMD-70672 and PDB model 9OOT. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



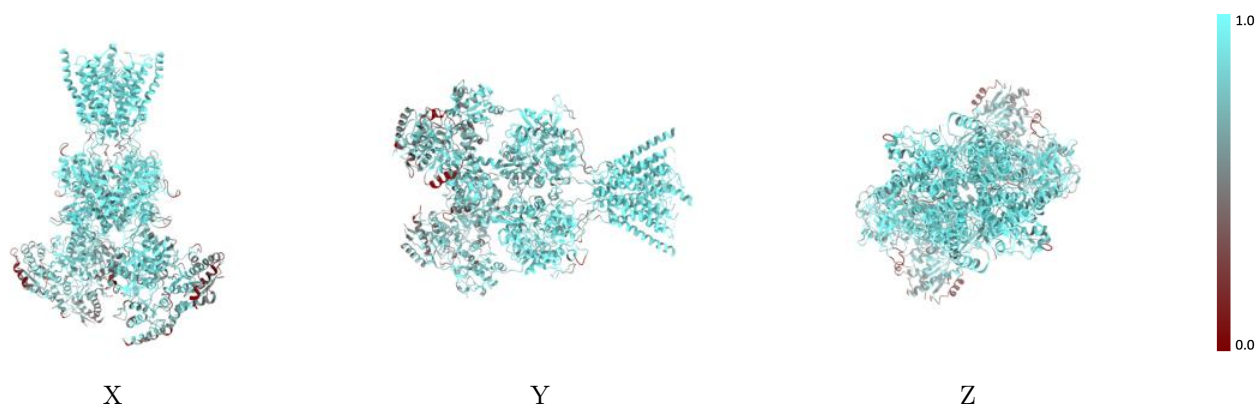
The images above show the 3D surface view of the map at the recommended contour level 0.048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



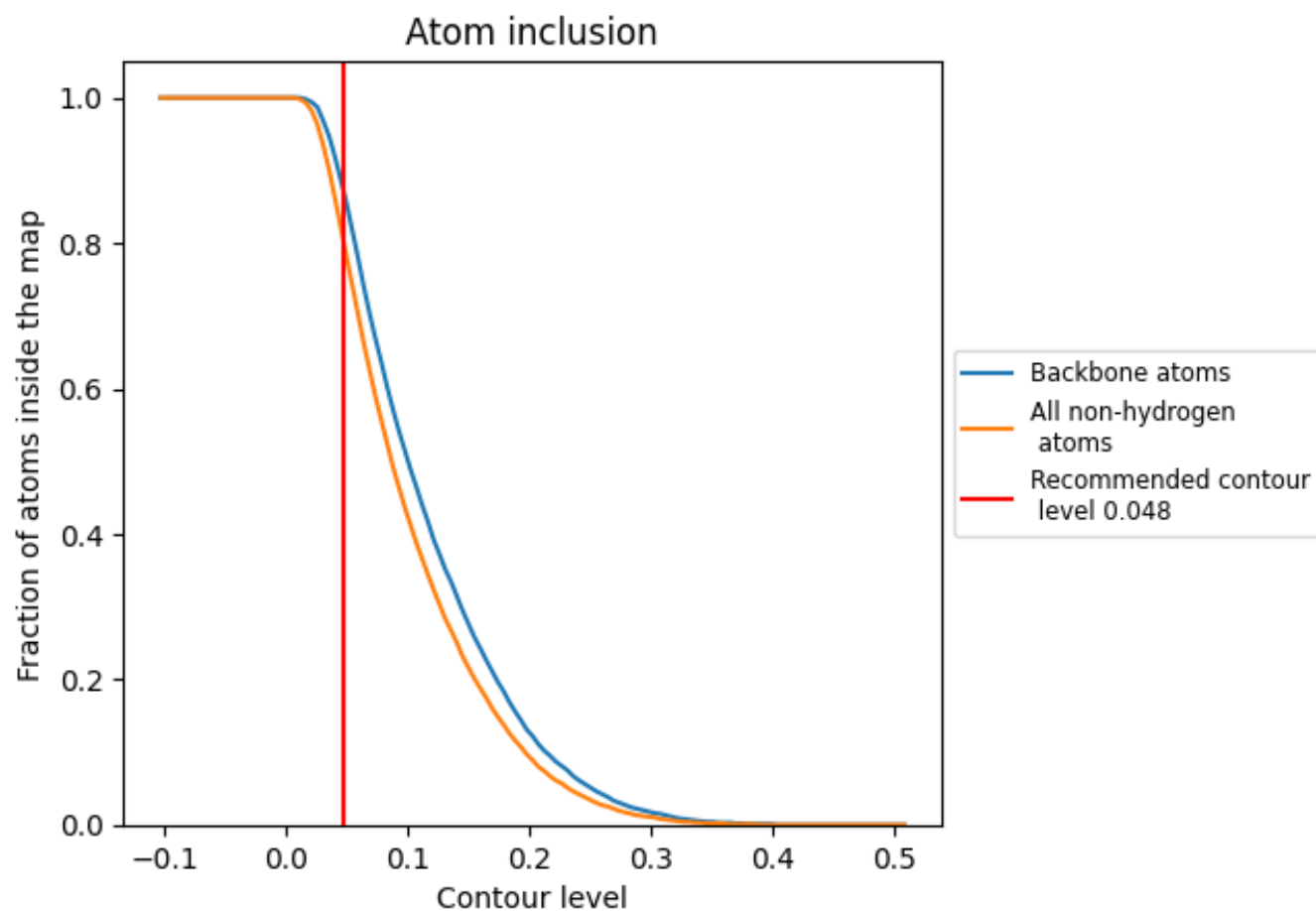
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.048).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 80% 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 (0.048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7970	<div></div> 0.4830
A	<div></div> 0.8100	<div></div> 0.4920
B	<div></div> 0.7790	<div></div> 0.4720
C	<div></div> 0.8140	<div></div> 0.4910
D	<div></div> 0.7840	<div></div> 0.4760

