



Full wwPDB EM Validation Report ⓘ

Dec 6, 2025 – 01:27 PM EST

PDB ID : 9OOQ / pdb_00009ooq
EMDB ID : EMD-70669
Title : Closed state of Gly/Glu/24S-HC bound hGluN1a-2B NMDAR
Authors : Hyunook, K.; Hiro, F.
Deposited on : 2025-05-16
Resolution : 3.20 Å(reported)
Based on initial model : 7saa

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

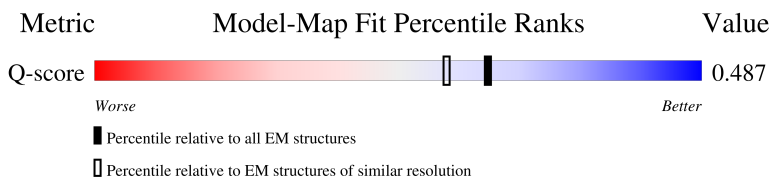
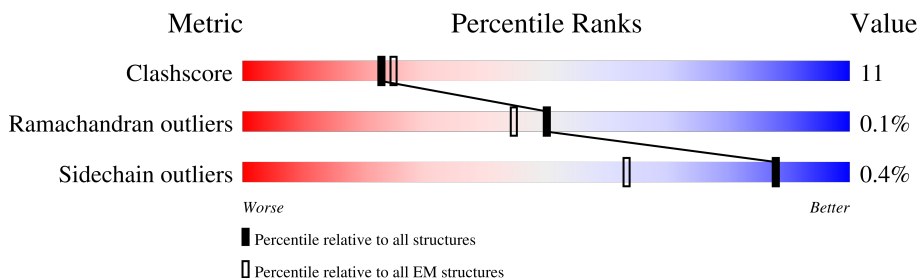
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	830	<div> <div>23%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	C	830	<div> <div>25%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
2	B	861	<div> <div>16%</div> <div>69%</div> <div>22%</div> <div>9%</div> </div>
2	D	861	<div> <div>25%</div> <div>66%</div> <div>24%</div> <div>10%</div> </div>

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	GLU	D	1000	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24897 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	799	Total	C	N	O	S	0	0
			6147	3927	1054	1132	34		
1	C	800	Total	C	N	O	S	0	0
			6158	3934	1052	1137	35		

There are 8 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	780	Total	C	N	O	S	0	0
			6063	3906	971	1146	40		
2	D	778	Total	C	N	O	S	0	0
			6012	3880	961	1131	40		

There are 76 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

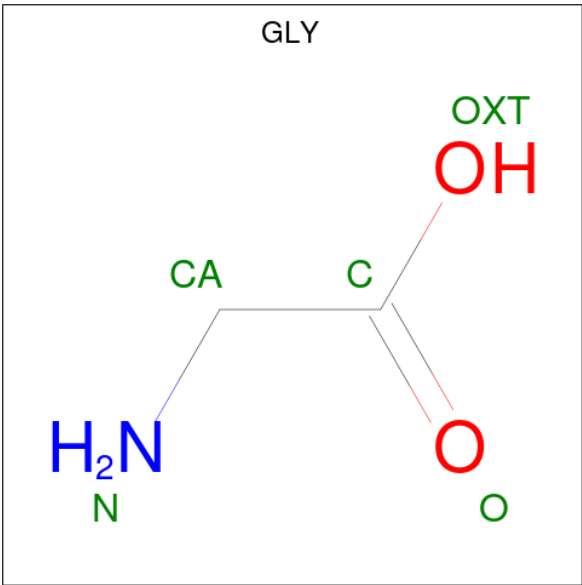
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	PHE	-	expression tag	UNP Q13224
B	-2	GLU	-	expression tag	UNP Q13224
B	-1	LYS	-	expression tag	UNP Q13224
B	0	GLY	-	expression tag	UNP Q13224
B	1	GLY	-	expression tag	UNP Q13224
B	2	GLY	-	expression tag	UNP Q13224
B	3	SER	-	expression tag	UNP Q13224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

Continued on next page...

Continued from previous page...

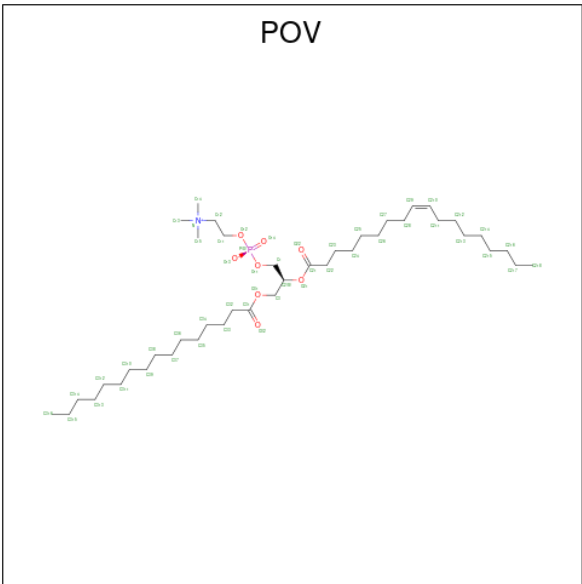
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP Q13224
D	2	GLY	-	expression tag	UNP Q13224
D	3	SER	-	expression tag	UNP Q13224
D	4	GLY	-	expression tag	UNP Q13224
D	5	GLY	-	expression tag	UNP Q13224
D	6	GLY	-	expression tag	UNP Q13224
D	7	SER	-	expression tag	UNP Q13224
D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

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



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

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



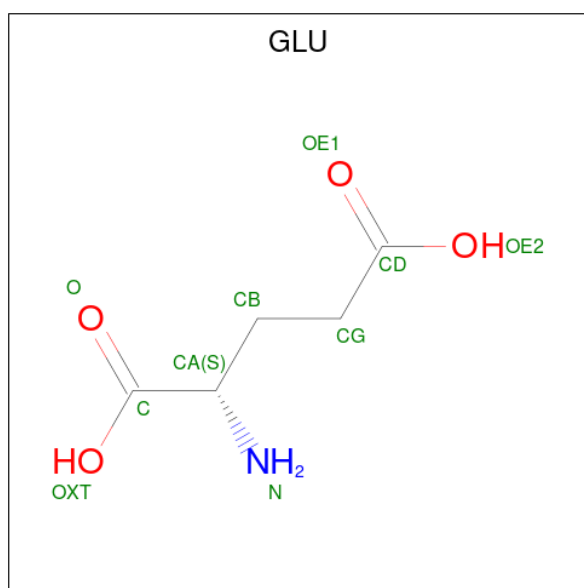
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

Continued on next page...

Continued from previous page...

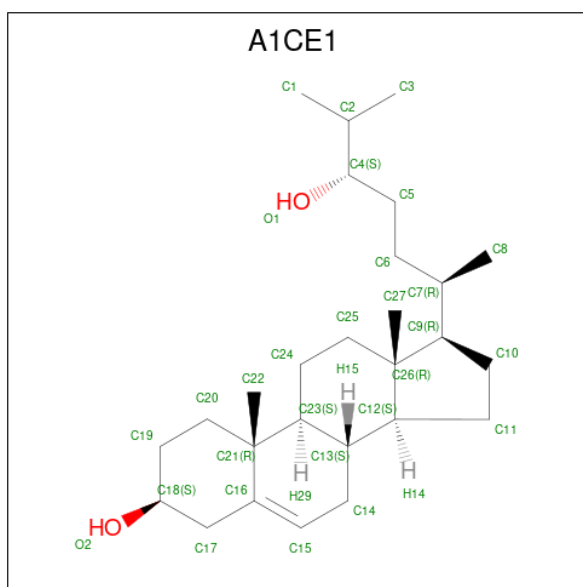
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 5 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 24S-hydroxycholesterol (CCD ID: A1CE1) (formula: $C_{27}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			29	27	2	
6	D	1	Total	C	O	0
			29	27	2	

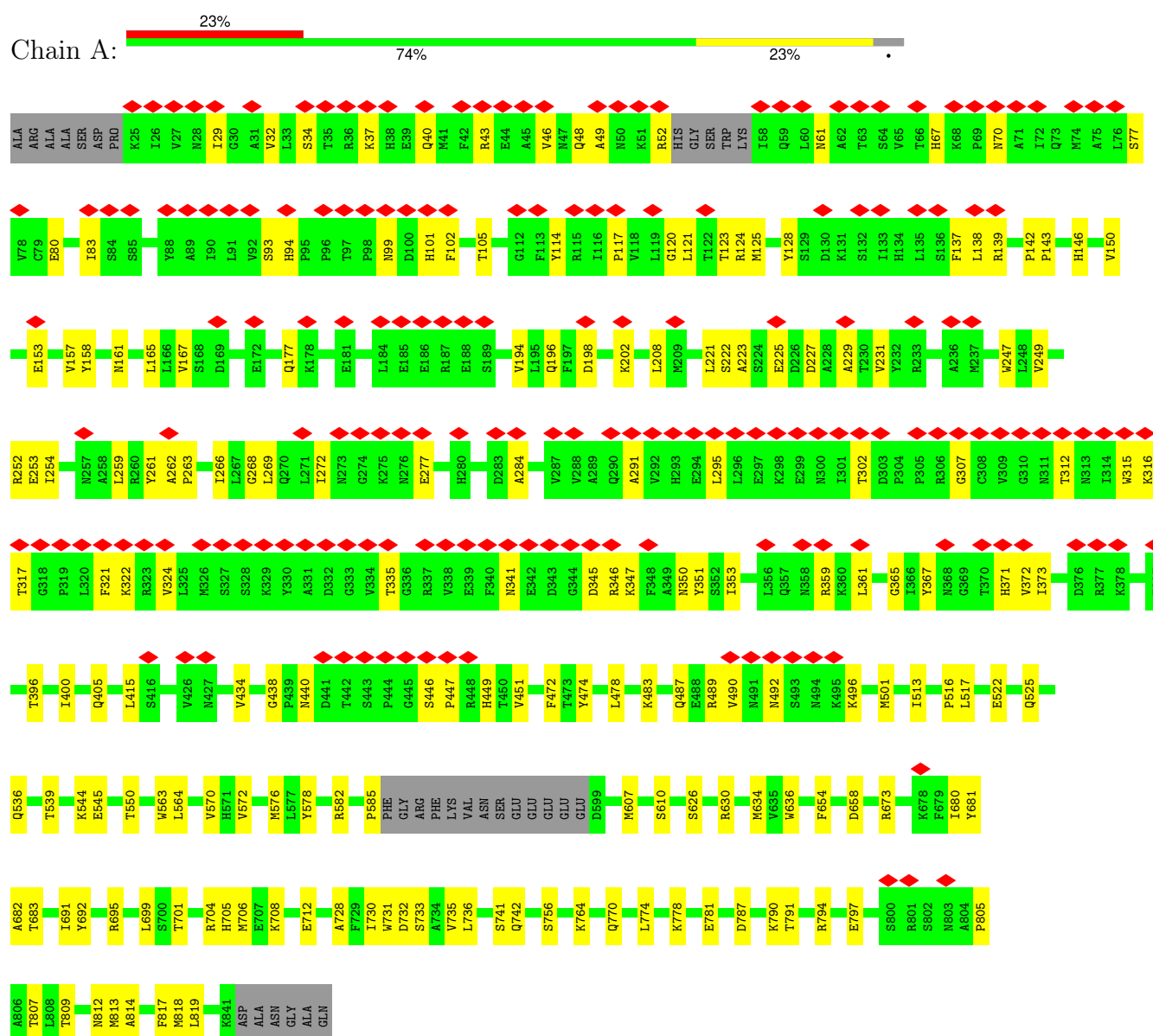
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	3	Total	O	0
			3	3	
7	B	4	Total	O	0
			4	4	
7	C	4	Total	O	0
			4	4	
7	D	2	Total	O	0
			2	2	

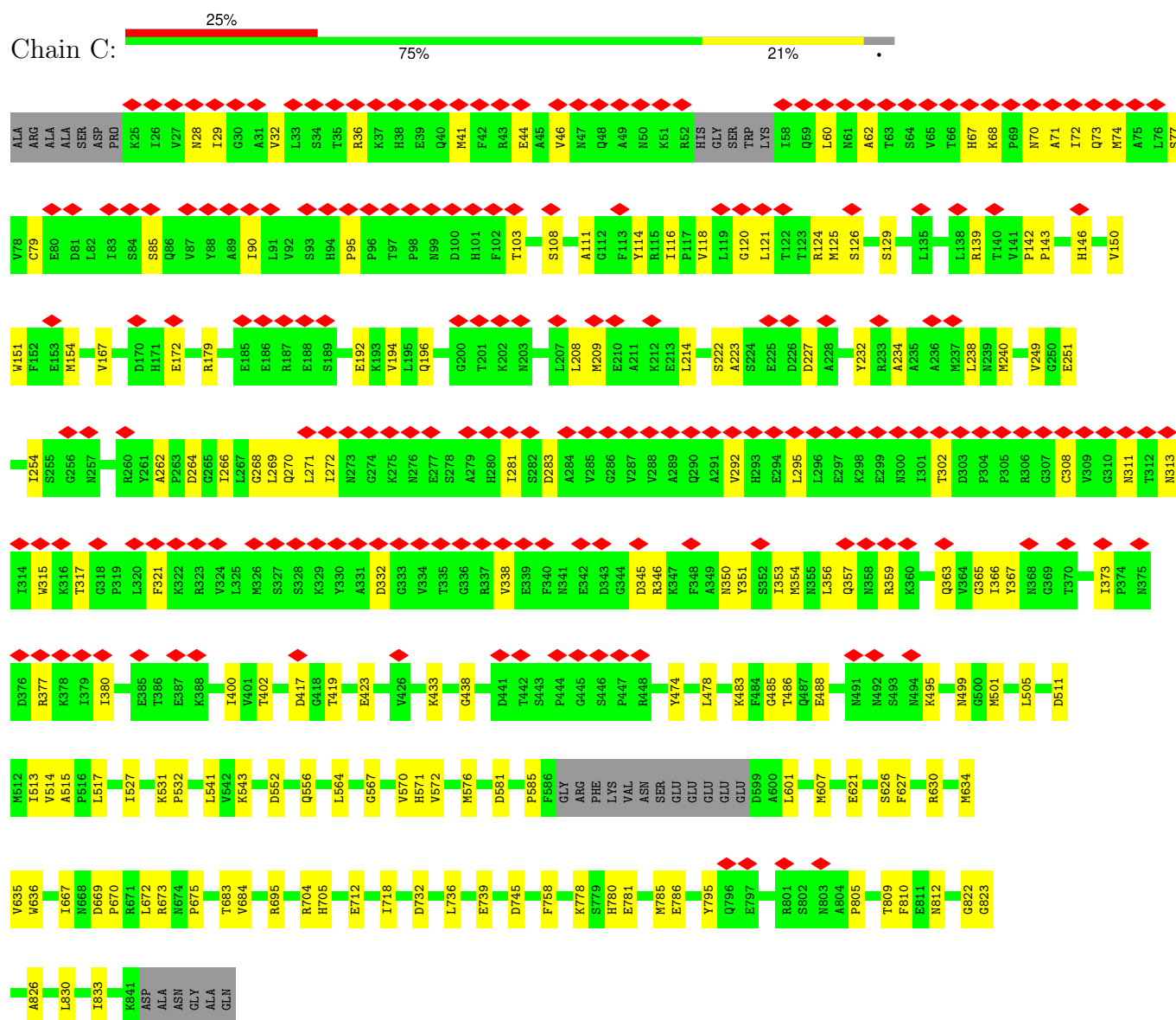
3 Residue-property plots

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.

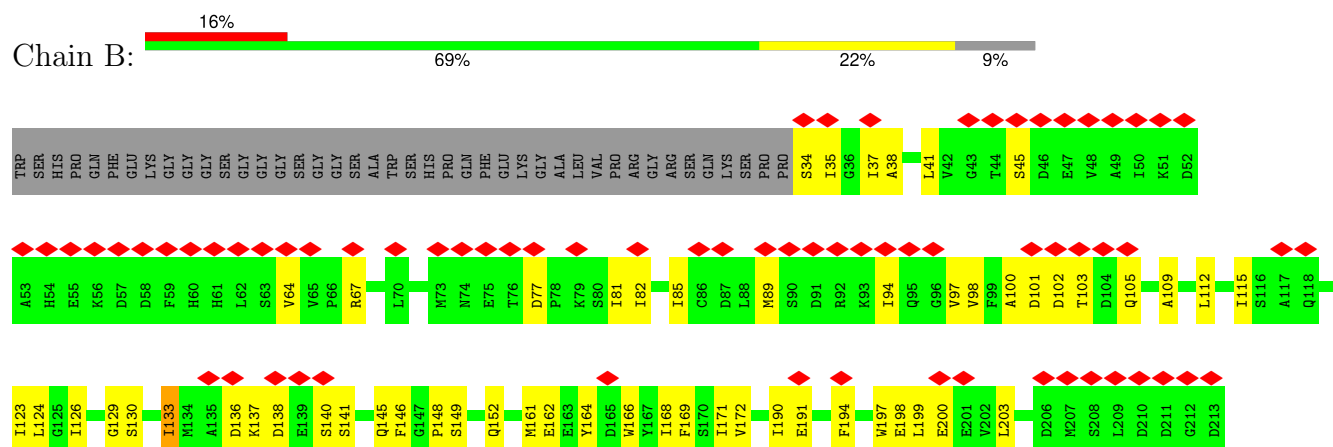
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

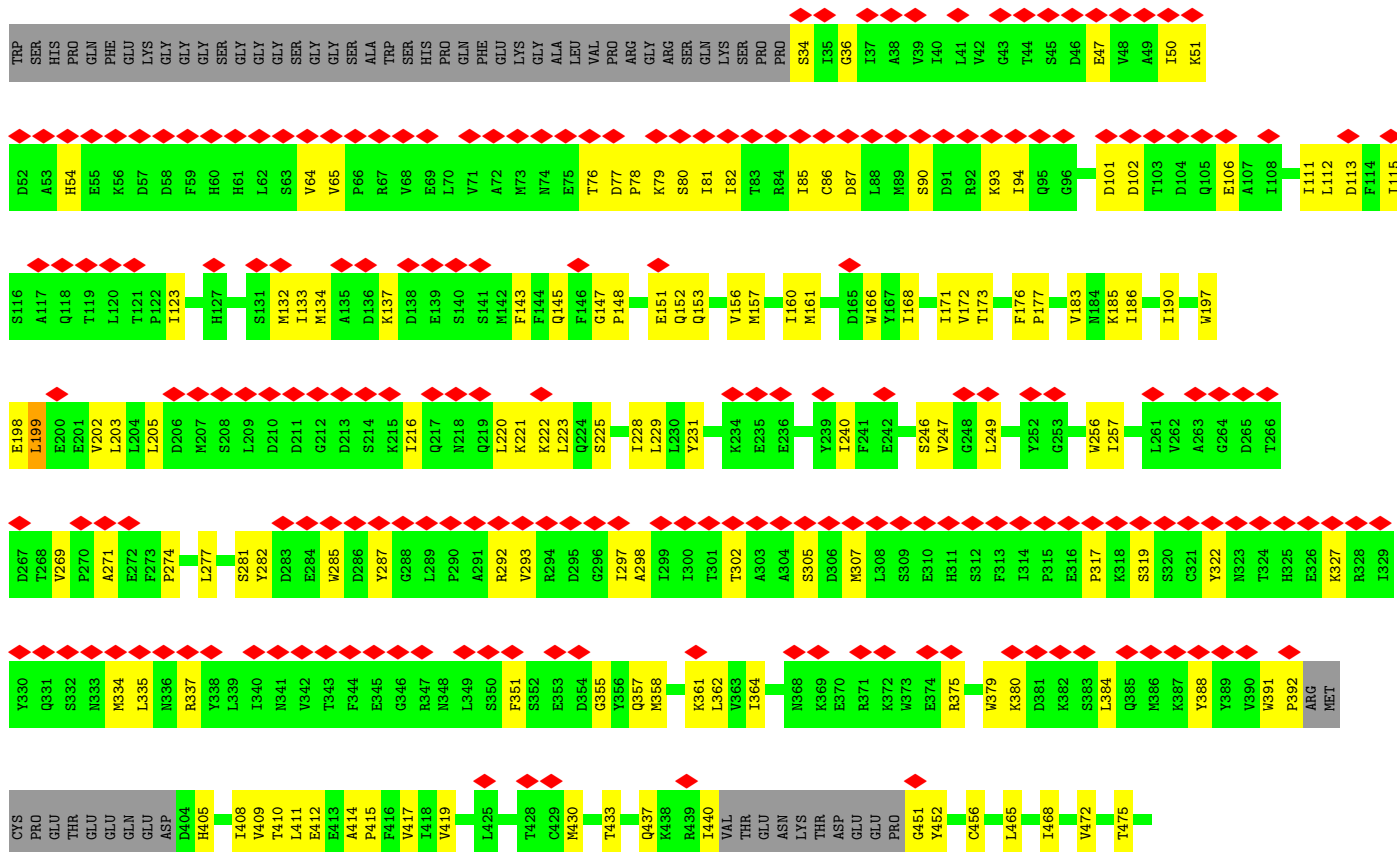


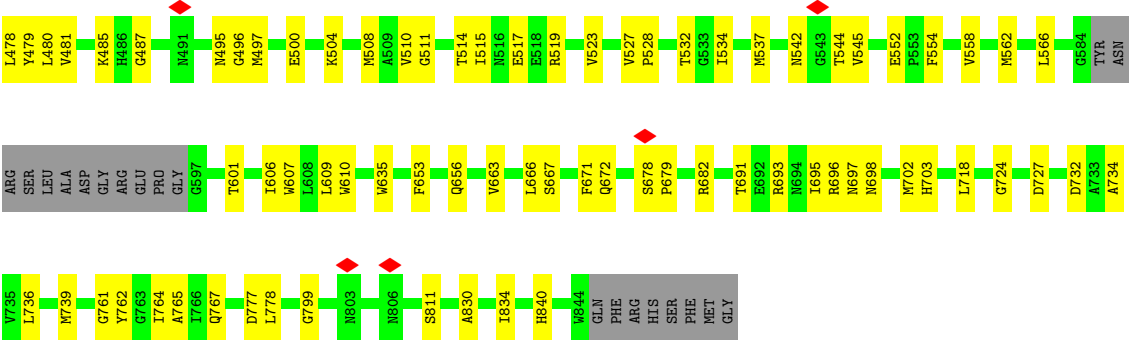
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



• Molecule 2: Glutamate receptor ionotropic, NMDA 2B







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	243459	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.645	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	330.80002, 330.80002, 330.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1CE1, POV

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	0.20	0/6285	0.27	0/8544
1	C	0.22	0/6296	0.27	0/8558
2	B	0.21	0/6198	0.30	0/8410
2	D	0.19	0/6147	0.28	0/8346
All	All	0.20	0/24926	0.28	0/33858

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	6147	0	6022	136	0
1	C	6158	0	6030	135	0
2	B	6063	0	5933	143	0
2	D	6012	0	5872	149	0
3	A	5	0	2	1	0
3	C	5	0	2	1	0
4	A	156	0	246	8	0
4	B	104	0	164	13	0
4	C	104	0	164	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	52	0	82	9	0
5	B	10	0	5	1	0
5	D	10	0	5	4	0
6	B	29	0	0	0	0
6	D	29	0	0	0	0
7	A	3	0	0	0	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
7	D	2	0	0	0	0
All	All	24897	0	24527	542	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 (542) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:ILE:HA	1:A:705:HIS:HE1	1.44	0.82
1:A:704:ARG:NH1	2:B:430:MET:SD	2.54	0.80
1:C:302:THR:H	1:C:317:THR:HG21	1.47	0.78
1:A:704:ARG:HH21	2:B:194:PHE:HB3	1.49	0.77
2:D:223:LEU:HD13	2:D:228:ILE:HG12	1.69	0.74
1:C:139:ARG:HH12	1:C:143:PRO:HB3	1.53	0.73
1:A:139:ARG:HB2	1:A:345:ASP:HA	1.71	0.72
2:B:198:GLU:N	2:B:198:GLU:OE1	2.23	0.72
1:A:302:THR:H	1:A:317:THR:HG21	1.54	0.72
1:A:259:LEU:HD21	1:A:361:LEU:HD21	1.71	0.72
1:C:108:SER:HA	1:C:118:VAL:HG21	1.70	0.71
4:D:1002:POV:H310	4:D:1002:POV:H21C	1.70	0.71
2:D:534:ILE:HG12	2:D:691:THR:HG22	1.71	0.71
2:B:138:ASP:HB3	2:B:141:SER:HB3	1.70	0.71
1:C:120:GLY:HA3	1:C:139:ARG:HG2	1.70	0.71
2:B:149:SER:H	2:B:152:GLN:HE21	1.37	0.70
2:D:379:TRP:HB2	2:D:384:LEU:HD12	1.73	0.70
2:B:161:MET:HB3	2:B:166:TRP:HB2	1.75	0.69
1:C:571:HIS:HB3	4:C:903:POV:H21A	1.74	0.69
2:D:334:MET:HA	2:D:337:ARG:HH21	1.58	0.68
2:D:545:VAL:HG23	2:D:811:SER:HB2	1.75	0.68
1:A:223:ALA:HB1	1:A:227:ASP:HB2	1.74	0.68
1:C:667:ILE:O	1:C:673:ARG:NH2	2.27	0.68
2:D:514:THR:HG22	2:D:762:TYR:HE1	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD21	1:A:284:ALA:HB2	1.76	0.67
2:D:64:VAL:HG12	2:D:305:SER:HB3	1.76	0.67
1:A:254:ILE:HD13	1:A:268:GLY:HA3	1.76	0.67
1:C:68:LYS:HB2	1:C:74:MET:HE1	1.78	0.67
1:C:251:GLU:HG2	1:C:270:GLN:HA	1.78	0.66
2:D:274:PRO:HD2	2:D:277:LEU:HD13	1.77	0.66
1:A:150:VAL:HG11	1:A:269:LEU:HD21	1.77	0.66
1:C:143:PRO:HD2	1:C:146:HIS:CD2	2.30	0.66
2:B:412:GLU:HG3	2:B:419:VAL:HG13	1.78	0.66
1:A:263:PRO:O	1:A:359:ARG:NH1	2.29	0.65
1:A:489:ARG:NH2	2:B:191:GLU:OE2	2.28	0.65
1:A:177:GLN:OE1	1:A:196:GLN:NE2	2.30	0.65
1:A:490:VAL:HG12	1:A:492:ASN:H	1.62	0.65
2:D:322:TYR:O	2:D:327:LYS:NZ	2.27	0.65
2:D:671:PHE:HB3	2:D:702:MET:HE2	1.78	0.65
2:D:307:MET:HG2	2:D:335:LEU:HD13	1.79	0.64
2:D:90:SER:HA	2:D:319:SER:HB2	1.79	0.64
2:B:682:ARG:NH1	2:B:724:GLY:O	2.31	0.64
1:A:70:ASN:ND2	2:B:321:CYS:O	2.31	0.64
1:C:146:HIS:HA	1:C:179:ARG:HH12	1.61	0.64
1:A:125:MET:O	1:A:139:ARG:NH2	2.31	0.64
2:B:534:ILE:HG12	2:B:691:THR:HG22	1.80	0.63
1:C:718:ILE:HD13	1:C:739:GLU:HG3	1.81	0.63
1:A:70:ASN:HD21	2:B:324:THR:HG23	1.63	0.63
2:B:219:GLN:OE1	2:B:219:GLN:N	2.25	0.62
2:D:610:TRP:CZ2	4:D:1002:POV:H212	2.35	0.62
2:B:771:GLY:O	2:B:775:GLN:NE2	2.33	0.62
2:D:161:MET:HE1	2:D:229:LEU:HD11	1.81	0.62
2:D:148:PRO:HG3	2:D:362:LEU:HD11	1.81	0.61
1:A:167:VAL:HG11	1:A:177:GLN:HB2	1.81	0.61
1:C:36:ARG:O	1:C:36:ARG:NH1	2.31	0.61
2:B:324:THR:HA	2:B:327:LYS:HD2	1.82	0.61
1:C:28:ASN:ND2	1:C:85:SER:O	2.33	0.61
2:D:50:ILE:HG23	2:D:293:VAL:HG11	1.81	0.61
2:D:79:LYS:HA	2:D:82:ILE:HD12	1.80	0.61
2:D:440:ILE:O	2:D:451:GLY:N	2.34	0.60
1:A:48:GLN:HG2	1:A:52:ARG:HH21	1.65	0.60
1:A:607:MET:HE3	4:A:1003:POV:H34A	1.82	0.60
1:C:621:GLU:OE2	1:C:621:GLU:N	2.35	0.60
1:A:40:GLN:HA	1:A:43:ARG:HH12	1.64	0.60
4:B:904:POV:H33A	4:C:903:POV:H37A	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:VAL:HG21	2:B:371:ARG:HB3	1.84	0.60
1:C:262:ALA:O	1:C:359:ARG:NH1	2.34	0.60
2:B:334:MET:SD	2:B:334:MET:N	2.75	0.60
1:A:563:TRP:HB3	4:A:1002:POV:H26A	1.83	0.59
1:A:634:MET:HG3	2:B:610:TRP:CD1	2.37	0.59
4:B:904:POV:H21E	4:C:902:POV:H311	1.84	0.59
1:C:634:MET:HG3	4:D:1002:POV:H27A	1.85	0.59
2:D:199:LEU:HD22	2:D:202:VAL:HG22	1.84	0.59
1:C:70:ASN:ND2	1:C:73:GLN:OE1	2.36	0.59
2:D:361:LYS:HG2	2:D:380:LYS:HD2	1.85	0.59
2:D:465:LEU:HD22	2:D:510:VAL:HG11	1.85	0.59
1:C:423:GLU:OE2	1:C:433:LYS:NZ	2.30	0.59
2:D:379:TRP:HD1	2:D:384:LEU:HB2	1.66	0.59
1:A:102:PHE:O	1:A:105:THR:OG1	2.22	0.58
1:C:543:LYS:NZ	1:C:745:ASP:OD2	2.28	0.58
2:D:47:GLU:HA	2:D:50:ILE:HD12	1.85	0.58
2:B:610:TRP:HE1	4:B:903:POV:H214	1.68	0.58
1:A:262:ALA:HB3	1:A:359:ARG:HH22	1.69	0.58
1:C:809:THR:H	1:C:812:ASN:HD22	1.50	0.58
2:D:732:ASP:OD2	5:D:1000:GLU:N	2.37	0.58
1:A:525:GLN:HG2	2:D:778:LEU:HD11	1.86	0.58
1:A:805:PRO:HG2	2:D:653:PHE:HA	1.86	0.58
2:D:727:ASP:OD1	2:D:727:ASP:N	2.36	0.58
1:A:522:GLU:CD	1:A:522:GLU:H	2.12	0.57
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.86	0.57
1:C:46:VAL:HG21	1:C:62:ALA:HB2	1.85	0.57
1:A:221:LEU:HD23	1:A:223:ALA:H	1.68	0.57
2:B:168:ILE:HB	2:B:226:PRO:HD2	1.86	0.57
2:D:36:GLY:HA3	2:D:94:ILE:HA	1.85	0.57
2:D:667:SER:HA	2:D:672:GLN:HE21	1.69	0.57
1:A:266:ILE:HD12	1:A:266:ILE:H	1.68	0.57
2:D:143:PHE:HE2	2:D:145:GLN:HG3	1.68	0.57
1:A:249:VAL:HG13	1:A:253:GLU:HB2	1.86	0.57
2:D:198:GLU:OE1	2:D:198:GLU:N	2.37	0.57
1:C:338:VAL:HA	1:C:346:ARG:NH1	2.19	0.57
2:D:106:GLU:HG3	2:D:132:MET:HE2	1.85	0.57
2:D:523:VAL:HG21	2:D:765:ALA:HB1	1.87	0.57
1:C:73:GLN:O	1:C:77:SER:N	2.36	0.57
1:C:129:SER:OG	1:C:345:ASP:OD2	2.23	0.57
1:A:536:GLN:NE2	1:A:756:SER:O	2.37	0.57
1:C:29:ILE:HD13	1:C:60:LEU:HD23	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:HD1	1:A:139:ARG:HH21	1.53	0.56
2:D:537:MET:HB2	2:D:736:LEU:HD13	1.86	0.56
2:D:269:VAL:HG12	2:D:271:ALA:H	1.70	0.56
1:C:732:ASP:OD2	3:C:901:GLY:N	2.39	0.56
1:C:513:ILE:HG21	1:C:517:LEU:HD22	1.87	0.56
1:A:680:ILE:HA	1:A:705:HIS:CE1	2.34	0.56
1:C:786:GLU:OE1	1:C:786:GLU:N	2.31	0.56
2:B:537:MET:HB2	2:B:736:LEU:HD13	1.87	0.56
2:B:171:ILE:HG12	2:B:229:LEU:HB2	1.87	0.56
2:D:414:ALA:HB3	2:D:415:PRO:HD3	1.86	0.56
1:A:120:GLY:N	1:A:138:LEU:O	2.29	0.55
1:A:682:ALA:HA	1:A:706:MET:HG2	1.87	0.55
2:D:173:THR:HG22	2:D:231:TYR:HB3	1.87	0.55
2:D:77:ASP:OD2	2:D:80:SER:N	2.39	0.55
2:B:229:LEU:HD22	2:B:257:ILE:HB	1.87	0.55
4:B:903:POV:H31B	4:B:903:POV:H21A	1.87	0.55
1:C:272:ILE:HD13	1:C:350:ASN:HD21	1.70	0.55
1:C:501:MET:HE3	1:C:517:LEU:HD13	1.88	0.55
1:A:229:ALA:HB1	1:A:261:TYR:HD2	1.72	0.55
1:C:311:ASN:HD22	1:C:315:TRP:HZ2	1.53	0.55
1:C:572:VAL:O	1:C:576:MET:HG3	2.07	0.55
1:A:124:ARG:NH2	1:A:142:PRO:O	2.38	0.55
2:B:465:LEU:HD22	2:B:510:VAL:HG11	1.89	0.55
2:B:352:SER:OG	2:B:358:MET:SD	2.58	0.55
2:D:485:LYS:O	2:D:496:GLY:HA3	2.06	0.55
2:B:100:ALA:HB2	2:B:126:ILE:HD11	1.89	0.55
2:B:166:TRP:HB3	2:B:227:ILE:HD11	1.88	0.55
1:C:350:ASN:HA	1:C:367:TYR:HD2	1.70	0.55
2:D:528:PRO:HB3	2:D:761:GLY:HA3	1.89	0.55
4:A:1001:POV:H216	4:A:1002:POV:H37A	1.89	0.54
2:B:389:TYR:HD1	2:B:390:VAL:HG13	1.71	0.54
1:C:121:LEU:HD11	1:C:281:ILE:HD13	1.89	0.54
1:C:552:ASP:HB3	1:C:556:GLN:HE21	1.71	0.54
2:B:479:TYR:OH	2:B:500:GLU:OE1	2.22	0.54
2:D:514:THR:HG22	2:D:762:TYR:CE1	2.42	0.54
2:D:663:VAL:HG11	2:D:671:PHE:HE2	1.73	0.54
1:A:501:MET:HE3	1:A:517:LEU:HD13	1.89	0.54
2:B:561:MET:SD	1:C:810:PHE:HE1	2.30	0.54
2:D:93:LYS:NZ	2:D:317:PRO:O	2.33	0.54
1:C:283:ASP:OD1	1:C:283:ASP:N	2.38	0.54
2:B:133:ILE:HA	2:B:145:GLN:HE22	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:GLN:NE2	2:D:246:SER:O	2.40	0.54
1:A:572:VAL:O	1:A:576:MET:HG3	2.08	0.54
1:C:60:LEU:HD11	1:C:292:VAL:HG11	1.90	0.54
2:D:220:LEU:HD11	2:D:240:ILE:HG23	1.89	0.54
2:D:411:LEU:HG	2:D:412:GLU:H	1.73	0.54
1:A:805:PRO:HG3	2:D:656:GLN:HG3	1.89	0.53
2:D:76:THR:OG1	2:D:77:ASP:N	2.38	0.53
2:D:351:PHE:HE1	2:D:357:GLN:HG2	1.73	0.53
1:A:335:THR:OG1	1:A:346:ARG:NH2	2.41	0.53
1:C:167:VAL:HA	1:C:222:SER:HB2	1.89	0.53
1:C:332:ASP:OD1	1:C:332:ASP:N	2.39	0.53
1:C:363:GLN:O	1:C:377:ARG:NH1	2.41	0.53
1:A:634:MET:HG3	2:B:610:TRP:HD1	1.73	0.53
2:B:296:GLY:HA2	2:B:299:ILE:HD12	1.91	0.53
1:C:704:ARG:NE	2:D:430:MET:SD	2.72	0.53
2:D:334:MET:SD	2:D:334:MET:N	2.81	0.53
1:A:70:ASN:OD1	2:B:324:THR:OG1	2.22	0.53
2:B:133:ILE:HA	2:B:145:GLN:NE2	2.23	0.53
4:A:1001:POV:H36A	4:A:1002:POV:H31H	1.90	0.53
2:D:137:LYS:HZ2	2:D:355:GLY:HA3	1.72	0.53
2:D:718:LEU:HD11	2:D:739:MET:HB3	1.91	0.53
2:B:553:PRO:HA	2:B:649:ASN:HD22	1.73	0.53
2:D:171:ILE:HG21	2:D:183:VAL:HG23	1.91	0.53
1:A:550:THR:OG1	1:A:658:ASP:OD2	2.24	0.52
2:B:610:TRP:NE1	2:B:614:PHE:HE2	2.07	0.52
1:C:353:ILE:HD12	1:C:365:GLY:HA3	1.91	0.52
2:D:186:ILE:O	2:D:190:ILE:HG12	2.09	0.52
2:D:334:MET:HA	2:D:337:ARG:NH2	2.22	0.52
2:D:532:THR:HG21	2:D:762:TYR:CZ	2.44	0.52
1:A:705:HIS:HA	1:A:708:LYS:HE2	1.90	0.52
2:B:126:ILE:HA	2:B:146:PHE:HD2	1.74	0.52
4:B:904:POV:H23A	1:C:607:MET:HG2	1.91	0.52
4:B:904:POV:H23	4:C:903:POV:H35	1.91	0.52
1:A:123:THR:HG21	1:A:137:PHE:HZ	1.74	0.52
1:A:778:LYS:HG3	2:D:517:GLU:HG2	1.90	0.52
4:A:1001:POV:H3A	4:A:1003:POV:H33	1.90	0.52
4:B:904:POV:H314	1:C:822:GLY:HA3	1.90	0.52
2:B:200:GLU:OE1	2:B:225:SER:OG	2.26	0.52
2:B:283:ASP:HB3	2:B:287:TYR:H	1.75	0.52
2:B:526:SER:O	1:C:531:LYS:NZ	2.42	0.52
1:A:673:ARG:NH1	2:B:795:LEU:O	2.37	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:OD1	1:A:161:ASN:N	2.43	0.52
1:A:814:ALA:O	1:A:818:MET:HG2	2.10	0.52
2:B:685:THR:OG1	2:B:730:ILE:O	2.25	0.52
2:D:519:ARG:NH2	5:D:1000:GLU:OXT	2.28	0.52
2:D:682:ARG:NH1	2:D:724:GLY:O	2.41	0.52
1:A:809:THR:H	1:A:812:ASN:HD22	1.56	0.52
2:B:41:LEU:HD22	2:B:45:SER:HB3	1.92	0.52
1:A:681:TYR:HB3	1:A:728:ALA:HB3	1.92	0.51
2:D:148:PRO:HG2	2:D:153:GLN:HE21	1.74	0.51
1:A:49:ALA:HA	1:A:52:ARG:HD2	1.93	0.51
2:B:98:VAL:HG22	2:B:124:LEU:HD12	1.92	0.51
1:C:29:ILE:HD11	1:C:46:VAL:HG13	1.92	0.51
1:C:683:THR:OG1	1:C:684:VAL:N	2.44	0.51
1:C:417:ASP:OD2	1:C:419:THR:OG1	2.22	0.51
1:A:449:HIS:CE1	1:A:451:VAL:HB	2.45	0.51
2:D:168:ILE:HG22	2:D:225:SER:HB3	1.92	0.51
1:A:578:TYR:OH	1:A:582:ARG:NH1	2.42	0.51
1:A:654:PHE:O	1:A:658:ASP:HB2	2.11	0.51
1:A:692:TYR:HA	1:A:695:ARG:HE	1.75	0.51
2:B:109:ALA:HB2	2:B:130:SER:HA	1.93	0.51
1:A:741:SER:OG	1:A:742:GLN:OE1	2.28	0.51
2:B:77:ASP:O	2:B:81:ILE:HG13	2.11	0.51
2:D:433:THR:HG22	2:D:456:CYS:HB3	1.93	0.51
1:C:67:HIS:CE1	1:C:95:PRO:HB3	2.46	0.51
2:D:34:SER:HA	2:D:65:VAL:HB	1.93	0.51
2:B:678:SER:HB2	2:B:679:PRO:HD2	1.93	0.50
1:C:209:MET:HE3	1:C:238:LEU:HD22	1.93	0.50
2:B:661:ASP:OD1	2:B:662:GLN:N	2.42	0.50
1:C:485:GLY:HA2	1:C:499:ASN:O	2.11	0.50
1:A:198:ASP:OD1	1:A:198:ASP:N	2.43	0.50
2:B:64:VAL:HG21	2:B:301:THR:HB	1.93	0.50
2:B:433:THR:HG23	2:B:458:LYS:HB3	1.92	0.50
2:B:544:THR:OG1	2:B:817:ASN:ND2	2.44	0.50
2:B:601:THR:HB	4:B:903:POV:H13B	1.93	0.50
1:A:446:SER:OG	1:A:447:PRO:HD3	2.12	0.50
2:B:485:LYS:O	2:B:496:GLY:HA3	2.12	0.50
2:B:243:VAL:O	2:B:246:SER:OG	2.30	0.50
2:B:406:LEU:HD11	2:B:474:PHE:CE2	2.47	0.50
1:C:351:TYR:H	1:C:367:TYR:HB3	1.77	0.49
2:D:133:ILE:HD11	2:D:147:GLY:HA3	1.93	0.49
2:D:176:PHE:CG	2:D:177:PRO:HD2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:VAL:HG13	2:D:205:LEU:HD11	1.93	0.49
1:C:438:GLY:HA3	1:C:478:LEU:HB2	1.94	0.49
2:D:558:VAL:O	2:D:562:MET:HG3	2.12	0.49
1:C:150:VAL:HG11	1:C:269:LEU:HD21	1.93	0.49
2:D:112:LEU:HB2	2:D:143:PHE:CE1	2.46	0.49
1:A:157:VAL:HG23	1:A:158:TYR:HD1	1.77	0.49
2:B:168:ILE:HD13	2:B:198:GLU:OE2	2.12	0.49
1:C:634:MET:SD	2:D:610:TRP:CD1	3.06	0.49
1:A:114:TYR:HB3	1:A:315:TRP:HD1	1.77	0.49
1:A:817:PHE:HD1	2:D:566:LEU:HD22	1.78	0.49
2:B:162:GLU:HG3	2:B:197:TRP:HZ2	1.77	0.49
2:B:164:TYR:CZ	2:B:386:MET:HG3	2.46	0.49
2:B:610:TRP:NE1	4:B:903:POV:H212	2.28	0.49
1:A:405:GLN:HE22	1:A:731:TRP:HE1	1.59	0.49
1:A:99:ASN:O	1:A:101:HIS:ND1	2.46	0.49
2:B:38:ALA:HB2	2:B:94:ILE:HD13	1.94	0.49
2:B:82:ILE:HG12	2:B:115:ILE:HD11	1.94	0.49
2:D:411:LEU:HD21	2:D:485:LYS:HG2	1.94	0.49
1:C:194:VAL:HG12	1:C:196:GLN:HE21	1.78	0.49
2:D:504:LYS:HE2	2:D:767:GLN:NE2	2.28	0.49
2:D:388:TYR:CZ	2:D:392:PRO:HD3	2.47	0.48
1:A:225:GLU:HG2	1:A:252:ARG:O	2.13	0.48
2:B:172:VAL:HG22	2:B:228:ILE:HG22	1.94	0.48
1:A:819:LEU:HD11	4:A:1001:POV:H21E	1.94	0.48
2:B:101:ASP:OD1	2:B:103:THR:N	2.46	0.48
1:C:114:TYR:OH	1:C:308:CYS:SG	2.71	0.48
1:A:790:LYS:HE3	1:A:794:ARG:HH21	1.78	0.48
2:D:542:ASN:O	2:D:544:THR:OG1	2.30	0.48
2:B:126:ILE:O	2:B:292:ARG:NH1	2.36	0.48
2:D:379:TRP:CD1	2:D:384:LEU:HB2	2.48	0.48
2:D:508:MET:HE3	2:D:764:ILE:HG21	1.95	0.48
1:A:585:PRO:HD3	2:B:840:HIS:CE1	2.49	0.48
1:A:434:VAL:HG21	1:A:474:TYR:HE1	1.78	0.48
1:C:353:ILE:C	1:C:354:MET:HE2	2.39	0.48
1:A:254:ILE:HD11	1:A:269:LEU:O	2.13	0.48
1:A:405:GLN:HG2	1:A:516:PRO:HG2	1.95	0.48
2:D:152:GLN:NE2	2:D:358:MET:O	2.46	0.48
1:C:146:HIS:HA	1:C:179:ARG:NH1	2.28	0.48
2:D:496:GLY:O	2:D:500:GLU:HG2	2.13	0.48
2:D:601:THR:HB	4:D:1002:POV:H13A	1.96	0.48
2:B:698:ASN:ND2	1:C:781:GLU:O	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:ILE:HG23	2:B:197:TRP:HB3	1.96	0.47
1:C:571:HIS:NE2	4:C:903:POV:H38	2.29	0.47
2:D:293:VAL:O	2:D:297:ILE:HG12	2.14	0.47
1:A:778:LYS:HB3	1:A:778:LYS:HE3	1.69	0.47
1:A:585:PRO:HD3	2:B:840:HIS:HE1	1.79	0.47
2:B:513:LEU:HA	2:B:513:LEU:HD23	1.76	0.47
2:D:190:ILE:HG23	2:D:197:TRP:HB3	1.96	0.47
2:D:440:ILE:HG13	2:D:451:GLY:HA3	1.96	0.47
2:D:419:VAL:HG21	2:D:480:LEU:HD11	1.97	0.47
1:A:77:SER:HA	1:A:80:GLU:HB2	1.96	0.47
2:B:166:TRP:HB3	2:B:227:ILE:CD1	2.45	0.47
1:A:101:HIS:HB3	1:A:125:MET:HE3	1.96	0.47
2:B:637:PHE:HE1	4:C:902:POV:H21E	1.80	0.47
2:B:782:GLN:HE21	1:C:695:ARG:HH22	1.62	0.47
1:C:292:VAL:HA	1:C:295:LEU:HD12	1.96	0.47
1:C:486:THR:HG23	1:C:488:GLU:HG2	1.97	0.47
2:D:358:MET:SD	2:D:358:MET:N	2.86	0.47
1:A:787:ASP:O	1:A:791:THR:HG23	2.15	0.47
2:B:136:ASP:OD1	2:B:136:ASP:N	2.47	0.47
1:A:525:GLN:O	1:A:764:LYS:NZ	2.43	0.47
2:B:794:ALA:O	2:B:798:THR:OG1	2.32	0.47
1:C:400:ILE:HD12	1:C:474:TYR:HB2	1.96	0.47
2:D:666:LEU:O	2:D:672:GLN:NE2	2.48	0.47
1:A:371:HIS:CE1	1:A:373:ILE:HG12	2.50	0.47
1:C:67:HIS:HE1	1:C:103:THR:HB	1.80	0.47
1:A:438:GLY:HA3	1:A:478:LEU:HD12	1.97	0.46
2:B:149:SER:HB3	2:B:152:GLN:HB2	1.96	0.46
1:C:124:ARG:NH1	1:C:271:LEU:HD22	2.30	0.46
1:C:495:LYS:HA	1:C:495:LYS:HD3	1.67	0.46
1:C:541:LEU:HB2	1:C:736:LEU:HD13	1.97	0.46
2:D:515:ILE:HD12	2:D:528:PRO:HG3	1.97	0.46
1:A:683:THR:HG22	1:A:730:ILE:HB	1.97	0.46
1:A:704:ARG:HH22	2:B:430:MET:HG3	1.80	0.46
2:B:35:ILE:O	2:B:67:ARG:N	2.42	0.46
2:B:308:LEU:HA	2:B:312:SER:HA	1.97	0.46
2:D:221:LYS:HB3	2:D:222:LYS:NZ	2.30	0.46
2:D:532:THR:HG22	2:D:734:ALA:HB2	1.98	0.46
2:B:97:VAL:O	2:B:123:ILE:HA	2.14	0.46
2:B:723:THR:OG1	2:B:725:LYS:NZ	2.39	0.46
1:C:402:THR:HG22	1:C:514:VAL:O	2.14	0.46
1:C:667:ILE:HG22	1:C:672:LEU:HD21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:609:LEU:O	2:D:635:TRP:NE1	2.48	0.46
1:A:157:VAL:HG23	1:A:158:TYR:CD1	2.49	0.46
2:B:226:PRO:O	2:B:255:THR:N	2.46	0.46
2:B:755:LYS:HD3	2:B:756:VAL:H	1.81	0.46
1:C:234:ALA:O	1:C:238:LEU:HG	2.14	0.46
1:A:732:ASP:OD2	3:A:1000:GLY:N	2.48	0.46
2:D:379:TRP:HA	2:D:384:LEU:HA	1.98	0.46
1:A:249:VAL:CG1	1:A:253:GLU:HB2	2.45	0.46
1:A:487:GLN:HG2	1:A:496:LYS:HB3	1.96	0.46
1:A:440:ASN:HD22	1:A:451:VAL:HG12	1.79	0.46
1:C:581:ASP:OD1	1:C:626:SER:OG	2.21	0.46
1:C:778:LYS:HB3	1:C:778:LYS:HE3	1.73	0.46
1:C:32:VAL:HG12	1:C:67:HIS:HB2	1.97	0.46
1:C:626:SER:O	1:C:630:ARG:HG3	2.16	0.46
1:C:208:LEU:HD12	1:C:208:LEU:O	2.16	0.46
2:D:409:VAL:HG22	2:D:479:TYR:CE2	2.51	0.46
2:D:287:TYR:HD2	2:D:292:ARG:HG3	1.81	0.46
1:A:34:SER:HB3	1:A:67:HIS:HB2	1.98	0.45
2:B:138:ASP:OD2	2:B:140:SER:OG	2.30	0.45
1:C:511:ASP:N	1:C:511:ASP:OD1	2.48	0.45
1:C:712:GLU:HA	1:C:712:GLU:OE1	2.16	0.45
2:D:285:TRP:HB2	2:D:375:ARG:HH12	1.80	0.45
1:A:351:TYR:H	1:A:367:TYR:HB3	1.80	0.45
4:C:902:POV:H34	4:C:902:POV:H23	1.97	0.45
2:D:86:CYS:SG	2:D:87:ASP:N	2.90	0.45
2:D:161:MET:HB2	2:D:166:TRP:HE3	1.80	0.45
2:B:306:ASP:OD1	2:B:306:ASP:N	2.47	0.45
2:B:676:ASP:OD1	2:B:676:ASP:N	2.48	0.45
2:B:782:GLN:HG3	1:C:695:ARG:NH2	2.32	0.45
2:B:783:LEU:HD12	2:B:789:MET:HE2	1.99	0.45
2:D:256:TRP:HB2	2:D:277:LEU:HD12	1.98	0.45
2:D:487:GLY:HA2	2:D:495:ASN:O	2.17	0.45
4:B:904:POV:H311	1:C:823:GLY:HA2	1.99	0.45
1:C:634:MET:SD	2:D:610:TRP:HD1	2.39	0.45
1:A:272:ILE:HD13	1:A:350:ASN:HB2	1.97	0.45
4:B:903:POV:H213	4:B:903:POV:H31D	1.97	0.45
1:C:41:MET:HA	1:C:44:GLU:HG2	1.98	0.45
2:B:738:TYR:HD2	2:B:739:MET:HE2	1.82	0.45
2:D:113:ASP:HB2	2:D:134:MET:HE1	1.98	0.45
2:D:151:GLU:HB3	2:D:185:LYS:HE3	1.99	0.45
1:A:770:GLN:O	1:A:774:LEU:HG	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:HD21	2:B:123:ILE:HG21	1.99	0.45
1:C:313:ASN:OD1	1:C:313:ASN:N	2.48	0.45
4:C:903:POV:H36	4:C:903:POV:H39	1.81	0.45
1:A:483:LYS:NZ	1:A:712:GLU:O	2.50	0.45
2:B:148:PRO:HB3	2:B:362:LEU:HD21	1.99	0.45
2:B:227:ILE:HA	2:B:255:THR:O	2.16	0.45
2:D:190:ILE:HD12	2:D:197:TRP:HB3	1.98	0.45
1:A:222:SER:O	1:A:222:SER:OG	2.34	0.45
1:A:405:GLN:HE21	1:A:735:VAL:HG21	1.81	0.45
1:A:626:SER:O	1:A:630:ARG:HG3	2.17	0.45
1:C:111:ALA:HB1	1:C:116:ILE:HB	1.99	0.45
1:C:295:LEU:HD11	1:C:321:PHE:CE1	2.52	0.45
2:B:161:MET:HE1	2:B:169:PHE:CE1	2.53	0.44
1:C:501:MET:HE1	1:C:515:ALA:HB3	1.99	0.44
2:B:101:ASP:CG	2:B:129:GLY:H	2.25	0.44
2:B:562:MET:HE1	2:B:642:PHE:HD1	1.81	0.44
1:A:83:ILE:HA	1:A:307:GLY:HA2	1.98	0.44
1:A:117:PRO:HG3	1:A:322:LYS:HB2	1.98	0.44
1:A:312:THR:OG1	2:B:105:GLN:OE1	2.35	0.44
2:B:515:ILE:HD12	2:B:528:PRO:HG3	1.98	0.44
2:D:112:LEU:HB3	2:D:123:ILE:HG21	1.99	0.44
1:A:353:ILE:N	1:A:365:GLY:O	2.50	0.44
2:D:112:LEU:HB2	2:D:143:PHE:HE1	1.83	0.44
2:B:112:LEU:HA	2:B:115:ILE:HD13	2.00	0.44
1:C:634:MET:HG2	2:D:607:TRP:CZ3	2.52	0.44
2:D:678:SER:HB3	2:D:679:PRO:HD2	1.99	0.44
2:B:41:LEU:HD11	2:B:289:LEU:HD21	2.00	0.44
2:B:89:MET:HE1	2:B:319:SER:HA	2.00	0.44
2:B:410:THR:HG22	2:B:411:LEU:H	1.81	0.44
2:B:663:VAL:HG11	2:B:671:PHE:HE2	1.83	0.44
1:C:483:LYS:HA	1:C:483:LYS:HD3	1.74	0.44
2:D:830:ALA:O	2:D:834:ILE:HG12	2.17	0.44
1:A:400:ILE:HD12	1:A:474:TYR:HB2	2.00	0.44
1:C:68:LYS:HB2	1:C:68:LYS:HE2	1.79	0.44
1:C:826:ALA:O	1:C:830:LEU:HB2	2.17	0.44
2:D:160:ILE:HD12	2:D:364:ILE:HD13	2.00	0.44
2:D:695:ILE:HG22	2:D:703:HIS:HB2	2.00	0.44
2:D:693:ARG:CZ	2:D:697:ASN:HD21	2.30	0.43
1:A:153:GLU:HB3	1:A:372:VAL:HG23	2.00	0.43
1:A:321:PHE:O	1:A:324:VAL:HG12	2.18	0.43
2:B:741:GLY:HA2	2:B:801:CYS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:MET:HE3	1:C:238:LEU:HD13	2.00	0.43
1:C:505:LEU:HD23	1:C:527:ILE:HG21	2.00	0.43
1:C:139:ARG:HH12	1:C:143:PRO:CB	2.26	0.43
2:D:51:LYS:HA	2:D:54:HIS:CD2	2.54	0.43
2:D:205:LEU:HB3	2:D:216:ILE:HD12	2.00	0.43
2:D:532:THR:HG21	2:D:762:TYR:CE1	2.53	0.43
1:A:570:VAL:HG13	1:A:610:SER:HB2	1.99	0.43
2:B:137:LYS:HZ3	2:B:355:GLY:HA3	1.84	0.43
2:B:389:TYR:CZ	2:B:452:TYR:HB2	2.53	0.43
1:A:94:HIS:CD2	1:A:94:HIS:C	2.96	0.43
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.81	0.43
2:B:430:MET:HE3	2:B:430:MET:HB2	1.81	0.43
2:B:782:GLN:HE21	1:C:695:ARG:NH2	2.17	0.43
1:C:70:ASN:OD1	1:C:71:ALA:N	2.48	0.43
1:C:124:ARG:HG2	1:C:142:PRO:O	2.19	0.43
2:D:468:ILE:O	2:D:472:VAL:HG23	2.19	0.43
1:A:291:ALA:O	1:A:295:LEU:N	2.52	0.43
1:A:539:THR:HG23	1:A:733:SER:HB3	2.00	0.43
1:A:539:THR:OG1	1:A:736:LEU:HD12	2.18	0.43
1:A:544:LYS:HG2	1:A:545:GLU:H	1.83	0.43
2:B:203:LEU:HB2	2:B:222:LYS:HZ1	1.84	0.43
1:C:585:PRO:HB3	2:D:840:HIS:HD2	1.83	0.43
2:D:410:THR:HG21	2:D:417:VAL:HG21	2.00	0.43
1:A:817:PHE:CD1	2:D:566:LEU:HD22	2.54	0.43
2:B:35:ILE:HD12	2:B:64:VAL:HB	2.00	0.43
2:B:320:SER:O	2:B:327:LYS:NZ	2.40	0.43
1:C:79:CYS:HB3	1:C:308:CYS:HB3	1.89	0.43
1:C:151:TRP:HD1	1:C:154:MET:HE3	1.83	0.43
2:D:405:HIS:ND1	2:D:475:THR:OG1	2.46	0.43
2:B:416:PHE:HB3	2:B:461:CYS:SG	2.59	0.43
1:C:264:ASP:HA	1:C:356:LEU:HD22	2.01	0.43
1:A:143:PRO:HD2	1:A:146:HIS:ND1	2.34	0.42
1:A:813:MET:SD	2:D:554:PHE:HE1	2.42	0.42
2:B:102:ASP:OD1	2:B:102:ASP:N	2.50	0.42
1:C:262:ALA:HB1	1:C:266:ILE:HD12	2.01	0.42
1:C:357:GLN:HG2	1:C:380:ILE:HB	2.01	0.42
1:C:366:ILE:N	1:C:373:ILE:O	2.48	0.42
1:C:564:LEU:HD12	4:C:902:POV:H27A	2.00	0.42
2:D:223:LEU:HD12	2:D:249:LEU:HD13	2.01	0.42
2:D:497:MET:HE1	2:D:511:GLY:HA3	2.01	0.42
2:D:610:TRP:HZ2	4:D:1002:POV:H212	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:780:HIS:CD2	1:C:785:MET:HG3	2.54	0.42
4:B:903:POV:H35A	4:B:903:POV:H25A	2.01	0.42
4:B:904:POV:H13B	4:B:904:POV:H11A	1.85	0.42
1:C:192:GLU:OE1	1:C:214:LEU:HD13	2.19	0.42
1:C:601:LEU:HD23	1:C:601:LEU:HA	1.88	0.42
1:C:669:ASP:N	1:C:669:ASP:OD1	2.53	0.42
2:D:76:THR:HG1	2:D:77:ASP:H	1.66	0.42
1:A:32:VAL:HG12	1:A:67:HIS:CD2	2.55	0.42
2:B:161:MET:HE3	2:B:197:TRP:HZ3	1.84	0.42
2:B:269:VAL:HA	2:B:270:PRO:HD3	1.90	0.42
2:B:126:ILE:HG22	2:B:146:PHE:CE2	2.55	0.42
2:B:379:TRP:HD1	2:B:384:LEU:HB2	1.83	0.42
1:C:532:PRO:HA	1:C:758:PHE:O	2.20	0.42
2:D:504:LYS:HE2	2:D:767:GLN:HE21	1.83	0.42
1:A:221:LEU:HD11	1:A:231:VAL:HG11	2.00	0.42
2:B:37:ILE:C	2:B:94:ILE:HD11	2.45	0.42
1:C:532:PRO:O	1:C:780:HIS:HE1	2.03	0.42
2:D:691:THR:HG1	5:D:1000:GLU:CD	2.27	0.42
2:B:577:PHE:HB3	2:B:627:THR:HG23	2.02	0.42
1:C:125:MET:HE3	1:C:125:MET:HB3	1.86	0.42
1:C:208:LEU:HD11	1:C:240:MET:SD	2.59	0.42
1:C:635:VAL:HG22	4:D:1002:POV:H213	2.02	0.42
1:A:202:LYS:HD3	1:A:202:LYS:HA	1.77	0.42
1:A:247:TRP:HB2	1:A:266:ILE:HG23	2.00	0.42
2:B:709:PHE:O	2:B:711:GLN:NE2	2.44	0.42
1:C:366:ILE:HB	1:C:373:ILE:HB	2.02	0.42
1:C:567:GLY:HA3	4:C:902:POV:H211	2.01	0.42
2:D:85:ILE:HD13	2:D:115:ILE:HG21	2.01	0.42
2:D:298:ALA:O	2:D:302:THR:OG1	2.29	0.42
1:A:114:TYR:HB3	1:A:315:TRP:CD1	2.55	0.42
1:A:781:GLU:O	2:D:698:ASN:ND2	2.46	0.42
2:B:34:SER:OG	2:B:67:ARG:NH2	2.53	0.42
2:D:282:TYR:OH	2:D:357:GLN:OE1	2.25	0.42
2:D:527:VAL:N	2:D:777:ASP:OD1	2.48	0.42
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.91	0.41
2:B:81:ILE:O	2:B:85:ILE:HG12	2.20	0.41
2:B:814:ASP:OD1	2:B:815:ILE:N	2.46	0.41
1:C:41:MET:HE3	1:C:41:MET:HB2	1.84	0.41
1:C:67:HIS:CE1	1:C:103:THR:HB	2.54	0.41
1:C:570:VAL:HG22	1:C:636:TRP:CZ2	2.55	0.41
4:C:903:POV:H315	4:C:903:POV:H31C	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:562:MET:HE1	2:B:642:PHE:CD1	2.55	0.41
1:A:513:ILE:HG21	1:A:517:LEU:HD22	2.01	0.41
2:B:813:LEU:O	2:B:817:ASN:HB2	2.21	0.41
4:C:903:POV:H212	4:C:903:POV:H316	2.03	0.41
2:D:409:VAL:CG1	2:D:481:VAL:HG22	2.50	0.41
2:D:610:TRP:CD1	2:D:610:TRP:C	2.98	0.41
2:B:169:PHE:HB3	2:B:199:LEU:HA	2.01	0.41
2:D:78:PRO:HB3	2:D:111:ILE:HD13	2.01	0.41
2:D:156:VAL:O	2:D:160:ILE:HG22	2.20	0.41
4:A:1001:POV:H21D	4:A:1002:POV:H212	2.03	0.41
2:B:115:ILE:H	2:B:115:ILE:HD12	1.86	0.41
1:C:627:PHE:HE1	4:D:1002:POV:H32	1.86	0.41
2:D:78:PRO:HA	2:D:81:ILE:HD12	2.02	0.41
2:D:203:LEU:HD21	2:D:223:LEU:HD21	2.02	0.41
1:A:37:LYS:HA	1:A:40:GLN:HE21	1.85	0.41
1:A:302:THR:OG1	1:A:317:THR:OG1	2.35	0.41
1:A:396:THR:O	1:A:472:PHE:HB2	2.21	0.41
2:B:513:LEU:O	2:B:762:TYR:HA	2.20	0.41
1:C:126:SER:N	1:C:172:GLU:OE1	2.34	0.41
1:C:630:ARG:HB3	4:D:1002:POV:H26	2.03	0.41
1:A:564:LEU:HD12	4:A:1002:POV:H27	2.03	0.41
1:A:807:THR:OG1	2:D:552:GLU:O	2.32	0.41
2:B:221:LYS:NZ	2:D:247:VAL:O	2.40	0.41
2:B:314:ILE:HA	2:B:315:PRO:HD3	1.93	0.41
1:C:72:ILE:HD13	1:C:72:ILE:HA	1.84	0.41
1:C:223:ALA:HB1	1:C:227:ASP:HB2	2.03	0.41
2:D:101:ASP:OD1	2:D:102:ASP:N	2.52	0.41
2:D:157:MET:HB3	2:D:257:ILE:HG21	2.03	0.41
2:D:478:LEU:HD23	2:D:478:LEU:HA	1.86	0.41
2:D:691:THR:OG1	5:D:1000:GLU:OE2	2.37	0.41
1:A:93:SER:HB3	1:A:277:GLU:OE2	2.20	0.41
1:C:572:VAL:HG22	4:C:903:POV:H215	2.03	0.41
2:D:160:ILE:HD12	2:D:364:ILE:HG21	2.03	0.41
2:D:693:ARG:HH11	2:D:696:ARG:HE	1.69	0.41
4:D:1002:POV:H36	4:D:1002:POV:H39	1.78	0.41
1:A:29:ILE:HD11	1:A:46:VAL:HG22	2.03	0.41
1:A:70:ASN:HB2	2:B:323:ASN:H	1.86	0.41
1:A:630:ARG:O	1:A:634:MET:HB2	2.21	0.41
2:B:433:THR:HG22	2:B:456:CYS:HB3	2.01	0.41
2:B:519:ARG:NH2	5:B:901:GLU:OXT	2.39	0.41
2:B:567:LEU:HD23	2:B:568:ILE:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ILE:HG23	1:C:118:VAL:HG13	2.02	0.41
1:C:232:TYR:OH	1:C:249:VAL:HG11	2.20	0.41
1:C:833:ILE:HD13	1:C:833:ILE:HA	1.84	0.41
2:D:437:GLN:HG2	2:D:452:TYR:HE1	1.85	0.41
1:A:316:LYS:H	1:A:316:LYS:HG2	1.58	0.41
1:C:67:HIS:HD2	1:C:74:MET:SD	2.44	0.41
2:D:281:SER:OG	2:D:282:TYR:N	2.54	0.41
2:D:606:ILE:O	2:D:610:TRP:HB3	2.20	0.41
1:A:229:ALA:HB1	1:A:261:TYR:CD2	2.55	0.40
1:A:341:ASN:CG	1:A:347:LYS:HG2	2.46	0.40
2:B:725:LYS:HB2	2:B:725:LYS:HE2	1.85	0.40
1:C:254:ILE:HD13	1:C:268:GLY:HA3	2.02	0.40
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.85	0.40
2:B:137:LYS:NZ	2:B:355:GLY:HA3	2.37	0.40
2:B:528:PRO:HB3	2:B:761:GLY:HA3	2.03	0.40
2:B:751:ILE:HD13	2:B:751:ILE:HA	1.91	0.40
1:A:570:VAL:HG22	1:A:636:TRP:CZ2	2.56	0.40
2:B:149:SER:HB2	2:B:356:TYR:CG	2.56	0.40
2:B:726:LEU:HD23	2:B:726:LEU:HA	1.86	0.40
2:B:747:LYS:HA	2:B:747:LYS:HD3	1.88	0.40
1:C:670:PRO:HG3	2:D:799:GLY:HA2	2.03	0.40
1:C:675:PRO:HB3	1:C:705:HIS:ND1	2.37	0.40
2:D:408:ILE:HD13	2:D:508:MET:HE2	2.04	0.40
1:A:194:VAL:HG12	1:A:194:VAL:O	2.21	0.40
2:B:653:PHE:HA	1:C:805:PRO:HG2	2.03	0.40
1:C:167:VAL:O	1:C:196:GLN:HA	2.22	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	793/830 (96%)	749 (94%)	43 (5%)	1 (0%)	48	80
1	C	794/830 (96%)	757 (95%)	37 (5%)	0	100	100
2	B	772/861 (90%)	717 (93%)	54 (7%)	1 (0%)	48	80
2	D	770/861 (89%)	720 (94%)	49 (6%)	1 (0%)	48	80
All	All	3129/3382 (92%)	2943 (94%)	183 (6%)	3 (0%)	50	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	797	GLU
2	B	660	VAL
2	D	391	TRP

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	652/712 (92%)	647 (99%)	5 (1%)	79	90
1	C	654/712 (92%)	653 (100%)	1 (0%)	92	97
2	B	660/744 (89%)	656 (99%)	4 (1%)	84	92
2	D	650/744 (87%)	649 (100%)	1 (0%)	92	97
All	All	2616/2912 (90%)	2605 (100%)	11 (0%)	88	94

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

Mol	Chain	Res	Type
1	A	61	ASN
1	A	208	LEU
1	A	691	ILE
1	A	699	LEU
1	A	701	THR
2	B	133	ILE
2	B	282	TYR
2	B	363	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	365	ILE
1	C	795	TYR
2	D	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	40	GLN
1	A	61	ASN
1	A	67	HIS
1	A	94	HIS
1	A	177	GLN
1	A	196	GLN
1	A	393	GLN
1	A	405	GLN
1	A	427	ASN
1	A	440	ASN
1	A	449	HIS
1	A	453	GLN
1	A	499	ASN
1	A	521	ASN
1	A	571	HIS
1	A	705	HIS
1	A	780	HIS
1	A	812	ASN
2	B	145	GLN
2	B	152	GLN
2	B	192	ASN
2	B	325	HIS
2	B	333	ASN
2	B	341	ASN
2	B	615	ASN
2	B	767	GLN
2	B	775	GLN
2	B	782	GLN
2	B	817	ASN
2	B	840	HIS
1	C	67	HIS
1	C	161	ASN
1	C	162	HIS
1	C	196	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	350	ASN
1	C	357	GLN
1	C	427	ASN
1	C	471	ASN
1	C	492	ASN
1	C	556	GLN
1	C	668	ASN
1	C	696	GLN
1	C	780	HIS
1	C	812	ASN
2	D	153	GLN
2	D	192	ASN
2	D	218	ASN
2	D	336	ASN
2	D	368	ASN
2	D	483	ASN
2	D	672	GLN
2	D	688	ASN
2	D	697	ASN
2	D	775	GLN
2	D	802	HIS
2	D	840	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GLU	D	1000	-	8,9,9	1.12	1 (12%)	8,11,11	1.18	1 (12%)
4	POV	B	904	-	51,51,51	0.51	0	57,59,59	0.47	0
4	POV	C	902	-	51,51,51	0.49	0	57,59,59	0.47	0
5	GLU	B	901	-	8,9,9	1.13	1 (12%)	8,11,11	1.16	1 (12%)
3	GLY	A	1000	-	4,4,4	1.22	1 (25%)	3,4,4	1.60	1 (33%)
4	POV	A	1002	-	51,51,51	0.50	0	57,59,59	0.46	0
3	GLY	C	901	-	4,4,4	1.23	1 (25%)	3,4,4	1.61	1 (33%)
4	POV	A	1001	-	51,51,51	0.50	0	57,59,59	0.47	0
4	POV	C	903	-	51,51,51	0.51	0	57,59,59	0.49	0
4	POV	A	1003	-	51,51,51	0.51	0	57,59,59	0.45	0
6	A1CE1	B	902	-	32,32,32	0.28	0	50,50,50	0.66	0
4	POV	B	903	-	51,51,51	0.50	0	57,59,59	0.48	0
4	POV	D	1002	-	51,51,51	0.50	0	57,59,59	0.44	0
6	A1CE1	D	1001	-	32,32,32	0.28	0	50,50,50	0.63	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	GLU	D	1000	-	-	2/9/9/9	-
4	POV	B	904	-	-	19/55/55/55	-
4	POV	C	902	-	-	19/55/55/55	-
5	GLU	B	901	-	-	2/9/9/9	-
3	GLY	A	1000	-	-	0/2/2/2	-
4	POV	A	1002	-	-	21/55/55/55	-
3	GLY	C	901	-	-	0/2/2/2	-
4	POV	A	1001	-	-	24/55/55/55	-
4	POV	C	903	-	-	22/55/55/55	-
4	POV	A	1003	-	-	19/55/55/55	-
6	A1CE1	B	902	-	-	4/13/71/71	0/4/4/4
4	POV	B	903	-	-	15/55/55/55	-
4	POV	D	1002	-	-	18/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1CE1	D	1001	-	-	4/13/71/71	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	GLU	OXT-C	-2.36	1.23	1.30
5	D	1000	GLU	OXT-C	-2.33	1.23	1.30
3	A	1000	GLY	OXT-C	-2.32	1.23	1.30
3	C	901	GLY	OXT-C	-2.31	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1000	GLU	OXT-C-O	-2.55	118.29	124.08
5	B	901	GLU	OXT-C-O	-2.50	118.42	124.08
3	A	1000	GLY	OXT-C-O	-2.10	117.94	123.33
3	C	901	GLY	OXT-C-O	-2.08	117.99	123.33

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	POV	C11-O12-P-O13
4	A	1001	POV	O12-C11-C12-N
4	A	1002	POV	C1-O11-P-O12
4	A	1002	POV	C1-O11-P-O13
4	A	1002	POV	C11-O12-P-O14
4	A	1002	POV	O11-C1-C2-O21
4	A	1003	POV	C1-O11-P-O12
4	A	1003	POV	C1-O11-P-O13
4	A	1003	POV	C1-O11-P-O14
4	A	1003	POV	C11-O12-P-O11
4	A	1003	POV	C11-O12-P-O13
4	A	1003	POV	O12-C11-C12-N
4	A	1003	POV	C12-C11-O12-P
4	B	903	POV	O12-C11-C12-N
4	B	904	POV	C1-O11-P-O13
4	B	904	POV	C11-O12-P-O13
4	B	904	POV	O12-C11-C12-N
4	B	904	POV	C12-C11-O12-P
4	C	903	POV	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	903	POV	C1-O11-P-O13
4	C	903	POV	C1-O11-P-O14
4	C	903	POV	C11-O12-P-O13
4	C	903	POV	O12-C11-C12-N
4	D	1002	POV	C11-O12-P-O11
4	D	1002	POV	C11-O12-P-O14
4	D	1002	POV	O11-C1-C2-O21
4	D	1002	POV	O12-C11-C12-N
4	C	903	POV	C2-C1-O11-P
4	C	902	POV	C32-C31-O31-C3
4	C	902	POV	O11-C1-C2-O21
4	B	903	POV	C11-C12-N-C15
4	B	903	POV	C21-C22-C23-C24
4	C	902	POV	O32-C31-O31-C3
4	A	1001	POV	C22-C21-O21-C2
4	A	1001	POV	O22-C21-O21-C2
4	A	1002	POV	C310-C311-C312-C313
4	C	902	POV	C24-C25-C26-C27
4	B	904	POV	C310-C311-C312-C313
4	A	1002	POV	C211-C212-C213-C214
4	D	1002	POV	C310-C311-C312-C313
4	A	1003	POV	C35-C36-C37-C38
4	A	1003	POV	C211-C212-C213-C214
4	C	903	POV	C33-C34-C35-C36
4	A	1003	POV	C2-C1-O11-P
4	C	902	POV	C31-C32-C33-C34
4	B	904	POV	C22-C23-C24-C25
4	C	903	POV	C310-C311-C312-C313
4	C	903	POV	C32-C33-C34-C35
4	A	1001	POV	C24-C25-C26-C27
4	B	903	POV	C11-C12-N-C14
4	B	903	POV	C26-C27-C28-C29
4	B	904	POV	C311-C310-C39-C38
4	A	1002	POV	C35-C36-C37-C38
4	A	1001	POV	C310-C311-C312-C313
4	B	903	POV	C11-C12-N-C13
4	B	904	POV	C26-C27-C28-C29
4	A	1002	POV	O11-C1-C2-C3
4	C	902	POV	O11-C1-C2-C3
4	D	1002	POV	O11-C1-C2-C3
4	C	903	POV	C39-C310-C311-C312
4	C	903	POV	C210-C211-C212-C213

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	903	POV	C34-C35-C36-C37
4	A	1002	POV	C212-C213-C214-C215
4	A	1002	POV	C11-C12-N-C15
4	A	1003	POV	C24-C25-C26-C27
4	A	1001	POV	C212-C213-C214-C215
4	B	904	POV	C23-C24-C25-C26
4	A	1003	POV	C311-C312-C313-C314
4	B	904	POV	C210-C211-C212-C213
4	C	902	POV	C210-C211-C212-C213
4	D	1002	POV	C210-C211-C212-C213
4	C	903	POV	C312-C313-C314-C315
4	D	1002	POV	C39-C310-C311-C312
6	D	1001	A1CE1	C8-C7-C9-C26
4	A	1001	POV	C214-C215-C216-C217
4	A	1001	POV	C23-C24-C25-C26
6	B	902	A1CE1	C8-C7-C9-C26
4	A	1002	POV	C11-C12-N-C14
4	C	902	POV	C33-C34-C35-C36
4	D	1002	POV	C34-C35-C36-C37
6	D	1001	A1CE1	C6-C7-C9-C26
4	B	904	POV	C212-C213-C214-C215
4	D	1002	POV	C212-C213-C214-C215
4	B	903	POV	C210-C211-C212-C213
4	A	1001	POV	C32-C33-C34-C35
4	D	1002	POV	C25-C26-C27-C28
4	A	1002	POV	C33-C34-C35-C36
4	A	1001	POV	C213-C214-C215-C216
4	D	1002	POV	C214-C215-C216-C217
6	B	902	A1CE1	C6-C7-C9-C26
4	A	1002	POV	O21-C2-C3-O31
4	A	1003	POV	O21-C2-C3-O31
4	D	1002	POV	C35-C36-C37-C38
4	A	1002	POV	C25-C26-C27-C28
4	C	902	POV	C215-C216-C217-C218
6	D	1001	A1CE1	C8-C7-C9-C10
4	A	1001	POV	O11-C1-C2-C3
4	C	903	POV	O11-C1-C2-C3
4	A	1003	POV	C37-C38-C39-C310
4	A	1001	POV	O11-C1-C2-O21
6	D	1001	A1CE1	C6-C7-C9-C10
4	C	903	POV	C211-C212-C213-C214
4	A	1001	POV	C12-C11-O12-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	903	POV	C12-C11-O12-P
4	C	903	POV	O21-C2-C3-O31
4	A	1002	POV	C214-C215-C216-C217
4	B	904	POV	C35-C36-C37-C38
4	A	1002	POV	O12-C11-C12-N
6	B	902	A1CE1	C6-C7-C9-C10
4	C	902	POV	C26-C27-C28-C29
6	B	902	A1CE1	C8-C7-C9-C10
4	A	1003	POV	C31-C32-C33-C34
4	B	904	POV	C32-C33-C34-C35
4	A	1002	POV	C215-C216-C217-C218
4	C	903	POV	O11-C1-C2-O21
4	A	1001	POV	C11-C12-N-C13
4	B	904	POV	C312-C313-C314-C315
4	C	902	POV	C35-C36-C37-C38
4	A	1002	POV	C1-C2-C3-O31
4	A	1001	POV	C1-O11-P-O12
4	A	1001	POV	C1-O11-P-O13
4	A	1001	POV	C1-O11-P-O14
4	A	1002	POV	C1-O11-P-O14
4	C	902	POV	C11-O12-P-O14
4	D	1002	POV	C11-O12-P-O13
4	C	903	POV	C23-C24-C25-C26
4	C	903	POV	C35-C36-C37-C38
4	D	1002	POV	C22-C23-C24-C25
4	A	1003	POV	C25-C26-C27-C28
4	C	902	POV	C23-C24-C25-C26
4	C	902	POV	C212-C213-C214-C215
4	B	903	POV	C24-C25-C26-C27
4	D	1002	POV	C36-C37-C38-C39
4	A	1001	POV	C39-C310-C311-C312
4	A	1002	POV	C11-C12-N-C13
4	B	904	POV	C34-C35-C36-C37
4	C	902	POV	C211-C212-C213-C214
4	B	903	POV	C39-C310-C311-C312
4	B	904	POV	C2-C1-O11-P
4	C	902	POV	C214-C215-C216-C217
4	D	1002	POV	C211-C212-C213-C214
4	D	1002	POV	C1-C2-C3-O31
4	B	903	POV	O11-C1-C2-O21
5	D	1000	GLU	OE2-CD-CG-CB
4	B	904	POV	C214-C215-C216-C217

Continued on next page...

Continued from previous page...

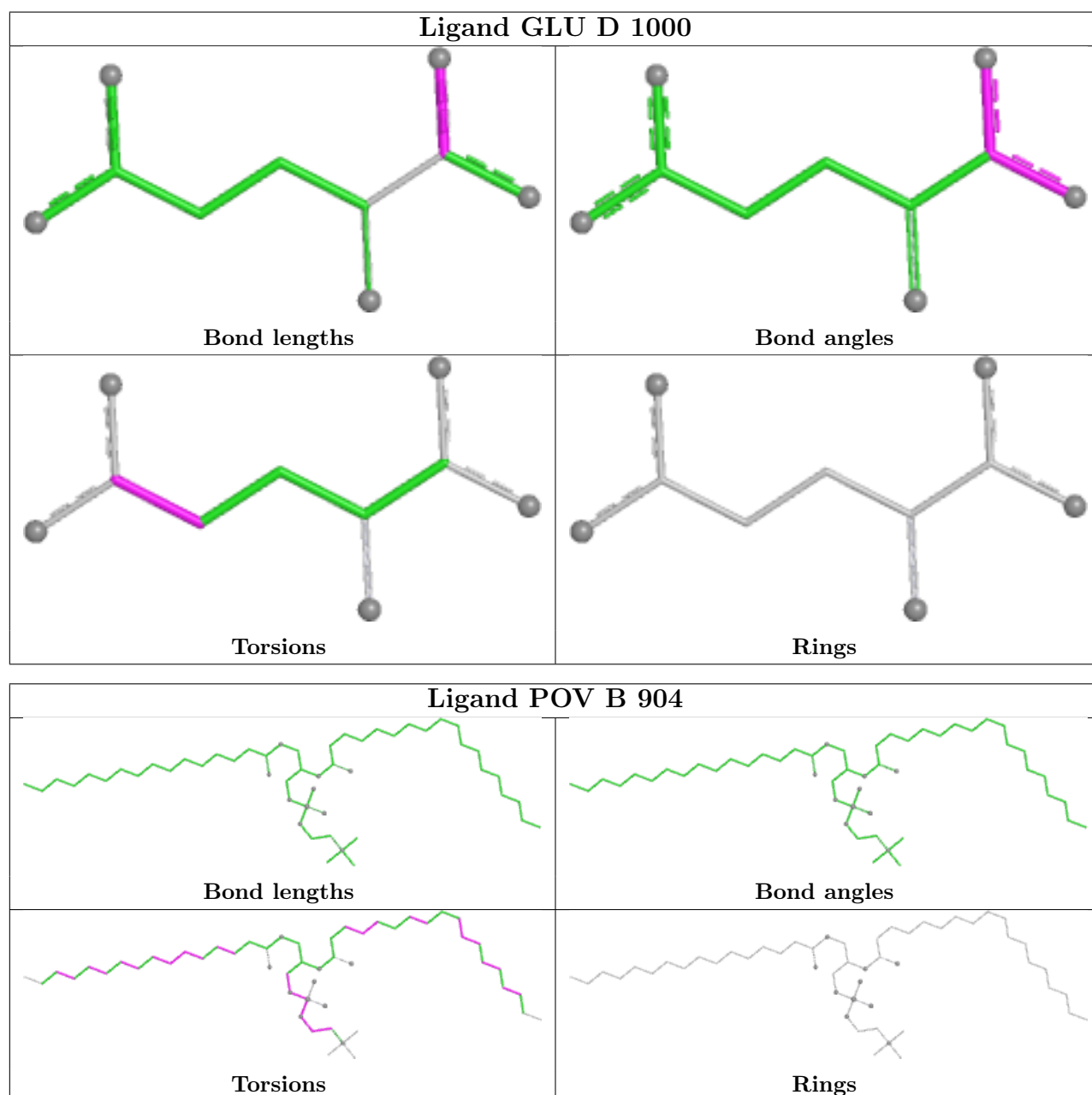
Mol	Chain	Res	Type	Atoms
4	B	903	POV	O11-C1-C2-C3
5	D	1000	GLU	OE1-CD-CG-CB
4	A	1003	POV	O21-C21-C22-C23
4	C	903	POV	C26-C27-C28-C29
4	C	902	POV	C311-C310-C39-C38
5	B	901	GLU	OE2-CD-CG-CB
5	B	901	GLU	OE1-CD-CG-CB
4	B	904	POV	C29-C210-C211-C212
4	C	902	POV	C36-C37-C38-C39
4	A	1002	POV	C24-C25-C26-C27
4	C	903	POV	C1-C2-C3-O31
4	A	1001	POV	C36-C37-C38-C39
4	A	1001	POV	C11-C12-N-C14
4	B	903	POV	C27-C28-C29-C210
4	A	1001	POV	C11-C12-N-C15
4	A	1003	POV	C1-C2-C3-O31
4	B	903	POV	C33-C34-C35-C36
4	A	1001	POV	C26-C27-C28-C29
4	B	904	POV	C36-C37-C38-C39
4	C	902	POV	C1-C2-C3-O31
4	A	1003	POV	C27-C28-C29-C210
4	C	903	POV	C36-C37-C38-C39
4	B	903	POV	O31-C31-C32-C33
4	A	1001	POV	O31-C31-C32-C33

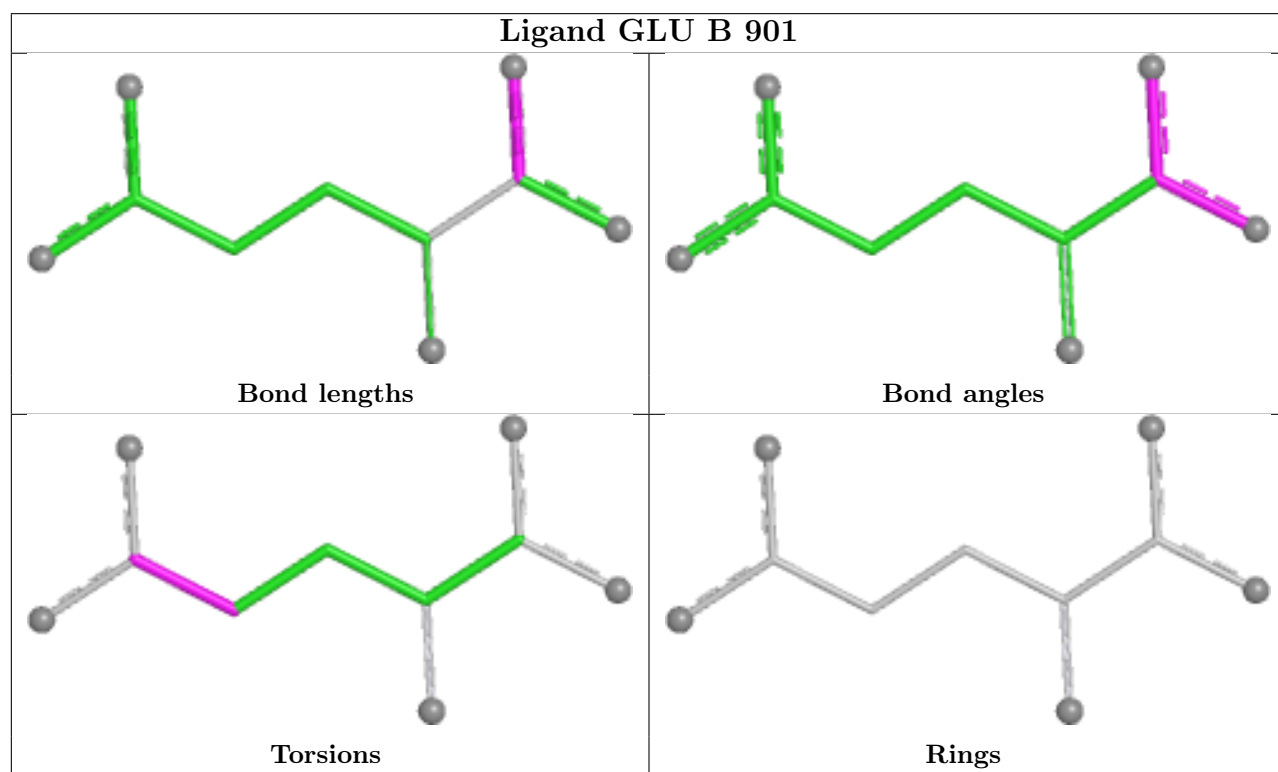
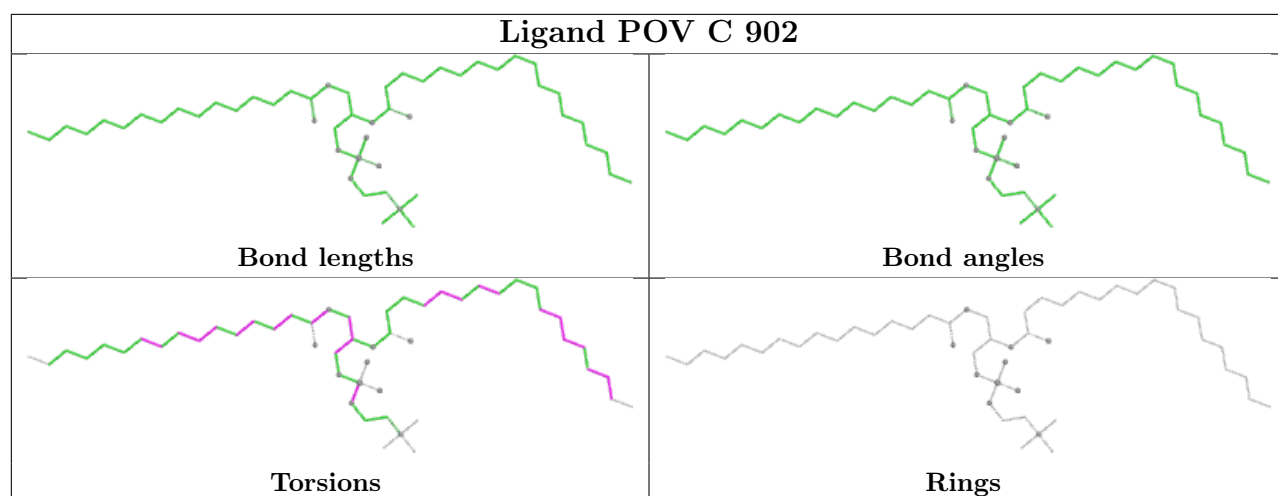
There are no ring outliers.

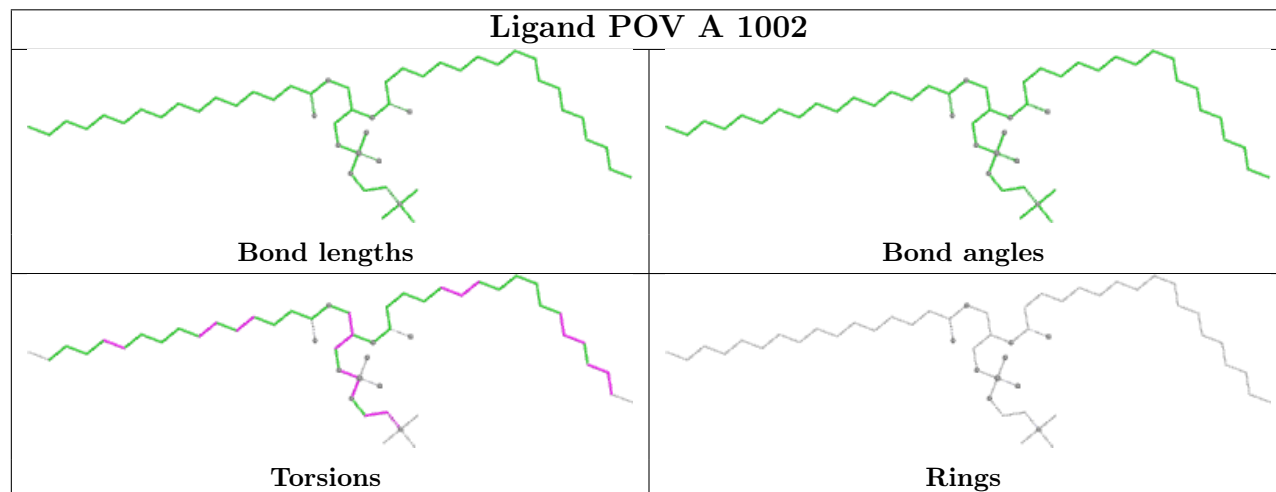
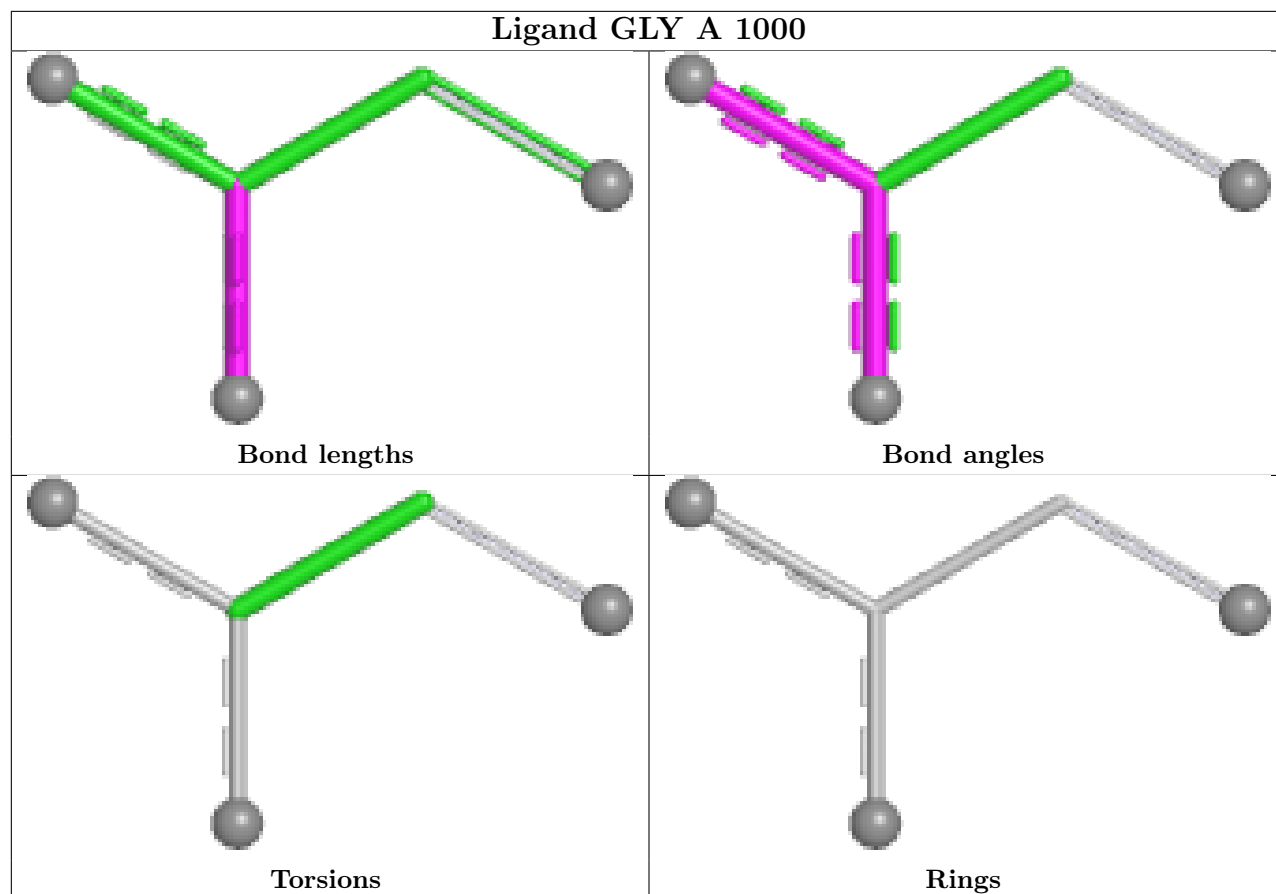
12 monomers are involved in 47 short contacts:

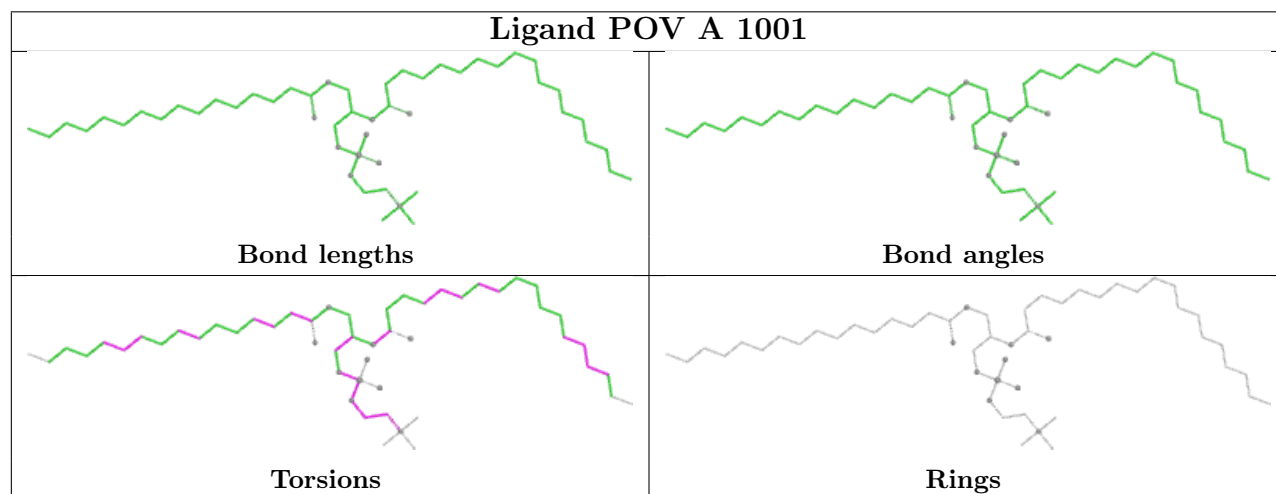
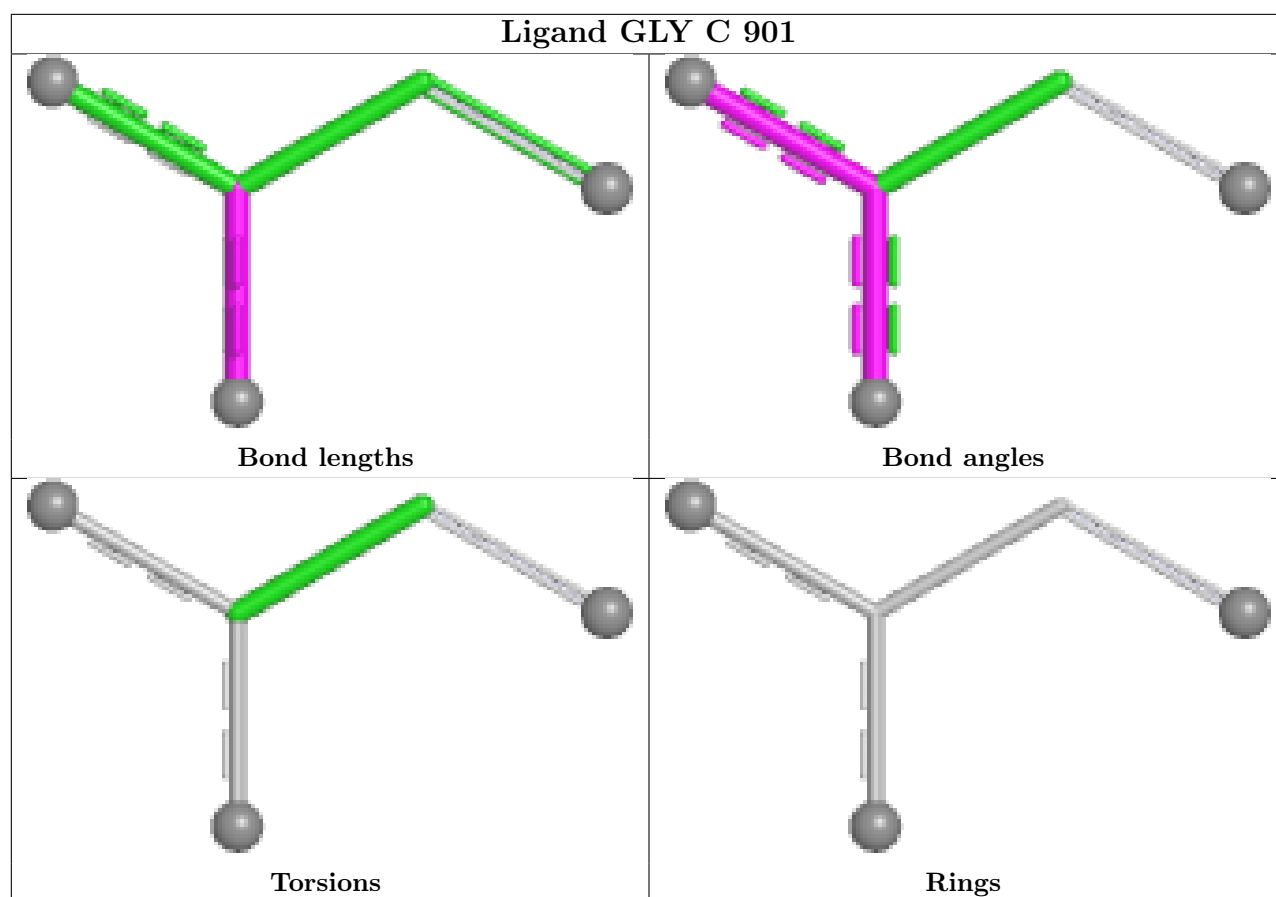
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1000	GLU	4	0
4	B	904	POV	7	0
4	C	902	POV	5	0
5	B	901	GLU	1	0
3	A	1000	GLY	1	0
4	A	1002	POV	5	0
3	C	901	GLY	1	0
4	A	1001	POV	5	0
4	C	903	POV	8	0
4	A	1003	POV	2	0
4	B	903	POV	6	0
4	D	1002	POV	9	0

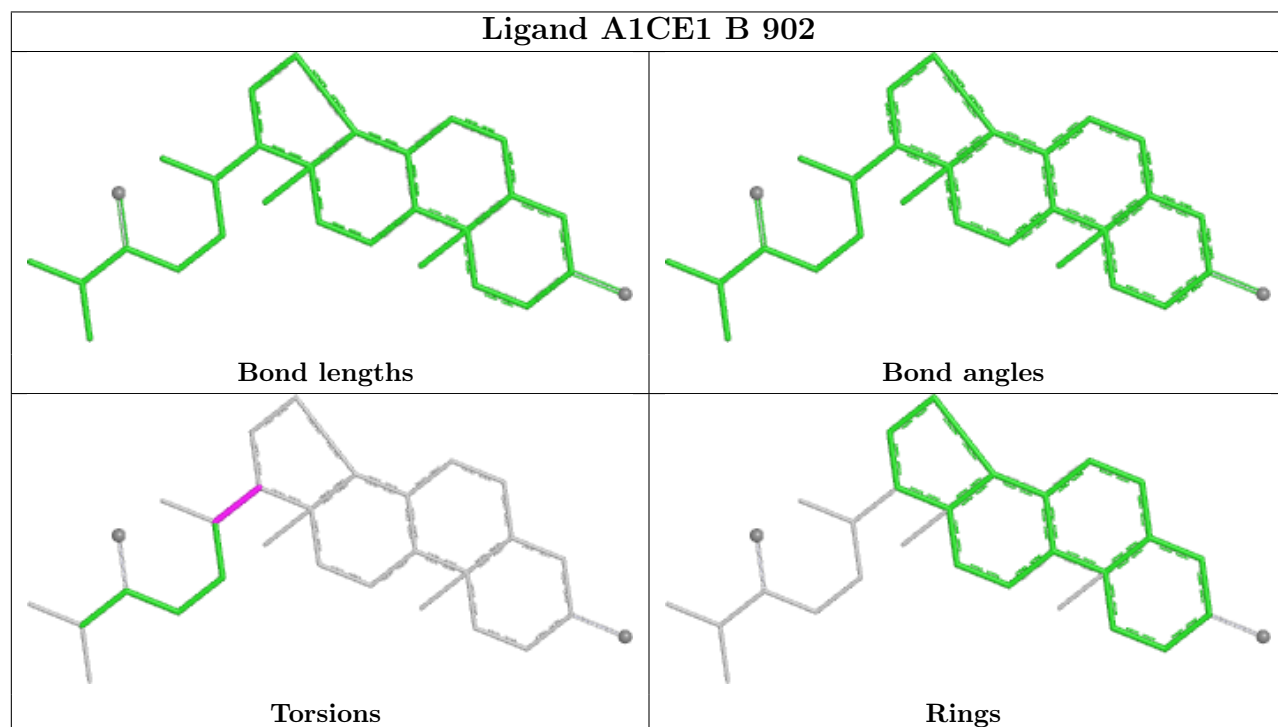
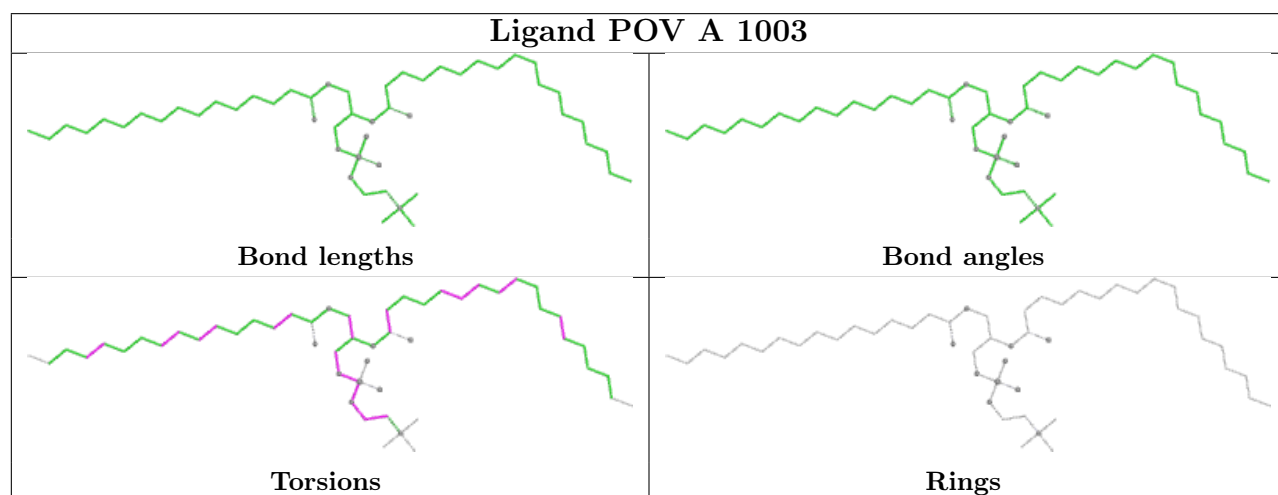
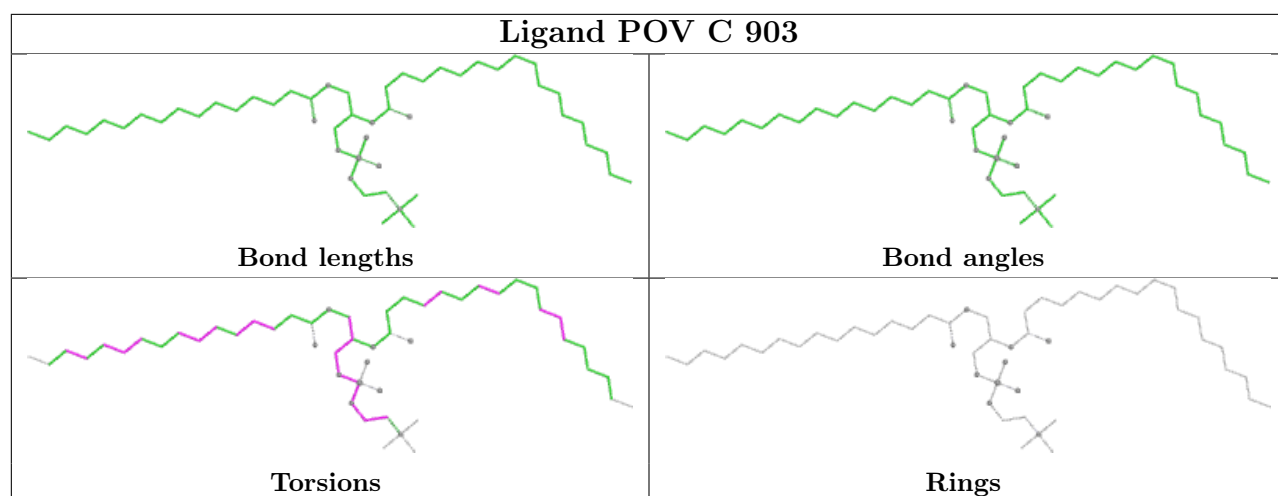
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

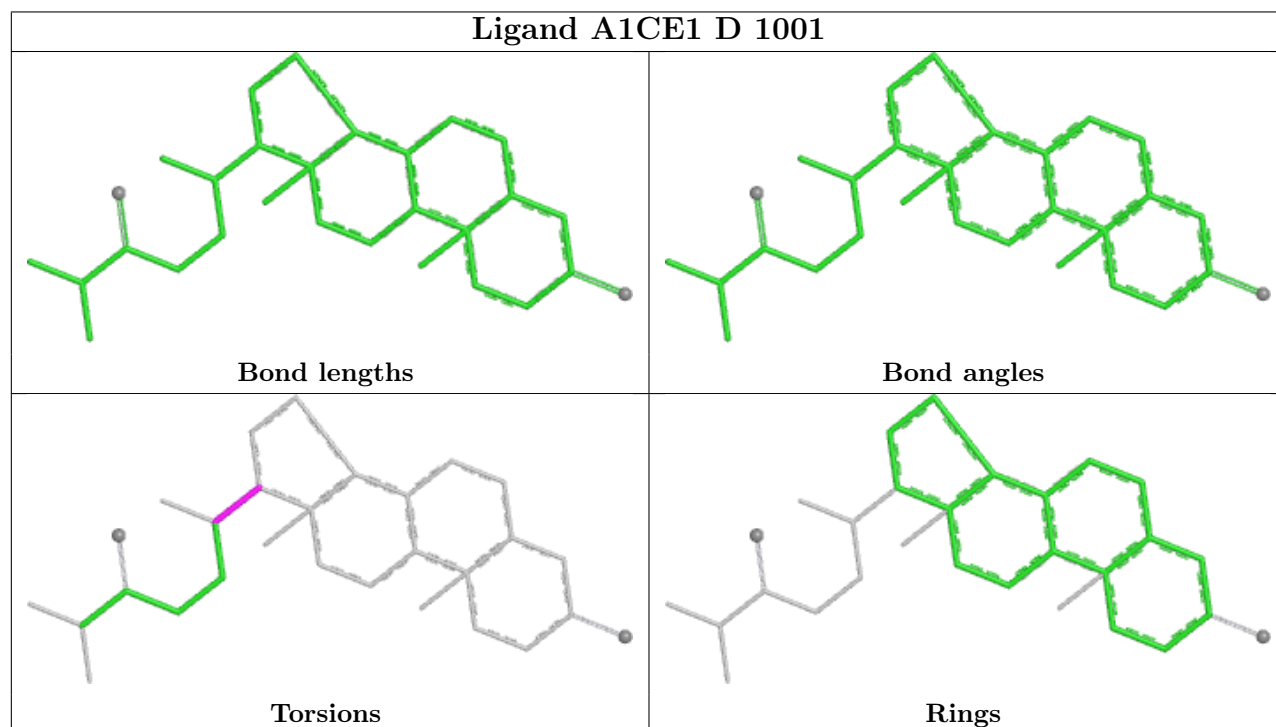
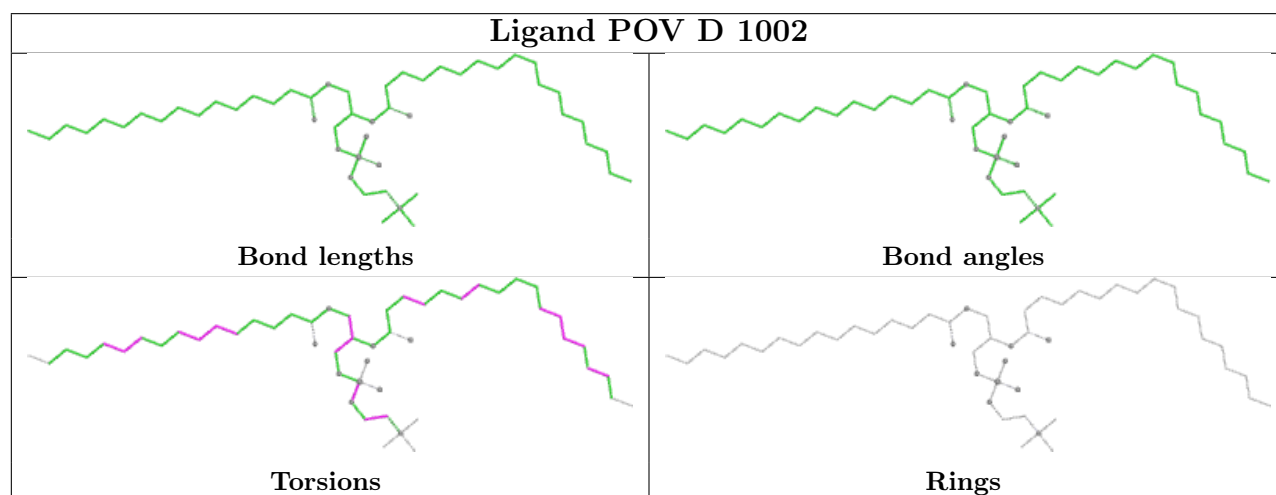
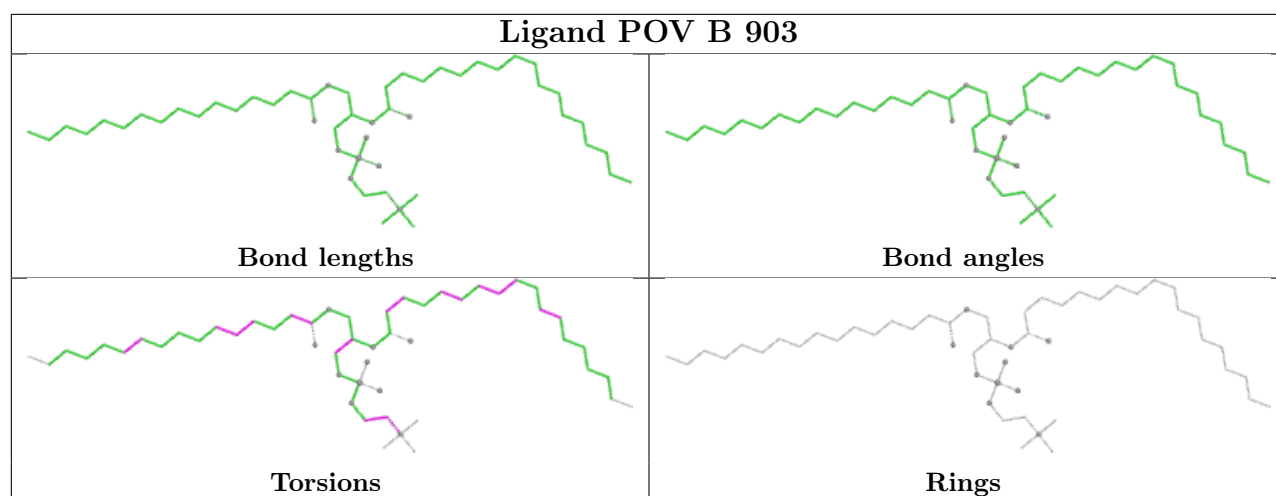












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

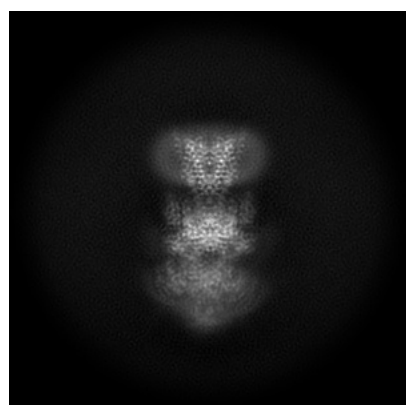
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70669. These allow visual inspection of the internal detail of the map and identification of artifacts.

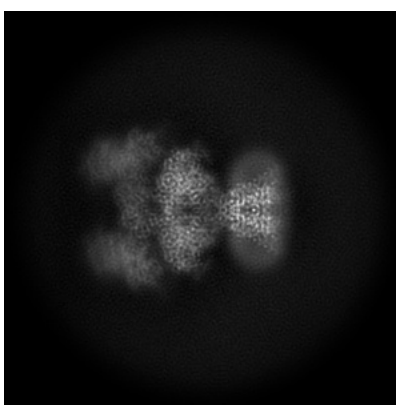
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

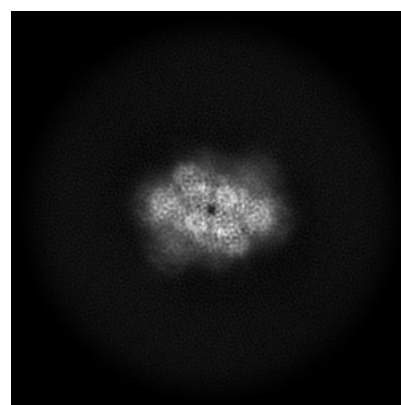
6.1.1 Primary map



X



Y



Z

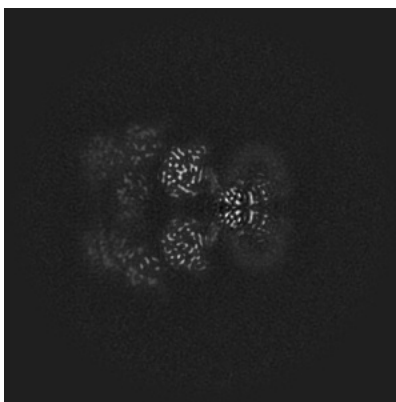
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

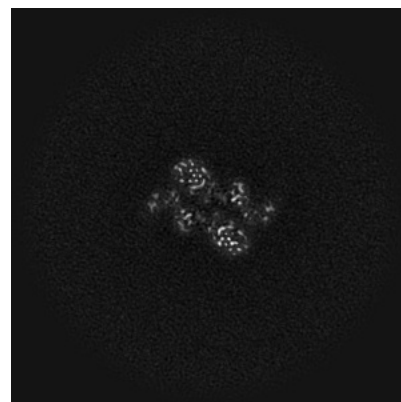
6.2.1 Primary map



X Index: 200



Y Index: 200

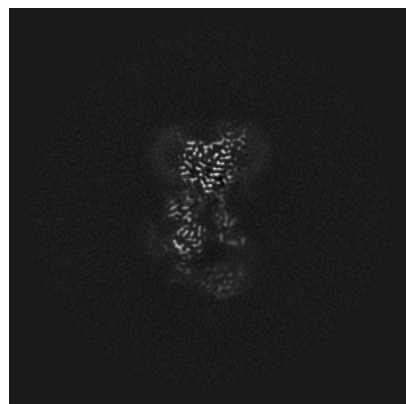


Z Index: 200

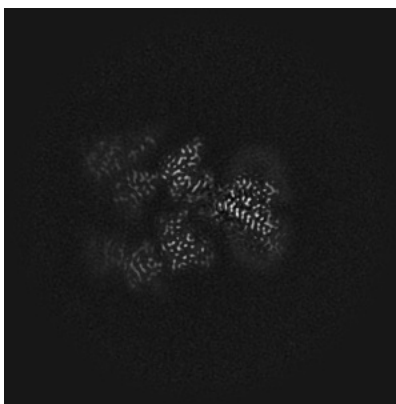
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

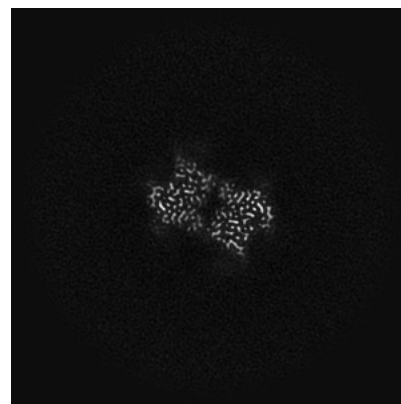
6.3.1 Primary map



X Index: 208



Y Index: 209

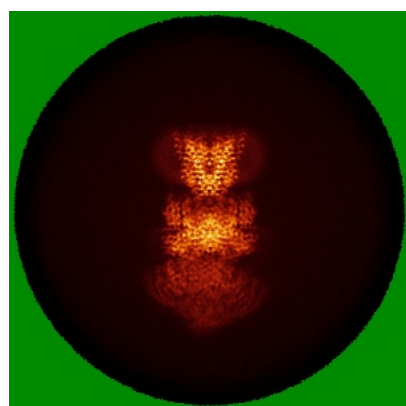


Z Index: 174

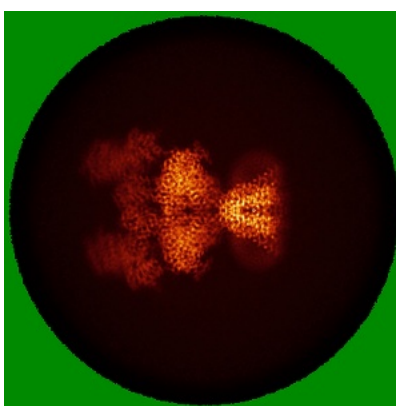
The images above show the largest variance slices of the map in three orthogonal directions.

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

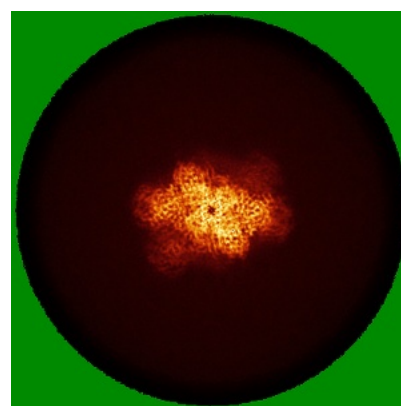
6.4.1 Primary map



X



Y

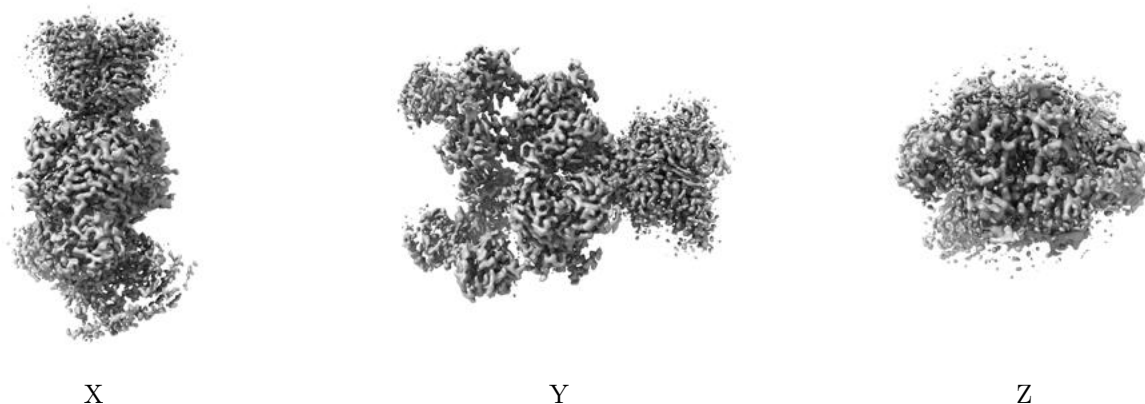


Z

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

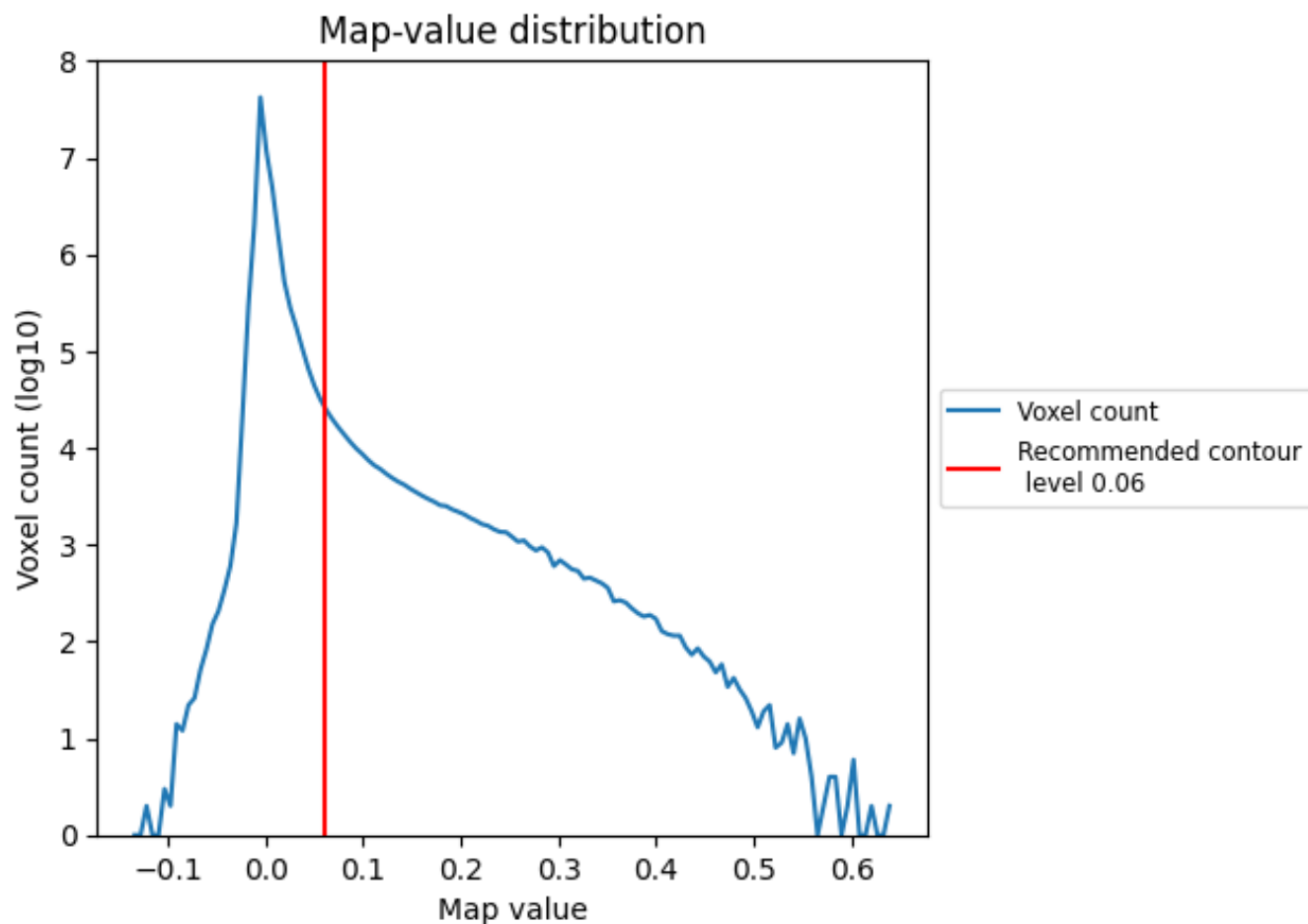
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

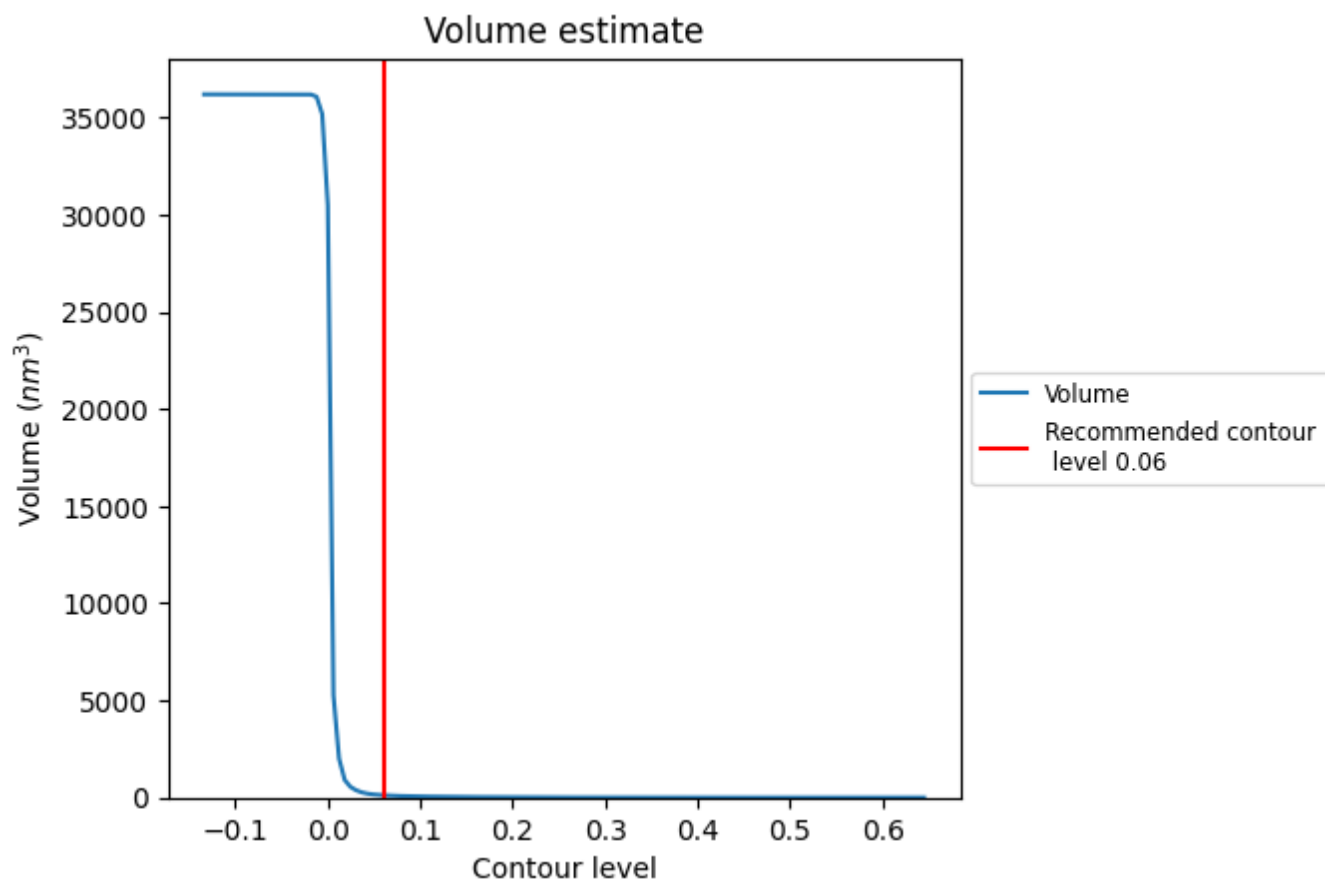
This section contains the results of statistical analysis of the map.

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.

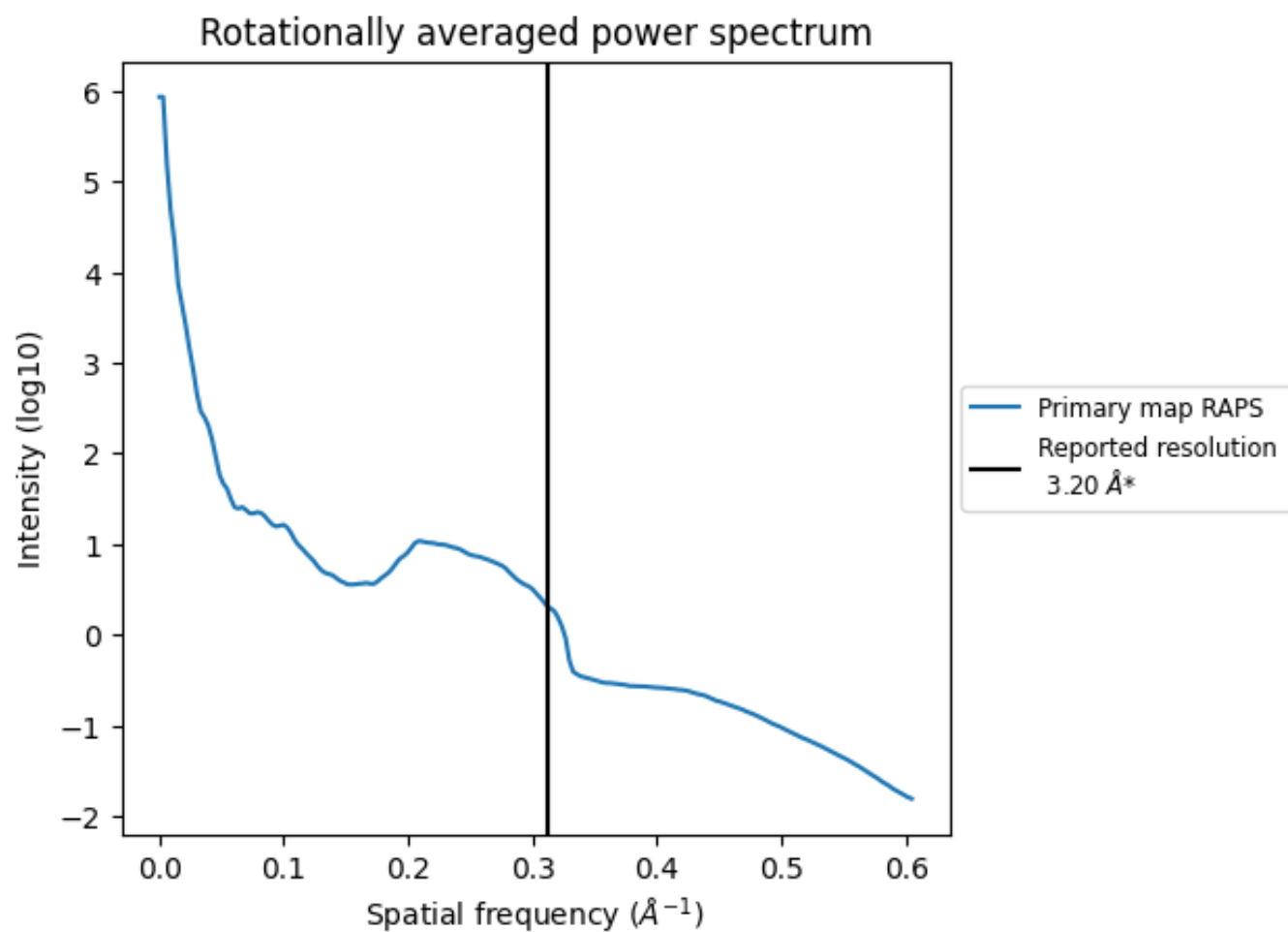
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 107 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 0.312 Å⁻¹

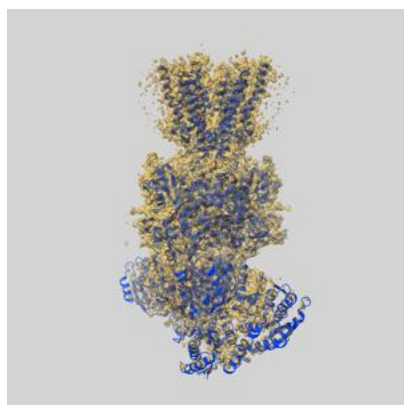
8 Fourier-Shell correlation ⓘ

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

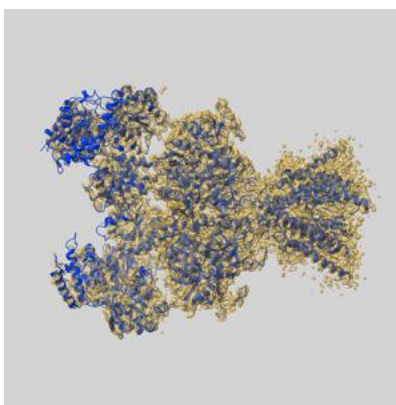
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70669 and PDB model 9OOQ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

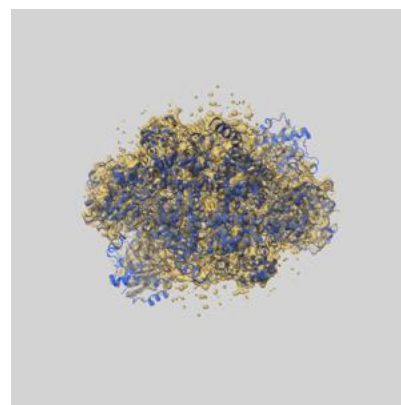
9.1 Map-model overlay [i](#)



X



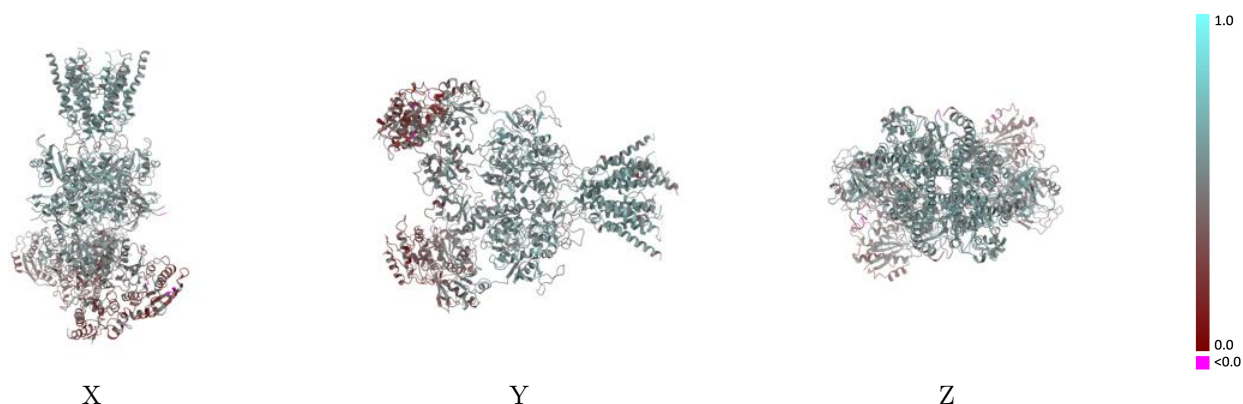
Y



Z

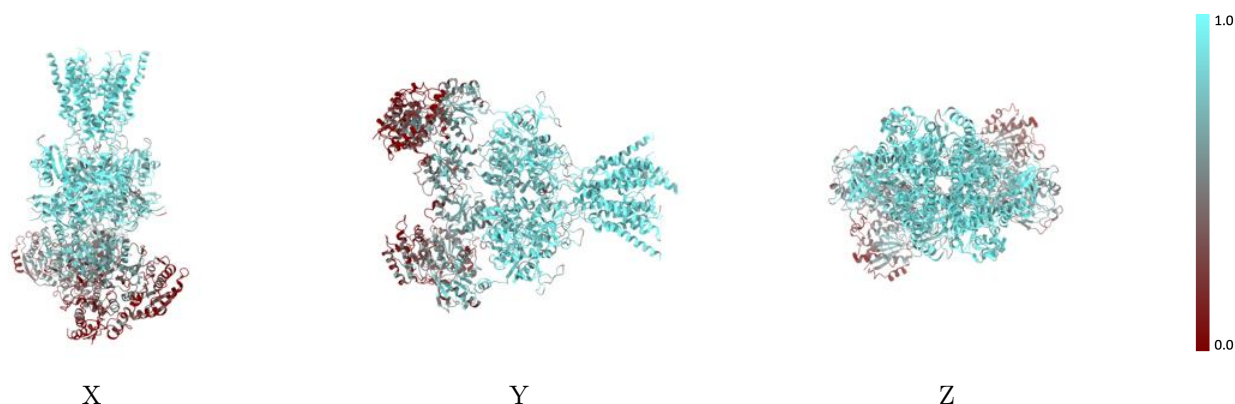
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



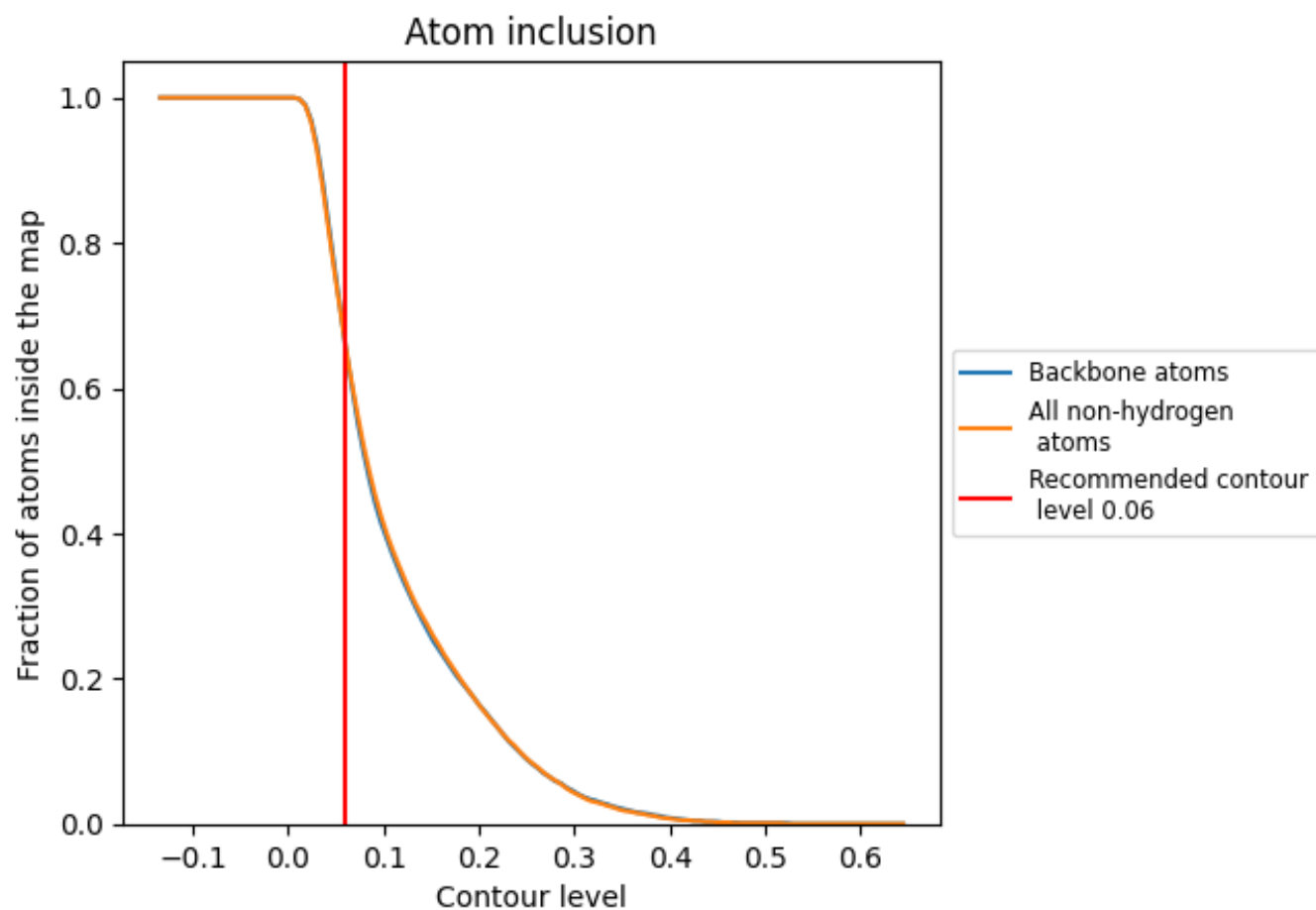
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6600	<div></div> 0.4870
A	<div></div> 0.6680	<div></div> 0.4770
B	<div></div> 0.7000	<div></div> 0.4960
C	<div></div> 0.6620	<div></div> 0.4980
D	<div></div> 0.6260	<div></div> 0.4760

