



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:10 AM UTC

PDB ID : 9D3C / pdb_00009d3c
EMDB ID : EMD-46531
Title : Gly-,Glu-, (S)-(+)-ketamine bound GluN1a-2B-2D NMDAR
Authors : Hyunook, K.; Hiro, F.
Deposited on : 2024-08-09
Resolution : 3.96 Å (reported)
Based on initial models : 7saa, 8e96

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

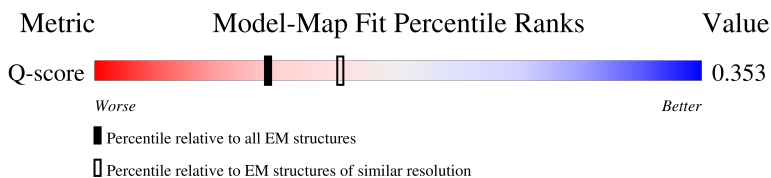
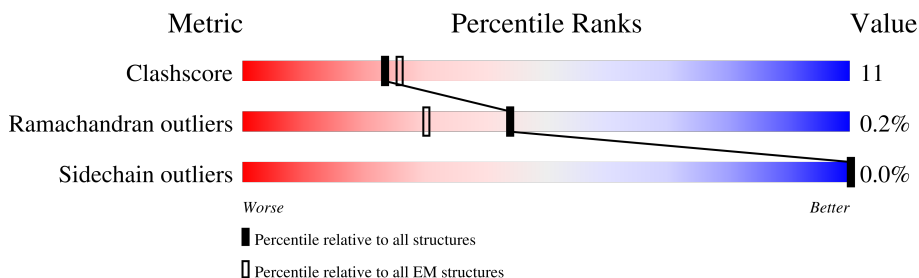
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.96 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	7646 (3.46 - 4.46)

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	825	
1	C	825	
2	B	884	
3	D	861	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GLY	A	901	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24194 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	779	Total	C	N	O	S	0	0
			6033	3841	1046	1114	32		
1	C	803	Total	C	N	O	S	0	0
			6254	3989	1070	1160	35		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	778	Total	C	N	O	S	0	0
			5969	3837	962	1131	39		

There are 61 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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
B	853	GLY	-	expression tag	UNP Q13224
B	854	PRO	-	expression tag	UNP Q13224
B	855	GLY	-	expression tag	UNP Q13224
B	856	SER	-	expression tag	UNP Q13224
B	857	GLY	-	expression tag	UNP Q13224
B	858	ALA	-	expression tag	UNP Q13224
B	859	THR	-	expression tag	UNP Q13224
B	860	ASN	-	expression tag	UNP Q13224
B	861	PHE	-	expression tag	UNP Q13224
B	862	SER	-	expression tag	UNP Q13224
B	863	LEU	-	expression tag	UNP Q13224
B	864	LEU	-	expression tag	UNP Q13224
B	865	LYS	-	expression tag	UNP Q13224

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	866	GLN	-	expression tag	UNP Q13224
B	867	ALA	-	expression tag	UNP Q13224
B	868	GLY	-	expression tag	UNP Q13224
B	869	ASP	-	expression tag	UNP Q13224
B	870	VAL	-	expression tag	UNP Q13224
B	871	GLU	-	expression tag	UNP Q13224
B	872	GLU	-	expression tag	UNP Q13224
B	873	ASN	-	expression tag	UNP Q13224
B	874	PRO	-	expression tag	UNP Q13224
B	875	GLY	-	expression tag	UNP Q13224

- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 2D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	755	Total	C	N	O	S	0	0
			5752	3690	980	1054	28		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	881	GLU	-	expression tag	UNP O15399
D	882	THR	-	expression tag	UNP O15399
D	883	SER	-	expression tag	UNP O15399
D	884	GLN	-	expression tag	UNP O15399
D	885	VAL	-	expression tag	UNP O15399
D	886	ALA	-	expression tag	UNP O15399
D	887	PRO	-	expression tag	UNP O15399
D	888	ALA	-	expression tag	UNP O15399

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



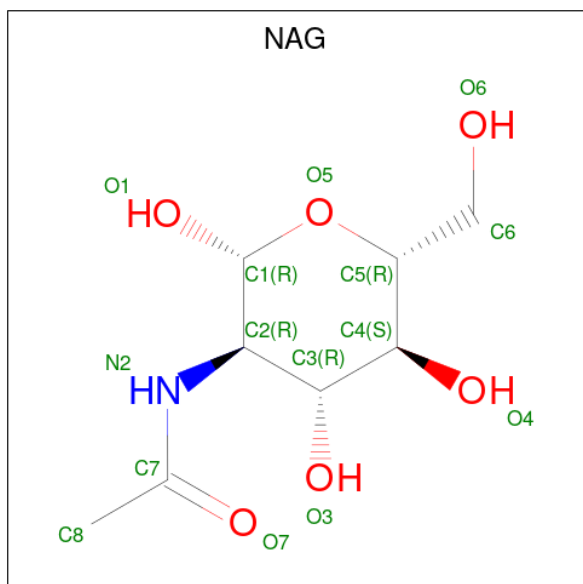
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



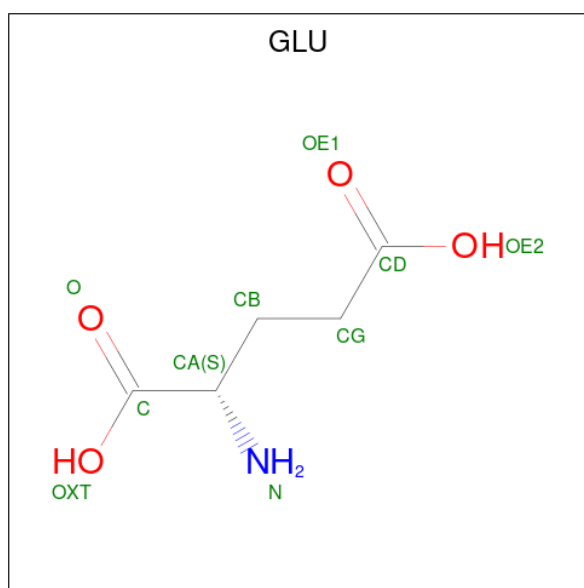
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

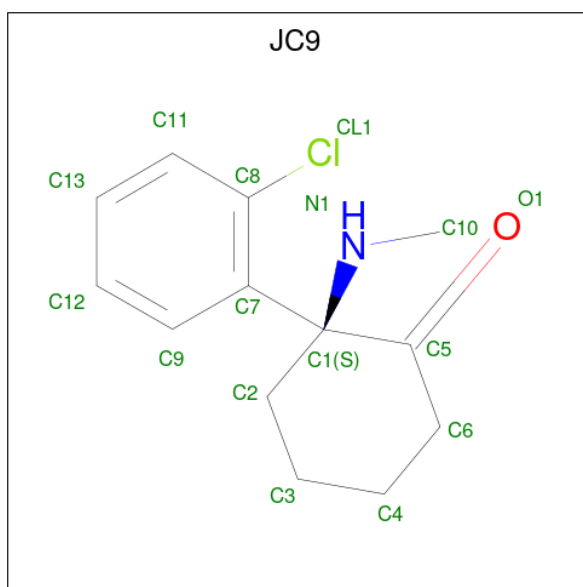
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			10	5	1	4	
7	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 8 is (2 {S})-2-(2-chlorophenyl)-2-(methylamino)cyclohexan-1-one (CCD ID: JC9) (formula: $C_{13}H_{16}ClNO$) (labeled as "Ligand of Interest" by depositor).

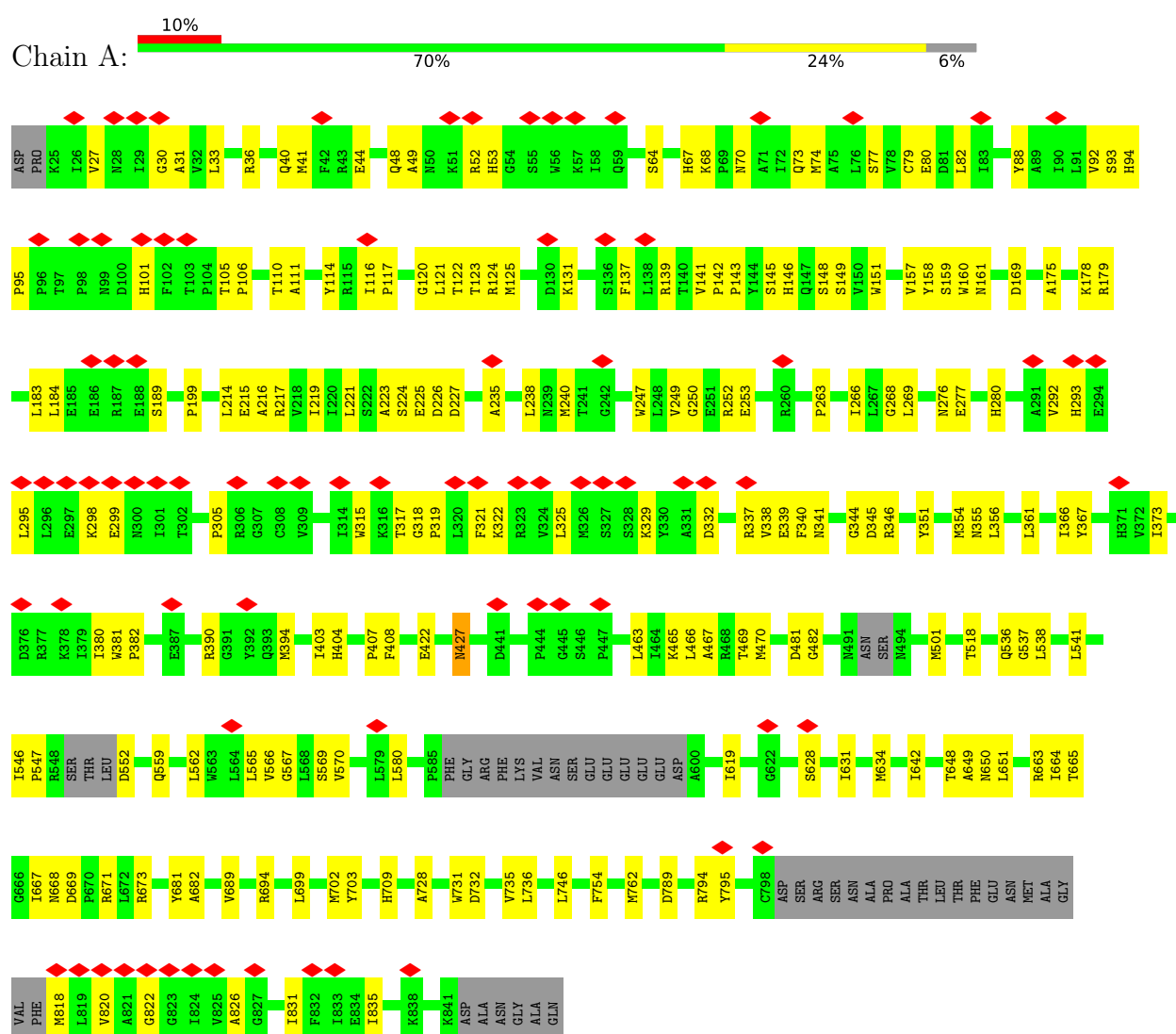


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
8	B	1	16	13	1	1	1	0

3 Residue-property plots

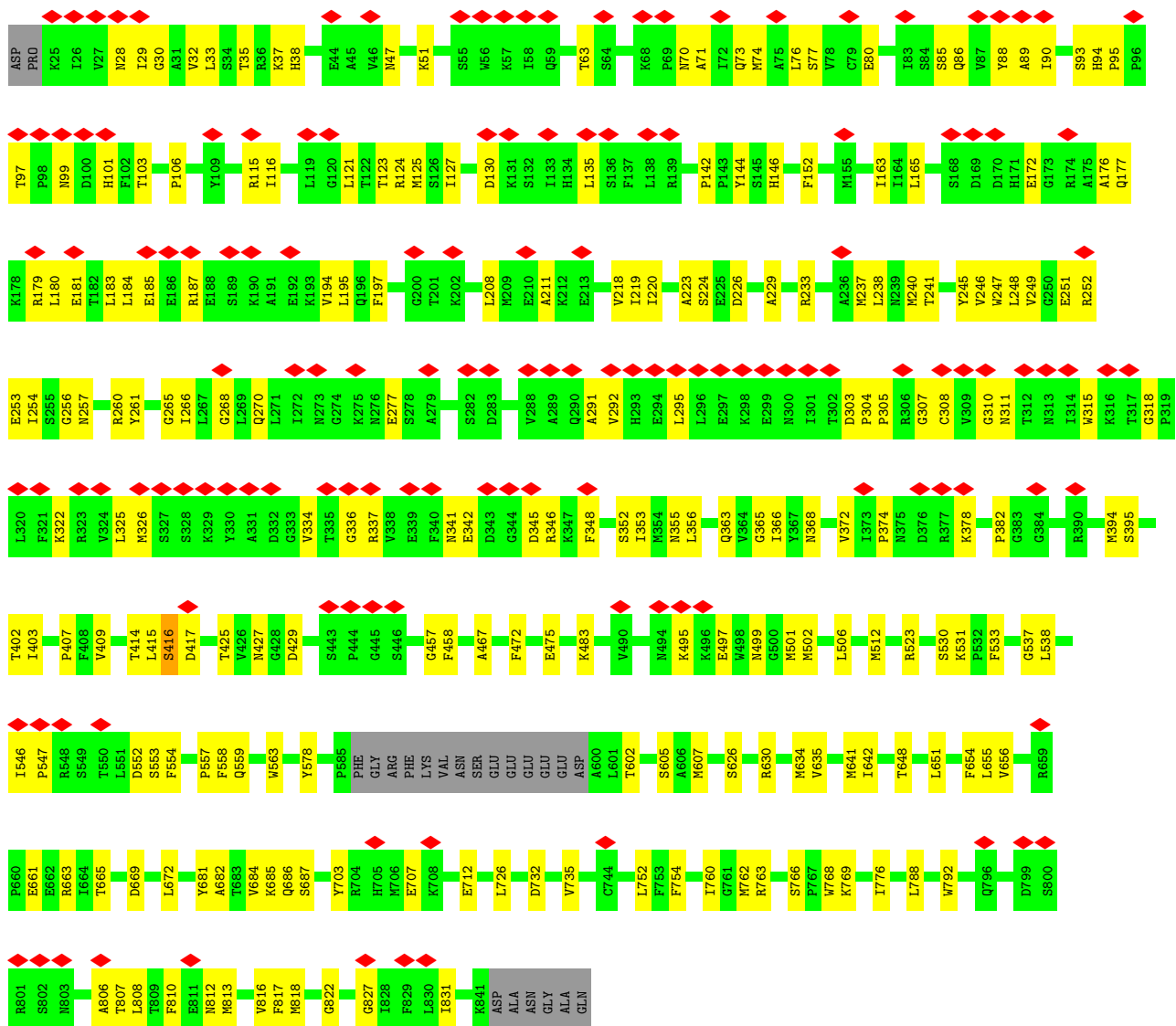
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

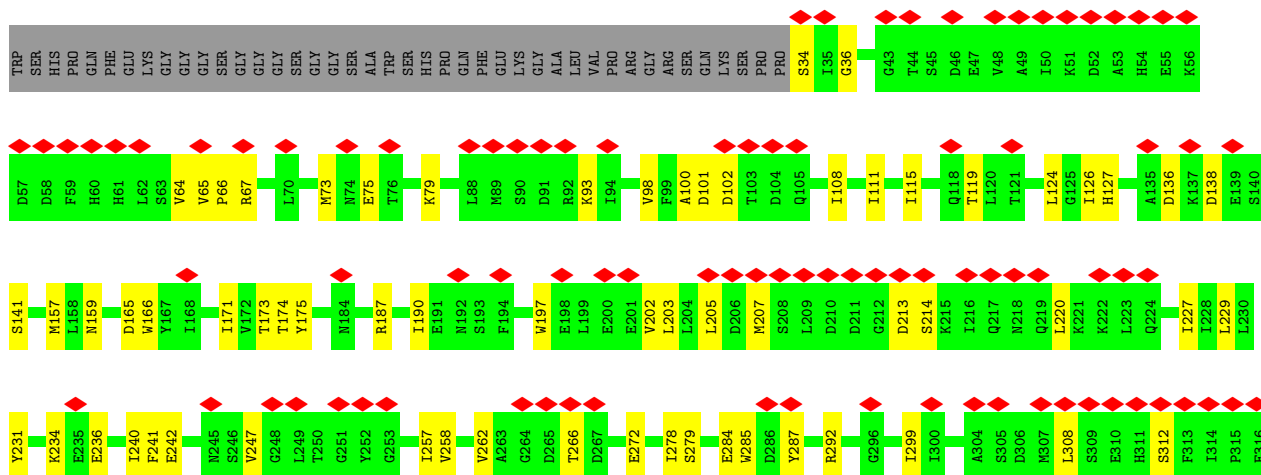


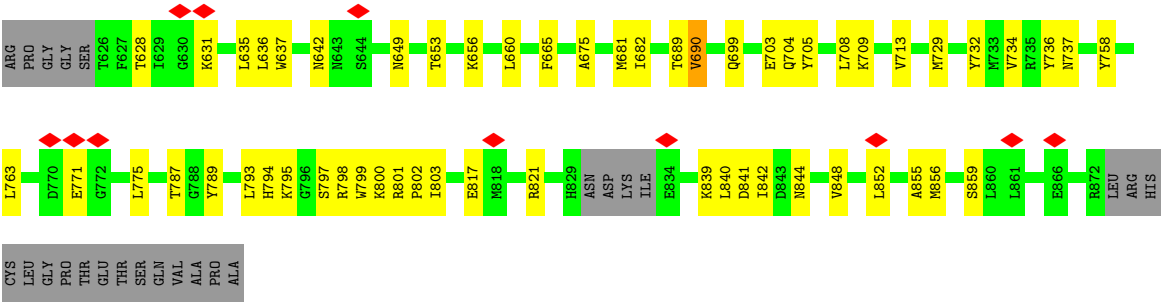
- Molecule 1: Glutamate receptor ionotropic, NMDA 1





● Molecule 2: Glutamate receptor ionotropic, NMDA 2B





● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	77.7	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	2.148	Depositor
Minimum map value	-0.385	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	342.4, 342.4, 342.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.856, 0.856, 0.856	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: NAG, JC9

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	0/6165	0.35	0/8365
1	C	0.21	0/6397	0.36	0/8685
2	B	0.20	0/6096	0.31	0/8279
3	D	0.19	0/5879	0.34	1/8003 (0.0%)
All	All	0.20	0/24537	0.34	1/33332 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	477	PRO	N-CA-CB	6.80	110.48	103.00

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	6033	0	5917	143	0
1	C	6254	0	6156	158	0
2	B	5969	0	5790	111	0
3	D	5752	0	5647	142	0
4	E	28	0	25	1	0
5	A	5	0	2	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	5	0	2	2	0
6	A	56	0	52	0	0
6	B	14	0	13	2	0
6	C	42	0	39	0	0
7	B	10	0	5	2	0
7	D	10	0	5	0	0
8	B	16	0	0	1	0
All	All	24194	0	23653	526	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 (526) 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:337:ARG:HE	1:C:348:PHE:HB3	1.36	0.85
2:B:813:LEU:HD13	2:B:818:MET:HE1	1.59	0.84
1:C:341:ASN:OD1	1:C:342:GLU:N	2.16	0.77
1:C:28:ASN:ND2	1:C:85:SER:OG	2.19	0.75
1:A:650:ASN:HD21	2:B:813:LEU:HD21	1.51	0.75
3:D:89:LEU:HD21	3:D:106:LEU:HG	1.70	0.73
3:D:194:ALA:O	3:D:197:HIS:ND1	2.22	0.73
2:B:649:ASN:HD22	1:C:655:LEU:HD13	1.53	0.73
8:B:903:JC9:N1	8:B:903:JC9:CL1	2.59	0.73
3:D:192:THR:HG1	3:D:248:CYS:HG	1.34	0.72
1:C:483:LYS:NZ	1:C:712:GLU:OE2	2.23	0.72
3:D:248:CYS:O	3:D:278:GLN:NE2	2.19	0.71
1:C:341:ASN:HB3	1:C:345:ASP:HB3	1.70	0.71
1:C:762:MET:HE1	1:C:768:TRP:HB2	1.73	0.71
3:D:239:VAL:HG21	3:D:244:ARG:HH21	1.56	0.70
1:C:363:GLN:NE2	1:C:365:GLY:O	2.25	0.69
1:A:160:TRP:HA	1:A:390:ARG:HH22	1.56	0.69
2:B:345:GLU:OE1	2:B:347:ARG:NH2	2.24	0.69
1:A:337:ARG:O	1:A:346:ARG:NH2	2.27	0.68
1:C:557:PRO:HG3	1:C:651:LEU:HD13	1.76	0.68
2:B:234:LYS:HG2	2:B:262:VAL:HA	1.76	0.67
1:A:341:ASN:OD1	1:A:345:ASP:N	2.28	0.67
1:A:559:GLN:H	1:A:562:LEU:HD12	1.60	0.67
1:A:631:ILE:HA	1:A:634:MET:HG2	1.75	0.67
3:D:53:VAL:HG21	3:D:324:VAL:HG23	1.77	0.67
1:C:684:VAL:O	1:C:687:SER:OG	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ALA:HB1	1:C:233:ARG:HH12	1.60	0.66
1:A:619:ILE:HD13	3:D:660:LEU:HD21	1.77	0.66
1:C:183:LEU:O	1:C:187:ARG:NH1	2.29	0.66
1:C:240:MET:SD	1:C:245:TYR:OH	2.52	0.66
2:B:683:PHE:HB3	2:B:728:ALA:HB3	1.78	0.66
3:D:653:THR:HA	3:D:656:LYS:HE3	1.78	0.66
1:C:523:ARG:NH2	5:C:901:GLY:OXT	2.30	0.65
1:A:427:ASN:O	1:A:427:ASN:ND2	2.28	0.65
1:A:117:PRO:HG3	1:A:322:LYS:HD2	1.79	0.65
1:A:649:ALA:HA	2:B:651:ALA:HB2	1.78	0.65
2:B:608:LEU:HD13	2:B:620:VAL:HG21	1.79	0.64
1:A:249:VAL:HG22	1:A:253:GLU:OE2	1.97	0.64
1:C:353:ILE:O	1:C:363:GLN:NE2	2.31	0.64
3:D:175:ILE:HD11	3:D:275:VAL:HG11	1.80	0.64
2:B:690:SER:N	7:B:901:GLU:OE2	2.31	0.64
3:D:313:ARG:O	3:D:319:ARG:NH2	2.24	0.64
3:D:300:LEU:O	3:D:396:ARG:NH2	2.30	0.63
1:A:36:ARG:O	1:A:40:GLN:NE2	2.32	0.63
1:C:74:MET:HE2	1:C:106:PRO:HG3	1.80	0.63
2:B:190:ILE:HG13	2:B:197:TRP:HB2	1.79	0.63
2:B:157:MET:HE1	2:B:229:LEU:HG	1.81	0.63
3:D:250:ARG:HH12	3:D:254:GLU:HG2	1.61	0.63
1:C:74:MET:HE1	3:D:132:PHE:CZ	2.34	0.63
1:A:74:MET:HA	1:A:77:SER:HB2	1.80	0.62
1:A:41:MET:HA	1:A:44:GLU:HB2	1.80	0.62
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.81	0.62
2:B:648:ALA:HB2	1:C:648:THR:HG23	1.82	0.62
1:A:403:ILE:CG1	1:A:501:MET:HE2	2.30	0.62
1:A:648:THR:HG23	3:D:675:ALA:HB2	1.80	0.62
2:B:159:ASN:HB3	2:B:384:LEU:HD11	1.82	0.62
2:B:688:ASN:OD1	6:B:902:NAG:N2	2.33	0.62
1:C:499:ASN:ND2	1:C:686:GLN:OE1	2.27	0.62
1:C:760:ILE:HD12	1:C:776:ILE:HD11	1.82	0.61
3:D:233:SER:OG	3:D:237:ARG:NH1	2.32	0.61
1:C:337:ARG:HH22	1:C:368:ASN:HB2	1.65	0.61
3:D:216:GLU:OE1	3:D:218:ARG:NH1	2.29	0.61
3:D:689:THR:HG22	3:D:690:VAL:HG23	1.83	0.61
1:A:518:THR:N	5:A:901:GLY:OXT	2.31	0.61
2:B:115:ILE:O	2:B:119:THR:OG1	2.16	0.61
1:C:352:SER:HA	1:C:366:ILE:HA	1.83	0.61
1:C:642:ILE:HG13	3:D:848:VAL:HG21	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ASN:OD1	1:A:673:ARG:NH1	2.34	0.61
3:D:249:ALA:HB3	3:D:252:GLU:HG2	1.82	0.61
3:D:437:LEU:HD21	3:D:512:LYS:HD3	1.83	0.61
3:D:150:LEU:HD21	3:D:279:LEU:HD22	1.82	0.61
1:A:355:ASN:HD21	1:A:380:ILE:HG22	1.66	0.60
2:B:561:MET:HE1	1:C:817:PHE:CE1	2.36	0.60
1:C:253:GLU:OE1	1:C:253:GLU:N	2.34	0.60
1:A:681:TYR:HB3	1:A:728:ALA:HB3	1.83	0.60
3:D:120:ASP:OD1	3:D:145:HIS:NE2	2.33	0.60
3:D:430:GLN:HB3	3:D:501:PHE:HA	1.84	0.60
1:A:139:ARG:HH22	1:A:143:PRO:HB3	1.67	0.59
1:A:322:LYS:HA	1:A:325:LEU:HD12	1.84	0.59
2:B:649:ASN:HD21	1:C:806:ALA:HB1	1.66	0.59
1:C:265:GLY:HA3	1:C:382:PRO:HD3	1.84	0.59
1:A:30:GLY:HA2	1:A:82:LEU:HD11	1.83	0.59
1:C:101:HIS:HB3	1:C:125:MET:HG2	1.84	0.59
1:C:372:VAL:HG12	1:C:374:PRO:HD3	1.84	0.59
2:B:101:ASP:O	2:B:127:HIS:ND1	2.33	0.59
1:C:732:ASP:OD2	5:C:901:GLY:N	2.36	0.59
3:D:310:ALA:O	3:D:319:ARG:NH2	2.35	0.59
2:B:258:VAL:O	2:B:279:SER:OG	2.15	0.58
2:B:433:THR:HG21	2:B:456:CYS:HB3	1.84	0.58
1:A:139:ARG:NH1	1:A:345:ASP:OD1	2.36	0.58
1:C:427:ASN:ND2	1:C:429:ASP:OD2	2.36	0.58
3:D:797:SER:O	3:D:798:ARG:HG3	2.03	0.58
1:C:116:ILE:HG12	1:C:315:TRP:HE1	1.69	0.58
2:B:207:MET:HE1	2:B:236:GLU:HB2	1.85	0.58
1:C:538:LEU:HD21	1:C:754:PHE:HB3	1.84	0.58
1:C:665:THR:OG1	1:C:669:ASP:OD1	2.20	0.58
1:A:114:TYR:O	1:A:315:TRP:NE1	2.36	0.58
1:C:251:GLU:OE2	1:C:270:GLN:NE2	2.32	0.58
1:C:355:ASN:OD1	1:C:356:LEU:N	2.36	0.58
3:D:221:LEU:HD21	3:D:235:GLN:HB2	1.84	0.58
1:A:546:ILE:HD12	1:A:547:PRO:HD2	1.85	0.57
1:A:124:ARG:NH1	1:A:142:PRO:O	2.37	0.57
3:D:140:PRO:HG3	3:D:360:LEU:HD13	1.85	0.57
1:C:94:HIS:CE1	1:C:123:THR:HA	2.39	0.57
3:D:347:ASP:HB2	3:D:350:ALA:HB2	1.86	0.57
1:A:263:PRO:HD2	1:A:266:ILE:HD11	1.86	0.57
1:A:566:VAL:O	1:A:569:SER:OG	2.19	0.57
1:A:216:ALA:O	1:A:217:ARG:NE	2.28	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:SER:O	1:C:630:ARG:NE	2.38	0.57
2:B:266:THR:OG1	2:B:284:GLU:OE1	2.23	0.56
1:C:415:LEU:O	1:C:417:ASP:N	2.38	0.56
1:A:123:THR:O	1:A:139:ARG:NH2	2.38	0.56
2:B:671:PHE:HB3	2:B:702:MET:HE1	1.87	0.56
1:A:699:LEU:HD22	1:A:702:MET:HE1	1.87	0.56
2:B:220:LEU:HD11	2:B:247:VAL:HG21	1.86	0.56
1:C:121:LEU:HD21	1:C:277:GLU:HB2	1.88	0.56
3:D:84:VAL:HG12	3:D:86:PRO:HD3	1.85	0.56
1:C:641:MET:HE1	3:D:642:ASN:HB2	1.87	0.56
3:D:313:ARG:HE	3:D:388:VAL:HG21	1.70	0.56
1:A:481:ASP:OD1	1:A:482:GLY:N	2.38	0.56
2:B:187:ARG:HA	2:B:190:ILE:HG22	1.88	0.56
3:D:306:ALA:HB3	3:D:390:ILE:HD11	1.87	0.56
1:A:149:SER:HA	1:A:183:LEU:HD11	1.88	0.56
3:D:596:VAL:HG13	3:D:636:LEU:HD11	1.86	0.56
3:D:402:GLY:HA3	3:D:411:LEU:HD12	1.86	0.56
3:D:437:LEU:HB2	3:D:524:MET:HE3	1.87	0.56
2:B:64:VAL:HG23	2:B:66:PRO:HD3	1.88	0.55
3:D:137:THR:HG23	3:D:139:LEU:H	1.70	0.55
3:D:709:LYS:HG3	3:D:736:TYR:CE2	2.41	0.55
1:A:319:PRO:HA	1:A:322:LYS:HE2	1.88	0.55
1:A:552:ASP:OD2	1:A:818:MET:N	2.40	0.55
1:A:665:THR:OG1	1:A:669:ASP:OD1	2.25	0.55
2:B:661:ASP:OD1	2:B:662:GLN:N	2.38	0.55
2:B:242:GLU:HG3	2:B:272:GLU:HG2	1.87	0.55
1:C:218:VAL:HG23	1:C:246:VAL:HG23	1.88	0.55
3:D:250:ARG:O	3:D:250:ARG:NH1	2.34	0.55
1:A:161:ASN:O	1:A:161:ASN:ND2	2.38	0.55
1:A:354:MET:HE2	1:A:361:LEU:HD13	1.89	0.55
2:B:404:ASP:O	2:B:475:THR:OG1	2.20	0.55
3:D:248:CYS:SG	3:D:249:ALA:N	2.80	0.55
1:A:541:LEU:HD11	1:A:746:LEU:HB3	1.89	0.55
1:C:224:SER:OG	1:C:226:ASP:OD1	2.22	0.55
2:B:299:ILE:HG23	2:B:342:VAL:HG11	1.89	0.55
3:D:445:VAL:HG21	3:D:507:LEU:HD21	1.87	0.55
3:D:793:LEU:HD11	3:D:803:ILE:HD11	1.89	0.55
3:D:97:ARG:NH1	3:D:98:SER:HB3	2.22	0.54
3:D:250:ARG:NH2	3:D:254:GLU:OE2	2.40	0.54
2:B:805:LYS:O	2:B:805:LYS:HG2	2.07	0.54
1:C:172:GLU:O	1:C:176:ALA:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:PRO:HG2	1:A:408:PHE:HD1	1.72	0.54
1:C:416:SER:OG	1:C:417:ASP:N	2.41	0.54
3:D:549:ILE:HG13	3:D:550:VAL:HG13	1.89	0.54
1:A:298:LYS:HD2	1:A:299:GLU:N	2.23	0.54
3:D:734:VAL:O	3:D:737:ASN:ND2	2.41	0.54
2:B:241:PHE:HB2	2:B:272:GLU:HG3	1.90	0.54
1:C:86:GLN:NE2	1:C:304:PRO:O	2.40	0.54
1:A:536:GLN:NE2	1:A:732:ASP:OD2	2.41	0.53
3:D:391:SER:OG	3:D:392:LEU:N	2.40	0.53
3:D:842:ILE:HG23	3:D:844:ASN:H	1.74	0.53
2:B:666:LEU:HG	2:B:757:PHE:CE2	2.43	0.53
3:D:699:GLN:HA	3:D:729:MET:HE1	1.89	0.53
1:A:403:ILE:HG22	1:A:404:HIS:H	1.73	0.53
1:C:93:SER:HB3	1:C:121:LEU:HD23	1.90	0.53
1:C:305:PRO:HD2	1:C:315:TRP:HD1	1.72	0.53
1:C:766:SER:O	1:C:769:LYS:HG2	2.07	0.53
1:A:175:ALA:HA	1:A:178:LYS:HB2	1.90	0.53
1:C:77:SER:HA	1:C:80:GLU:HB2	1.90	0.53
1:C:763:ARG:O	1:C:769:LYS:NZ	2.42	0.53
2:B:67:ARG:HH12	2:B:93:LYS:HB2	1.74	0.53
1:C:233:ARG:HH11	1:C:261:TYR:HD2	1.56	0.53
1:A:121:LEU:HD23	1:A:122:THR:HG23	1.91	0.52
3:D:68:ARG:HH21	3:D:69:LEU:HD23	1.74	0.52
1:C:310:GLY:HA2	3:D:95:ASP:HB3	1.91	0.52
3:D:107:LEU:HA	3:D:112:VAL:HG22	1.90	0.52
3:D:817:GLU:HG2	3:D:821:ARG:HH21	1.73	0.52
1:A:565:LEU:HD22	2:B:815:ILE:HD12	1.91	0.52
2:B:391:TRP:CD2	2:B:392:PRO:HD2	2.44	0.52
1:C:76:LEU:HD21	3:D:101:LEU:HG	1.90	0.52
1:C:249:VAL:HG13	1:C:253:GLU:HG2	1.90	0.52
1:C:99:ASN:HD21	1:C:103:THR:HG23	1.75	0.52
1:C:95:PRO:HG3	1:C:103:THR:HG21	1.92	0.52
3:D:559:THR:OG1	3:D:787:THR:O	2.21	0.52
2:B:777:ASP:OD1	2:B:777:ASP:N	2.41	0.52
2:B:258:VAL:HG11	2:B:262:VAL:HB	1.92	0.52
1:C:71:ALA:HA	1:C:74:MET:HG2	1.92	0.52
2:B:532:THR:OG1	2:B:732:ASP:OD1	2.28	0.52
1:C:808:LEU:HG	1:C:812:ASN:HD21	1.75	0.52
1:C:47:ASN:O	1:C:51:LYS:NZ	2.32	0.51
1:A:151:TRP:HZ2	1:A:250:GLY:HA2	1.75	0.51
3:D:393:THR:HB	3:D:397:THR:HB	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:572:VAL:HG12	3:D:840:LEU:HD11	1.92	0.51
1:A:329:LYS:HG3	1:A:339:GLU:HG2	1.92	0.51
1:A:731:TRP:CG	1:A:732:ASP:H	2.28	0.51
2:B:73:MET:SD	2:B:75:GLU:N	2.84	0.51
2:B:668:ASP:OD1	2:B:669:LYS:N	2.42	0.51
3:D:713:VAL:HB	3:D:758:TYR:HE1	1.74	0.51
1:A:53:HIS:HB2	1:A:293:HIS:HE1	1.76	0.51
1:C:30:GLY:HA3	1:C:90:ILE:HG22	1.90	0.51
1:A:111:ALA:HB1	1:A:116:ILE:HB	1.91	0.51
1:C:88:TYR:OH	1:C:303:ASP:OD1	2.26	0.51
3:D:531:GLN:HG3	3:D:794:HIS:NE2	2.26	0.51
3:D:578:LEU:HD12	3:D:578:LEU:H	1.75	0.51
3:D:242:GLN:HB2	3:D:270:TYR:HA	1.93	0.51
3:D:430:GLN:O	3:D:502:SER:N	2.34	0.51
1:A:214:LEU:O	1:A:217:ARG:NH2	2.43	0.51
2:B:536:VAL:HG22	2:B:730:ILE:HG12	1.92	0.51
3:D:63:ALA:HA	3:D:90:VAL:HG21	1.92	0.51
3:D:95:ASP:OD1	3:D:95:ASP:N	2.43	0.51
3:D:437:LEU:HG	3:D:438:GLU:H	1.76	0.50
2:B:464:ILE:HD11	2:B:789:MET:HE1	1.92	0.50
3:D:709:LYS:HG3	3:D:736:TYR:CD2	2.47	0.50
1:A:366:ILE:O	1:A:373:ILE:N	2.40	0.50
2:B:618:VAL:O	2:B:620:VAL:HG13	2.11	0.50
2:B:673:ARG:HD3	2:B:676:ASP:OD2	2.11	0.50
1:C:635:VAL:HG11	3:D:855:ALA:HB1	1.93	0.50
3:D:635:LEU:HD22	3:D:649:ASN:HA	1.93	0.50
2:B:171:ILE:HG22	2:B:229:LEU:HB2	1.93	0.50
1:C:165:LEU:HD21	1:C:194:VAL:HG13	1.94	0.50
1:C:812:ASN:OD1	1:C:813:MET:N	2.45	0.50
1:A:403:ILE:HG12	1:A:501:MET:HE2	1.94	0.50
1:A:315:TRP:CH2	1:A:318:GLY:HA2	2.47	0.50
1:C:195:LEU:HD21	1:C:211:ALA:HB2	1.93	0.50
2:B:34:SER:HA	2:B:65:VAL:HG11	1.94	0.49
3:D:330:GLY:HA2	3:D:363:TYR:CZ	2.47	0.49
1:A:298:LYS:HD2	1:A:299:GLU:H	1.77	0.49
2:B:171:ILE:HG13	2:B:202:VAL:HG13	1.93	0.49
1:A:53:HIS:HB2	1:A:293:HIS:CE1	2.47	0.49
2:B:379:TRP:HD1	2:B:384:LEU:HG	1.78	0.49
2:B:796:TRP:HB2	2:B:797:LEU:HD12	1.94	0.49
1:C:558:PHE:HD2	1:C:563:TRP:HE1	1.60	0.49
3:D:377:ASN:OD1	3:D:380:GLY:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:128:PRO:O	3:D:132:PHE:N	2.45	0.49
1:A:122:THR:HG22	1:A:141:VAL:HG21	1.93	0.49
3:D:244:ARG:HH22	3:D:270:TYR:HD2	1.61	0.49
1:A:33:LEU:HD23	1:A:93:SER:HB3	1.94	0.49
1:A:169:ASP:HB3	1:A:199:PRO:HD3	1.94	0.49
2:B:101:ASP:OD1	2:B:102:ASP:N	2.45	0.49
1:A:355:ASN:OD1	1:A:356:LEU:N	2.45	0.49
2:B:477:ASP:OD1	2:B:477:ASP:N	2.45	0.49
1:C:241:THR:HG22	1:C:247:TRP:CZ2	2.48	0.49
1:C:656:VAL:HG21	3:D:682:ILE:HD11	1.95	0.49
1:C:70:ASN:OD1	1:C:73:GLN:NE2	2.41	0.49
1:C:322:LYS:HD2	1:C:325:LEU:HD12	1.95	0.49
3:D:311:GLY:C	3:D:319:ARG:HH22	2.21	0.49
1:A:789:ASP:OD2	1:A:794:ARG:NH1	2.40	0.48
1:A:762:MET:SD	1:A:762:MET:N	2.86	0.48
1:C:146:HIS:HD2	1:C:179:ARG:HH12	1.60	0.48
3:D:597:VAL:O	3:D:600:THR:OG1	2.25	0.48
3:D:601:VAL:HA	3:D:604:PHE:HD2	1.78	0.48
1:A:682:ALA:HB2	1:A:709:HIS:HB2	1.95	0.48
2:B:213:ASP:OD1	2:B:214:SER:N	2.45	0.48
2:B:257:ILE:HG13	2:B:278:ILE:HG23	1.96	0.48
3:D:840:LEU:HD12	3:D:841:ASP:N	2.28	0.48
1:A:31:ALA:HB3	1:A:64:SER:HA	1.95	0.48
1:C:177:GLN:O	1:C:180:LEU:N	2.42	0.48
1:C:208:LEU:HD23	1:C:238:LEU:HD12	1.95	0.48
3:D:302:ALA:HB2	3:D:394:ARG:HD2	1.95	0.48
3:D:369:TRP:CD1	3:D:370:ASP:N	2.80	0.48
1:A:146:HIS:HA	1:A:179:ARG:NH1	2.28	0.48
1:C:546:ILE:N	1:C:547:PRO:HD2	2.28	0.48
2:B:709:PHE:O	2:B:711:GLN:NE2	2.40	0.48
1:C:402:THR:HG21	1:C:409:VAL:HG11	1.94	0.48
1:A:143:PRO:HD2	1:A:146:HIS:ND1	2.28	0.48
1:C:74:MET:HE1	3:D:132:PHE:HZ	1.75	0.48
1:A:184:LEU:HD21	1:A:189:SER:HB3	1.96	0.48
1:A:664:ILE:HG23	1:A:671:ARG:HD2	1.95	0.48
1:C:93:SER:HA	1:C:121:LEU:HB3	1.96	0.48
1:A:121:LEU:HD11	1:A:277:GLU:HB2	1.95	0.48
1:A:226:ASP:OD1	1:A:227:ASP:N	2.47	0.48
1:C:224:SER:HA	1:C:252:ARG:HE	1.79	0.48
3:D:223:LEU:HD12	3:D:232:LEU:HD22	1.95	0.48
1:A:315:TRP:CZ3	1:A:317:THR:HG23	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:ALA:HA	1:C:472:PHE:CE1	2.49	0.48
3:D:840:LEU:HD12	3:D:842:ILE:H	1.79	0.47
2:B:108:ILE:HA	2:B:111:ILE:HD12	1.95	0.47
2:B:555:SER:HB3	1:C:807:THR:HG22	1.96	0.47
1:C:103:THR:O	1:C:106:PRO:HD2	2.14	0.47
1:C:607:MET:HE2	1:C:607:MET:HA	1.97	0.47
3:D:465:GLN:OE1	3:D:478:ARG:HG2	2.14	0.47
1:A:215:GLU:HG3	1:A:394:MET:H	1.79	0.47
2:B:36:GLY:HA3	2:B:67:ARG:HB2	1.96	0.47
1:A:235:ALA:HB1	1:A:240:MET:HB2	1.95	0.47
2:B:616:ASN:CG	2:B:617:SER:H	2.22	0.47
1:C:414:THR:OG1	1:C:415:LEU:N	2.45	0.47
1:C:457:GLY:O	1:C:792:TRP:NE1	2.47	0.47
1:C:495:LYS:O	1:C:497:GLU:HG2	2.15	0.47
3:D:496:ALA:HA	3:D:501:PHE:CE1	2.49	0.47
2:B:414:ALA:HB1	2:B:415:PRO:HD2	1.97	0.47
2:B:464:ILE:CD1	2:B:789:MET:HE1	2.45	0.47
1:C:403:ILE:HB	1:C:501:MET:HE3	1.97	0.47
3:D:551:ASP:OD2	3:D:800:LYS:HE2	2.15	0.47
1:C:181:GLU:O	1:C:185:GLU:HG2	2.15	0.47
1:C:194:VAL:HG12	1:C:194:VAL:O	2.15	0.47
1:C:256:GLY:O	1:C:260:ARG:NH1	2.48	0.47
1:A:221:LEU:HB3	1:A:249:VAL:HG23	1.96	0.47
1:A:276:ASN:O	1:A:280:HIS:ND1	2.40	0.47
1:C:29:ILE:O	1:C:63:THR:OG1	2.33	0.47
1:C:180:LEU:O	1:C:183:LEU:HG	2.15	0.47
1:C:307:GLY:O	1:C:311:ASN:ND2	2.48	0.47
1:C:530:SER:OG	1:C:531:LYS:N	2.48	0.47
3:D:405:GLU:OE2	3:D:408:THR:OG1	2.23	0.47
1:A:157:VAL:HG12	1:A:158:TYR:HD1	1.80	0.47
1:C:28:ASN:ND2	1:C:63:THR:HG21	2.29	0.47
1:A:305:PRO:HD3	1:A:315:TRP:CG	2.50	0.46
1:C:326:MET:SD	1:C:326:MET:N	2.88	0.46
2:B:439:ARG:HB3	2:B:482:THR:HG21	1.97	0.46
1:C:30:GLY:N	1:C:89:ALA:O	2.39	0.46
1:C:346:ARG:NH1	1:C:348:PHE:O	2.48	0.46
3:D:771:GLU:HB3	3:D:775:LEU:HB2	1.96	0.46
3:D:799:TRP:O	3:D:802:PRO:HD2	2.16	0.46
1:A:277:GLU:HA	1:A:280:HIS:HB2	1.97	0.46
2:B:98:VAL:HG22	2:B:124:LEU:HB2	1.96	0.46
2:B:284:GLU:HB3	2:B:285:TRP:CE3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:THR:HB	1:A:106:PRO:HD3	1.95	0.46
1:C:602:THR:O	1:C:605:SER:OG	2.29	0.46
2:B:727:ASP:OD1	2:B:727:ASP:N	2.46	0.46
1:A:223:ALA:O	1:A:252:ARG:NH2	2.49	0.46
2:B:73:MET:SD	2:B:75:GLU:HB2	2.56	0.46
2:B:136:ASP:OD1	2:B:136:ASP:N	2.48	0.46
1:C:219:ILE:HD11	1:C:247:TRP:CE2	2.51	0.46
1:A:67:HIS:ND1	1:A:68:LYS:O	2.49	0.46
2:B:100:ALA:HB2	2:B:126:ILE:HD11	1.98	0.46
1:A:70:ASN:HD22	1:A:73:GLN:HE22	1.64	0.46
1:A:110:THR:HG22	2:B:79:LYS:NZ	2.31	0.46
3:D:54:ALA:HB3	3:D:115:VAL:HG22	1.98	0.46
3:D:300:LEU:HB2	3:D:396:ARG:HH12	1.81	0.46
1:A:250:GLY:N	1:A:253:GLU:OE2	2.49	0.46
1:A:292:VAL:HA	1:A:295:LEU:HB3	1.98	0.46
3:D:559:THR:HG21	3:D:789:TYR:CE1	2.51	0.46
1:C:249:VAL:HG21	1:C:266:ILE:HD12	1.99	0.46
1:A:92:VAL:HG23	1:A:120:GLY:HA2	1.98	0.45
1:A:148:SER:HA	1:A:151:TRP:CE3	2.51	0.45
1:A:117:PRO:HG2	1:A:321:PHE:HD2	1.81	0.45
1:C:305:PRO:HD2	1:C:315:TRP:CD1	2.51	0.45
1:C:818:MET:HE2	1:C:818:MET:HA	1.97	0.45
1:A:253:GLU:H	1:A:253:GLU:CD	2.22	0.45
1:A:642:ILE:HG21	2:B:821:VAL:HG11	1.98	0.45
1:A:184:LEU:HD23	1:A:184:LEU:O	2.17	0.45
1:A:541:LEU:HD22	1:A:736:LEU:HD22	1.99	0.45
2:B:386:MET:SD	2:B:386:MET:N	2.90	0.45
1:C:101:HIS:O	1:C:101:HIS:ND1	2.48	0.45
3:D:184:TRP:HB3	3:D:243:ILE:HG13	1.99	0.45
3:D:463:ARG:NE	3:D:478:ARG:HD2	2.32	0.45
1:A:407:PRO:HG2	1:A:408:PHE:CD1	2.52	0.45
2:B:561:MET:HE2	1:C:810:PHE:CZ	2.51	0.45
1:C:394:MET:HE3	1:C:395:SER:H	1.81	0.45
3:D:708:LEU:O	3:D:732:TYR:OH	2.28	0.45
2:B:205:LEU:HD23	2:B:205:LEU:H	1.81	0.45
2:B:488:LYS:NZ	6:B:902:NAG:O6	2.42	0.45
1:C:163:ILE:HG22	1:C:218:VAL:HG11	1.99	0.45
3:D:73:VAL:HG13	3:D:324:VAL:HG11	1.99	0.45
3:D:369:TRP:HD1	3:D:370:ASP:N	2.14	0.45
1:A:407:PRO:HG3	1:A:735:VAL:HA	1.98	0.45
1:A:422:GLU:OE1	1:A:422:GLU:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:PRO:HB2	1:C:97:THR:HG23	1.99	0.45
3:D:117:PHE:HE2	3:D:148:ALA:HB3	1.81	0.45
1:C:318:GLY:O	1:C:322:LYS:HG2	2.17	0.45
1:C:458:PHE:CE1	1:C:788:LEU:HB3	2.52	0.45
1:C:35:THR:HG22	1:C:37:LYS:H	1.83	0.44
1:C:183:LEU:HD12	1:C:184:LEU:HG	1.98	0.44
1:C:703:TYR:O	1:C:707:GLU:HB2	2.16	0.44
1:A:27:VAL:HG13	1:A:88:TYR:CD2	2.52	0.44
1:A:49:ALA:HB1	1:A:53:HIS:CE1	2.52	0.44
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.81	0.44
2:B:813:LEU:HD13	2:B:818:MET:CE	2.40	0.44
3:D:162:LEU:HD21	3:D:376:PHE:CD2	2.51	0.44
3:D:504:ASP:N	3:D:504:ASP:OD1	2.50	0.44
3:D:188:VAL:O	3:D:244:ARG:HA	2.17	0.44
1:A:48:GLN:HB3	1:A:52:ARG:HH12	1.82	0.44
1:A:145:SER:O	1:A:179:ARG:NH1	2.49	0.44
1:A:332:ASP:OD1	1:A:332:ASP:N	2.50	0.44
1:A:831:ILE:O	1:A:835:ILE:N	2.51	0.44
1:C:71:ALA:HB3	3:D:349:ARG:CZ	2.48	0.44
1:C:672:LEU:HD13	1:C:681:TYR:CZ	2.52	0.44
1:C:827:GLY:O	1:C:831:ILE:HG13	2.18	0.44
3:D:434:VAL:HG12	3:D:535:MET:HB2	2.00	0.44
4:E:2:NAG:O7	4:E:2:NAG:O4	2.23	0.44
1:A:101:HIS:NE2	1:A:125:MET:HG2	2.32	0.44
2:B:507:TYR:HH	2:B:772:TRP:CD1	2.36	0.44
1:C:816:VAL:HG13	1:C:817:PHE:HD2	1.83	0.44
3:D:156:GLU:O	3:D:159:SER:OG	2.23	0.44
3:D:801:ARG:HB3	3:D:802:PRO:HD3	2.00	0.44
1:A:238:LEU:HB2	1:A:240:MET:HG3	2.00	0.44
1:A:469:THR:C	1:A:470:MET:HG2	2.43	0.44
2:B:165:ASP:OD2	2:B:435:PRO:HG3	2.18	0.44
3:D:125:ALA:O	3:D:128:PRO:HD2	2.18	0.44
1:A:224:SER:HA	1:A:252:ARG:HH22	1.81	0.44
1:C:101:HIS:HB2	1:C:127:ILE:HD11	2.00	0.44
3:D:540:LEU:HD12	3:D:540:LEU:HA	1.83	0.44
3:D:848:VAL:O	3:D:852:LEU:N	2.50	0.44
1:A:131:LYS:NZ	1:A:137:PHE:O	2.51	0.44
2:B:308:LEU:O	2:B:312:SER:OG	2.22	0.44
1:C:220:ILE:HG13	1:C:248:LEU:HB2	1.98	0.44
1:C:578:TYR:HE2	1:C:602:THR:HA	1.82	0.43
3:D:443:VAL:HG13	3:D:443:VAL:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:MET:HE1	3:D:132:PHE:CE2	2.52	0.43
1:C:197:PHE:HZ	1:C:223:ALA:HB2	1.83	0.43
3:D:95:ASP:OD1	3:D:98:SER:OG	2.34	0.43
1:C:334:VAL:C	1:C:336:GLY:H	2.27	0.43
3:D:145:HIS:CE1	3:D:316:LEU:HB2	2.54	0.43
3:D:543:ASN:OD1	3:D:544:GLU:N	2.49	0.43
2:B:805:LYS:NZ	2:B:807:GLU:HA	2.33	0.43
1:C:124:ARG:NE	1:C:142:PRO:O	2.43	0.43
1:C:152:PHE:CG	1:C:183:LEU:HD13	2.53	0.43
1:C:661:GLU:O	1:C:663:ARG:NH1	2.51	0.43
1:A:159:SER:O	1:A:390:ARG:NH1	2.40	0.43
1:A:820:VAL:HG22	3:D:665:PHE:HD1	1.83	0.43
2:B:406:LEU:O	2:B:476:TYR:HA	2.18	0.43
1:C:71:ALA:HB3	3:D:349:ARG:NH1	2.33	0.43
1:C:237:MET:SD	1:C:237:MET:N	2.88	0.43
1:C:554:PHE:CD1	1:C:816:VAL:HB	2.54	0.43
1:A:403:ILE:HG22	1:A:404:HIS:N	2.34	0.43
1:A:628:SER:O	1:A:631:ILE:HG22	2.18	0.43
1:C:73:GLN:HA	1:C:76:LEU:HB2	2.00	0.43
1:C:552:ASP:OD1	1:C:553:SER:N	2.52	0.43
3:D:55:LEU:HD13	3:D:57:PHE:HE1	1.83	0.43
3:D:600:THR:O	3:D:603:ILE:HG22	2.18	0.43
3:D:856:MET:O	3:D:859:SER:OG	2.27	0.43
2:B:666:LEU:HG	2:B:757:PHE:CD2	2.54	0.43
1:C:682:ALA:HB3	1:C:726:LEU:HD21	2.01	0.43
3:D:363:TYR:CG	3:D:364:PHE:N	2.87	0.43
1:C:308:CYS:SG	3:D:97:ARG:HD2	2.59	0.43
1:C:537:GLY:HA3	1:C:752:LEU:HD12	2.00	0.43
3:D:57:PHE:HB3	3:D:62:TYR:CD2	2.54	0.43
3:D:134:SER:HA	3:D:137:THR:HG22	2.01	0.43
1:A:465:LYS:HA	1:A:465:LYS:HD2	1.79	0.43
1:A:794:ARG:HG2	1:A:795:TYR:HD1	1.84	0.43
2:B:67:ARG:NH1	2:B:93:LYS:HB2	2.33	0.43
2:B:672:GLN:HB3	2:B:673:ARG:NH2	2.34	0.43
1:C:130:ASP:OD1	1:C:130:ASP:N	2.50	0.43
3:D:244:ARG:HD2	3:D:272:TRP:CH2	2.54	0.43
3:D:542:ILE:O	3:D:787:THR:HG21	2.19	0.43
1:A:94:HIS:ND1	1:A:95:PRO:HD2	2.34	0.42
3:D:124:PRO:HA	3:D:148:ALA:HA	2.01	0.42
1:A:151:TRP:CZ2	1:A:250:GLY:HA2	2.54	0.42
1:C:475:GLU:O	1:C:475:GLU:HG3	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:601:VAL:HA	3:D:604:PHE:HB2	2.02	0.42
1:A:694:ARG:HD3	1:A:703:TYR:OH	2.20	0.42
1:A:123:THR:O	1:A:123:THR:OG1	2.37	0.42
1:A:351:TYR:HD1	1:A:367:TYR:HD2	1.66	0.42
2:B:691:THR:N	7:B:901:GLU:OE2	2.44	0.42
2:B:774:ARG:HH21	2:B:778:LEU:HD21	1.84	0.42
1:C:257:ASN:HA	1:C:260:ARG:CZ	2.49	0.42
3:D:703:GLU:HG3	3:D:704:GLN:H	1.84	0.42
1:A:822:GLY:O	1:A:826:ALA:N	2.52	0.42
2:B:755:LYS:HG3	2:B:757:PHE:CE1	2.54	0.42
3:D:628:THR:HG23	3:D:631:LYS:H	1.84	0.42
3:D:636:LEU:HD23	3:D:636:LEU:O	2.20	0.42
2:B:173:THR:OG1	2:B:231:TYR:HB3	2.19	0.42
3:D:142:VAL:HG22	3:D:162:LEU:HB3	2.01	0.42
2:B:138:ASP:HB3	2:B:141:SER:HB2	2.02	0.42
2:B:460:PHE:HB2	2:B:796:TRP:CG	2.55	0.42
2:B:537:MET:SD	2:B:736:LEU:HD22	2.58	0.42
2:B:561:MET:O	2:B:564:VAL:HG12	2.20	0.42
2:B:602:ILE:HD12	2:B:605:ALA:HB3	2.02	0.42
2:B:672:GLN:HB3	2:B:673:ARG:CZ	2.49	0.42
2:B:755:LYS:HG3	2:B:757:PHE:HE1	1.84	0.42
3:D:390:ILE:HD12	3:D:398:TRP:NE1	2.35	0.42
1:A:79:CYS:SG	1:A:80:GLU:N	2.93	0.42
1:A:538:LEU:HD21	1:A:689:VAL:HG12	2.01	0.42
1:C:292:VAL:HA	1:C:295:LEU:HD12	2.01	0.42
1:C:685:LYS:HG2	1:C:686:GLN:HG3	2.02	0.42
1:C:32:VAL:C	1:C:33:LEU:HD12	2.45	0.42
3:D:392:LEU:HD13	3:D:398:TRP:CE3	2.55	0.42
3:D:564:MET:SD	3:D:763:LEU:HD22	2.59	0.42
1:A:338:VAL:HG12	1:A:346:ARG:NH1	2.35	0.41
2:B:545:VAL:HG12	2:B:547:PRO:HD3	2.02	0.41
2:B:641:ILE:HG21	1:C:554:PHE:HE1	1.84	0.41
1:C:115:ARG:HH21	1:C:135:LEU:HD21	1.85	0.41
1:A:667:ILE:HD12	1:A:667:ILE:HA	1.93	0.41
2:B:829:MET:O	2:B:832:SER:OG	2.31	0.41
3:D:127:ALA:HB3	3:D:128:PRO:HD3	2.02	0.41
1:A:117:PRO:HG2	1:A:321:PHE:CD2	2.54	0.41
1:A:567:GLY:O	1:A:570:VAL:HG12	2.19	0.41
2:B:287:TYR:CE2	2:B:292:ARG:HB3	2.55	0.41
2:B:685:THR:HG22	2:B:706:MET:HE1	2.03	0.41
1:C:291:ALA:O	1:C:295:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:794:HIS:O	3:D:795:LYS:HG2	2.21	0.41
3:D:797:SER:C	3:D:799:TRP:H	2.27	0.41
1:A:263:PRO:CD	1:A:266:ILE:HD11	2.51	0.41
1:A:537:GLY:HA2	1:A:754:PHE:O	2.20	0.41
2:B:498:ILE:HA	2:B:498:ILE:HD13	1.83	0.41
1:C:38:HIS:NE2	1:C:277:GLU:OE2	2.53	0.41
1:C:254:ILE:HD11	1:C:268:GLY:HA3	2.01	0.41
1:C:425:THR:HG22	1:C:429:ASP:O	2.21	0.41
1:A:41:MET:SD	1:A:41:MET:N	2.93	0.41
1:A:219:ILE:HG21	1:A:247:TRP:CZ3	2.56	0.41
2:B:718:LEU:HD23	2:B:718:LEU:HA	1.92	0.41
3:D:553:SER:OG	3:D:554:VAL:N	2.53	0.41
1:A:340:PHE:HB3	1:A:344:GLY:HA2	2.03	0.41
1:A:619:ILE:O	1:A:619:ILE:HG13	2.21	0.41
1:A:731:TRP:CG	1:A:732:ASP:N	2.89	0.41
2:B:464:ILE:HD13	2:B:464:ILE:HA	1.86	0.41
1:C:378:LYS:HD2	1:C:378:LYS:HA	1.97	0.41
1:A:463:LEU:O	1:A:467:ALA:N	2.44	0.41
2:B:784:PHE:HE1	2:B:789:MET:HG2	1.85	0.41
1:C:394:MET:HE3	1:C:395:SER:N	2.35	0.41
1:C:407:PRO:HG3	1:C:735:VAL:HA	2.02	0.41
1:C:634:MET:SD	3:D:637:TRP:CD1	3.14	0.41
1:A:315:TRP:CZ2	1:A:318:GLY:HA2	2.55	0.41
1:A:762:MET:HE3	1:A:762:MET:HB3	1.96	0.41
2:B:174:THR:OG1	2:B:175:TYR:N	2.53	0.41
2:B:207:MET:SD	2:B:240:ILE:HD11	2.61	0.41
2:B:408:ILE:HB	2:B:478:LEU:HD23	2.02	0.41
2:B:755:LYS:HD2	2:B:755:LYS:HA	1.92	0.41
1:C:502:MET:O	1:C:506:LEU:HD23	2.20	0.41
1:C:654:PHE:HZ	3:D:839:LYS:CB	2.33	0.41
1:A:225:GLU:OE2	1:A:252:ARG:HB3	2.21	0.41
1:A:651:LEU:HA	1:A:651:LEU:HD13	1.87	0.41
1:C:559:GLN:OE1	3:D:842:ILE:HD12	2.20	0.41
3:D:272:TRP:CD1	3:D:301:PRO:HG2	2.56	0.41
3:D:274:MET:HB2	3:D:304:LEU:HD12	2.03	0.41
1:A:403:ILE:HG13	1:A:501:MET:HE2	2.03	0.40
1:A:580:LEU:HD23	1:A:580:LEU:HA	1.86	0.40
2:B:573:ALA:HA	2:B:576:VAL:HB	2.01	0.40
3:D:594:LEU:O	3:D:597:VAL:HG12	2.22	0.40
1:A:268:GLY:C	1:A:269:LEU:HD12	2.46	0.40
1:C:533:PHE:CE1	1:C:760:ILE:HG13	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TRP:HB3	1:A:382:PRO:HD2	2.03	0.40
3:D:681:MET:O	3:D:681:MET:HG2	2.21	0.40
2:B:203:LEU:HD21	2:B:220:LEU:HA	2.03	0.40
2:B:654:MET:HE3	2:B:654:MET:HB2	1.90	0.40
1:C:125:MET:HE2	1:C:125:MET:HA	2.03	0.40
1:C:512:MET:HE3	1:C:512:MET:HB2	1.91	0.40
1:C:818:MET:O	1:C:822:GLY:N	2.41	0.40
1:C:144:TYR:CE2	1:C:252:ARG:HD3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	769/825 (93%)	694 (90%)	74 (10%)	1 (0%)	48	81
1	C	799/825 (97%)	724 (91%)	74 (9%)	1 (0%)	48	81
2	B	770/884 (87%)	709 (92%)	60 (8%)	1 (0%)	48	81
3	D	741/861 (86%)	667 (90%)	72 (10%)	2 (0%)	36	69
All	All	3079/3395 (91%)	2794 (91%)	280 (9%)	5 (0%)	44	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	416	SER
1	A	663	ARG
3	D	690	VAL
2	B	414	ALA
3	D	705	TYR

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	641/710 (90%)	640 (100%)	1 (0%)	87	87
1	C	674/710 (95%)	674 (100%)	0	100	100
2	B	638/760 (84%)	638 (100%)	0	100	100
3	D	599/701 (85%)	599 (100%)	0	100	100
All	All	2552/2881 (89%)	2551 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	427	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	70	ASN
1	A	177	GLN
1	A	273	ASN
1	A	293	HIS
1	A	525	GLN
2	B	74	ASN
2	B	180	GLN
2	B	649	ASN
2	B	698	ASN
2	B	817	ASN
1	C	28	ASN
1	C	134	HIS
1	C	161	ASN
1	C	196	GLN
1	C	257	ASN
1	C	290	GLN
1	C	363	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	571	HIS
1	C	650	ASN
1	C	696	GLN
3	D	407	GLN
3	D	809	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides 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	$\# Z > 2$
4	NAG	E	1	4,3	14,14,15	0.50	0	17,19,21	0.64	0
4	NAG	E	2	4	14,14,15	0.64	1 (7%)	17,19,21	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	O5-C1	-2.26	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

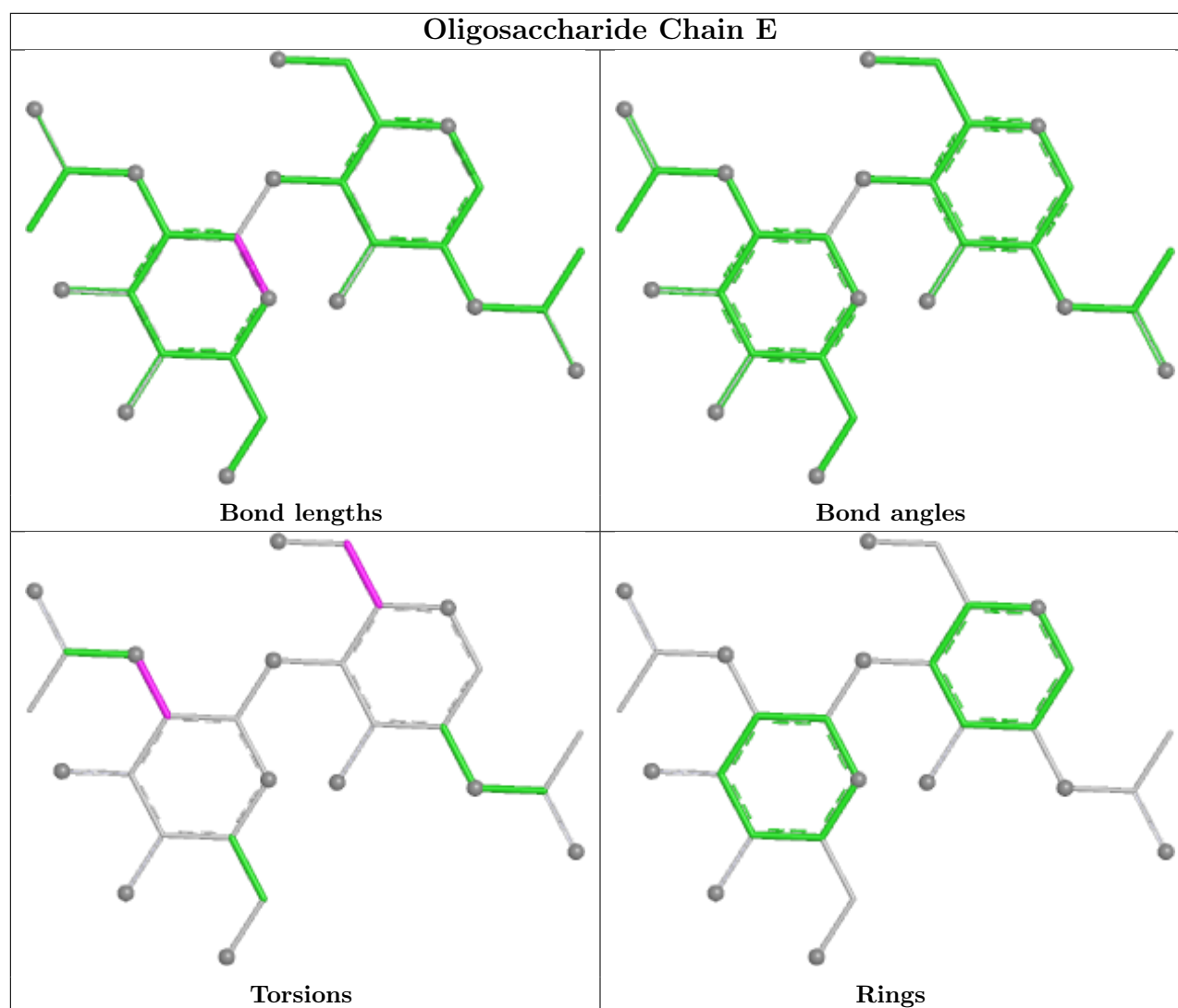
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	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 oligosaccharide.



5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
6	NAG	A	902	1	14,14,15	0.22	0	17,19,21	0.44	0
7	GLU	D	901	-	8,9,9	1.13	1 (12%)	8,11,11	1.19	1 (12%)
6	NAG	A	903	1	14,14,15	0.28	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	904	1	14,14,15	0.23	0	17,19,21	0.54	0
8	JC9	B	903	-	15,17,17	1.44	2 (13%)	15,24,24	1.50	2 (13%)
6	NAG	B	902	2	14,14,15	0.58	1 (7%)	17,19,21	0.64	0
6	NAG	C	902	1	14,14,15	0.29	0	17,19,21	0.32	0
5	GLY	C	901	-	4,4,4	1.17	1 (25%)	3,4,4	1.65	1 (33%)
7	GLU	B	901	-	8,9,9	1.12	1 (12%)	8,11,11	1.29	1 (12%)
6	NAG	A	905	1	14,14,15	0.51	0	17,19,21	0.95	1 (5%)
6	NAG	A	904	1	14,14,15	0.24	0	17,19,21	0.44	0
5	GLY	A	901	-	4,4,4	1.20	1 (25%)	3,4,4	1.75	2 (66%)
6	NAG	C	903	1	14,14,15	0.45	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	902	1	-	1/6/23/26	0/1/1/1
7	GLU	D	901	-	-	0/9/9/9	-
6	NAG	A	903	1	-	4/6/23/26	0/1/1/1
6	NAG	C	904	1	-	3/6/23/26	0/1/1/1
8	JC9	B	903	-	-	3/6/23/23	0/2/2/2
6	NAG	B	902	2	-	4/6/23/26	0/1/1/1
6	NAG	C	902	1	-	2/6/23/26	0/1/1/1
5	GLY	C	901	-	-	0/2/2/2	-
7	GLU	B	901	-	-	0/9/9/9	-
6	NAG	A	905	1	-	1/6/23/26	0/1/1/1
6	NAG	A	904	1	-	2/6/23/26	0/1/1/1
5	GLY	A	901	-	-	2/2/2/2	-
6	NAG	C	903	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	903	JC9	C6-C5	4.01	1.56	1.50
7	B	901	GLU	OXT-C	-2.37	1.23	1.30
5	A	901	GLY	OXT-C	-2.28	1.23	1.30
7	D	901	GLU	OXT-C	-2.26	1.23	1.30
5	C	901	GLY	OXT-C	-2.23	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	903	JC9	C8-CL1	2.13	1.78	1.73
6	B	902	NAG	C1-C2	2.10	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	903	JC9	C9-C7-C8	3.48	120.21	116.51
8	B	903	JC9	C1-C7-C8	-3.31	120.40	123.43
7	B	901	GLU	OXT-C-O	-2.75	117.84	124.08
7	D	901	GLU	OXT-C-O	-2.61	118.15	124.08
6	A	905	NAG	C2-N2-C7	2.60	126.39	122.90
5	A	901	GLY	OXT-C-O	-2.19	117.70	123.33
5	C	901	GLY	OXT-C-O	-2.11	117.90	123.33
5	A	901	GLY	OXT-C-CA	2.07	121.61	113.38

There are no chirality outliers.

All (22) torsion outliers are listed below:

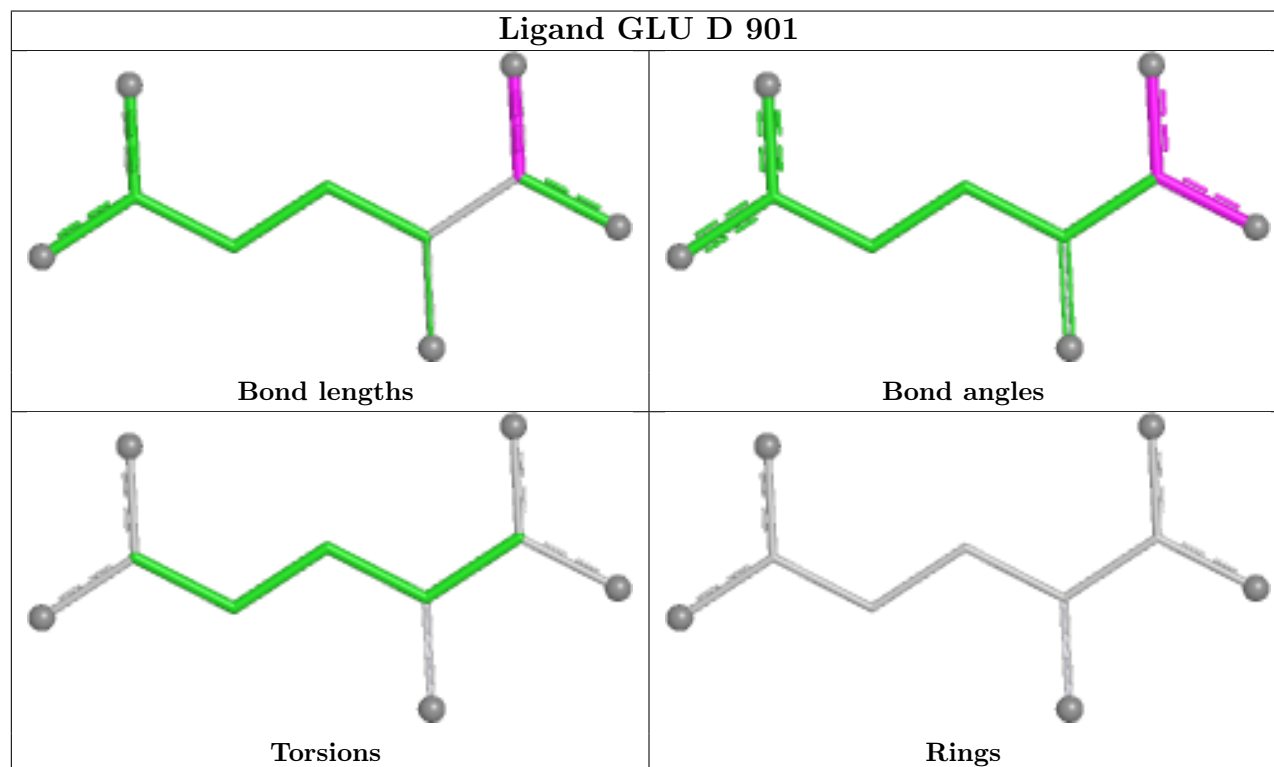
Mol	Chain	Res	Type	Atoms
5	A	901	GLY	O-C-CA-N
5	A	901	GLY	OXT-C-CA-N
6	A	905	NAG	C1-C2-N2-C7
8	B	903	JC9	N1-C1-C7-C8
8	B	903	JC9	C5-C1-C7-C8
8	B	903	JC9	C5-C1-C7-C9
6	A	903	NAG	O5-C5-C6-O6
6	C	904	NAG	O5-C5-C6-O6
6	B	902	NAG	O5-C5-C6-O6
6	A	903	NAG	C4-C5-C6-O6
6	C	904	NAG	C4-C5-C6-O6
6	C	902	NAG	O5-C5-C6-O6
6	B	902	NAG	C4-C5-C6-O6
6	A	902	NAG	O5-C5-C6-O6
6	C	902	NAG	C4-C5-C6-O6
6	A	904	NAG	C4-C5-C6-O6
6	A	904	NAG	O5-C5-C6-O6
6	A	903	NAG	C3-C2-N2-C7
6	B	902	NAG	C3-C2-N2-C7
6	A	903	NAG	C1-C2-N2-C7
6	B	902	NAG	C1-C2-N2-C7
6	C	904	NAG	C3-C2-N2-C7

There are no ring outliers.

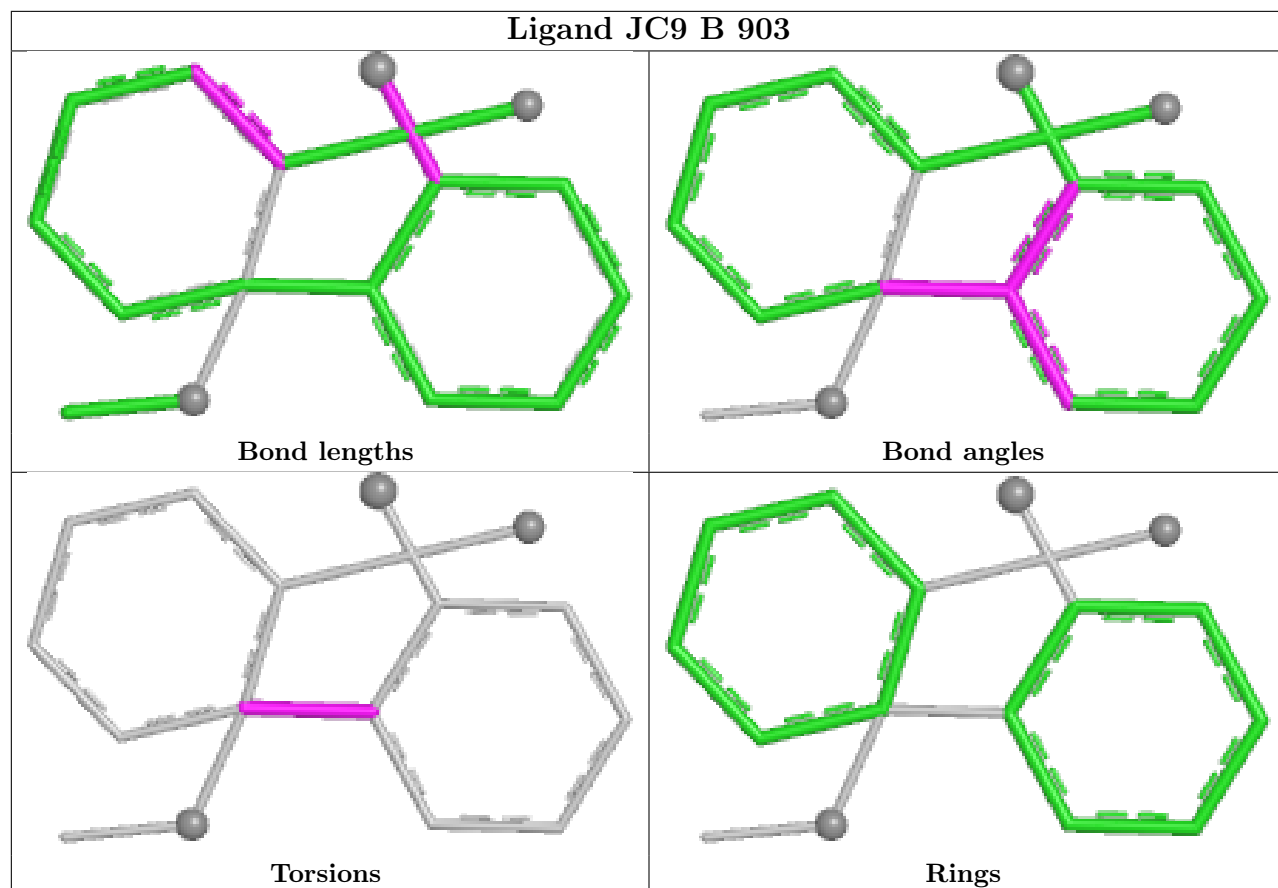
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	903	JC9	1	0
6	B	902	NAG	2	0
5	C	901	GLY	2	0
7	B	901	GLU	2	0
5	A	901	GLY	1	0

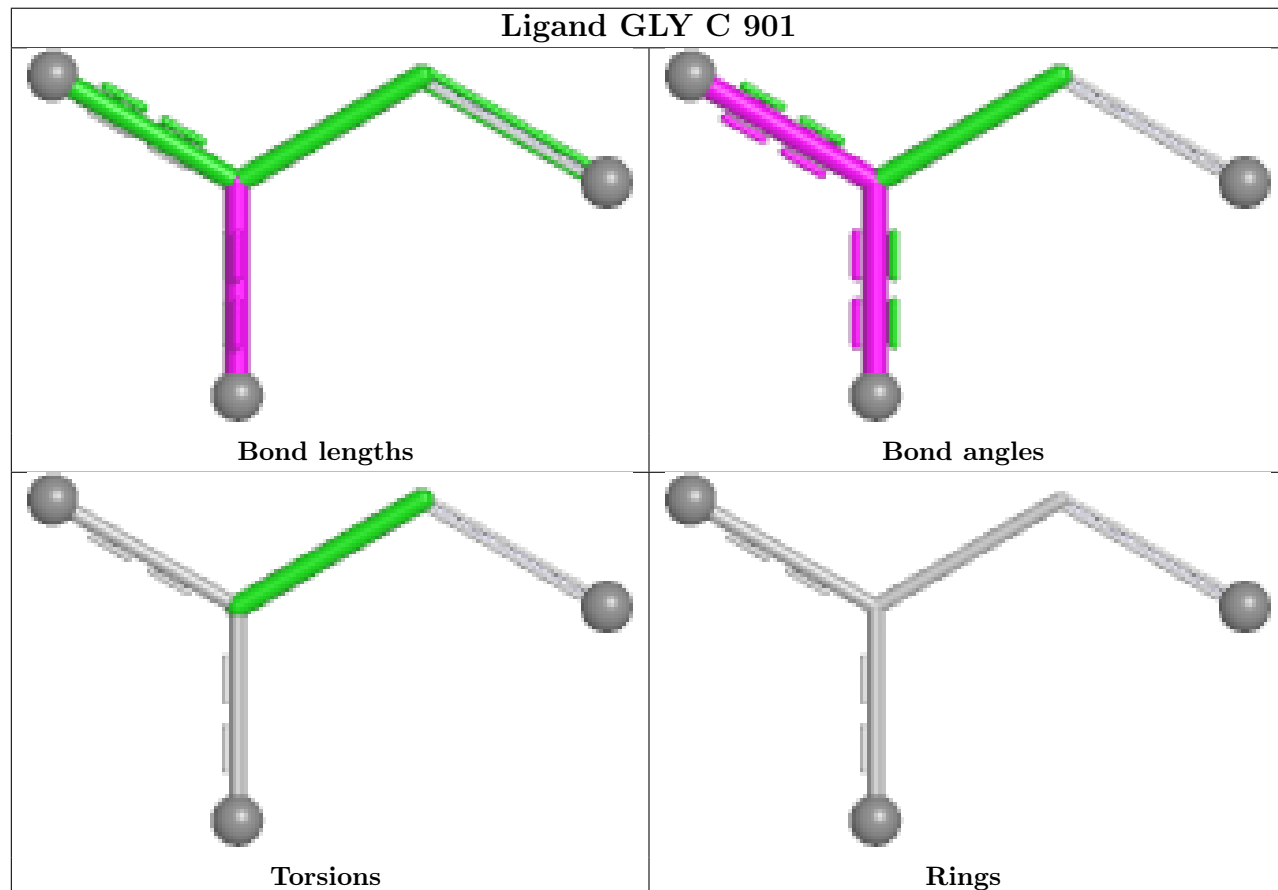
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

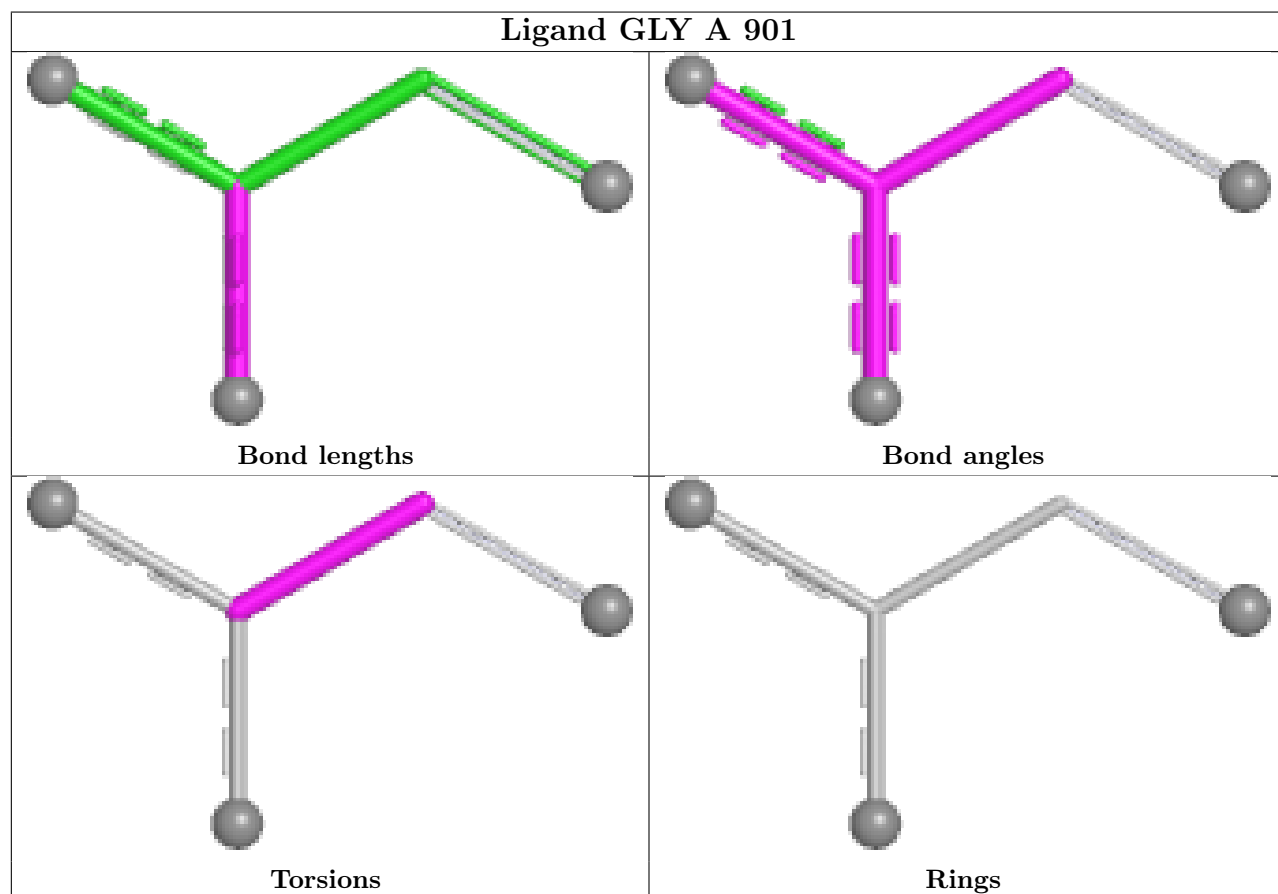
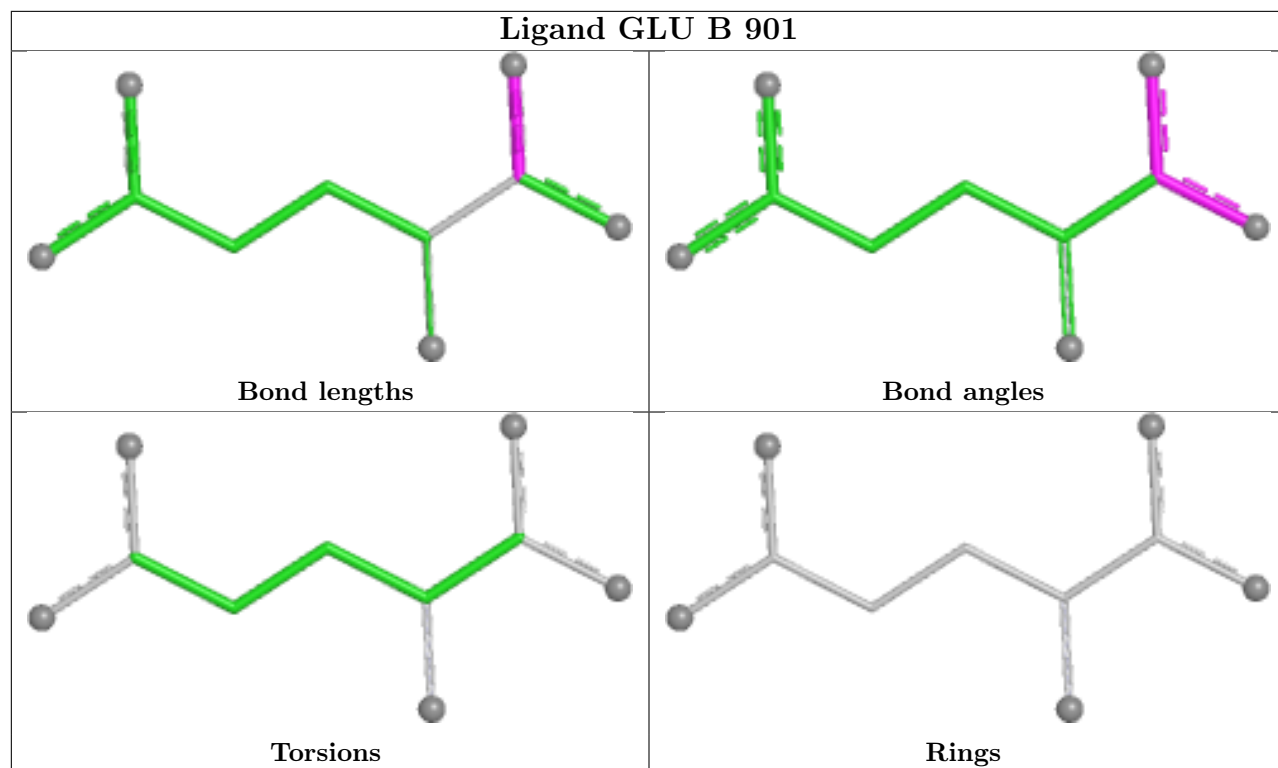


Ligand JC9 B 903



Ligand GLY C 901





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.

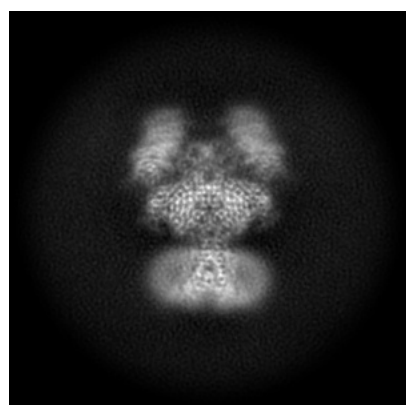
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46531. These allow visual inspection of the internal detail of the map and identification of artifacts.

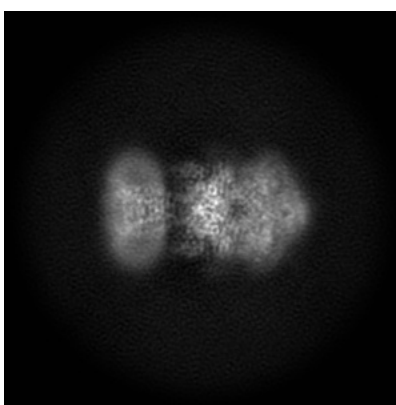
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

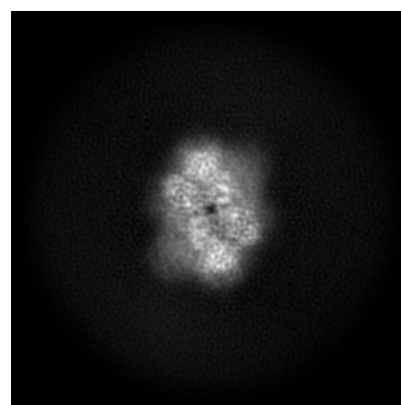
6.1.1 Primary map



X



Y

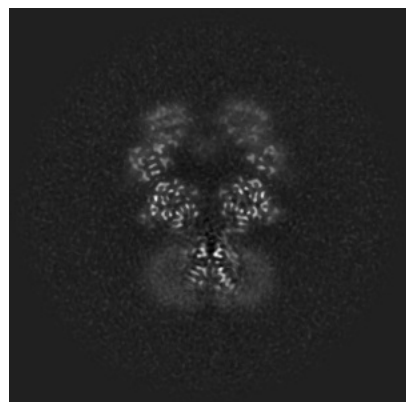


Z

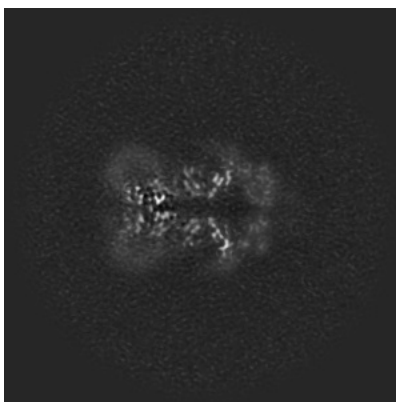
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

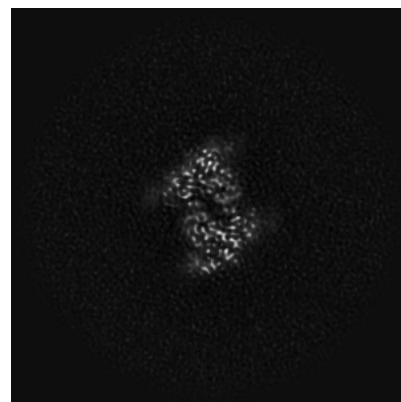
6.2.1 Primary map



X Index: 200



Y Index: 200

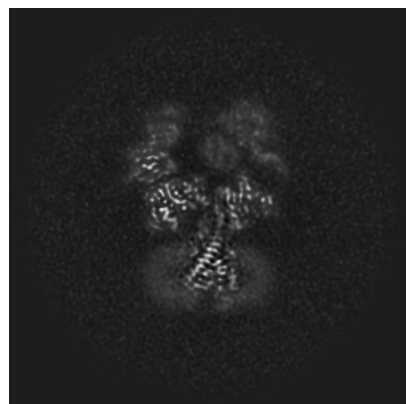


Z Index: 200

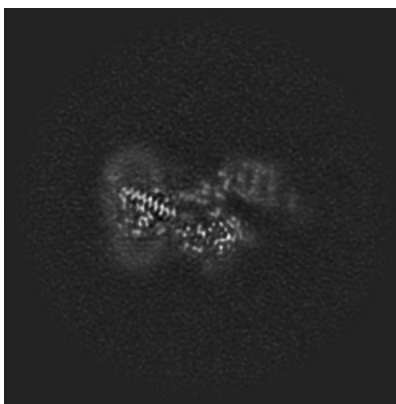
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

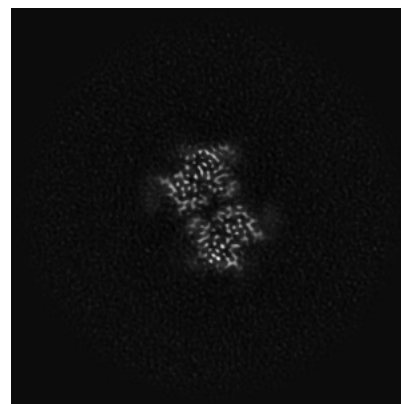
6.3.1 Primary map



X Index: 209



Y Index: 210

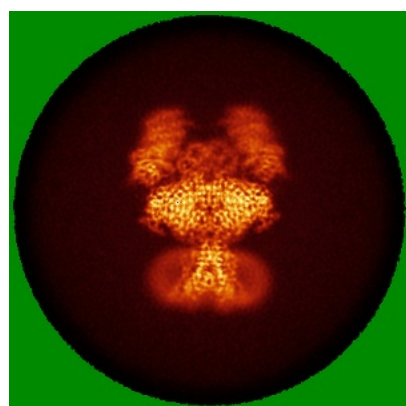


Z Index: 210

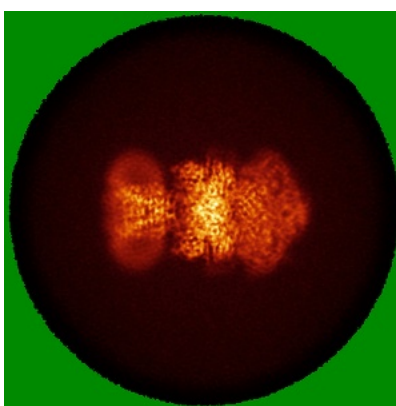
The images above show the largest variance slices of the map in three orthogonal directions.

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

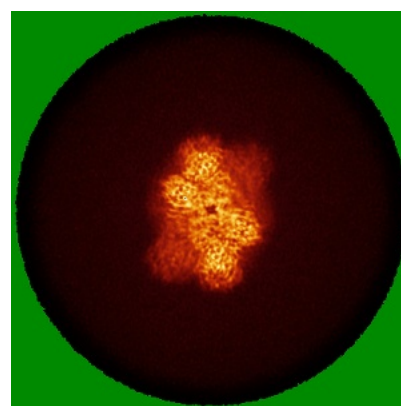
6.4.1 Primary map



X



Y

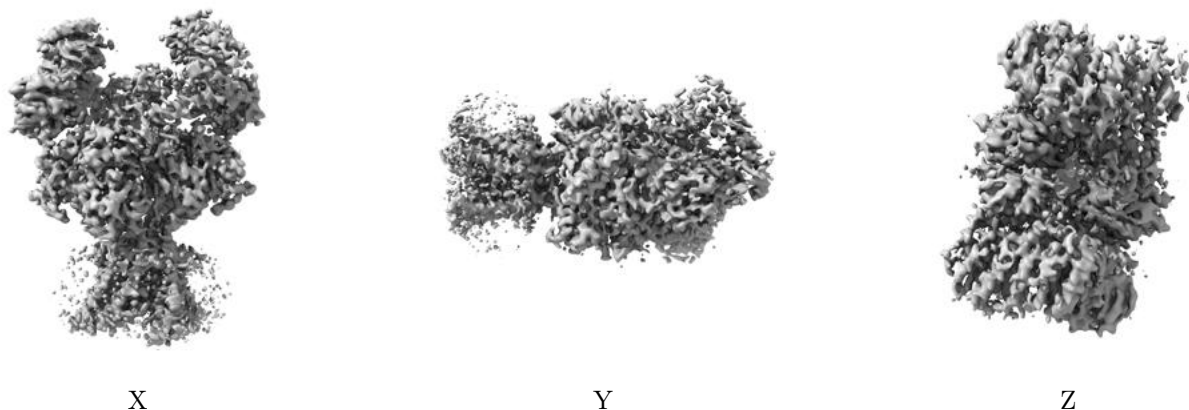


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

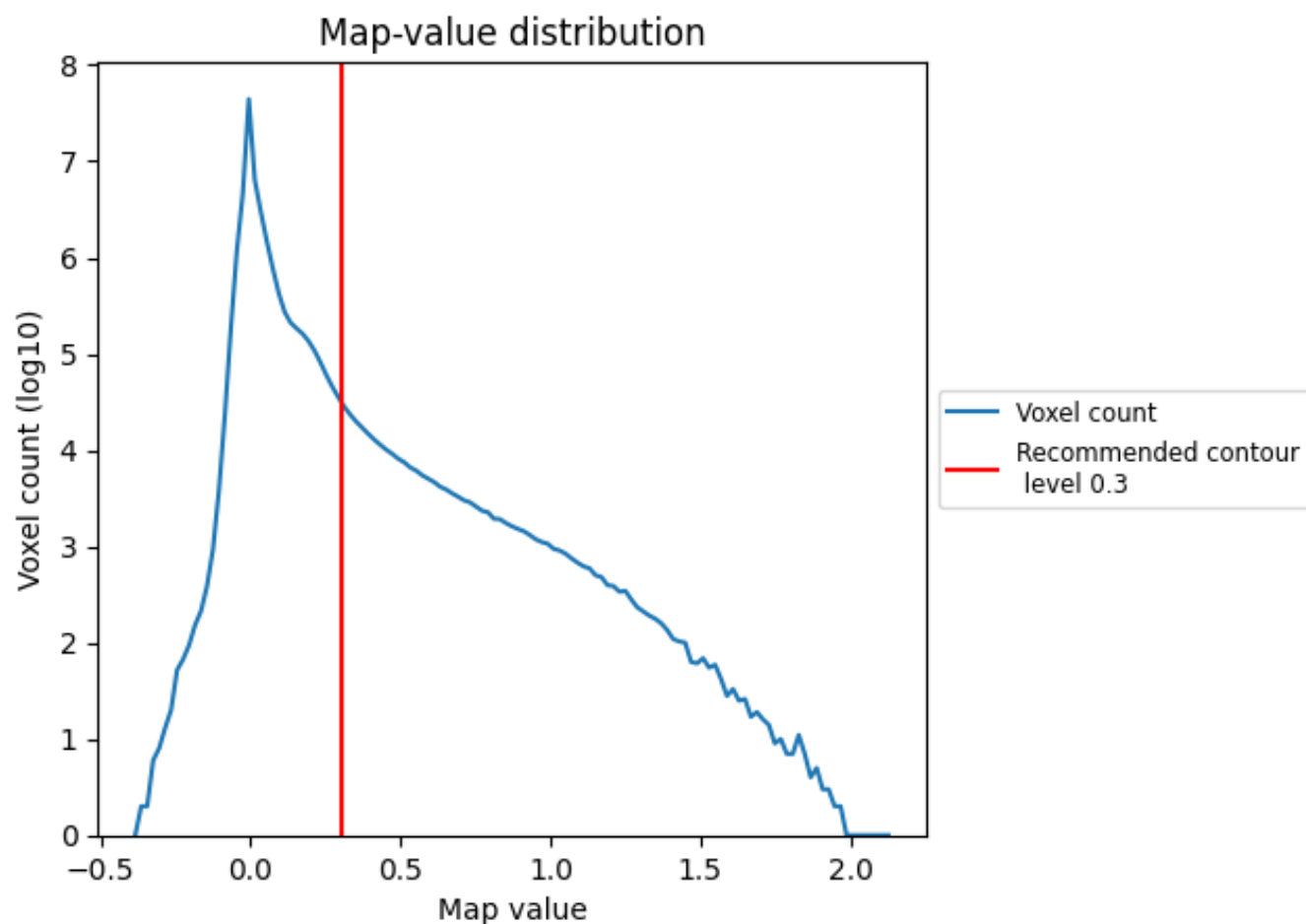
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

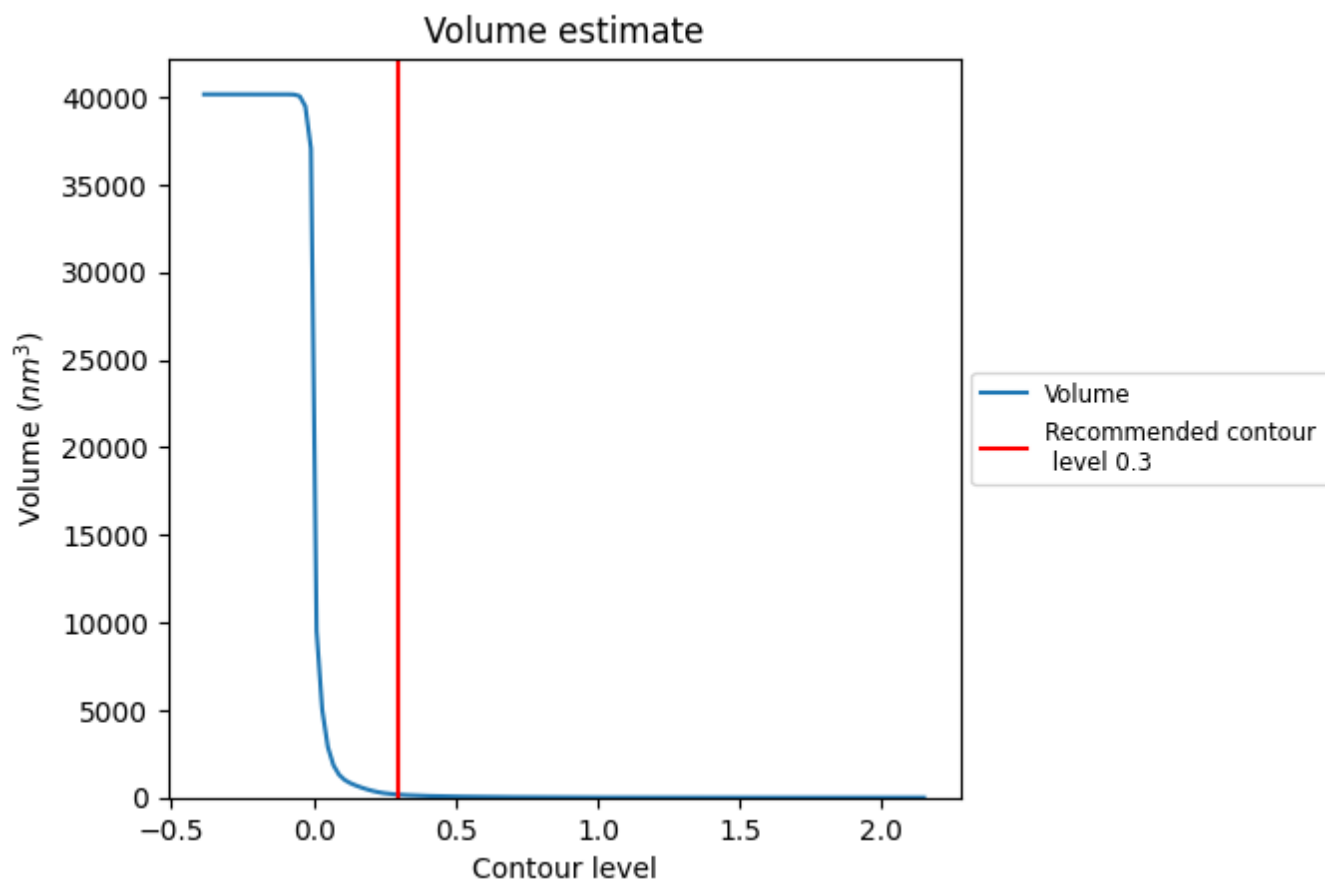
This section contains the results of statistical analysis of the map.

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.

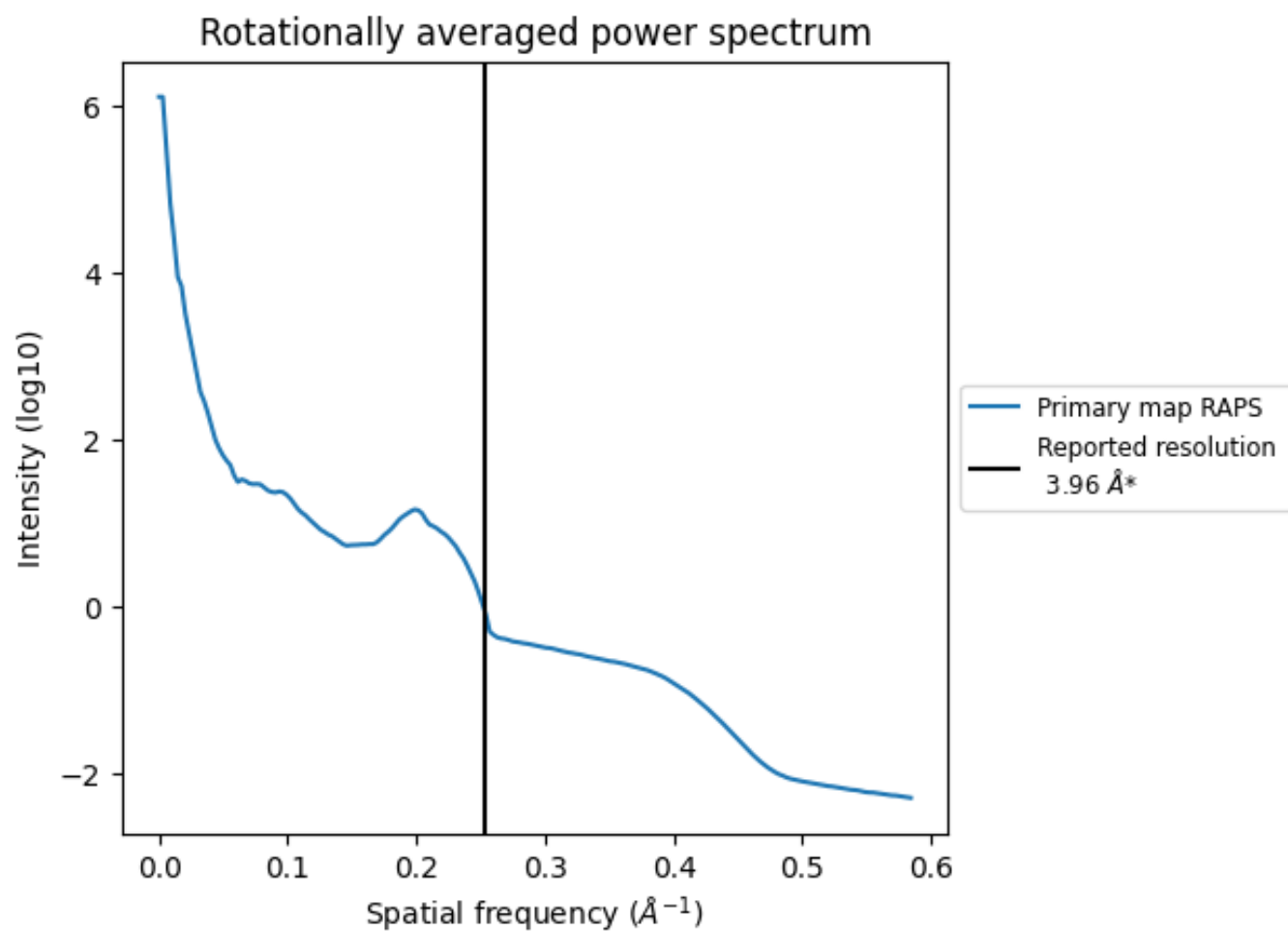
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm³; this corresponds to an approximate mass of 150 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 ⓘ

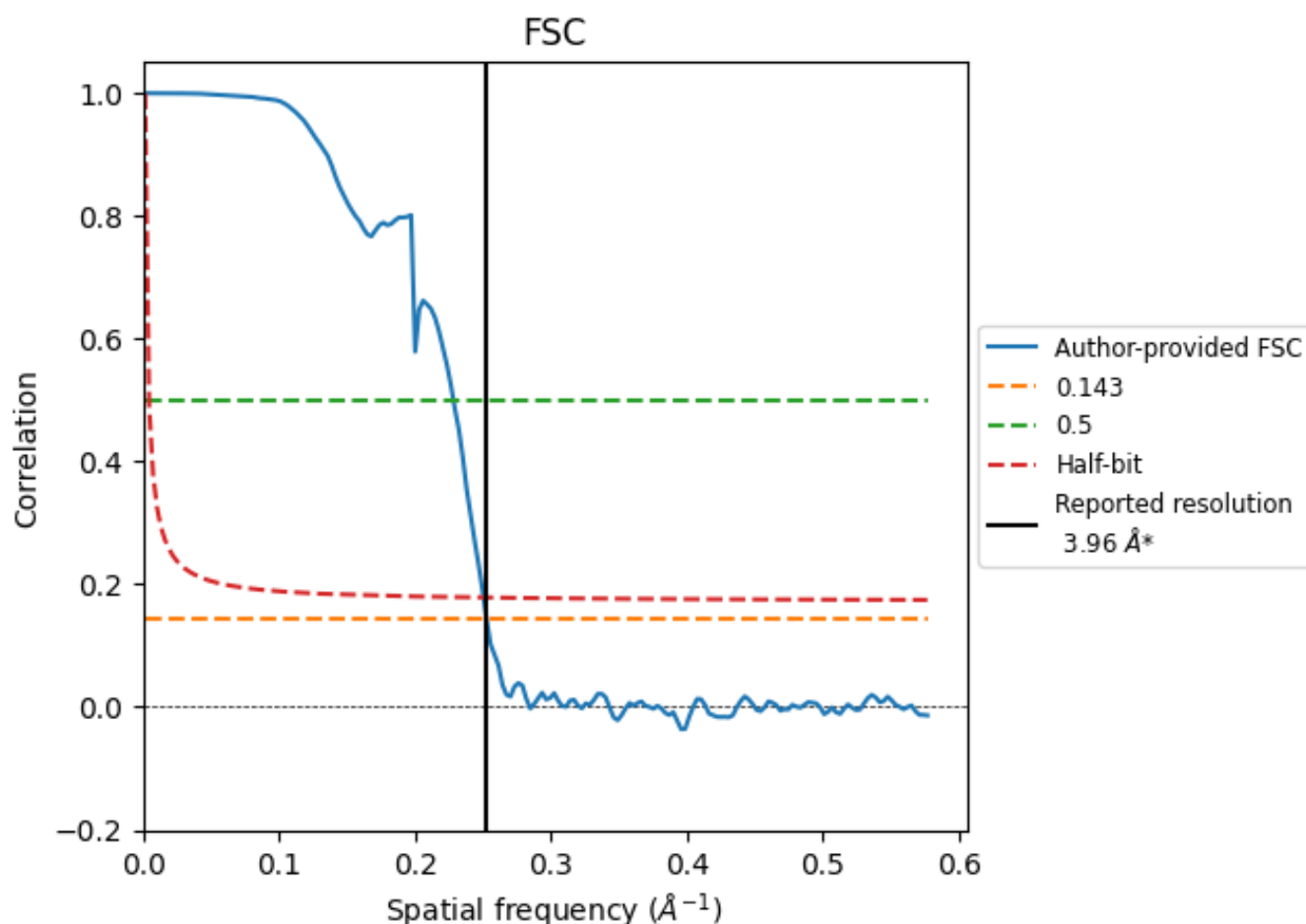


*Reported resolution corresponds to spatial frequency of 0.253 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

8.2 Resolution estimates [i](#)

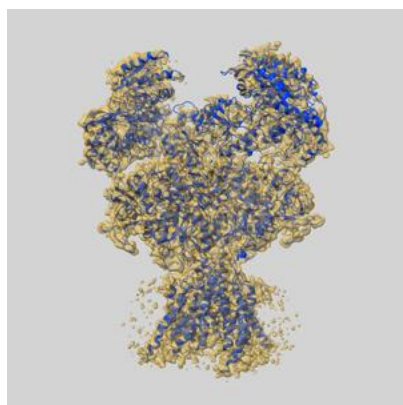
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	3.96	4.38	3.99
Unmasked-calculated*	-	-	-

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

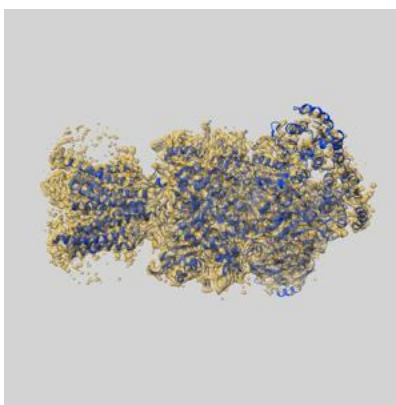
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46531 and PDB model 9D3C. Per-residue inclusion information can be found in section [3](#) on page [10](#).

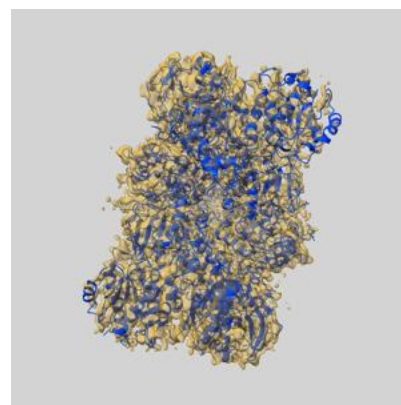
9.1 Map-model overlay [i](#)



X



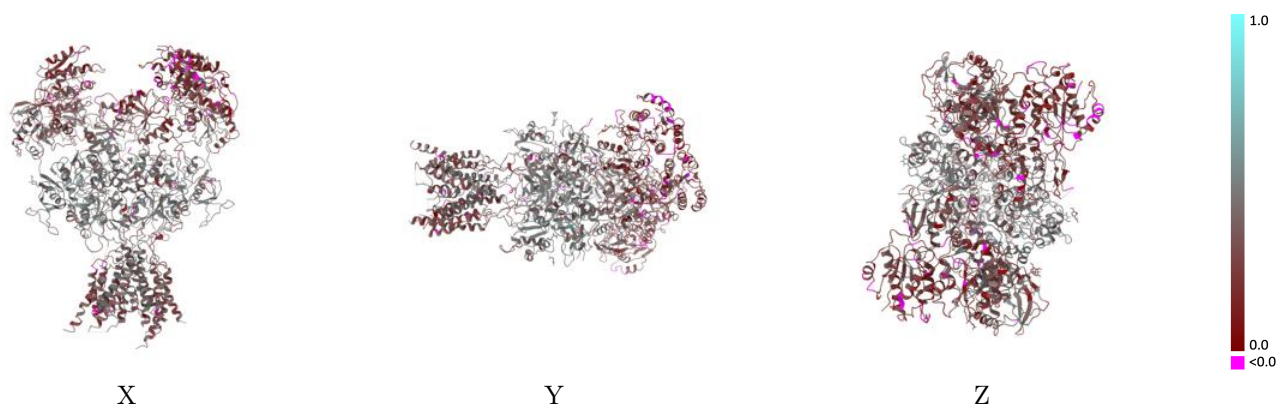
Y



Z

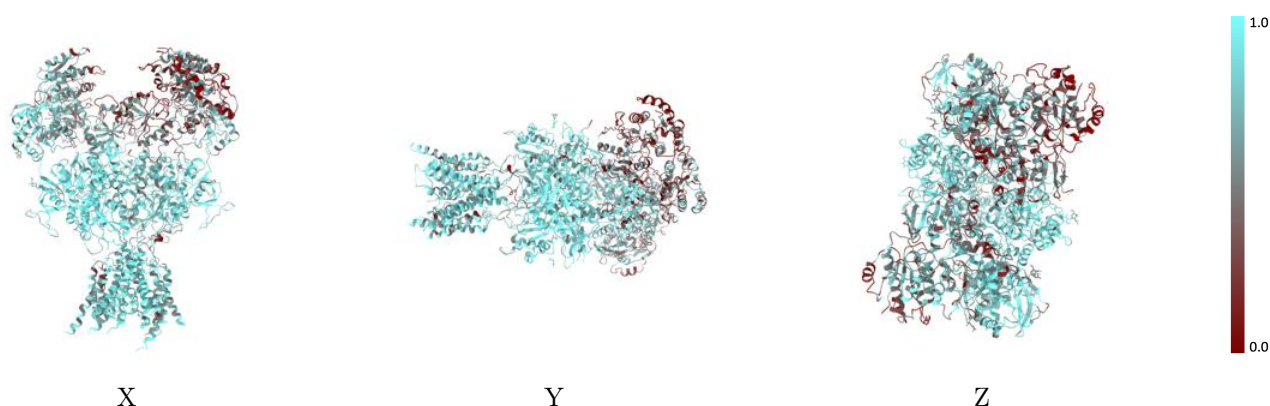
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



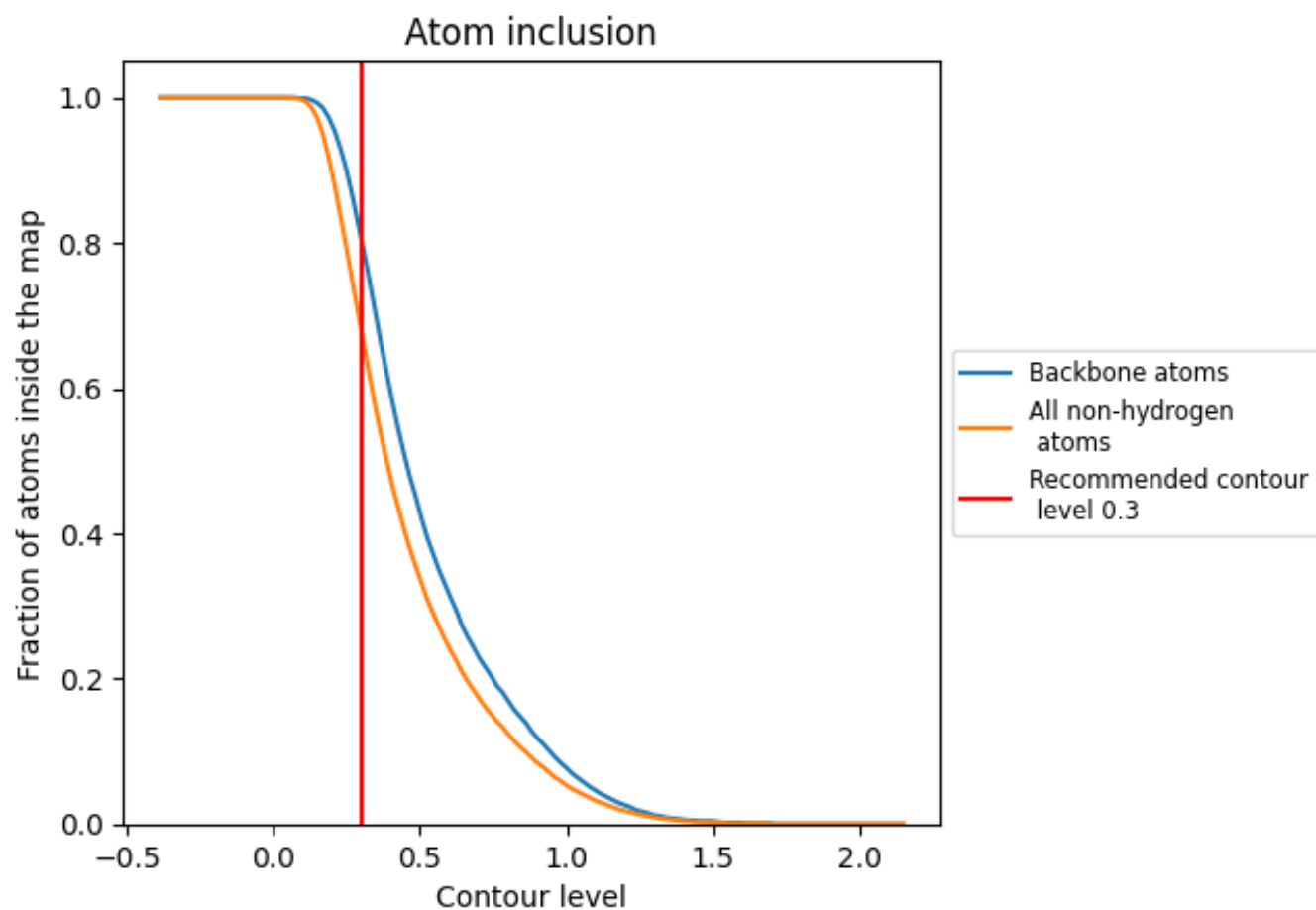
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6800	0.3530
A	0.7490	0.3700
B	0.6850	0.3560
C	0.6830	0.3500
D	0.5980	0.3360
E	0.7860	0.4160

