



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 05:47 PM UTC

PDB ID : 9D39 / pdb_00009d39
EMDB ID : EMD-46528
Title : Gly-,PPDA- bound GluN1a-2B-2D NMDAR
Authors : Hyunook, K.; Hiro, F.
Deposited on : 2024-08-09
Resolution : 3.65 Å(reported)
Based on initial models : 8E96, 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.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

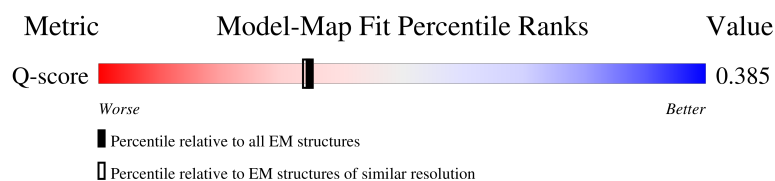
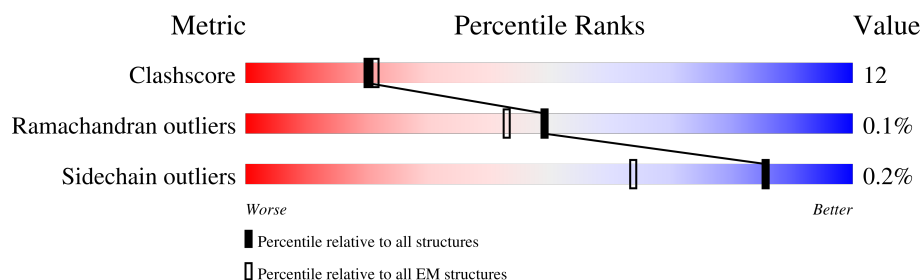
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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	11564 (3.15 - 4.15)

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	7% 68% 28% .
1	C	825	26% 71% 26% .
2	B	884	12% 63% 24% 12%
3	D	861	38% 68% 21% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24275 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	794	Total	C	N	O	S	0	0
			6196	3954	1068	1140	34		
1	C	799	Total	C	N	O	S	0	0
			6235	3981	1066	1153	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	775	Total	C	N	O	S	0	0
			5852	3778	947	1091	36		

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	764	Total	C	N	O	S	0	0
			5884	3779	1001	1075	29		

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



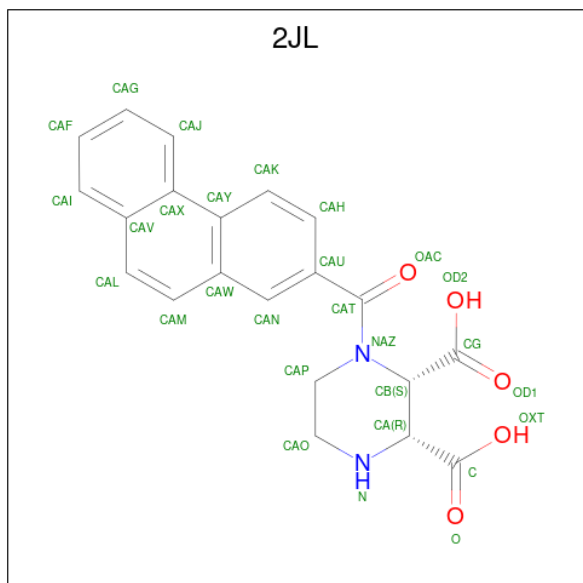
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

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

- Molecule 6 is (2S,3R)-1-(phenanthren-2-ylcarbonyl)piperazine-2,3-dicarboxylic acid (CCD ID: 2JL) (formula: C₂₁H₁₈N₂O₅) (labeled as "Ligand of Interest" by depositor).

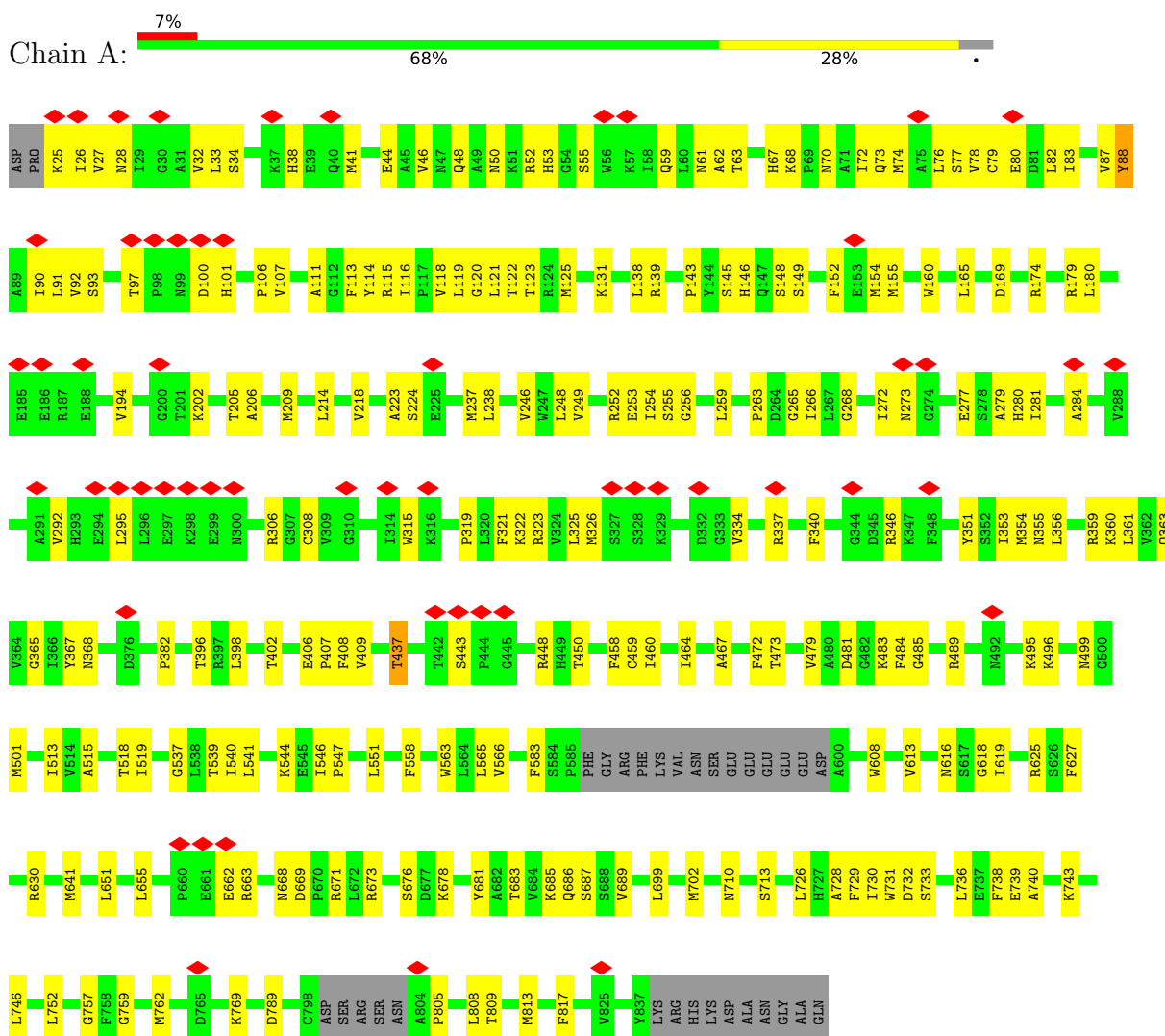


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			28	21	2	5	
6	D	1	Total	C	N	O	0
			28	21	2	5	

3 Residue-property plots [i](#)

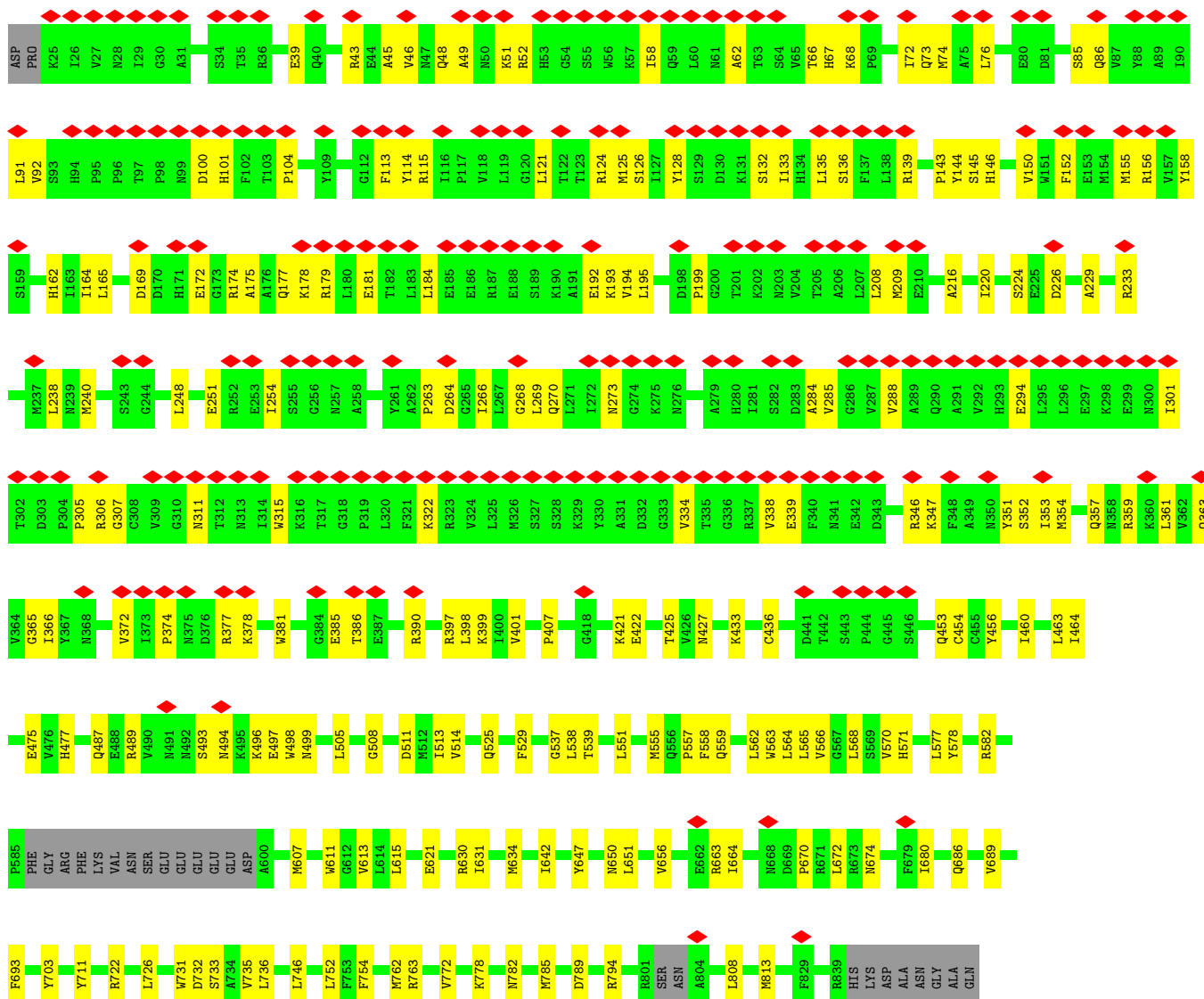
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

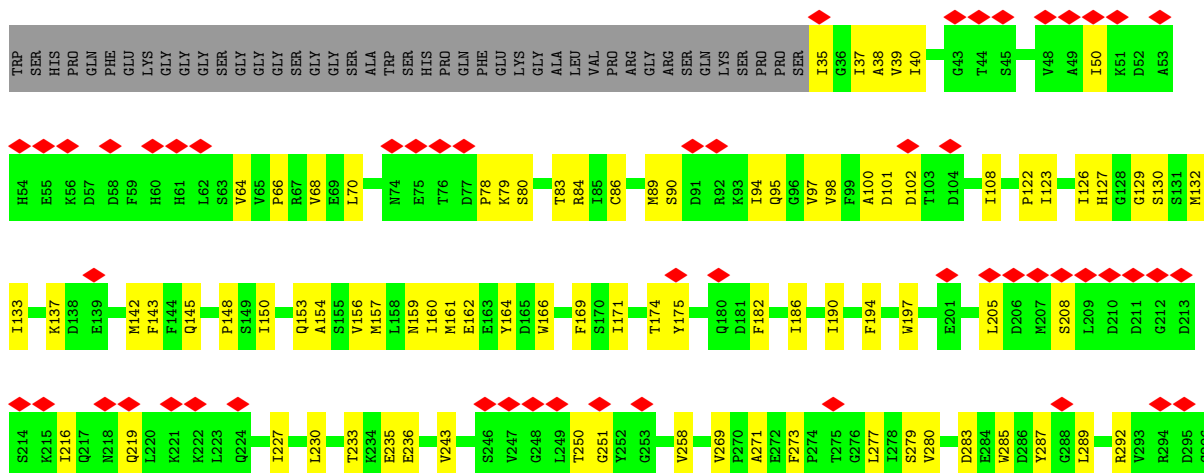


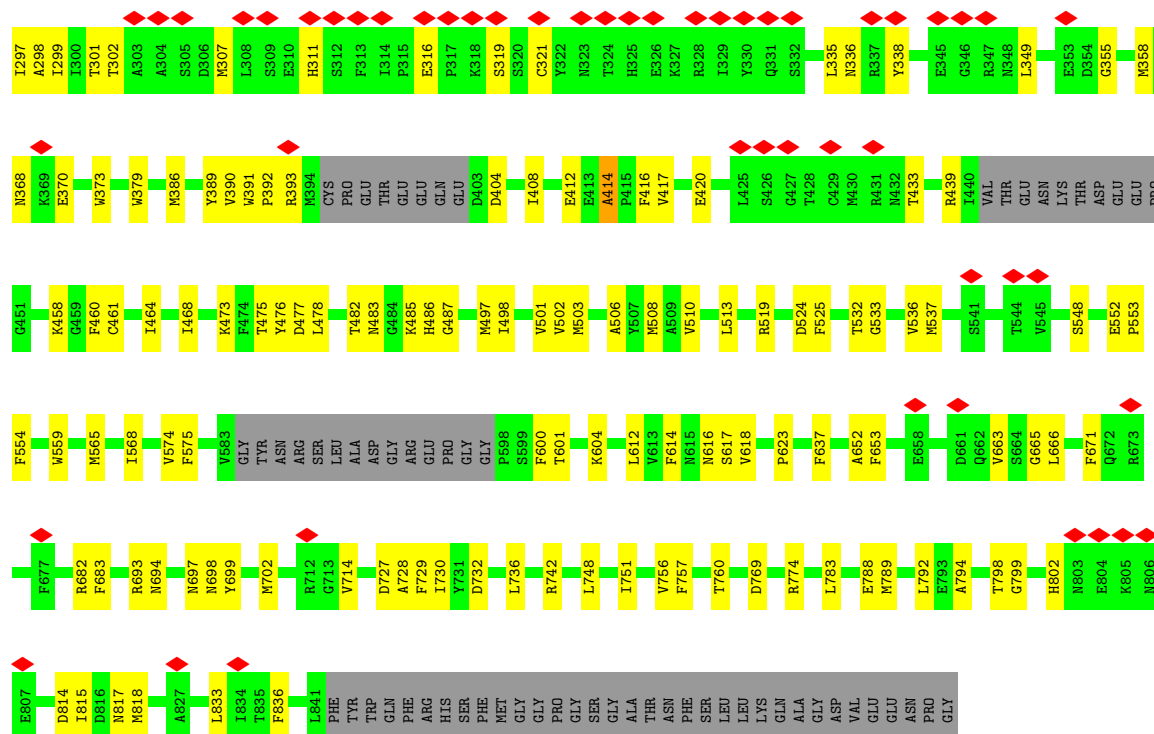
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



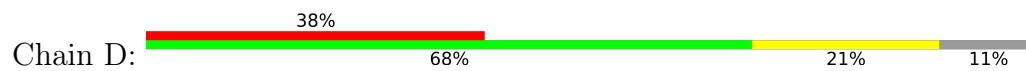


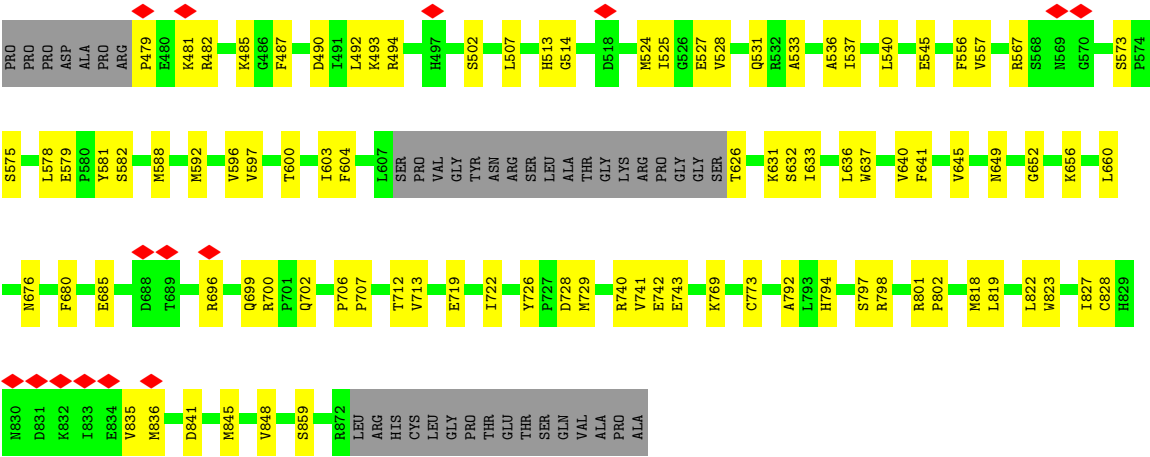
• Molecule 2: Glutamate receptor ionotropic, NMDA 2B





• Molecule 3: Glutamate receptor ionotropic, NMDA 2D





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72214	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 ($e^-/\text{\AA}^2$)	59.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.554	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	330.80002, 330.80002, 330.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: 2JL, NAG

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	0.12	0/6335	0.30	0/8594
1	C	0.11	0/6376	0.29	0/8652
2	B	0.11	0/5978	0.28	0/8130
3	D	0.10	0/6021	0.28	0/8193
All	All	0.11	0/24710	0.29	0/33569

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	6196	0	6141	171	0
1	C	6235	0	6164	168	0
2	B	5852	0	5652	157	0
3	D	5884	0	5784	128	0
4	A	5	0	2	2	0
4	C	5	0	2	1	0
5	A	28	0	26	0	0
5	C	14	0	13	0	0
6	B	28	0	16	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	28	0	16	6	0
All	All	24275	0	23816	590	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 12.

All (590) 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)
2:B:552:GLU:HG2	2:B:553:PRO:HD3	1.60	0.81
1:A:155:MET:HB2	1:A:160:TRP:HB2	1.63	0.80
2:B:205:LEU:HB2	2:B:219:GLN:HE22	1.46	0.80
1:A:655:LEU:HD13	3:D:676:ASN:HD22	1.48	0.76
1:C:399:LYS:HZ3	1:C:475:GLU:HG3	1.52	0.75
1:C:693:PHE:HB3	1:C:703:TYR:HB2	1.69	0.72
1:C:670:PRO:O	1:C:674:ASN:ND2	2.23	0.72
2:B:132:MET:SD	2:B:132:MET:N	2.57	0.72
2:B:160:ILE:HD11	2:B:364:ILE:HG12	1.71	0.71
1:A:149:SER:HB2	1:A:179:ARG:HH21	1.55	0.71
2:B:90:SER:HA	2:B:319:SER:HB3	1.72	0.71
1:A:546:ILE:HD12	1:A:547:PRO:HD2	1.74	0.70
1:C:557:PRO:HG3	1:C:651:LEU:HD13	1.73	0.70
1:A:120:GLY:N	1:A:138:LEU:O	2.25	0.70
1:A:326:MET:SD	1:A:326:MET:N	2.63	0.70
2:B:666:LEU:HD21	2:B:757:PHE:HB2	1.75	0.69
3:D:194:ALA:HB3	3:D:197:HIS:HB3	1.73	0.69
2:B:159:ASN:HD22	2:B:379:TRP:HE1	1.39	0.68
2:B:307:MET:SD	2:B:307:MET:N	2.67	0.68
1:A:279:ALA:HB1	1:A:334:VAL:HG21	1.74	0.67
3:D:365:MET:SD	3:D:365:MET:N	2.68	0.67
1:C:499:ASN:ND2	1:C:686:GLN:OE1	2.29	0.66
1:A:73:GLN:O	1:A:77:SER:N	2.29	0.66
1:A:668:ASN:HA	1:A:673:ARG:HD3	1.76	0.66
1:A:537:GLY:HA3	1:A:752:LEU:HB3	1.77	0.65
1:A:115:ARG:HH22	1:A:321:PHE:HB3	1.60	0.65
2:B:794:ALA:HA	2:B:798:THR:HB	1.77	0.65
3:D:597:VAL:HG11	3:D:633:ILE:HG12	1.76	0.65
1:C:731:TRP:HB3	1:C:736:LEU:HD21	1.77	0.65
3:D:155:LYS:NZ	3:D:161:PHE:O	2.29	0.65
1:A:789:ASP:N	1:A:789:ASP:OD1	2.30	0.65
2:B:154:ALA:HA	2:B:157:MET:HE2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:PRO:HG2	3:D:680:PHE:HA	1.78	0.65
1:C:551:LEU:HD23	1:C:808:LEU:HD11	1.79	0.65
2:B:122:PRO:HA	2:B:142:MET:HB3	1.79	0.65
1:C:73:GLN:HA	1:C:76:LEU:HD12	1.79	0.64
1:A:272:ILE:O	1:A:273:ASN:ND2	2.30	0.64
2:B:408:ILE:HG13	2:B:508:MET:HB3	1.79	0.64
1:A:121:LEU:HD12	1:A:122:THR:HG23	1.80	0.64
2:B:694:ASN:O	2:B:698:ASN:ND2	2.30	0.64
1:C:363:GLN:NE2	1:C:365:GLY:O	2.30	0.64
1:A:668:ASN:OD1	1:A:673:ARG:NH1	2.31	0.64
1:C:177:GLN:HE21	1:C:194:VAL:HG11	1.63	0.64
3:D:740:ARG:HB3	3:D:743:GLU:HB3	1.78	0.64
1:A:50:ASN:HD21	1:A:59:GLN:HB2	1.61	0.64
2:B:287:TYR:HD2	2:B:292:ARG:HG2	1.64	0.63
1:A:152:PHE:HA	1:A:155:MET:HE3	1.80	0.63
1:C:115:ARG:O	1:C:315:TRP:NE1	2.32	0.63
1:C:357:GLN:NE2	1:C:378:LYS:O	2.31	0.63
1:A:739:GLU:OE1	1:A:743:LYS:NZ	2.31	0.63
2:B:150:ILE:HD11	2:B:182:PHE:HB2	1.81	0.63
1:C:307:GLY:O	1:C:311:ASN:ND2	2.32	0.62
1:C:752:LEU:HD12	1:C:752:LEU:H	1.64	0.62
2:B:473:LYS:HD2	2:B:473:LYS:O	1.98	0.62
1:A:165:LEU:HB2	1:A:194:VAL:HG12	1.81	0.62
1:A:123:THR:O	1:A:139:ARG:NH2	2.32	0.62
2:B:38:ALA:HB3	2:B:97:VAL:HG12	1.81	0.61
1:C:352:SER:HA	1:C:366:ILE:HA	1.81	0.61
1:A:259:LEU:O	1:A:359:ARG:NH2	2.27	0.61
1:A:616:ASN:ND2	2:B:617:SER:OG	2.33	0.61
1:A:224:SER:HA	1:A:252:ARG:HD2	1.82	0.61
2:B:487:GLY:HA3	2:B:498:ILE:HD12	1.82	0.61
3:D:410:ARG:O	3:D:410:ARG:NH1	2.33	0.61
3:D:119:ASP:HB3	3:D:146:GLY:HA3	1.81	0.61
3:D:445:VAL:HG21	3:D:507:LEU:HD21	1.82	0.61
1:C:67:HIS:HB2	1:C:74:MET:HE1	1.81	0.61
1:C:421:LYS:NZ	1:C:422:GLU:O	2.34	0.61
3:D:836:MET:HE2	3:D:836:MET:HA	1.81	0.61
2:B:307:MET:HE1	2:B:338:TYR:HD2	1.65	0.61
2:B:637:PHE:HB2	1:C:615:LEU:HD23	1.83	0.61
1:A:292:VAL:HA	1:A:295:LEU:HB3	1.82	0.60
3:D:536:ALA:HB3	3:D:792:ALA:HB3	1.83	0.60
3:D:726:TYR:HB2	3:D:729:MET:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:HE1	2:B:78:PRO:HG3	1.67	0.60
2:B:439:ARG:HB2	2:B:482:THR:HG21	1.84	0.59
3:D:236:LEU:O	3:D:244:ARG:NH1	2.35	0.59
2:B:142:MET:HE2	2:B:142:MET:HA	1.85	0.59
1:A:625:ARG:HA	1:A:630:ARG:HH21	1.68	0.59
1:C:354:MET:HE3	1:C:354:MET:HA	1.85	0.59
1:A:115:ARG:HE	1:A:319:PRO:HA	1.68	0.59
1:A:91:LEU:HD12	1:A:121:LEU:HD23	1.84	0.58
1:A:736:LEU:HA	1:A:739:GLU:HB2	1.85	0.58
1:C:208:LEU:HD11	1:C:238:LEU:HD12	1.85	0.58
1:A:539:THR:HG23	1:A:733:SER:HB2	1.85	0.58
2:B:714:VAL:HG11	6:B:901:2JL:H8	1.85	0.58
1:C:778:LYS:HE3	1:C:782:ASN:HD21	1.67	0.58
1:C:169:ASP:H	1:C:199:PRO:HD3	1.68	0.58
1:C:571:HIS:HA	1:C:607:MET:HE1	1.85	0.58
2:B:95:GLN:NE2	2:B:316:GLU:OE2	2.37	0.58
1:C:365:GLY:HA2	1:C:374:PRO:HD2	1.85	0.58
1:A:732:ASP:OD2	4:A:901:GLY:N	2.36	0.58
1:A:115:ARG:HG3	1:A:315:TRP:HE1	1.69	0.58
1:A:28:ASN:ND2	1:A:63:THR:OG1	2.37	0.58
3:D:696:ARG:HA	3:D:699:GLN:HB2	1.86	0.57
1:C:135:LEU:O	1:C:322:LYS:NZ	2.33	0.57
3:D:115:VAL:HB	3:D:141:ILE:HG23	1.86	0.57
2:B:414:ALA:HB2	6:B:901:2JL:H10	1.86	0.57
1:C:45:ALA:HB1	1:C:285:VAL:HG21	1.87	0.57
1:A:540:ILE:HG13	1:A:730:ILE:HG12	1.86	0.57
3:D:409:LEU:HD13	3:D:411:LEU:HD21	1.86	0.57
2:B:416:PHE:HA	2:B:460:PHE:HB3	1.87	0.57
1:C:114:TYR:OH	1:C:311:ASN:ND2	2.37	0.57
1:C:73:GLN:CD	1:C:73:GLN:H	2.12	0.57
1:C:125:MET:HE3	1:C:125:MET:HA	1.86	0.57
1:C:557:PRO:O	1:C:650:ASN:ND2	2.37	0.57
1:A:518:THR:N	4:A:901:GLY:O	2.35	0.56
3:D:797:SER:O	3:D:798:ARG:HG3	2.05	0.56
3:D:155:LYS:NZ	3:D:379:ASP:O	2.33	0.56
2:B:299:ILE:HD11	2:B:349:LEU:HB3	1.87	0.56
1:C:224:SER:OG	1:C:226:ASP:OD1	2.22	0.56
1:C:456:TYR:HA	1:C:460:ILE:HG21	1.88	0.56
1:C:178:LYS:H	1:C:178:LYS:HD3	1.71	0.56
1:A:319:PRO:O	1:A:323:ARG:N	2.36	0.56
2:B:287:TYR:CD2	2:B:292:ARG:HG2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:GLU:OE1	1:C:294:GLU:N	2.33	0.55
3:D:313:ARG:NH1	3:D:314:ASP:OD1	2.39	0.55
1:A:618:GLY:O	3:D:649:ASN:ND2	2.39	0.55
1:A:113:PHE:CE1	2:B:78:PRO:HG3	2.42	0.55
2:B:783:LEU:HB3	2:B:789:MET:HE3	1.88	0.55
1:C:238:LEU:HB2	1:C:240:MET:HE1	1.88	0.55
1:A:143:PRO:HD2	1:A:146:HIS:HD2	1.72	0.55
1:C:91:LEU:HD12	1:C:121:LEU:HD23	1.88	0.55
1:A:32:VAL:HB	1:A:93:SER:HB3	1.89	0.55
1:A:78:VAL:HG12	1:A:83:ILE:HG23	1.89	0.55
2:B:477:ASP:OD1	2:B:477:ASP:N	2.40	0.55
1:C:92:VAL:HG11	1:C:104:PRO:HB3	1.89	0.55
1:C:139:ARG:HE	1:C:143:PRO:HD3	1.72	0.55
1:C:564:LEU:HD12	1:C:564:LEU:H	1.71	0.55
3:D:185:THR:OG1	3:D:214:GLY:O	2.25	0.55
1:C:305:PRO:HD3	1:C:315:TRP:HB3	1.89	0.55
1:C:493:SER:OG	1:C:494:ASN:N	2.39	0.55
1:C:732:ASP:OD2	4:C:901:GLY:N	2.40	0.55
1:C:209:MET:HE3	1:C:209:MET:O	2.07	0.55
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.89	0.54
2:B:39:VAL:HA	2:B:98:VAL:HG23	1.89	0.54
2:B:79:LYS:O	2:B:83:THR:OG1	2.22	0.54
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.88	0.54
1:C:220:ILE:HG12	1:C:248:LEU:HB2	1.89	0.54
1:C:511:ASP:OD1	1:C:763:ARG:NH2	2.41	0.54
3:D:728:ASP:N	3:D:728:ASP:OD1	2.39	0.54
1:C:680:ILE:HG22	1:C:726:LEU:HD13	1.90	0.54
1:C:139:ARG:HH21	1:C:143:PRO:HG3	1.72	0.54
2:B:774:ARG:NH2	1:C:525:GLN:O	2.39	0.54
1:C:489:ARG:HA	1:C:496:LYS:HA	1.89	0.54
1:A:206:ALA:HA	1:A:209:MET:HE1	1.88	0.54
1:A:662:GLU:O	1:A:671:ARG:NH1	2.40	0.54
3:D:524:MET:HG2	3:D:536:ALA:HB1	1.90	0.54
3:D:685:GLU:HA	3:D:835:VAL:HG22	1.90	0.54
2:B:699:TYR:HB3	2:B:702:MET:HB3	1.88	0.54
1:C:48:GLN:OE1	1:C:52:ARG:NH2	2.41	0.54
1:C:555:MET:HE3	1:C:555:MET:HA	1.90	0.54
2:B:174:THR:OG1	2:B:175:TYR:N	2.40	0.53
2:B:233:THR:HB	2:B:236:GLU:HG2	1.90	0.53
2:B:742:ARG:HG3	2:B:799:GLY:HA2	1.89	0.53
1:A:353:ILE:C	1:A:354:MET:HE2	2.33	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ASP:O	1:C:101:HIS:ND1	2.41	0.53
3:D:712:THR:OG1	3:D:713:VAL:N	2.42	0.53
1:A:281:ILE:HA	1:A:284:ALA:HB3	1.90	0.53
2:B:148:PRO:HB3	2:B:360:PRO:HG2	1.90	0.53
1:A:92:VAL:HG12	1:A:107:VAL:HG21	1.90	0.53
2:B:732:ASP:O	2:B:736:LEU:HB2	2.09	0.53
1:A:351:TYR:HB2	1:A:367:TYR:HB3	1.90	0.52
1:A:681:TYR:HB3	1:A:728:ALA:HB3	1.90	0.52
3:D:362:ARG:HH21	3:D:363:TYR:HB3	1.73	0.52
3:D:578:LEU:HD23	3:D:578:LEU:H	1.73	0.52
1:A:354:MET:HB3	1:A:361:LEU:HD12	1.91	0.52
1:A:437:THR:O	1:A:437:THR:OG1	2.27	0.52
2:B:814:ASP:H	2:B:817:ASN:HB2	1.74	0.52
3:D:430:GLN:O	3:D:502:SER:N	2.38	0.52
2:B:433:THR:HG22	2:B:458:LYS:HB3	1.91	0.52
2:B:612:LEU:HA	2:B:616:ASN:HB2	1.90	0.52
2:B:788:GLU:O	2:B:792:LEU:HD12	2.09	0.52
1:C:497:GLU:OE2	1:C:498:TRP:N	2.42	0.52
1:A:145:SER:O	1:A:148:SER:OG	2.28	0.52
1:A:619:ILE:HD12	3:D:656:LYS:HG3	1.92	0.52
2:B:64:VAL:HG13	2:B:66:PRO:HD3	1.92	0.52
2:B:663:VAL:HG13	2:B:665:GLY:H	1.75	0.52
3:D:514:GLY:HA3	3:D:525:ILE:HB	1.92	0.52
1:A:114:TYR:HE2	2:B:78:PRO:HD3	1.75	0.52
2:B:156:VAL:HG11	2:B:280:VAL:HG21	1.91	0.52
1:C:397:ARG:NE	1:C:475:GLU:OE1	2.43	0.52
2:B:161:MET:HE1	2:B:169:PHE:CD2	2.45	0.52
2:B:519:ARG:HB2	2:B:525:PHE:HE2	1.75	0.52
2:B:574:VAL:HG23	2:B:575:PHE:CD2	2.45	0.52
1:C:505:LEU:O	1:C:763:ARG:NH1	2.43	0.52
3:D:245:LEU:HA	3:D:273:PHE:HB3	1.91	0.52
2:B:416:PHE:HB3	2:B:461:CYS:SG	2.49	0.51
2:B:537:MET:HB2	2:B:729:PHE:HB3	1.92	0.51
1:C:178:LYS:HD3	1:C:178:LYS:N	2.25	0.51
2:B:365:ILE:HG12	2:B:373:TRP:HB3	1.91	0.51
1:C:254:ILE:HD11	1:C:268:GLY:HA3	1.91	0.51
1:C:49:ALA:HB1	1:C:58:ILE:HG22	1.93	0.51
3:D:388:VAL:HB	3:D:400:VAL:HG13	1.92	0.51
1:C:538:LEU:HD13	1:C:754:PHE:HB3	1.91	0.51
1:C:674:ASN:HD21	3:D:827:ILE:HG22	1.76	0.51
1:C:785:MET:HE2	1:C:785:MET:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:818:MET:HA	3:D:818:MET:HE3	1.93	0.51
2:B:64:VAL:HG23	2:B:301:THR:HG21	1.93	0.51
3:D:494:ARG:HH22	3:D:819:LEU:HD21	1.76	0.51
2:B:283:ASP:OD2	2:B:287:TYR:N	2.37	0.51
1:C:425:THR:HG23	1:C:427:ASN:H	1.75	0.51
2:B:536:VAL:HG22	2:B:730:ILE:HG12	1.92	0.50
1:C:86:GLN:OE1	1:C:306:ARG:NH2	2.37	0.50
3:D:223:LEU:HD13	3:D:232:LEU:HD13	1.92	0.50
3:D:741:VAL:HG21	6:D:901:2JL:H8	1.93	0.50
1:A:263:PRO:HG2	1:A:266:ILE:HD11	1.94	0.50
1:A:813:MET:HE1	3:D:581:TYR:HE1	1.76	0.50
2:B:142:MET:HE1	2:B:336:ASN:HB2	1.93	0.50
1:A:33:LEU:HD22	1:A:38:HIS:CE1	2.47	0.50
1:C:611:TRP:O	1:C:615:LEU:HD12	2.11	0.50
1:A:669:ASP:OD2	1:A:671:ARG:NH2	2.44	0.50
1:A:762:MET:HE1	1:A:769:LYS:HA	1.94	0.50
3:D:742:GLU:OE1	3:D:742:GLU:N	2.40	0.50
1:A:683:THR:HA	1:A:729:PHE:HE1	1.75	0.50
2:B:565:MET:HA	2:B:568:ILE:HG12	1.94	0.50
1:C:128:TYR:O	1:C:139:ARG:NH1	2.33	0.50
1:A:499:ASN:ND2	1:A:686:GLN:OE1	2.30	0.49
1:C:162:HIS:HD2	1:C:216:ALA:HA	1.77	0.49
3:D:626:THR:O	3:D:631:LYS:NZ	2.33	0.49
1:C:399:LYS:NZ	1:C:477:HIS:HD2	2.10	0.49
3:D:391:SER:HB3	3:D:401:VAL:HG11	1.95	0.49
1:C:634:MET:SD	3:D:637:TRP:HD1	2.35	0.49
1:A:111:ALA:HB1	1:A:116:ILE:HB	1.93	0.49
2:B:798:THR:O	2:B:802:HIS:ND1	2.45	0.49
1:C:284:ALA:O	1:C:288:VAL:HG23	2.13	0.49
1:A:26:ILE:HG12	1:A:59:GLN:HE21	1.78	0.49
1:A:254:ILE:HD11	1:A:268:GLY:HA3	1.93	0.49
1:A:519:ILE:HD11	1:A:759:GLY:HA3	1.93	0.49
2:B:420:GLU:N	2:B:420:GLU:OE1	2.46	0.49
3:D:368:THR:HG22	3:D:373:ASP:HA	1.94	0.49
2:B:216:ILE:HG13	2:B:243:VAL:HG11	1.94	0.49
2:B:693:ARG:O	2:B:697:ASN:ND2	2.46	0.49
1:C:401:VAL:HG23	1:C:513:ILE:HG23	1.93	0.49
1:A:154:MET:HE3	1:A:248:LEU:HG	1.94	0.49
3:D:440:ARG:HB3	6:D:901:2JL:H7	1.95	0.49
1:C:126:SER:N	1:C:172:GLU:OE1	2.39	0.49
1:A:78:VAL:HA	1:A:82:LEU:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:N	1:A:253:GLU:OE2	2.34	0.48
1:A:813:MET:HE1	3:D:581:TYR:CE1	2.48	0.48
1:C:39:GLU:OE2	1:C:66:THR:OG1	2.26	0.48
1:C:124:ARG:NH1	1:C:251:GLU:OE1	2.46	0.48
1:A:608:TRP:CE2	3:D:656:LYS:HD2	2.48	0.48
2:B:101:ASP:OD1	2:B:102:ASP:N	2.46	0.48
2:B:501:VAL:HG22	2:B:506:ALA:HB3	1.96	0.48
1:C:558:PHE:HB2	1:C:563:TRP:HE1	1.79	0.48
1:C:762:MET:HE1	1:C:772:VAL:HG11	1.95	0.48
1:C:789:ASP:OD1	1:C:794:ARG:NH1	2.46	0.48
1:C:372:VAL:HG12	1:C:374:PRO:HD3	1.96	0.48
3:D:513:HIS:HA	3:D:524:MET:HE3	1.94	0.48
3:D:527:GLU:O	3:D:533:ALA:N	2.45	0.48
1:A:541:LEU:HD11	1:A:746:LEU:HD12	1.95	0.48
1:C:263:PRO:HD2	1:C:266:ILE:HD11	1.94	0.48
1:C:338:VAL:HG12	1:C:346:ARG:HE	1.77	0.48
3:D:53:VAL:HG11	3:D:324:VAL:HG11	1.95	0.48
3:D:556:PHE:HD1	3:D:557:VAL:HG23	1.78	0.48
1:C:193:LYS:HG2	1:C:195:LEU:HD22	1.96	0.48
1:C:578:TYR:CZ	1:C:582:ARG:HD2	2.49	0.48
3:D:384:ASN:OD1	3:D:406:GLN:NE2	2.47	0.48
3:D:244:ARG:HB2	3:D:272:TRP:CD1	2.49	0.47
3:D:604:PHE:HE1	3:D:652:GLY:H	1.62	0.47
3:D:187:PHE:CD1	3:D:187:PHE:C	2.92	0.47
2:B:148:PRO:HG2	2:B:153:GLN:HE21	1.80	0.47
3:D:190:VAL:HG22	3:D:221:LEU:HG	1.97	0.47
2:B:169:PHE:HZ	2:B:190:ILE:HG13	1.79	0.47
2:B:389:TYR:HD1	2:B:390:VAL:HG13	1.77	0.47
2:B:548:SER:O	2:B:548:SER:OG	2.26	0.47
1:C:150:VAL:HG21	1:C:351:TYR:HD2	1.80	0.47
1:C:354:MET:HG3	1:C:361:LEU:HD13	1.96	0.47
1:A:165:LEU:HD21	1:A:180:LEU:HD23	1.97	0.47
1:A:450:THR:O	1:A:450:THR:OG1	2.31	0.47
1:C:164:ILE:HG22	1:C:192:GLU:HB2	1.95	0.47
1:C:381:TRP:HB2	1:C:385:GLU:HG3	1.96	0.47
3:D:100:VAL:HG12	3:D:133:LEU:HD22	1.95	0.47
1:A:83:ILE:HA	1:A:87:VAL:HG12	1.95	0.47
1:A:496:LYS:HE3	2:B:194:PHE:HA	1.96	0.47
2:B:783:LEU:HB3	2:B:789:MET:CE	2.45	0.47
2:B:833:LEU:HA	2:B:836:PHE:HB3	1.96	0.47
1:C:133:ILE:HD13	3:D:152:LEU:HG	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LEU:HD21	1:C:194:VAL:HG13	1.97	0.47
3:D:137:THR:HA	3:D:356:ARG:HH12	1.78	0.47
3:D:194:ALA:O	3:D:197:HIS:ND1	2.48	0.47
1:A:41:MET:HE1	1:A:281:ILE:HD11	1.97	0.47
1:A:407:PRO:HB3	1:A:738:PHE:CD2	2.50	0.47
1:A:408:PHE:HA	1:A:458:PHE:HB3	1.97	0.47
1:A:485:GLY:HA2	1:A:499:ASN:O	2.15	0.47
1:A:558:PHE:HB2	1:A:563:TRP:CE2	2.50	0.47
1:A:762:MET:HE3	1:A:762:MET:HB2	1.78	0.47
2:B:123:ILE:HG23	2:B:143:PHE:HD1	1.80	0.47
2:B:235:GLU:OE1	2:B:235:GLU:HA	2.14	0.47
1:C:113:PHE:HA	3:D:125:ALA:HB1	1.95	0.47
1:C:390:ARG:HA	1:C:390:ARG:HD2	1.59	0.47
1:C:642:ILE:HG21	3:D:848:VAL:HG21	1.95	0.47
3:D:545:GLU:OE1	3:D:545:GLU:N	2.46	0.47
1:C:68:LYS:HG2	1:C:73:GLN:HB2	1.97	0.47
2:B:250:THR:OG1	2:B:251:GLY:N	2.48	0.47
1:A:354:MET:HE2	1:A:354:MET:N	2.29	0.47
2:B:652:ALA:HA	1:C:656:VAL:HG22	1.95	0.47
1:A:25:LYS:HB2	1:A:25:LYS:HE3	1.68	0.46
1:A:34:SER:HA	1:A:67:HIS:HB2	1.98	0.46
1:A:481:ASP:N	1:A:481:ASP:OD1	2.48	0.46
2:B:175:TYR:HE2	2:B:208:SER:HB2	1.79	0.46
3:D:349:ARG:HH21	3:D:352:ASN:HA	1.81	0.46
1:A:70:ASN:HB2	1:A:72:ILE:HG12	1.96	0.46
1:A:809:THR:HA	3:D:582:SER:HB3	1.97	0.46
1:C:269:LEU:HB3	1:C:353:ILE:HG22	1.97	0.46
3:D:223:LEU:HD12	3:D:256:VAL:HG12	1.96	0.46
3:D:363:TYR:HA	3:D:365:MET:HE1	1.97	0.46
2:B:86:CYS:HB3	2:B:321:CYS:HB3	1.62	0.46
3:D:184:TRP:CE3	3:D:243:ILE:HD11	2.50	0.46
3:D:441:PRO:HD3	6:D:901:2JL:H10	1.97	0.46
3:D:845:MET:O	3:D:848:VAL:HG12	2.15	0.46
1:A:27:VAL:O	1:A:61:ASN:N	2.32	0.46
1:A:409:VAL:HG22	1:A:459:CYS:HB3	1.98	0.46
1:C:264:ASP:HA	1:C:359:ARG:HH22	1.80	0.46
2:B:50:ILE:HD11	2:B:289:LEU:HB3	1.96	0.46
3:D:52:ASN:ND2	3:D:110:LEU:O	2.49	0.46
3:D:333:ALA:HA	3:D:336:ARG:HE	1.81	0.46
3:D:421:ARG:O	3:D:423:LEU:N	2.49	0.46
2:B:130:SER:O	2:B:145:GLN:NE2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:PRO:HG3	1:C:735:VAL:HA	1.97	0.46
3:D:481:LYS:HD2	3:D:481:LYS:C	2.41	0.46
1:A:91:LEU:HD13	1:A:119:LEU:HB2	1.97	0.46
1:C:72:ILE:HB	3:D:349:ARG:HH11	1.81	0.46
1:C:398:LEU:HD12	1:C:398:LEU:HA	1.78	0.46
1:C:494:ASN:HB2	3:D:211:SER:HA	1.97	0.46
1:A:565:LEU:HD13	2:B:815:ILE:HG12	1.97	0.46
2:B:137:LYS:HZ2	2:B:355:GLY:HA3	1.81	0.46
1:C:174:ARG:C	1:C:178:LYS:HZ3	2.23	0.46
1:C:487:GLN:HB2	1:C:498:TRP:CE2	2.49	0.46
3:D:490:ASP:HA	3:D:493:LYS:HG2	1.97	0.46
1:C:263:PRO:O	1:C:266:ILE:HG12	2.16	0.46
3:D:444:ILE:N	3:D:485:LYS:O	2.45	0.46
1:A:218:VAL:HA	1:A:246:VAL:HG23	1.98	0.45
2:B:68:VAL:HG23	2:B:68:VAL:O	2.16	0.45
1:C:135:LEU:HD13	3:D:195:PRO:HB3	1.98	0.45
1:C:436:CYS:O	1:C:453:GLN:N	2.44	0.45
1:C:778:LYS:HB3	1:C:778:LYS:HE2	1.76	0.45
3:D:160:THR:HG23	3:D:360:LEU:HD23	1.99	0.45
3:D:528:VAL:HG21	3:D:536:ALA:HB2	1.98	0.45
1:A:205:THR:HG21	1:A:237:MET:HE2	1.97	0.45
1:A:255:SER:OG	1:A:256:GLY:N	2.49	0.45
2:B:137:LYS:NZ	2:B:355:GLY:HA3	2.31	0.45
2:B:666:LEU:HA	2:B:671:PHE:CD2	2.51	0.45
1:C:49:ALA:HA	1:C:52:ARG:HD3	1.99	0.45
3:D:128:PRO:HG3	3:D:152:LEU:HD21	1.97	0.45
3:D:440:ARG:O	3:D:444:ILE:HD11	2.15	0.45
1:A:484:PHE:HB2	1:A:687:SER:HA	1.97	0.45
2:B:554:PHE:O	2:B:559:TRP:NE1	2.50	0.45
2:B:600:PHE:CE2	2:B:623:PRO:HB3	2.51	0.45
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.84	0.45
1:A:544:LYS:H	1:A:746:LEU:HA	1.82	0.45
2:B:532:THR:HG23	2:B:732:ASP:OD1	2.17	0.45
2:B:537:MET:HE2	2:B:748:LEU:HD12	1.99	0.45
1:C:433:LYS:HD3	1:C:454:CYS:SG	2.56	0.45
1:C:663:ARG:HD3	1:C:663:ARG:HA	1.64	0.45
1:C:101:HIS:C	1:C:104:PRO:HD2	2.41	0.45
1:C:463:LEU:HD13	1:C:514:VAL:HG11	1.98	0.45
3:D:600:THR:HA	3:D:603:ILE:HG22	1.99	0.45
3:D:822:LEU:HB3	3:D:823:TRP:CE3	2.51	0.45
1:A:563:TRP:HA	1:A:566:VAL:HG12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ARG:HG2	1:C:378:LYS:N	2.31	0.45
1:A:131:LYS:HA	1:A:131:LYS:HD3	1.85	0.45
1:C:557:PRO:HG2	1:C:647:TYR:CZ	2.51	0.45
3:D:351:GLN:HE22	3:D:356:ARG:HH21	1.64	0.45
1:A:676:SER:C	1:A:678:LYS:H	2.23	0.45
1:A:169:ASP:O	1:A:174:ARG:NH1	2.50	0.45
1:A:495:LYS:HA	1:A:495:LYS:HD2	1.75	0.45
2:B:175:TYR:CE2	2:B:208:SER:HB2	2.51	0.45
2:B:552:GLU:HG3	2:B:653:PHE:CG	2.52	0.45
1:C:162:HIS:CD2	1:C:216:ALA:HA	2.51	0.45
1:C:613:VAL:HG22	3:D:645:VAL:HG12	1.99	0.45
2:B:307:MET:HE1	2:B:338:TYR:CD2	2.49	0.45
2:B:483:ASN:OD1	2:B:483:ASN:N	2.49	0.45
1:A:34:SER:N	1:A:93:SER:HB2	2.32	0.44
1:A:70:ASN:OD1	1:A:70:ASN:N	2.49	0.44
2:B:273:PHE:HB3	2:B:277:LEU:HD23	1.99	0.44
1:C:145:SER:HB2	1:C:175:ALA:HB1	1.99	0.44
1:C:558:PHE:HB2	1:C:563:TRP:NE1	2.32	0.44
3:D:442:PHE:O	3:D:487:PHE:N	2.50	0.44
1:A:409:VAL:HG13	1:A:460:ILE:HG12	1.98	0.44
2:B:230:LEU:HB3	2:B:258:VAL:HG12	2.00	0.44
3:D:719:GLU:HA	3:D:722:ILE:HG22	2.00	0.44
1:A:209:MET:SD	1:A:209:MET:N	2.87	0.44
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.84	0.44
2:B:186:ILE:O	2:B:190:ILE:HG12	2.17	0.44
2:B:358:MET:HE3	2:B:358:MET:HB3	1.89	0.44
2:B:508:MET:HE3	2:B:508:MET:HB2	1.75	0.44
1:C:577:LEU:HD23	1:C:577:LEU:HA	1.83	0.44
3:D:567:ARG:NH2	3:D:773:CYS:SG	2.91	0.44
1:A:53:HIS:ND1	1:A:55:SER:OG	2.48	0.44
1:A:663:ARG:HD3	1:A:663:ARG:HA	1.71	0.44
1:C:156:ARG:HA	1:C:156:ARG:NE	2.33	0.44
1:C:352:SER:O	1:C:352:SER:OG	2.30	0.44
1:C:651:LEU:HD12	1:C:651:LEU:HA	1.78	0.44
1:A:74:MET:HB3	1:A:106:PRO:HG3	1.99	0.44
1:C:499:ASN:N	1:C:499:ASN:OD1	2.51	0.44
1:A:467:ALA:HA	1:A:472:PHE:CE1	2.52	0.44
1:C:51:LYS:C	1:C:52:ARG:HD2	2.43	0.44
3:D:597:VAL:HG13	3:D:632:SER:HB3	1.99	0.44
2:B:307:MET:HE2	2:B:335:LEU:HA	1.99	0.44
2:B:414:ALA:HB2	6:B:901:2JL:CAL	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ARG:NH1	1:C:136:SER:HB2	2.33	0.44
1:C:621:GLU:OE1	1:C:621:GLU:N	2.50	0.44
1:A:115:ARG:HH21	1:A:319:PRO:HA	1.82	0.44
1:A:263:PRO:O	1:A:266:ILE:HG12	2.17	0.44
1:A:685:LYS:HG2	1:A:710:ASN:HB3	2.00	0.44
2:B:35:ILE:HG23	2:B:95:GLN:HB2	2.00	0.44
1:A:641:MET:HE3	2:B:614:PHE:CD1	2.53	0.44
3:D:223:LEU:HD22	3:D:232:LEU:HD22	2.00	0.44
1:A:48:GLN:HB2	1:A:52:ARG:HH22	1.83	0.43
1:A:80:GLU:OE1	1:A:80:GLU:N	2.43	0.43
1:A:363:GLN:OE1	1:A:365:GLY:N	2.51	0.43
2:B:98:VAL:HB	2:B:126:ILE:HD11	1.99	0.43
2:B:258:VAL:HG23	2:B:279:SER:HB2	2.00	0.43
1:C:254:ILE:HG21	1:C:361:LEU:HD11	2.00	0.43
3:D:103:LEU:HD13	3:D:133:LEU:HD23	1.99	0.43
1:A:101:HIS:CD2	1:A:125:MET:HE3	2.53	0.43
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.78	0.43
1:A:308:CYS:SG	2:B:78:PRO:HD2	2.58	0.43
1:A:681:TYR:HA	1:A:726:LEU:HD11	1.99	0.43
1:A:752:LEU:HD12	1:A:752:LEU:H	1.83	0.43
3:D:573:SER:O	3:D:575:SER:N	2.51	0.43
1:C:559:GLN:HB2	3:D:841:ASP:HA	1.99	0.43
1:A:72:ILE:HD12	2:B:321:CYS:O	2.18	0.43
1:A:443:SER:O	1:A:443:SER:OG	2.31	0.43
2:B:601:THR:HG23	2:B:604:LYS:H	1.83	0.43
1:C:51:LYS:O	1:C:52:ARG:NH1	2.45	0.43
1:C:565:LEU:HA	1:C:568:LEU:HD23	2.00	0.43
2:B:80:SER:HB2	2:B:84:ARG:NH2	2.33	0.43
2:B:498:ILE:O	2:B:502:VAL:HG12	2.19	0.43
1:C:301:ILE:O	1:C:301:ILE:HG22	2.17	0.43
1:C:381:TRP:NE1	1:C:386:THR:O	2.50	0.43
1:C:537:GLY:HA3	1:C:752:LEU:HB3	2.00	0.43
3:D:699:GLN:HA	3:D:729:MET:HE2	1.99	0.43
1:A:337:ARG:NH2	1:A:368:ASN:O	2.51	0.43
1:A:731:TRP:HB3	1:A:736:LEU:HD11	2.00	0.43
2:B:101:ASP:HB3	2:B:129:GLY:H	1.83	0.43
1:A:519:ILE:HG12	1:A:757:GLY:O	2.19	0.43
2:B:503:MET:HE2	2:B:503:MET:N	2.34	0.43
1:C:132:SER:OG	3:D:153:THR:O	2.37	0.43
1:A:76:LEU:HB3	1:A:80:GLU:OE2	2.19	0.43
1:A:396:THR:O	1:A:473:THR:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLU:HA	1:A:280:HIS:HB2	2.00	0.43
1:A:683:THR:HA	1:A:729:PHE:CE1	2.54	0.43
2:B:133:ILE:HD13	2:B:133:ILE:HA	1.90	0.43
2:B:298:ALA:O	2:B:302:THR:HG22	2.19	0.43
2:B:498:ILE:HD11	2:B:513:LEU:HD21	2.01	0.43
2:B:524:ASP:OD2	2:B:769:ASP:N	2.51	0.43
1:C:115:ARG:HG3	1:C:315:TRP:HE1	1.82	0.43
1:C:269:LEU:HA	1:C:354:MET:H	1.83	0.43
3:D:706:PRO:HA	3:D:707:PRO:HD3	1.89	0.43
2:B:464:ILE:O	2:B:468:ILE:HG12	2.19	0.43
2:B:532:THR:HB	2:B:760:THR:O	2.18	0.43
1:A:306:ARG:NH1	1:A:306:ARG:HA	2.34	0.42
1:A:817:PHE:CZ	3:D:588:MET:HE1	2.54	0.42
1:C:115:ARG:HA	1:C:115:ARG:HD2	1.92	0.42
1:C:181:GLU:HA	1:C:184:LEU:HB2	2.01	0.42
1:C:607:MET:HE3	1:C:607:MET:HA	2.00	0.42
3:D:441:PRO:CD	6:D:901:2JL:H10	2.49	0.42
1:A:44:GLU:H	1:A:44:GLU:HG3	1.73	0.42
1:A:360:LYS:HD2	1:A:360:LYS:HA	1.73	0.42
1:A:406:GLU:HB3	1:A:407:PRO:HD3	2.00	0.42
1:A:651:LEU:HD12	1:A:651:LEU:HA	1.93	0.42
1:A:736:LEU:O	1:A:740:ALA:N	2.50	0.42
3:D:464:SER:HB2	3:D:482:ARG:NH2	2.34	0.42
3:D:660:LEU:HD23	3:D:660:LEU:HA	1.90	0.42
1:A:340:PHE:HE1	1:A:346:ARG:HB2	1.83	0.42
2:B:157:MET:HE1	2:B:182:PHE:CZ	2.54	0.42
2:B:307:MET:O	2:B:311:HIS:N	2.51	0.42
2:B:818:MET:HE2	2:B:818:MET:HB3	1.89	0.42
1:C:789:ASP:O	1:C:794:ARG:N	2.49	0.42
3:D:540:LEU:HD12	3:D:540:LEU:HA	1.82	0.42
1:A:46:VAL:HG11	1:A:62:ALA:HB2	2.01	0.42
1:A:265:GLY:O	1:A:382:PRO:HD3	2.19	0.42
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.91	0.42
2:B:404:ASP:O	2:B:475:THR:OG1	2.27	0.42
1:C:630:ARG:O	1:C:634:MET:HB2	2.20	0.42
1:A:460:ILE:O	1:A:464:ILE:HG12	2.19	0.42
2:B:127:HIS:CG	2:B:289:LEU:HD21	2.55	0.42
2:B:565:MET:HE3	2:B:565:MET:HB2	1.89	0.42
2:B:682:ARG:HB2	2:B:727:ASP:H	1.84	0.42
1:C:266:ILE:HD13	1:C:266:ILE:HA	1.88	0.42
1:C:273:ASN:ND2	1:C:346:ARG:HH12	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:789:MET:N	2:B:789:MET:HE2	2.35	0.42
1:C:155:MET:HA	1:C:158:TYR:HB2	2.02	0.42
1:C:631:ILE:HD11	3:D:859:SER:HA	2.01	0.42
3:D:98:SER:HA	3:D:101:LEU:HB2	2.02	0.42
3:D:416:TRP:HB3	3:D:479:PRO:HG2	2.01	0.42
3:D:656:LYS:HB2	3:D:656:LYS:HE3	1.51	0.42
6:D:901:2JL:H8	6:D:901:2JL:H9	1.83	0.42
1:A:61:ASN:OD1	1:A:62:ALA:N	2.49	0.42
1:A:152:PHE:CD1	1:A:152:PHE:C	2.97	0.42
1:A:551:LEU:HD23	1:A:808:LEU:HD11	2.02	0.42
2:B:277:LEU:HD12	2:B:277:LEU:HA	1.82	0.42
2:B:368:ASN:ND2	2:B:370:GLU:OE1	2.53	0.42
1:C:339:GLU:HB2	1:C:347:LYS:HB2	2.01	0.42
3:D:174:VAL:HG11	3:D:387:LEU:HD13	2.01	0.42
3:D:575:SER:O	3:D:579:GLU:HG3	2.20	0.42
3:D:592:MET:O	3:D:596:VAL:HG23	2.19	0.42
1:A:483:LYS:HG3	1:A:686:GLN:HG3	2.01	0.42
1:A:613:VAL:HG22	2:B:618:VAL:HG12	2.02	0.42
3:D:252:GLU:C	3:D:255:PRO:HD2	2.44	0.42
3:D:597:VAL:HG23	3:D:636:LEU:HD12	2.01	0.42
1:C:143:PRO:HD2	1:C:146:HIS:ND1	2.35	0.42
1:C:146:HIS:CE1	1:C:179:ARG:HH22	2.37	0.42
1:C:152:PHE:HA	1:C:155:MET:HE1	2.02	0.42
3:D:168:THR:HA	3:D:171:GLN:HB2	2.02	0.42
3:D:361:HIS:NE2	3:D:377:ASN:O	2.53	0.42
1:C:270:GLN:HB2	1:C:354:MET:SD	2.59	0.41
1:C:722:ARG:HG2	1:C:746:LEU:HD21	2.01	0.41
3:D:260:ALA:HB2	3:D:272:TRP:CH2	2.55	0.41
3:D:531:GLN:OE1	3:D:794:HIS:NE2	2.53	0.41
1:A:90:ILE:HG22	1:A:118:VAL:HG13	2.01	0.41
2:B:37:ILE:HG21	2:B:297:ILE:HG13	2.01	0.41
2:B:391:TRP:HA	2:B:392:PRO:HD3	1.91	0.41
2:B:461:CYS:HB3	2:B:510:VAL:HG22	2.00	0.41
2:B:476:TYR:HD2	2:B:478:LEU:HD13	1.86	0.41
3:D:700:ARG:HE	3:D:702:GLN:HE22	1.67	0.41
1:A:27:VAL:HG13	1:A:88:TYR:HD2	1.86	0.41
1:A:79:CYS:HA	1:A:83:ILE:HG12	2.00	0.41
2:B:683:PHE:HA	2:B:728:ALA:O	2.20	0.41
1:C:273:ASN:HD21	1:C:334:VAL:HG21	1.85	0.41
1:A:68:LYS:H	1:A:74:MET:HE1	1.86	0.41
1:A:249:VAL:HG22	1:A:268:GLY:HA2	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:HA	1:A:702:MET:HE1	2.02	0.41
2:B:164:TYR:OH	2:B:386:MET:SD	2.64	0.41
1:C:813:MET:HE3	1:C:813:MET:HB3	1.78	0.41
3:D:335:LEU:HD12	3:D:335:LEU:HA	1.90	0.41
1:A:202:LYS:HA	1:A:202:LYS:HD2	1.75	0.41
1:A:489:ARG:HD2	2:B:194:PHE:HB2	2.02	0.41
1:A:627:PHE:HD1	1:A:627:PHE:O	2.03	0.41
2:B:391:TRP:HE1	2:B:393:ARG:HH21	1.68	0.41
1:C:46:VAL:HG21	1:C:62:ALA:HB2	2.01	0.41
1:C:124:ARG:CZ	1:C:144:TYR:HE1	2.33	0.41
3:D:492:LEU:HD22	3:D:537:ILE:HG21	2.01	0.41
1:A:25:LYS:O	1:A:59:GLN:HG3	2.20	0.41
1:A:322:LYS:O	1:A:325:LEU:HB2	2.21	0.41
1:A:402:THR:HG23	1:A:515:ALA:HB2	2.02	0.41
2:B:40:ILE:O	2:B:100:ALA:N	2.50	0.41
2:B:663:VAL:HG12	2:B:751:ILE:HG12	2.02	0.41
2:B:736:LEU:HD12	2:B:736:LEU:HA	1.80	0.41
1:C:150:VAL:HG21	1:C:351:TYR:CD2	2.55	0.41
3:D:822:LEU:HB3	3:D:823:TRP:H	1.75	0.41
2:B:814:ASP:OD1	2:B:815:ILE:N	2.43	0.41
1:C:538:LEU:HD21	1:C:689:VAL:HG22	2.02	0.41
1:C:539:THR:HG23	1:C:733:SER:HB2	2.03	0.41
1:A:254:ILE:O	1:A:259:LEU:HG	2.21	0.41
1:A:259:LEU:HD21	1:A:361:LEU:HD21	2.02	0.41
3:D:74:ALA:O	3:D:78:ARG:NH2	2.47	0.41
3:D:640:VAL:HG13	3:D:641:PHE:CD1	2.56	0.41
1:A:501:MET:HB3	1:A:513:ILE:HD13	2.03	0.41
2:B:161:MET:HE2	2:B:197:TRP:HZ3	1.86	0.41
2:B:162:GLU:HG2	2:B:197:TRP:HH2	1.86	0.41
2:B:285:TRP:HZ3	2:B:363:VAL:HG21	1.86	0.41
1:C:85:SER:O	1:C:85:SER:OG	2.33	0.41
1:C:229:ALA:O	1:C:233:ARG:NH1	2.52	0.41
1:C:562:LEU:O	1:C:565:LEU:HG	2.21	0.41
1:A:97:THR:OG1	1:A:100:ASP:OD2	2.32	0.41
1:A:406:GLU:HG2	1:A:739:GLU:OE2	2.20	0.41
2:B:89:MET:HA	2:B:94:ILE:HG12	2.03	0.41
1:C:43:ARG:HA	1:C:46:VAL:HG22	2.03	0.41
1:A:583:PHE:O	1:A:583:PHE:CD2	2.74	0.40
1:A:683:THR:OG1	1:A:689:VAL:HG21	2.21	0.40
2:B:533:GLY:HA3	2:B:756:VAL:HG21	2.03	0.40
2:B:714:VAL:HG11	6:B:901:2JL:CAJ	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:GLY:HA2	1:C:763:ARG:HH12	1.85	0.40
2:B:485:LYS:HE2	2:B:485:LYS:HB2	1.99	0.40
1:C:194:VAL:O	1:C:194:VAL:HG12	2.21	0.40
3:D:769:LYS:HE3	3:D:769:LYS:HB3	1.64	0.40
3:D:827:ILE:HG13	3:D:828:CYS:N	2.35	0.40
1:A:68:LYS:H	1:A:68:LYS:HG2	1.62	0.40
1:A:115:ARG:NH2	1:A:322:LYS:H	2.19	0.40
1:A:355:ASN:OD1	1:A:356:LEU:N	2.54	0.40
1:A:448:ARG:HH11	1:A:448:ARG:HA	1.87	0.40
2:B:269:VAL:HG12	2:B:271:ALA:H	1.86	0.40
2:B:502:VAL:HG13	2:B:503:MET:CE	2.51	0.40
1:C:731:TRP:HA	1:C:731:TRP:CE3	2.56	0.40
2:B:412:GLU:HA	2:B:417:VAL:HG12	2.02	0.40
1:C:39:GLU:HB3	1:C:43:ARG:HH21	1.86	0.40
1:C:664:ILE:HD13	1:C:672:LEU:HD21	2.04	0.40
1:C:711:TYR:HE2	1:C:726:LEU:HD22	1.87	0.40
3:D:513:HIS:CG	6:D:901:2JL:H3	2.56	0.40
2:B:68:VAL:HB	2:B:70:LEU:HD21	2.04	0.40
2:B:108:ILE:HD12	2:B:108:ILE:HA	1.87	0.40
2:B:497:MET:O	2:B:501:VAL:HG23	2.21	0.40
1:C:399:LYS:HA	1:C:399:LYS:HD2	1.80	0.40
1:C:566:VAL:O	1:C:570:VAL:HG23	2.20	0.40
3:D:307:VAL:HG22	3:D:389:VAL:HA	2.04	0.40
3:D:351:GLN:HE22	3:D:356:ARG:HE	1.69	0.40
3:D:801:ARG:HB3	3:D:802:PRO:HD3	2.02	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	788/825 (96%)	725 (92%)	62 (8%)	1 (0%)	48 78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	793/825 (96%)	732 (92%)	61 (8%)	0	100	100
2	B	767/884 (87%)	721 (94%)	44 (6%)	2 (0%)	36	64
3	D	754/861 (88%)	691 (92%)	62 (8%)	1 (0%)	48	78
All	All	3102/3395 (91%)	2869 (92%)	229 (7%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	713	SER
2	B	486	HIS
3	D	418	ARG
2	B	414	ALA

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	667/710 (94%)	664 (100%)	3 (0%)	84	79
1	C	673/710 (95%)	671 (100%)	2 (0%)	86	81
2	B	611/760 (80%)	611 (100%)	0	100	100
3	D	616/701 (88%)	616 (100%)	0	100	100
All	All	2567/2881 (89%)	2562 (100%)	5 (0%)	85	84

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

Mol	Chain	Res	Type
1	A	88	TYR
1	A	437	THR
1	A	479	VAL
1	C	464	ILE
1	C	529	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	101	HIS
1	A	146	HIS
1	A	171	HIS
1	A	239	ASN
1	A	290	GLN
1	A	293	HIS
1	A	311	ASN
1	A	358	ASN
1	A	440	ASN
1	A	487	GLN
1	A	709	HIS
1	A	742	GLN
1	A	780	HIS
2	B	118	GLN
2	B	159	ASN
2	B	357	GLN
2	B	359	HIS
2	B	694	ASN
2	B	697	ASN
2	B	710	ASN
2	B	737	ASN
2	B	782	GLN
1	C	177	GLN
1	C	273	ASN
1	C	311	ASN
1	C	453	GLN
1	C	477	HIS
1	C	674	ASN
1	C	705	HIS
1	C	724	ASN
1	C	727	HIS
1	C	782	ASN
3	D	170	GLN
3	D	173	GLN
3	D	351	GLN
3	D	407	GLN
3	D	430	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	NAG	A	903	1	14,14,15	0.40	0	17,19,21	0.40	0
5	NAG	A	902	1	14,14,15	0.20	0	17,19,21	0.47	0
6	2JL	B	901	-	29,31,31	1.83	5 (17%)	39,45,45	1.58	6 (15%)
4	GLY	A	901	-	4,4,4	1.19	1 (25%)	3,4,4	1.61	0
6	2JL	D	901	-	29,31,31	1.80	5 (17%)	39,45,45	1.52	7 (17%)
4	GLY	C	901	-	4,4,4	1.16	1 (25%)	3,4,4	1.71	2 (66%)
5	NAG	C	902	1	14,14,15	0.40	0	17,19,21	0.53	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
5	NAG	A	903	1	-	4/6/23/26	0/1/1/1
5	NAG	A	902	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	2JL	B	901	-	-	5/15/30/30	0/4/4/4
4	GLY	A	901	-	-	1/2/2/2	-
6	2JL	D	901	-	-	4/15/30/30	0/4/4/4
4	GLY	C	901	-	-	0/2/2/2	-
5	NAG	C	902	1	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	2JL	CAT-NAZ	6.20	1.49	1.34
6	D	901	2JL	CAT-NAZ	6.05	1.48	1.34
6	B	901	2JL	CAU-CAT	3.99	1.56	1.50
6	D	901	2JL	CAU-CAT	3.80	1.56	1.50
6	D	901	2JL	CAY-CAW	-2.70	1.37	1.42
6	B	901	2JL	CAY-CAW	-2.65	1.37	1.42
6	B	901	2JL	CAX-CAV	-2.52	1.37	1.42
6	D	901	2JL	CAX-CAV	-2.47	1.37	1.42
4	A	901	GLY	OXT-C	-2.25	1.23	1.30
6	D	901	2JL	CA-C	2.23	1.56	1.52
4	C	901	GLY	OXT-C	-2.21	1.23	1.30
6	B	901	2JL	CA-C	2.20	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	901	2JL	OD2-CG-CB	5.17	120.48	111.92
6	D	901	2JL	OD2-CG-CB	4.71	119.71	111.92
6	B	901	2JL	OD1-CG-CB	-2.57	119.73	123.45
6	B	901	2JL	CAP-NAZ-CB	-2.40	108.53	116.24
6	D	901	2JL	CAM-CAW-CAN	-2.40	117.88	122.00
6	D	901	2JL	CAK-CAY-CAW	2.39	121.25	117.66
6	B	901	2JL	CAM-CAW-CAN	-2.37	117.92	122.00
6	B	901	2JL	CAK-CAY-CAW	2.29	121.08	117.66
6	D	901	2JL	CAH-CAK-CAY	-2.17	118.29	121.62
6	D	901	2JL	OD1-CG-CB	-2.16	120.32	123.45
6	B	901	2JL	CAH-CAK-CAY	-2.15	118.32	121.62
4	C	901	GLY	OXT-C-O	-2.13	117.85	123.33
6	D	901	2JL	CAP-NAZ-CB	-2.07	109.59	116.24
6	D	901	2JL	CAK-CAY-CAX	-2.04	118.23	122.35
4	C	901	GLY	OXT-C-CA	2.01	121.38	113.38

There are no chirality outliers.

All (16) torsion outliers are listed below:

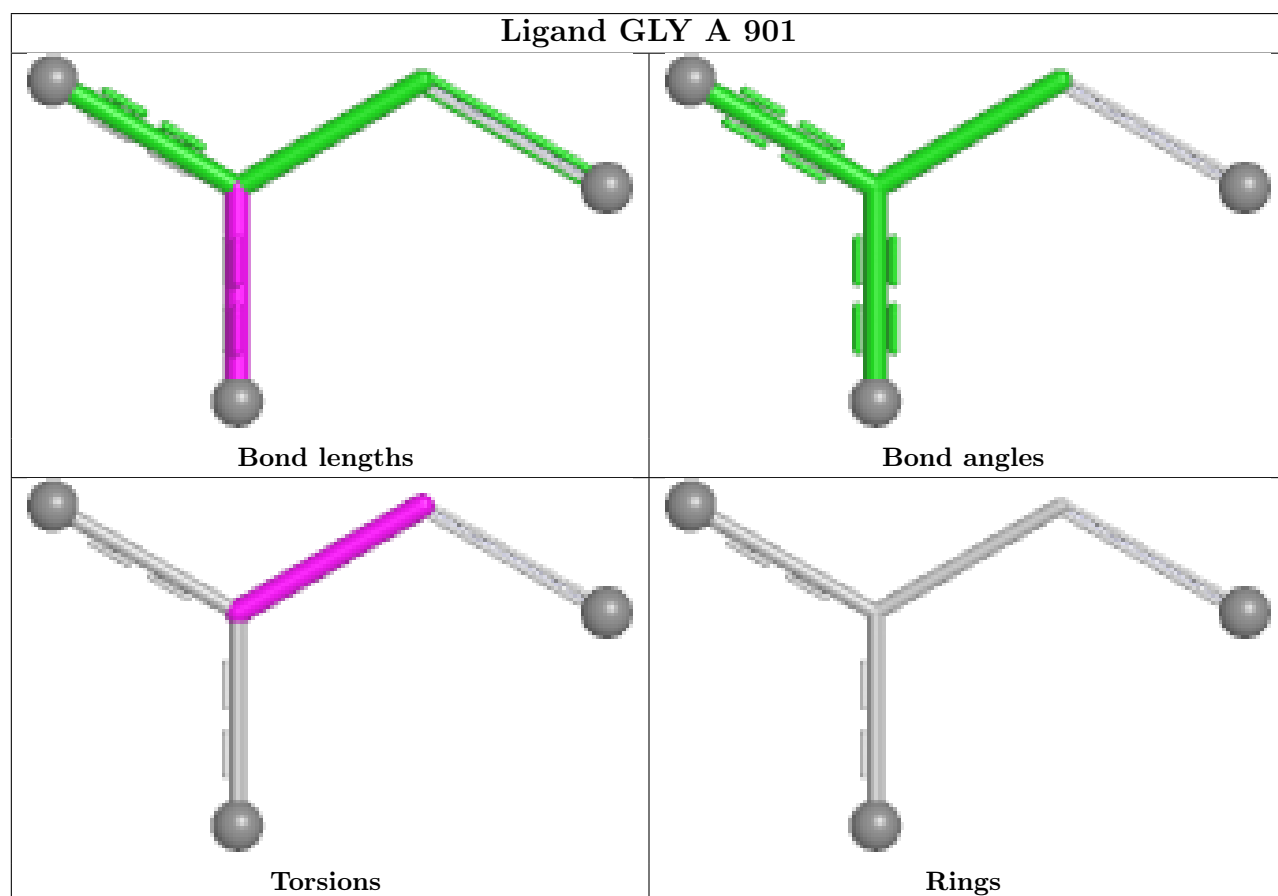
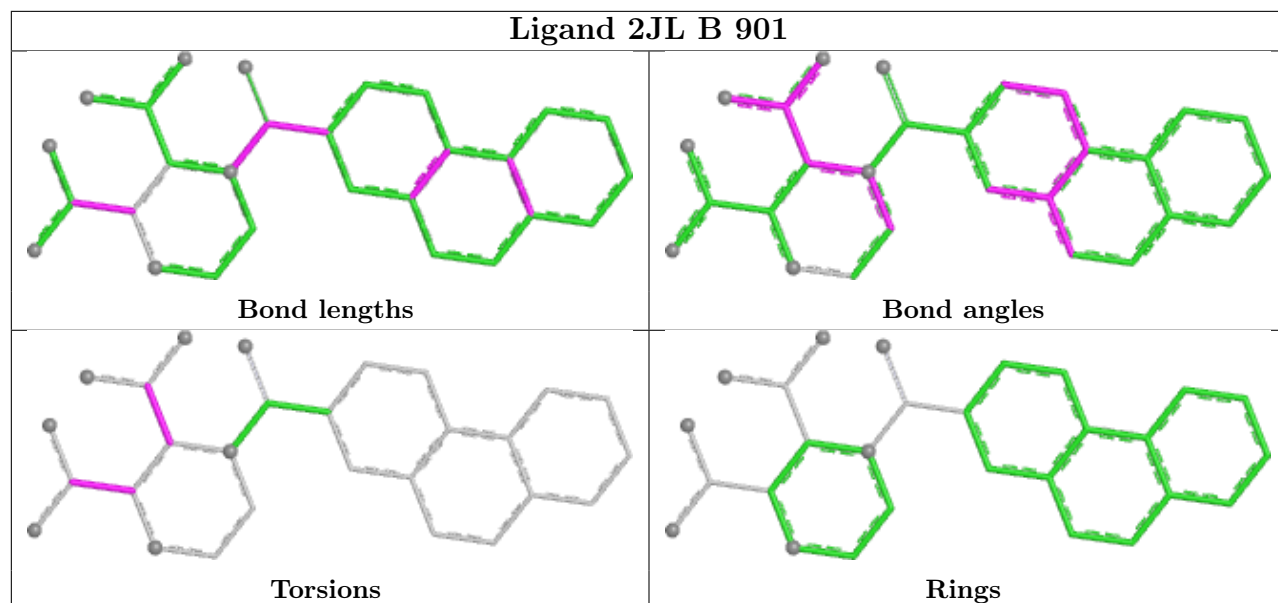
Mol	Chain	Res	Type	Atoms
6	B	901	2JL	CA-CB-CG-OD1
6	B	901	2JL	CA-CB-CG-OD2
6	B	901	2JL	NAZ-CB-CG-OD1
6	B	901	2JL	NAZ-CB-CG-OD2
6	D	901	2JL	NAZ-CB-CG-OD2
5	A	903	NAG	O5-C5-C6-O6
5	A	903	NAG	C4-C5-C6-O6
5	A	902	NAG	C4-C5-C6-O6
5	A	903	NAG	C8-C7-N2-C2
5	A	903	NAG	O7-C7-N2-C2
5	A	902	NAG	O5-C5-C6-O6
6	B	901	2JL	O-C-CA-N
6	D	901	2JL	NAZ-CB-CG-OD1
6	D	901	2JL	OXT-C-CA-CB
4	A	901	GLY	OXT-C-CA-N
6	D	901	2JL	O-C-CA-CB

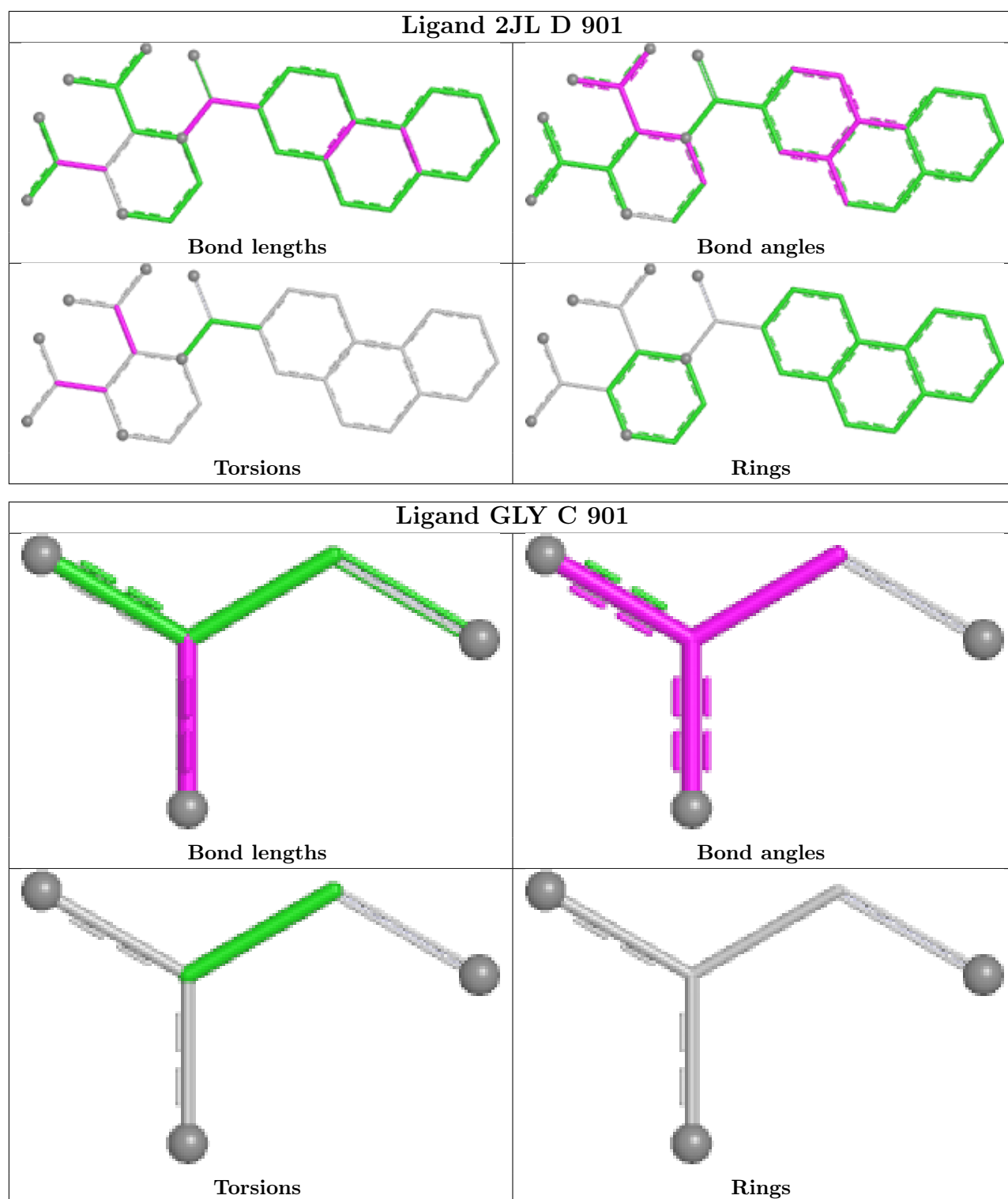
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	901	2JL	4	0
4	A	901	GLY	2	0
6	D	901	2JL	6	0
4	C	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

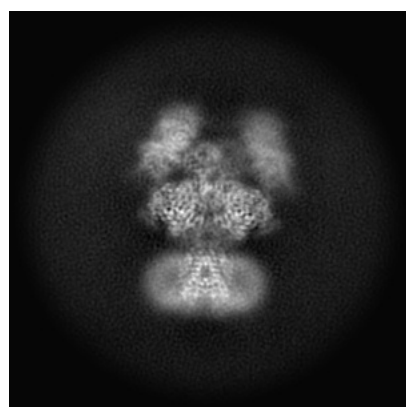
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46528. These allow visual inspection of the internal detail of the map and identification of artifacts.

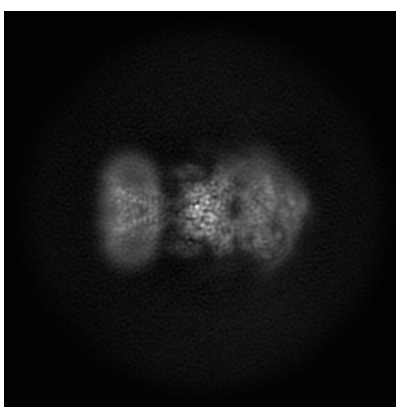
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

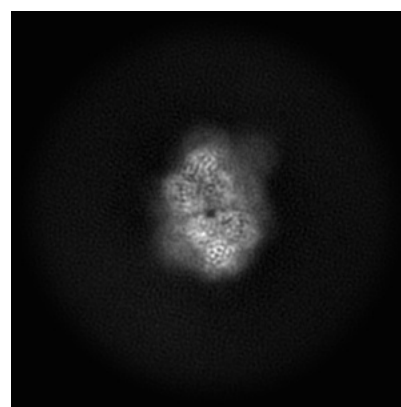
6.1.1 Primary map



X



Y

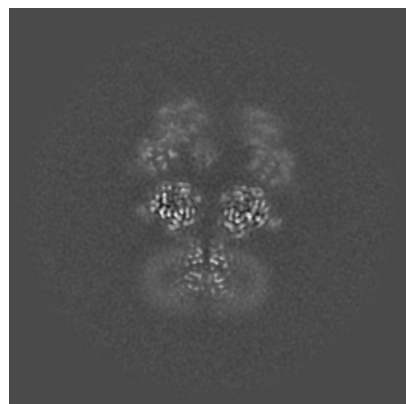


Z

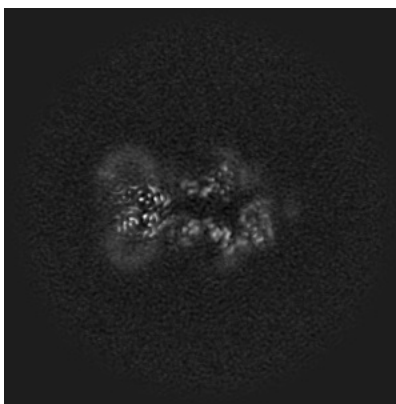
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

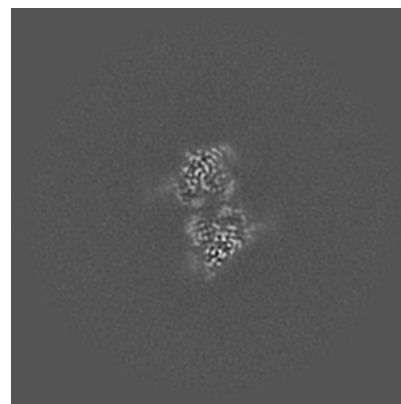
6.2.1 Primary map



X Index: 200



Y Index: 200

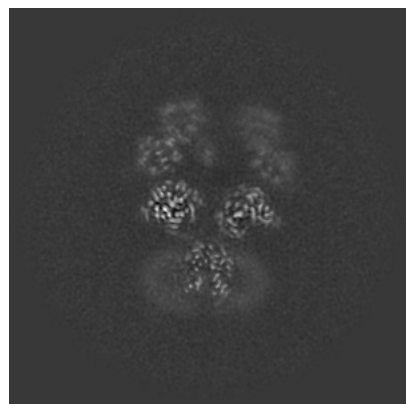


Z Index: 200

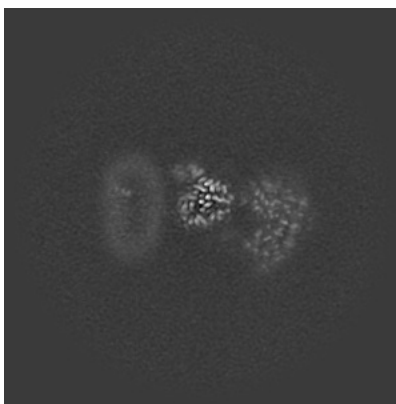
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

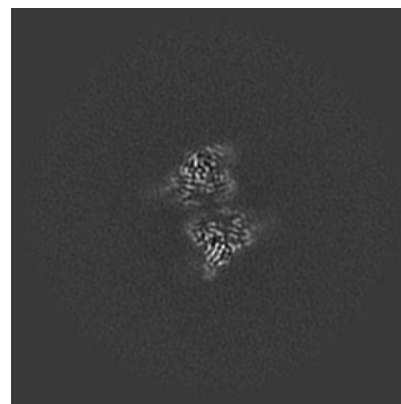
6.3.1 Primary map



X Index: 203



Y Index: 163

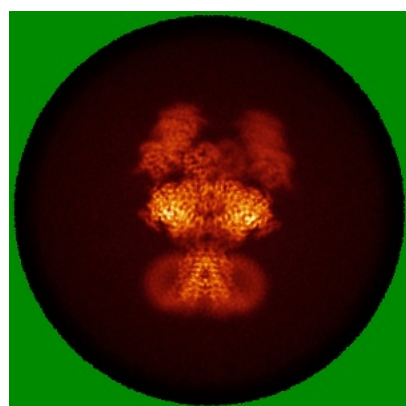


Z Index: 197

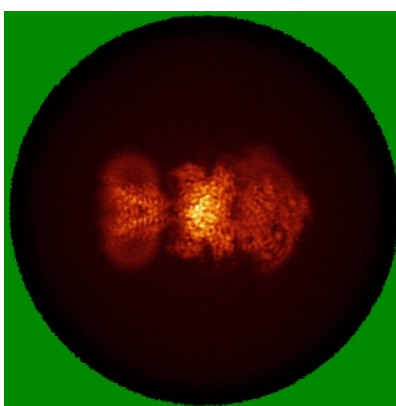
The images above show the largest variance slices of the map in three orthogonal directions.

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

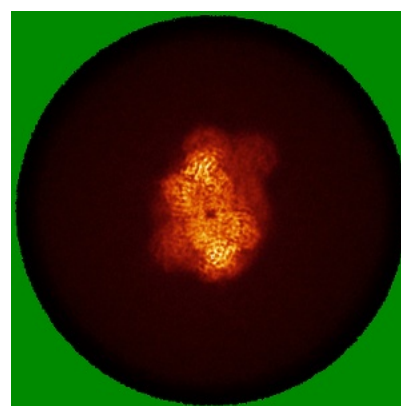
6.4.1 Primary map



X



Y

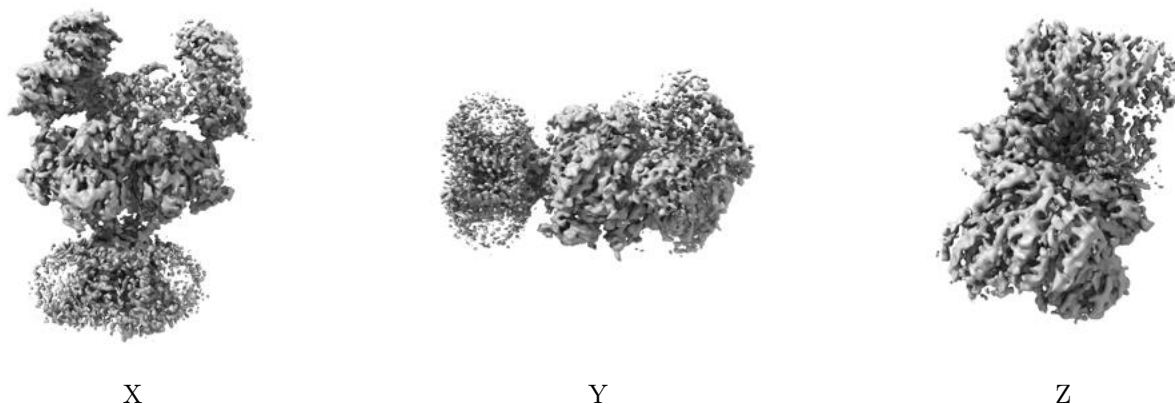


Z

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

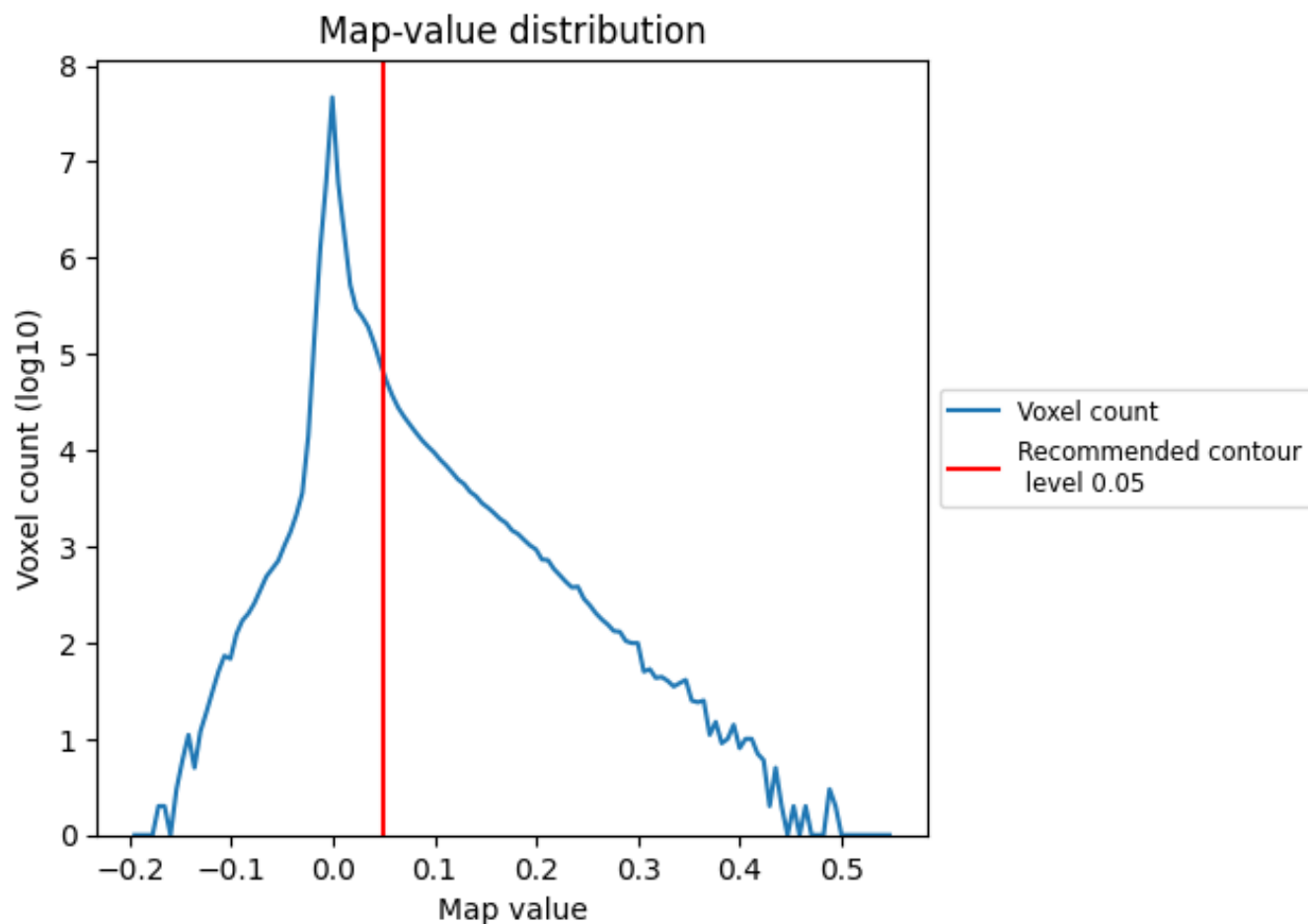
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

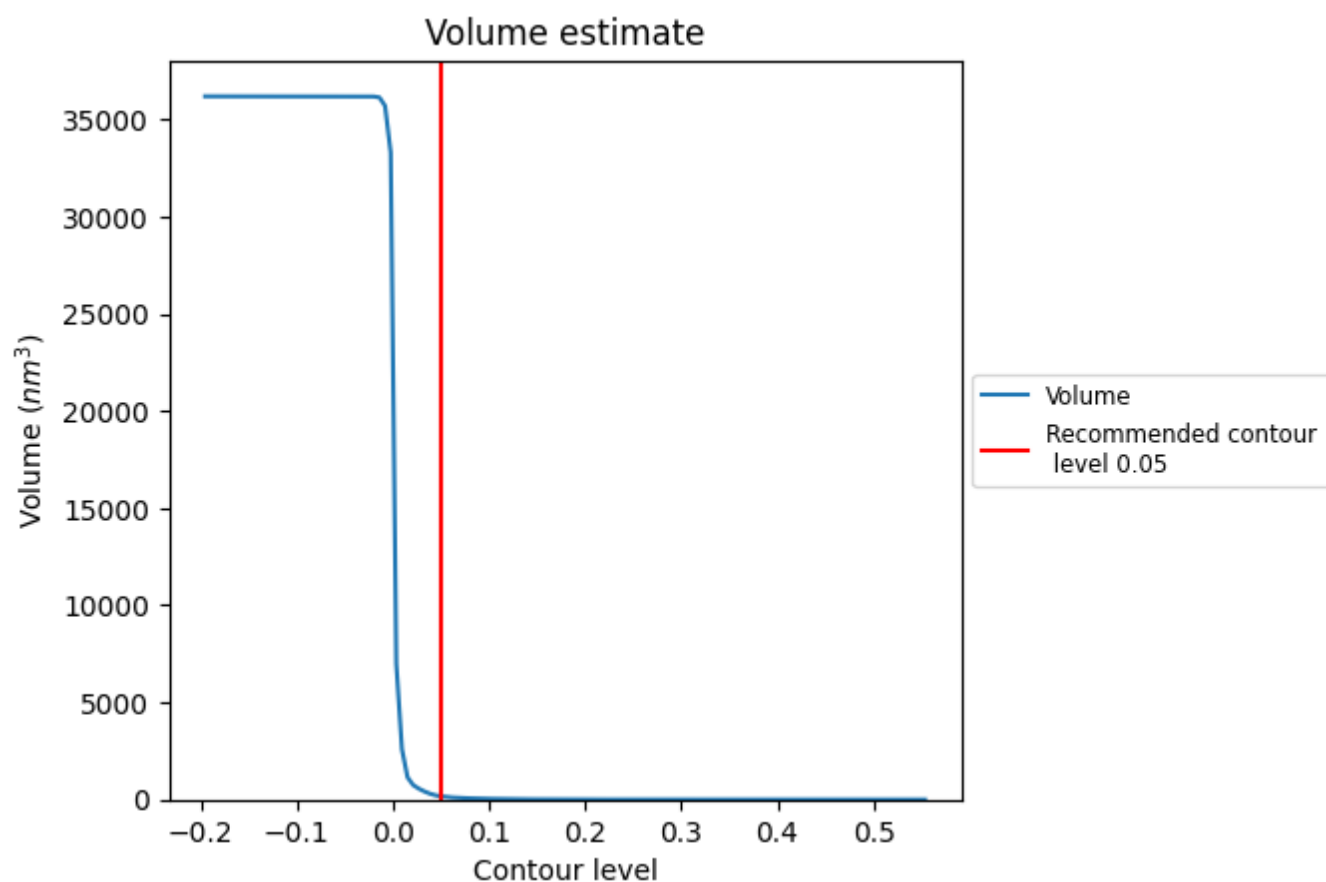
This section contains the results of statistical analysis of the map.

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.

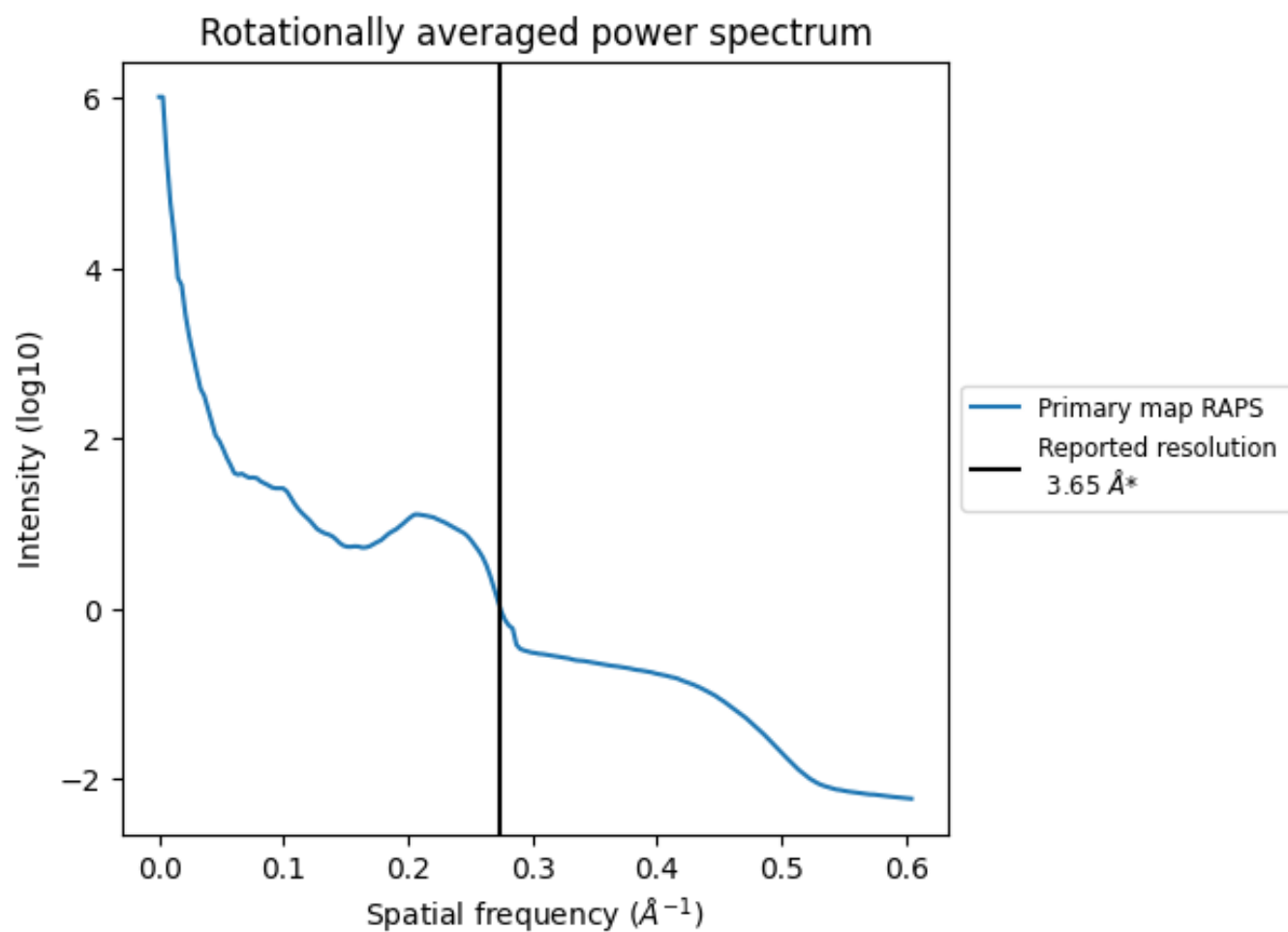
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm^3 ; this corresponds to an approximate mass of 152 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 0.274 Å⁻¹

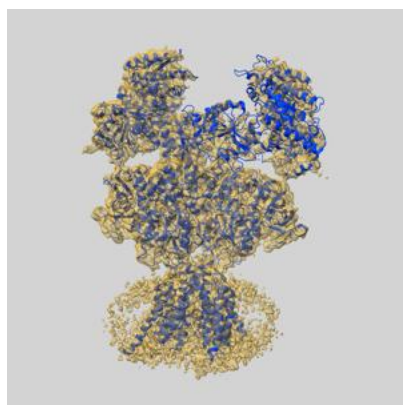
8 Fourier-Shell correlation ⓘ

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

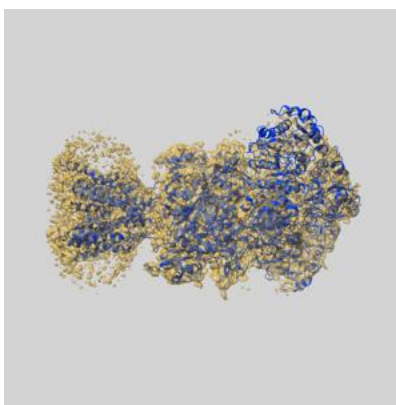
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46528 and PDB model 9D39. Per-residue inclusion information can be found in section [3](#) on page [8](#).

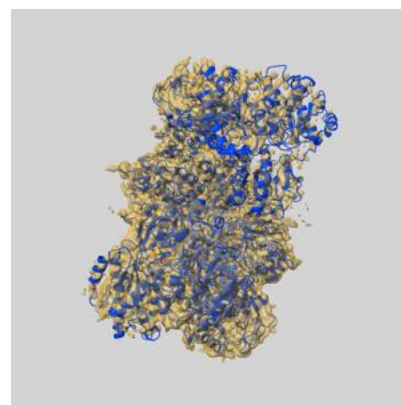
9.1 Map-model overlay [i](#)



X



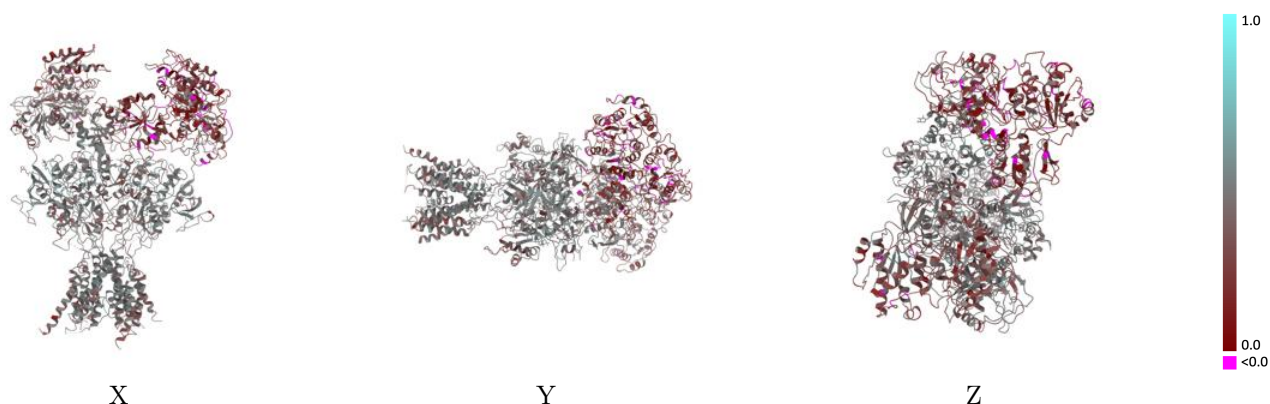
Y



Z

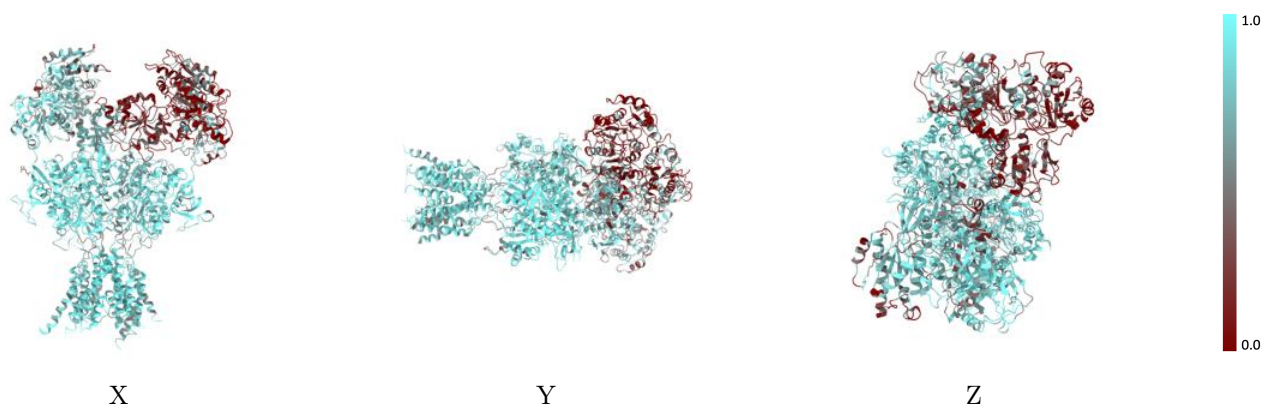
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



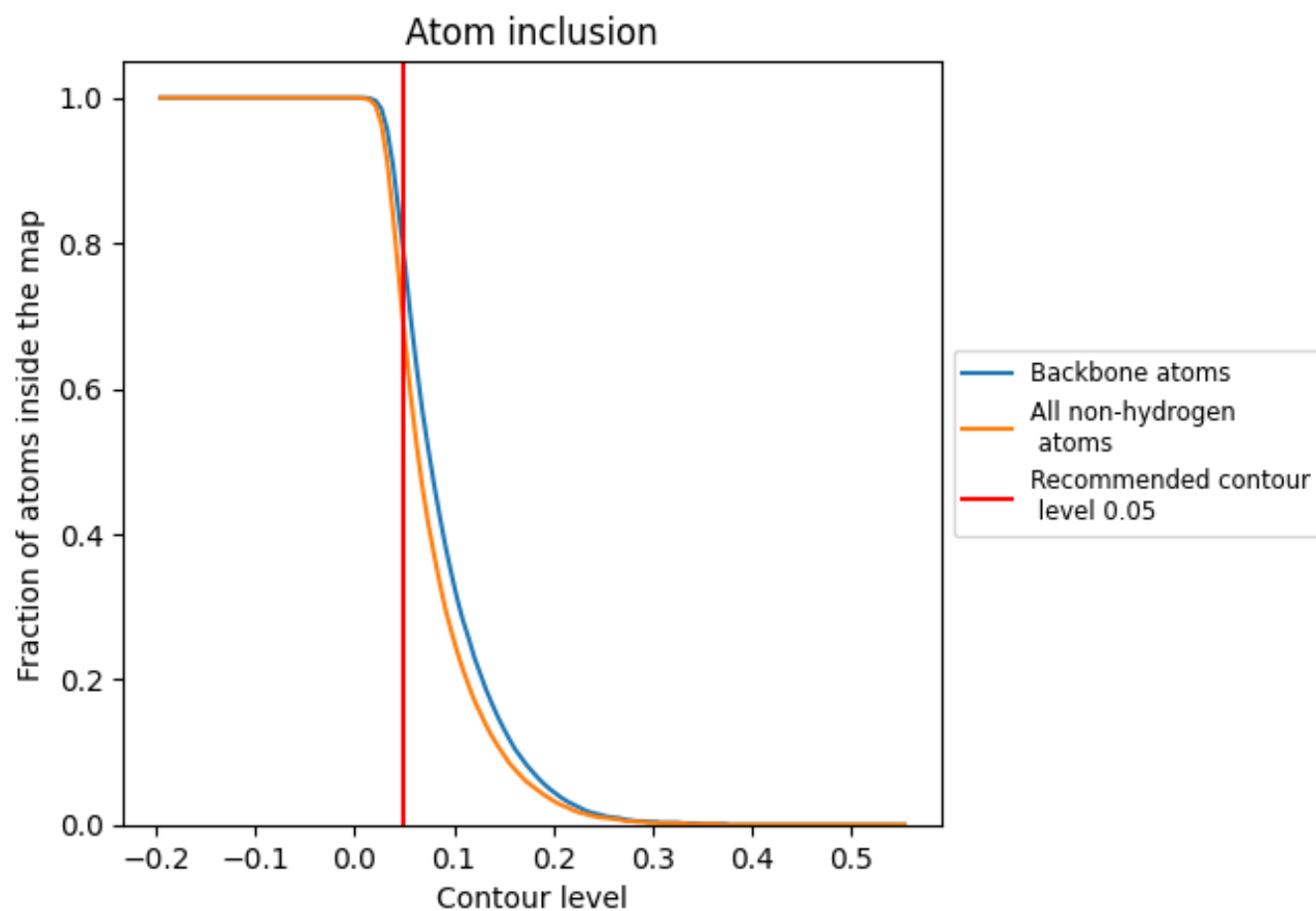
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6760	0.3850
A	0.7910	0.4210
B	0.7410	0.4060
C	0.6440	0.3670
D	0.5210	0.3460

