



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:47 AM UTC

PDB ID : 7EOR / pdb_00007eor
EMDB ID : EMD-31228
Title : Structure of the human GluN1/GluN2A NMDA receptor in the glycine/glutamate/GNE-6901 bound state
Authors : Wang, H.; Zhu, S.
Deposited on : 2021-04-22
Resolution : 4.00 Å(reported)
Based on initial model : 6IRA

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:

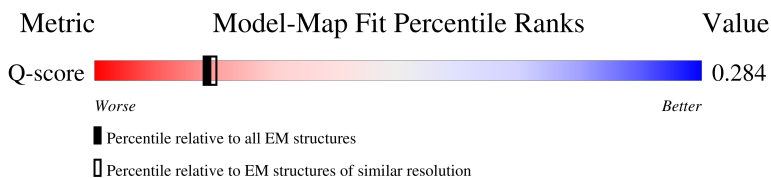
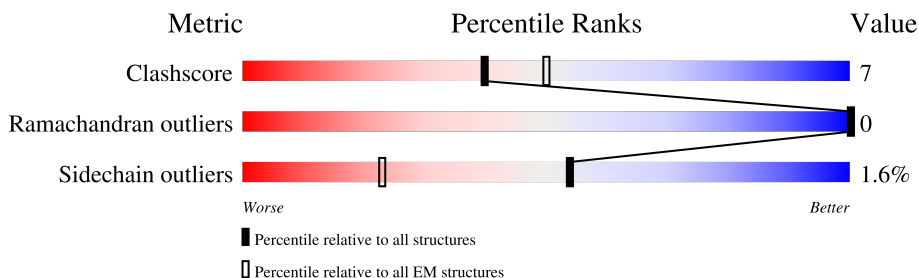
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.00 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	7587 (3.50 - 4.50)

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	853	11% 70% 17% 13%
1	C	853	10% 69% 17% 13%
2	B	847	11% 76% 15% 9%
2	D	847	11% 75% 15% 9%

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
4	6RM	A	902	-	-	X	-
4	6RM	C	902	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24232 atoms, of which 28 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 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	745	Total	C	N	O	S	0	0
			5886	3802	959	1085	40		
1	C	745	Total	C	N	O	S	0	0
			5886	3802	959	1085	40		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	794	CYS	LEU	engineered mutation	UNP Q12879
A	843	LYS	-	expression tag	UNP Q12879
A	844	SER	-	expression tag	UNP Q12879
A	845	ARG	-	expression tag	UNP Q12879
A	846	ALA	-	expression tag	UNP Q12879
A	847	GLU	-	expression tag	UNP Q12879
A	848	ALA	-	expression tag	UNP Q12879
A	849	LYS	-	expression tag	UNP Q12879
A	850	ARG	-	expression tag	UNP Q12879
A	851	MET	-	expression tag	UNP Q12879
A	852	LYS	-	expression tag	UNP Q12879
A	853	GLY	-	expression tag	UNP Q12879
C	794	CYS	LEU	engineered mutation	UNP Q12879
C	843	LYS	-	expression tag	UNP Q12879
C	844	SER	-	expression tag	UNP Q12879
C	845	ARG	-	expression tag	UNP Q12879
C	846	ALA	-	expression tag	UNP Q12879
C	847	GLU	-	expression tag	UNP Q12879
C	848	ALA	-	expression tag	UNP Q12879
C	849	LYS	-	expression tag	UNP Q12879
C	850	ARG	-	expression tag	UNP Q12879
C	851	MET	-	expression tag	UNP Q12879
C	852	LYS	-	expression tag	UNP Q12879
C	853	GLY	-	expression tag	UNP Q12879

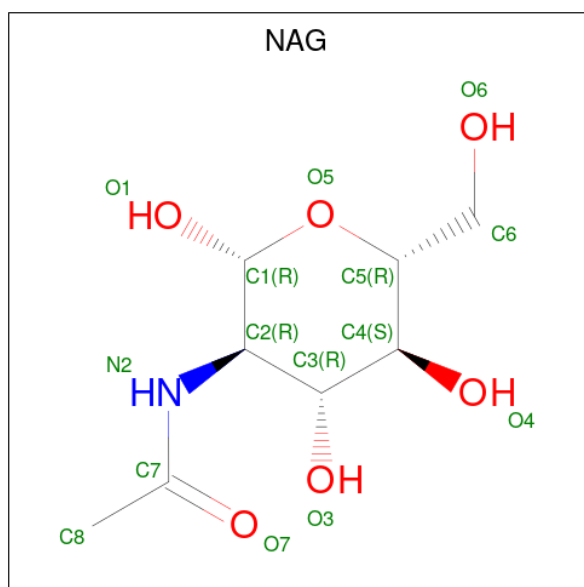
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	770	Total	C	N	O	S	1	0
			6093	3896	1052	1111	34		
2	D	770	Total	C	N	O	S	1	0
			6093	3896	1052	1111	34		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	698	CYS	GLU	engineered mutation	UNP Q05586
D	698	CYS	GLU	engineered mutation	UNP Q05586

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



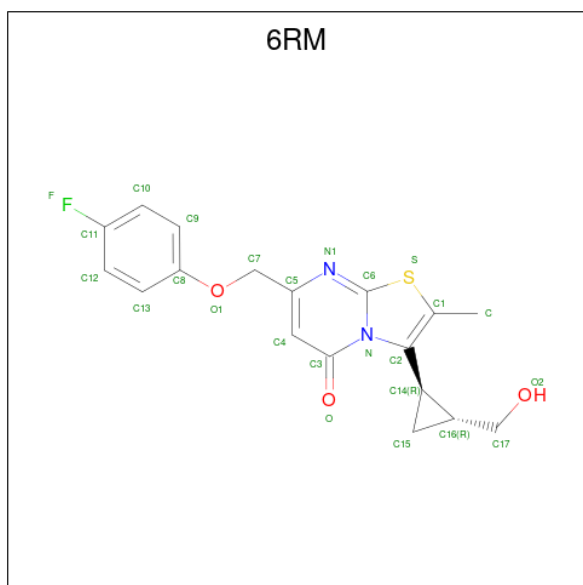
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O		0
			14	8	1	5		
3	B	1	Total	C	N	O		0
			14	8	1	5		
3	B	1	Total	C	N	O		0
			14	8	1	5		
3	B	1	Total	C	N	O		0
			14	8	1	5		
3	B	1	Total	C	N	O		0
			14	8	1	5		
3	B	1	Total	C	N	O		0
			14	8	1	5		

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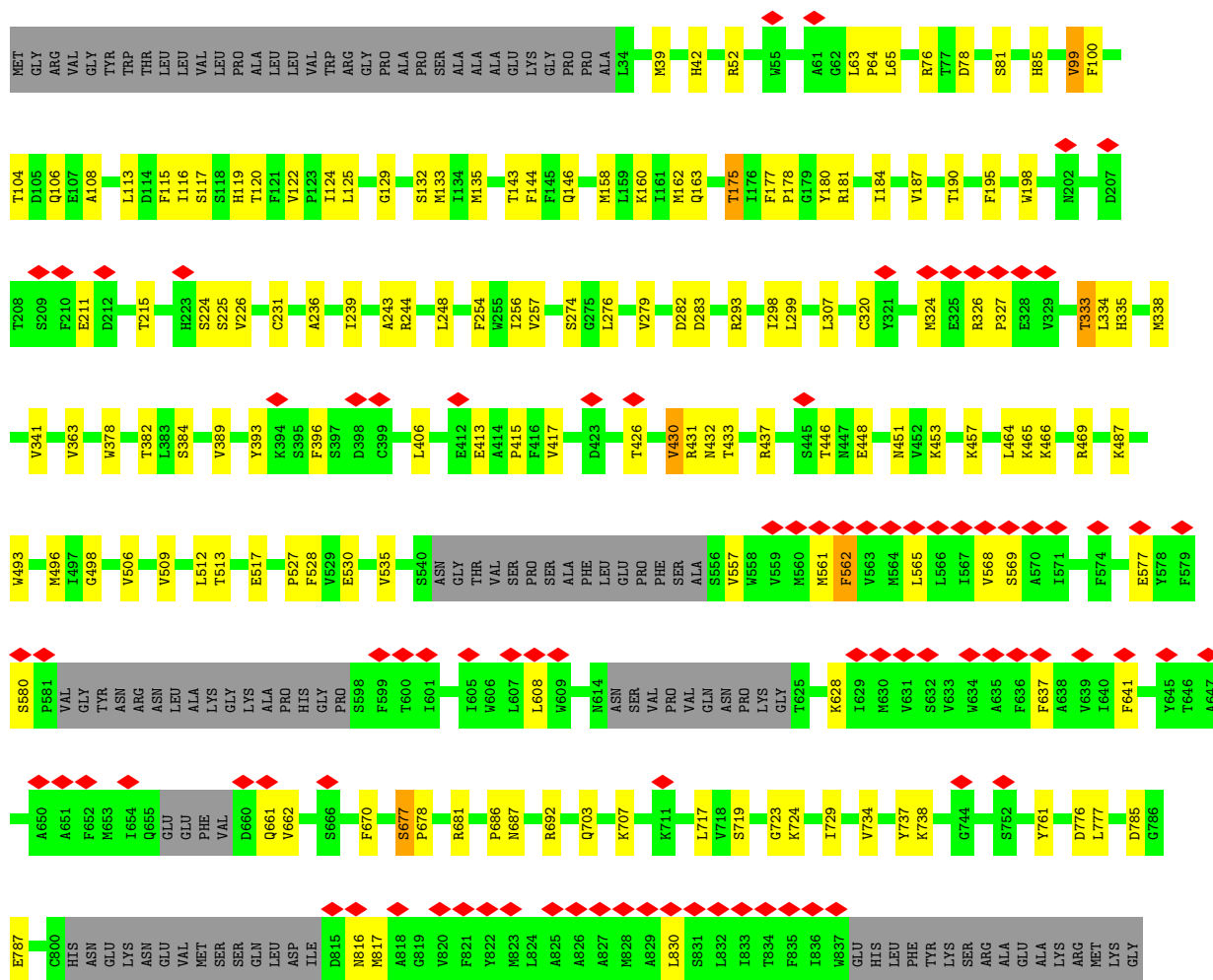
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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

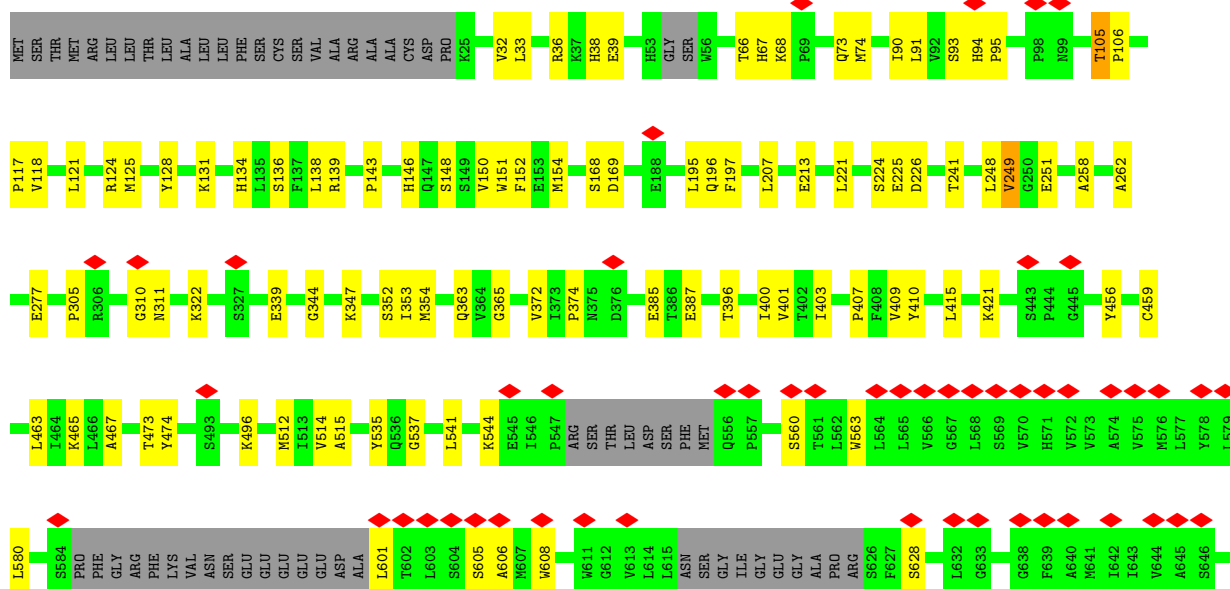
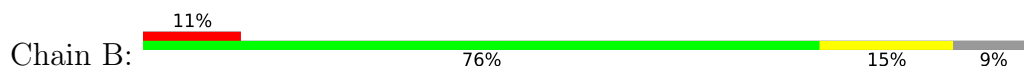
- Molecule 4 is 7-[(4-fluoranylphenoxy)methyl]-3-[(1 {R},2 {R})-2-(hydroxymethyl)cyclopropyl]-2-methyl-[1,3]thiazolo[3,2-a]pyrimidin-5-one (CCD ID: 6RM) (formula: C₁₈H₁₇FN₂O₃S) (labeled as "Ligand of Interest" by depositor).

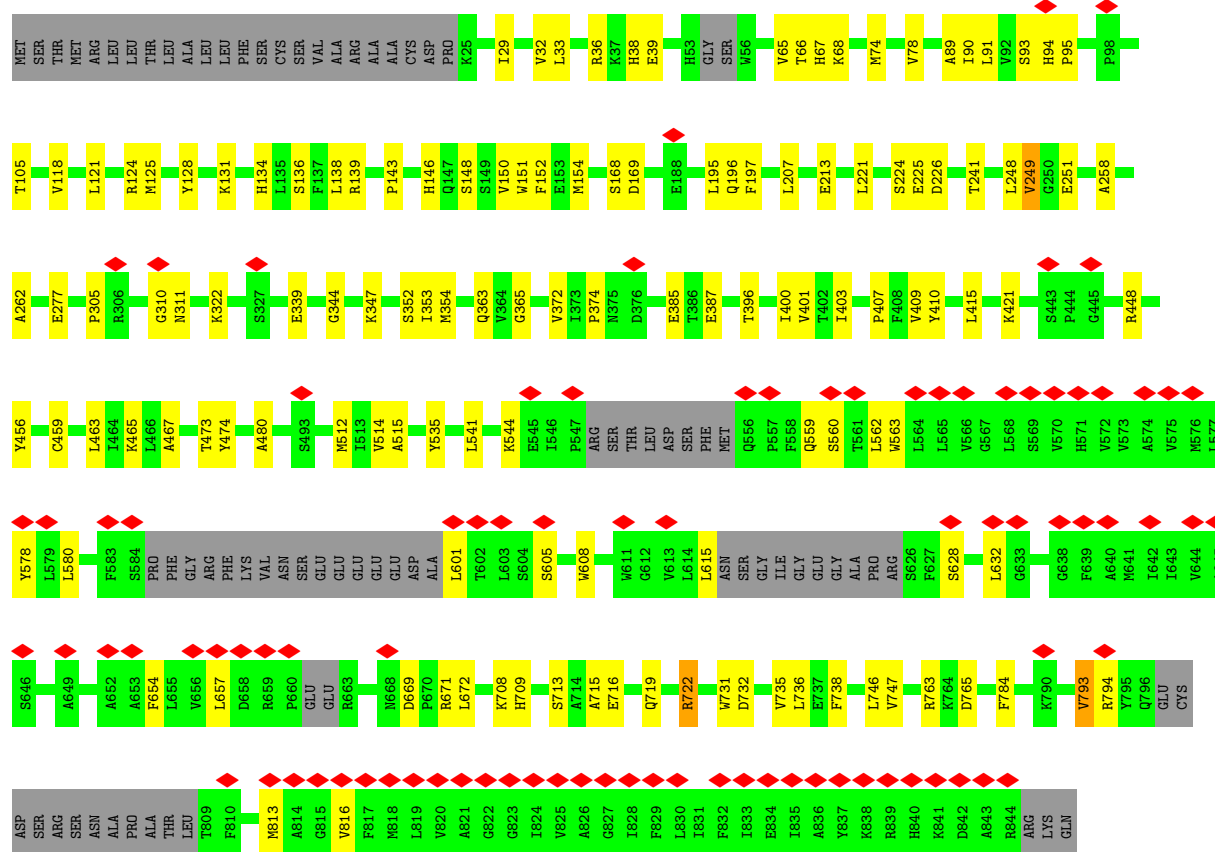


Mol	Chain	Residues	Atoms							AltConf
4	A	1	Total	C	F	H	N	O	S	0
			39	18	1	14	2	3	1	
4	C	1	Total	C	F	H	N	O	S	0
			39	18	1	14	2	3	1	



• Molecule 2: Glutamate receptor ionotropic, NMDA 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	69419	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.039	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0081	Depositor
Map size ($\text{\AA}$)	263.64, 263.64, 263.64	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.014, 1.014, 1.014	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 6RM

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	0.08	0/6026	0.23	0/8177
1	C	0.08	0/6026	0.23	0/8177
2	B	0.08	0/6229	0.21	0/8433
2	D	0.08	0/6229	0.21	0/8433
All	All	0.08	0/24510	0.22	0/33220

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	5886	0	5821	91	0
1	C	5886	0	5821	96	0
2	B	6093	0	6085	83	0
2	D	6093	0	6085	86	0
3	A	14	0	13	1	0
3	B	84	0	77	0	0
3	C	14	0	13	1	0
3	D	84	0	77	0	0
4	A	25	14	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	25	14	0	15	0
All	All	24204	28	23992	343	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 7.

All (343) 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)
4:C:902:6RM:C6	2:D:535:TYR:CD1	2.75	0.69
1:A:527:PRO:HG3	4:A:902:6RM:C12	2.24	0.68
1:C:527:PRO:HG3	4:C:902:6RM:C12	2.25	0.67
1:C:162:MET:HE1	1:C:226:VAL:HG21	1.79	0.65
2:B:68:LYS:HB2	2:B:74:MET:HB3	1.78	0.65
2:D:560:SER:HA	2:D:563:TRP:HD1	1.61	0.65
2:D:68:LYS:HB2	2:D:74:MET:HB3	1.78	0.64
1:A:162:MET:HE1	1:A:226:VAL:HG21	1.78	0.64
2:D:125:MET:O	2:D:139:ARG:NH2	2.32	0.63
2:B:33:LEU:HD13	2:B:38:HIS:HB3	1.80	0.62
1:A:717:LEU:HD11	1:A:738:LYS:HD2	1.81	0.62
1:A:178:PRO:HG3	2:D:131:LYS:HB3	1.81	0.62
2:B:125:MET:O	2:B:139:ARG:NH2	2.33	0.62
4:C:902:6RM:C2	2:D:535:TYR:HE1	2.12	0.62
2:B:131:LYS:HB3	1:C:178:PRO:HG3	1.82	0.62
2:B:560:SER:HA	2:B:563:TRP:HD1	1.64	0.61
1:A:117:SER:HB2	1:A:143:THR:H	1.64	0.61
4:A:902:6RM:C6	2:B:535:TYR:CD1	2.83	0.61
1:A:52:ARG:HG3	1:A:293:ARG:HH21	1.66	0.61
1:C:52:ARG:HG3	1:C:293:ARG:HH21	1.66	0.61
2:D:33:LEU:HD13	2:D:38:HIS:HB3	1.80	0.61
2:B:385:GLU:HG3	2:B:387:GLU:H	1.66	0.61
1:C:437:ARG:HH11	1:C:451:ASN:HB3	1.66	0.60
2:D:385:GLU:HG3	2:D:387:GLU:H	1.66	0.60
1:C:641:PHE:HE1	2:D:813:MET:HG2	1.67	0.60
2:D:669:ASP:OD2	2:D:671:ARG:NH1	2.35	0.60
2:B:138:LEU:HD22	2:B:344:GLY:HA3	1.83	0.60
2:B:669:ASP:OD2	2:B:671:ARG:NH1	2.35	0.60
1:A:437:ARG:HH11	1:A:451:ASN:HB3	1.67	0.59
2:D:353:ILE:HB	2:D:365:GLY:H	1.67	0.59
1:A:641:PHE:HE1	2:B:813:MET:HG2	1.67	0.59
2:B:353:ILE:HB	2:B:365:GLY:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:LEU:HD22	2:D:344:GLY:HA3	1.84	0.59
2:D:738:PHE:HE1	2:D:793:VAL:HG23	1.68	0.59
1:C:717:LEU:HD11	1:C:738:LYS:HD2	1.85	0.59
2:B:221:LEU:HB3	2:B:249:VAL:HG13	1.85	0.58
2:D:407:PRO:HG3	2:D:735:VAL:HG13	1.85	0.58
2:D:221:LEU:HB3	2:D:249:VAL:HG13	1.85	0.58
1:C:117:SER:HB2	1:C:143:THR:H	1.68	0.58
4:C:902:6RM:C6	2:D:535:TYR:CE1	2.87	0.58
2:B:407:PRO:HG3	2:B:735:VAL:HG13	1.84	0.58
2:B:738:PHE:HE1	2:B:793:VAL:HG23	1.69	0.58
1:C:115:PHE:O	1:C:119:HIS:ND1	2.36	0.58
2:D:580:LEU:HD21	2:D:628:SER:HB3	1.85	0.58
1:A:662:VAL:HG11	1:A:670:PHE:HE1	1.69	0.57
1:C:334:LEU:HB3	1:C:338:MET:HE3	1.86	0.57
1:A:334:LEU:HB3	1:A:338:MET:HE3	1.87	0.57
1:A:406:LEU:HD22	1:A:506:VAL:HG11	1.87	0.57
1:A:244:ARG:HH12	1:A:396:PHE:HB3	1.70	0.57
4:C:902:6RM:C1	2:D:535:TYR:HE1	2.18	0.57
1:C:175:THR:HG1	1:C:231:CYS:HG	1.54	0.56
1:C:244:ARG:HH12	1:C:396:PHE:HB3	1.70	0.56
1:C:406:LEU:HD22	1:C:506:VAL:HG11	1.87	0.56
1:C:662:VAL:HG11	1:C:670:PHE:HE1	1.71	0.56
1:A:681:ARG:NH1	1:A:723:GLY:O	2.38	0.56
1:C:681:ARG:NH1	1:C:723:GLY:O	2.39	0.56
2:D:195:LEU:HD13	2:D:207:LEU:HB3	1.88	0.56
2:B:396:THR:O	2:B:473:THR:OG1	2.23	0.56
2:D:354:MET:SD	2:D:363:GLN:NE2	2.79	0.55
1:A:326:ARG:HD2	1:A:327:PRO:HD2	1.88	0.55
1:C:326:ARG:HD2	1:C:327:PRO:HD2	1.88	0.55
2:D:396:THR:O	2:D:473:THR:OG1	2.23	0.55
1:A:577:GLU:O	1:A:580:SER:OG	2.23	0.55
2:D:465:LYS:HZ3	2:D:784:PHE:HB3	1.72	0.55
2:B:124:ARG:HH12	2:B:251:GLU:HG2	1.72	0.55
2:D:38:HIS:NE2	2:D:277:GLU:OE1	2.41	0.54
1:C:530:GLU:HB3	4:C:902:6RM:N1	2.22	0.54
1:A:703:GLN:O	1:A:707:LYS:NZ	2.40	0.54
2:B:38:HIS:NE2	2:B:277:GLU:OE1	2.41	0.54
1:A:324:MET:SD	1:A:324:MET:N	2.79	0.54
1:C:274:SER:HB3	1:C:396:PHE:HE1	1.72	0.54
2:D:169:ASP:OD1	2:D:196:GLN:NE2	2.34	0.54
1:C:577:GLU:O	1:C:580:SER:OG	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:PHE:HE2	2:B:816:VAL:HG22	1.73	0.54
1:C:132:SER:OG	1:C:133:MET:SD	2.59	0.54
2:B:354:MET:SD	2:B:363:GLN:NE2	2.81	0.53
1:C:703:GLN:O	1:C:707:LYS:NZ	2.41	0.53
4:A:902:6RM:C2	2:B:535:TYR:HE1	2.21	0.53
2:B:195:LEU:HD13	2:B:207:LEU:HB3	1.88	0.53
1:A:378:TRP:HD1	1:A:384:SER:HB2	1.74	0.53
2:B:169:ASP:OD1	2:B:196:GLN:NE2	2.34	0.53
1:A:274:SER:HB3	1:A:396:PHE:HE1	1.72	0.53
2:D:124:ARG:HH12	2:D:251:GLU:HG2	1.72	0.53
2:D:168:SER:HA	2:D:197:PHE:HB2	1.92	0.52
1:A:132:SER:OG	1:A:133:MET:SD	2.59	0.52
2:D:793:VAL:HG13	2:D:794:ARG:HG3	1.91	0.52
2:B:36:ARG:HH22	2:B:66:THR:HG22	1.75	0.52
1:C:104:THR:HG22	1:C:106:GLN:H	1.75	0.52
2:D:467:ALA:HB2	2:D:474:TYR:HE2	1.74	0.52
1:A:487:LYS:HD3	1:A:687:ASN:HA	1.92	0.52
1:C:378:TRP:HD1	1:C:384:SER:HB2	1.74	0.52
2:D:36:ARG:HH22	2:D:66:THR:HG22	1.75	0.52
2:D:601:LEU:HA	2:D:605:SER:HB2	1.92	0.52
2:B:465:LYS:HZ3	2:B:784:PHE:HB3	1.75	0.51
2:D:541:LEU:HD11	2:D:746:LEU:HB2	1.91	0.51
2:B:793:VAL:HG13	2:B:794:ARG:HG3	1.91	0.51
1:C:496:MET:HE3	1:C:512:LEU:HD11	1.92	0.51
2:B:496:LYS:HD3	1:C:195:PHE:HB3	1.92	0.51
1:A:104:THR:HG22	1:A:106:GLN:H	1.75	0.51
2:B:467:ALA:HB2	2:B:474:TYR:HE2	1.75	0.51
4:C:902:6RM:C3	2:D:535:TYR:HD1	2.23	0.51
4:C:902:6RM:S	2:D:535:TYR:CE1	3.04	0.51
2:D:224:SER:OG	2:D:226:ASP:OD1	2.28	0.51
1:C:487:LYS:HD3	1:C:687:ASN:HA	1.92	0.51
4:A:902:6RM:C1	2:B:535:TYR:HE1	2.23	0.51
2:B:463:LEU:HD21	2:B:514:VAL:HG21	1.93	0.51
1:C:106:GLN:HG2	1:C:108:ALA:H	1.77	0.50
2:B:541:LEU:HD11	2:B:746:LEU:HB2	1.93	0.50
1:C:637:PHE:HE2	2:D:816:VAL:HG22	1.76	0.50
1:C:324:MET:SD	1:C:324:MET:N	2.79	0.50
1:A:115:PHE:O	1:A:119:HIS:ND1	2.39	0.50
1:A:496:MET:HE3	1:A:512:LEU:HD11	1.93	0.50
2:D:463:LEU:HD21	2:D:514:VAL:HG21	1.93	0.50
1:A:106:GLN:HG2	1:A:108:ALA:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:GLN:NE2	1:C:320:CYS:O	2.43	0.50
1:C:113:LEU:HD23	1:C:124:ILE:HD12	1.94	0.50
1:C:513:THR:HA	1:C:761:TYR:HB3	1.94	0.50
1:A:225:SER:O	1:A:254:PHE:N	2.45	0.49
2:D:719:GLN:OE1	2:D:722:ARG:NH2	2.45	0.49
2:D:91:LEU:HB3	2:D:121:LEU:HD21	1.94	0.49
1:C:415:PRO:HG2	1:C:734:VAL:HG13	1.93	0.49
2:D:400:ILE:HG12	2:D:512:MET:HB3	1.94	0.49
2:B:91:LEU:HB3	2:B:121:LEU:HD21	1.93	0.49
2:D:258:ALA:O	2:D:262:ALA:HB2	2.12	0.49
1:A:530:GLU:HB3	4:A:902:6RM:N1	2.28	0.49
2:B:258:ALA:O	2:B:262:ALA:HB2	2.13	0.49
2:B:719:GLN:OE1	2:B:722:ARG:NH2	2.45	0.49
1:C:225:SER:O	1:C:254:PHE:N	2.45	0.49
1:C:628:LYS:HB2	2:D:608:TRP:HH2	1.77	0.49
2:B:32:VAL:O	2:B:67:HIS:NE2	2.45	0.49
2:B:400:ILE:HG12	2:B:512:MET:HB3	1.95	0.49
1:A:113:LEU:HD23	1:A:124:ILE:HD12	1.94	0.48
1:A:279:VAL:HG12	1:A:363:VAL:HG22	1.95	0.48
1:A:65:LEU:HD11	1:A:307:LEU:HD11	1.95	0.48
1:A:465:LYS:O	1:A:469:ARG:NE	2.46	0.48
4:A:902:6RM:C6	2:B:535:TYR:CE1	2.96	0.48
2:D:410:TYR:N	2:D:456:TYR:O	2.42	0.48
1:A:187:VAL:HA	1:A:190:THR:HG22	1.95	0.48
1:A:513:THR:HA	1:A:761:TYR:HB3	1.96	0.48
2:B:168:SER:HA	2:B:197:PHE:HB2	1.95	0.48
1:C:279:VAL:HG12	1:C:363:VAL:HG22	1.95	0.48
1:C:528:PHE:C	4:C:902:6RM:S	2.96	0.48
4:C:902:6RM:N	2:D:535:TYR:CD1	2.82	0.48
1:C:187:VAL:HA	1:C:190:THR:HG22	1.95	0.48
1:A:466:LYS:HA	1:A:469:ARG:HH21	1.79	0.48
1:C:517:GLU:OE1	1:C:692:ARG:NE	2.31	0.48
1:A:565:LEU:HA	1:A:568:VAL:HG22	1.94	0.48
1:C:65:LEU:HD11	1:C:307:LEU:HD11	1.94	0.48
2:B:225:GLU:OE2	2:B:258:ALA:N	2.46	0.48
1:C:493:TRP:HB3	1:C:498:GLY:HA2	1.96	0.48
1:C:466:LYS:HA	1:C:469:ARG:HH21	1.79	0.47
2:D:32:VAL:O	2:D:67:HIS:NE2	2.44	0.47
1:A:432:ASN:OD1	1:A:457:LYS:NZ	2.47	0.47
2:B:713:SER:HB3	2:B:716:GLU:HG2	1.96	0.47
1:C:465:LYS:O	1:C:469:ARG:NE	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:SER:HA	1:C:608:LEU:HD11	1.96	0.47
1:A:493:TRP:HB3	1:A:498:GLY:HA2	1.95	0.47
1:C:243:ALA:HB1	1:C:248:LEU:HB2	1.97	0.47
1:C:437:ARG:HD2	1:C:451:ASN:HB3	1.97	0.47
1:C:565:LEU:HA	1:C:568:VAL:HG22	1.95	0.47
2:D:225:GLU:OE2	2:D:258:ALA:N	2.47	0.47
2:D:403:ILE:HG22	2:D:515:ALA:HB1	1.96	0.47
2:D:544:LYS:HE2	2:D:747:VAL:HG13	1.97	0.47
1:A:628:LYS:HB2	2:B:608:TRP:HZ2	1.80	0.47
2:B:305:PRO:HB3	2:B:311:ASN:HD22	1.80	0.47
1:C:528:PHE:O	4:C:902:6RM:C	2.63	0.47
2:B:541:LEU:HD22	2:B:736:LEU:HD22	1.96	0.47
1:C:776:ASP:OD1	1:C:777:LEU:N	2.48	0.47
1:A:76:ARG:CZ	2:D:310:GLY:H	2.28	0.47
1:A:129:GLY:O	1:A:132:SER:OG	2.33	0.47
1:A:464:LEU:HD21	1:A:509:VAL:HG21	1.97	0.47
1:A:528:PHE:C	4:A:902:6RM:S	2.98	0.47
1:C:211:GLU:HB2	1:C:215:THR:HG23	1.96	0.47
1:A:163:GLN:NE2	1:A:426:THR:O	2.48	0.46
1:A:530:GLU:OE1	4:A:902:6RM:S	2.73	0.46
2:B:36:ARG:NH2	2:B:39:GLU:OE2	2.46	0.46
1:C:129:GLY:O	1:C:132:SER:OG	2.33	0.46
2:D:148:SER:HA	2:D:151:TRP:CD1	2.50	0.46
1:A:437:ARG:HD2	1:A:451:ASN:HB3	1.97	0.46
2:D:541:LEU:HD22	2:D:736:LEU:HD22	1.96	0.46
1:A:181:ARG:HE	1:A:184:ILE:HD12	1.81	0.46
2:B:601:LEU:N	2:B:605:SER:HB3	2.30	0.46
1:A:211:GLU:HB2	1:A:215:THR:HG23	1.97	0.46
2:B:148:SER:HA	2:B:151:TRP:CD1	2.50	0.46
2:D:713:SER:HB3	2:D:716:GLU:HG2	1.96	0.46
1:A:243:ALA:HB1	1:A:248:LEU:HB2	1.97	0.46
2:B:601:LEU:HD12	2:B:606:ALA:HB2	1.98	0.46
2:B:669:ASP:HB3	2:B:672:LEU:HD13	1.98	0.46
1:C:530:GLU:OE1	4:C:902:6RM:S	2.73	0.46
4:C:902:6RM:C2	2:D:535:TYR:CE1	2.96	0.46
2:D:36:ARG:NH2	2:D:39:GLU:OE2	2.46	0.46
2:B:403:ILE:HG22	2:B:515:ALA:HB1	1.97	0.46
2:B:544:LYS:HE2	2:B:747:VAL:HG13	1.98	0.46
1:C:464:LEU:HD21	1:C:509:VAL:HG21	1.98	0.46
1:A:776:ASP:OD1	1:A:777:LEU:N	2.48	0.46
2:B:410:TYR:N	2:B:456:TYR:O	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:LEU:HD11	2:B:628:SER:HB3	1.97	0.46
1:C:122:VAL:O	1:C:143:THR:OG1	2.32	0.46
2:D:143:PRO:HD2	2:D:146:HIS:CE1	2.51	0.46
2:B:143:PRO:HD2	2:B:146:HIS:CE1	2.51	0.45
1:C:257:VAL:HB	1:C:276:LEU:HD21	1.98	0.45
1:C:163:GLN:NE2	1:C:426:THR:O	2.48	0.45
2:D:353:ILE:HD12	2:D:365:GLY:HA3	1.98	0.45
1:C:135:MET:SD	1:C:135:MET:N	2.90	0.45
1:C:76:ARG:NH2	1:C:78:ASP:OD1	2.48	0.45
2:D:195:LEU:HD22	2:D:207:LEU:HD22	1.99	0.45
1:A:76:ARG:NH2	1:A:78:ASP:OD1	2.45	0.45
2:B:731:TRP:CG	2:B:732:ASP:H	2.35	0.45
1:C:446:THR:OG1	1:C:448:GLU:OE1	2.23	0.45
1:A:81:SER:O	1:A:85:HIS:ND1	2.50	0.45
1:A:135:MET:SD	1:A:135:MET:N	2.90	0.45
1:A:144:PHE:HB3	1:A:146:GLN:HE22	1.81	0.45
1:A:233:LYS:HA	1:A:261:VAL:HG13	1.97	0.45
2:D:654:PHE:HA	2:D:657:LEU:HG	1.97	0.45
4:A:902:6RM:S	2:B:535:TYR:CE1	3.10	0.44
1:C:163:GLN:HB2	1:C:198:TRP:HH2	1.81	0.44
1:C:413:GLU:O	1:C:417:VAL:N	2.45	0.44
1:A:517:GLU:OE1	1:A:692:ARG:NE	2.31	0.44
1:C:144:PHE:HB3	1:C:146:GLN:HE22	1.81	0.44
1:C:181:ARG:HE	1:C:184:ILE:HD12	1.81	0.44
2:D:94:HIS:HB3	2:D:95:PRO:HD3	2.00	0.44
2:D:139:ARG:NH1	2:D:143:PRO:HB3	2.33	0.44
2:B:372:VAL:HG12	2:B:374:PRO:HD3	1.98	0.44
2:D:352:SER:HB2	2:D:363:GLN:HE22	1.83	0.44
2:D:459:CYS:HB2	2:D:514:VAL:HG12	2.00	0.44
1:A:528:PHE:O	4:A:902:6RM:C	2.66	0.44
2:B:654:PHE:HA	2:B:657:LEU:HG	1.99	0.44
1:A:535:VAL:HG12	1:A:729:ILE:HG12	2.00	0.44
1:C:282:ASP:OD1	1:C:283:ASP:N	2.50	0.44
2:D:93:SER:HA	2:D:121:LEU:HB2	1.99	0.44
2:B:136:SER:HA	2:B:322:LYS:HE2	2.00	0.44
1:C:81:SER:O	1:C:85:HIS:ND1	2.50	0.43
1:C:686:PRO:HG2	3:C:901:NAG:H82	2.00	0.43
4:C:902:6RM:C1	2:D:535:TYR:CE1	3.00	0.43
1:C:63:LEU:HD12	1:C:64:PRO:HD2	2.00	0.43
1:C:298:ILE:HG23	1:C:341:VAL:HG11	2.00	0.43
2:D:372:VAL:HG12	2:D:374:PRO:HD3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:731:TRP:CG	2:D:732:ASP:H	2.35	0.43
1:A:430:VAL:HG23	1:A:431:ARG:H	1.84	0.43
1:C:99:VAL:HB	1:C:125:LEU:HB2	2.00	0.43
1:A:600:THR:OG1	1:A:601:ILE:N	2.50	0.43
2:B:94:HIS:HB3	2:B:95:PRO:HD3	1.99	0.43
2:B:93:SER:HA	2:B:121:LEU:HB2	2.00	0.43
2:B:339:GLU:HB2	2:B:347:LYS:HB3	2.00	0.43
2:B:353:ILE:HD12	2:B:365:GLY:HA3	2.00	0.43
2:D:136:SER:HA	2:D:322:LYS:HE2	2.01	0.43
2:D:669:ASP:HB3	2:D:672:LEU:HD13	2.00	0.43
2:B:195:LEU:HD22	2:B:207:LEU:HD22	1.99	0.43
1:C:160:LYS:NZ	1:C:378:TRP:HE1	2.16	0.43
4:C:902:6RM:N	2:D:535:TYR:CE1	2.87	0.43
1:A:163:GLN:HB2	1:A:198:TRP:HH2	1.83	0.43
1:A:413:GLU:O	1:A:417:VAL:N	2.45	0.43
4:A:902:6RM:C3	2:B:535:TYR:HD1	2.32	0.43
2:B:139:ARG:NH1	2:B:143:PRO:HB3	2.33	0.43
1:A:333:THR:HB	1:A:335:HIS:ND1	2.34	0.43
1:C:116:ILE:O	1:C:120:THR:OG1	2.37	0.43
1:A:63:LEU:HD12	1:A:64:PRO:HD2	2.00	0.43
1:A:99:VAL:HB	1:A:125:LEU:HB2	2.00	0.43
1:A:816:ASN:OD1	1:A:817:MET:N	2.52	0.43
1:C:133:MET:SD	1:C:133:MET:N	2.92	0.43
2:D:559:GLN:HG2	2:D:562:LEU:HD22	1.99	0.43
2:B:763:ARG:NE	2:B:765:ASP:OD1	2.51	0.42
1:C:160:LYS:NZ	1:C:382:THR:O	2.52	0.42
1:A:298:ILE:HG23	1:A:341:VAL:HG11	2.00	0.42
2:D:415:LEU:HD11	2:D:421:LYS:HB3	2.01	0.42
1:A:686:PRO:HG2	3:A:901:NAG:H82	2.01	0.42
1:A:719:SER:O	1:A:724:LYS:N	2.52	0.42
2:B:117:PRO:HA	2:B:136:SER:HB3	2.01	0.42
2:B:415:LEU:HD11	2:B:421:LYS:HB3	2.01	0.42
1:C:333:THR:HB	1:C:335:HIS:ND1	2.34	0.42
1:C:415:PRO:HB3	1:C:737:TYR:HD2	1.83	0.42
2:B:459:CYS:HB2	2:B:514:VAL:HG12	2.00	0.42
1:A:569:SER:HA	1:A:608:LEU:HD11	2.01	0.42
1:C:430:VAL:HG23	1:C:431:ARG:H	1.84	0.42
2:D:29:ILE:HD12	2:D:89:ALA:HB3	2.02	0.42
1:A:446:THR:OG1	1:A:448:GLU:OE1	2.23	0.42
1:C:333:THR:HG22	1:C:334:LEU:H	1.85	0.42
1:C:816:ASN:OD1	1:C:817:MET:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:339:GLU:HB2	2:D:347:LYS:HB3	2.02	0.42
1:A:160:LYS:NZ	1:A:378:TRP:HE1	2.17	0.42
1:A:133:MET:SD	1:A:133:MET:N	2.92	0.42
1:A:236:ALA:HA	1:A:239:ILE:HG22	2.02	0.42
2:B:352:SER:HB2	2:B:363:GLN:HE22	1.83	0.42
2:B:467:ALA:HB2	2:B:474:TYR:CE2	2.55	0.42
2:B:544:LYS:HE3	2:B:746:LEU:H	1.85	0.42
1:C:39:MET:HB3	1:C:100:PHE:CD1	2.54	0.42
1:C:719:SER:O	1:C:724:LYS:N	2.53	0.42
2:D:151:TRP:CZ3	2:D:248:LEU:HB3	2.55	0.42
1:C:562:PHE:HD1	1:C:562:PHE:HA	1.74	0.42
2:D:150:VAL:O	2:D:154:MET:HG2	2.20	0.42
2:B:105:THR:N	2:B:106:PRO:HD2	2.35	0.42
1:C:100:PHE:CD2	1:C:113:LEU:HD21	2.55	0.42
2:D:128:TYR:HA	2:D:134:HIS:CD2	2.54	0.42
1:A:363:VAL:HB	1:A:376:GLY:H	1.85	0.41
1:C:557:VAL:HG22	1:C:561:MET:HE3	2.02	0.41
2:D:708:LYS:HG3	2:D:709:HIS:ND1	2.35	0.41
1:C:432:ASN:OD1	1:C:457:LYS:NZ	2.54	0.41
1:C:535:VAL:HG12	1:C:729:ILE:HG12	2.02	0.41
2:D:90:ILE:HB	2:D:118:VAL:HG13	2.01	0.41
2:B:90:ILE:HB	2:B:118:VAL:HG13	2.01	0.41
1:C:236:ALA:HA	1:C:239:ILE:HG22	2.02	0.41
2:D:465:LYS:NZ	2:D:784:PHE:HB3	2.35	0.41
1:A:39:MET:HB3	1:A:100:PHE:CD1	2.55	0.41
1:A:100:PHE:CD2	1:A:113:LEU:HD21	2.55	0.41
1:A:226:VAL:HA	1:A:254:PHE:HB2	2.02	0.41
1:A:677:SER:OG	1:A:678:PRO:HD3	2.20	0.41
2:B:151:TRP:CZ3	2:B:248:LEU:HB3	2.55	0.41
2:D:763:ARG:NE	2:D:765:ASP:OD1	2.51	0.41
2:D:448:ARG:NH1	2:D:480:ALA:O	2.54	0.41
2:B:128:TYR:HA	2:B:134:HIS:CD2	2.55	0.41
1:C:226:VAL:HA	1:C:254:PHE:HB2	2.02	0.41
2:B:150:VAL:O	2:B:154:MET:HG2	2.20	0.41
2:B:310:GLY:H	1:C:76:ARG:CZ	2.33	0.41
2:B:708:LYS:HG3	2:B:709:HIS:ND1	2.36	0.41
1:C:158:MET:HG3	1:C:256:ILE:HG21	2.03	0.41
1:A:224:SER:OG	1:A:225:SER:N	2.53	0.41
1:C:224:SER:OG	1:C:225:SER:N	2.53	0.41
1:C:628:LYS:HB2	2:D:608:TRP:CH2	2.56	0.41
1:A:139:ASP:OD1	1:A:139:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASP:OD1	1:A:283:ASP:N	2.50	0.41
1:A:333:THR:HG22	1:A:334:LEU:H	1.85	0.41
1:A:393:TYR:HD1	1:A:396:PHE:HE2	1.69	0.41
1:A:557:VAL:HG22	1:A:561:MET:HE3	2.02	0.41
1:A:737:TYR:CZ	1:A:796:LEU:HD13	2.55	0.41
1:C:393:TYR:HD1	1:C:396:PHE:HE2	1.68	0.41
2:D:305:PRO:HB3	2:D:311:ASN:HD22	1.85	0.41
1:A:528:PHE:HA	4:A:902:6RM:C	2.51	0.41
2:B:537:GLY:HA2	2:B:755:ARG:HA	2.02	0.41
1:C:177:PHE:HB3	1:C:180:TYR:CE2	2.56	0.41
1:C:677:SER:OG	1:C:678:PRO:HD3	2.20	0.41
1:A:177:PHE:HB3	1:A:180:TYR:CE2	2.56	0.40
1:A:785:ASP:HB3	1:A:787:GLU:OE1	2.21	0.40
2:B:224:SER:OG	2:B:226:ASP:OD1	2.29	0.40
1:C:437:ARG:HH21	1:C:453:LYS:HE3	1.86	0.40
2:D:65:VAL:HG11	2:D:78:VAL:HG12	2.03	0.40
2:B:465:LYS:NZ	2:B:784:PHE:HB3	2.36	0.40
1:C:785:ASP:HB3	1:C:787:GLU:OE1	2.21	0.40
2:D:580:LEU:HD23	2:D:632:LEU:HD11	2.03	0.40
1:A:49:ARG:HA	1:A:49:ARG:HD3	1.94	0.40
1:A:94:ARG:NH2	1:A:316:ALA:O	2.53	0.40
4:A:902:6RM:N	2:B:535:TYR:CD1	2.89	0.40
2:D:715:ALA:O	2:D:719:GLN:HG2	2.22	0.40
2:D:544:LYS:HE3	2:D:746:LEU:H	1.87	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	733/853 (86%)	701 (96%)	32 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	733/853 (86%)	702 (96%)	31 (4%)	0	100	100
2	B	757/847 (89%)	743 (98%)	14 (2%)	0	100	100
2	D	757/847 (89%)	739 (98%)	18 (2%)	0	100	100
All	All	2980/3400 (88%)	2885 (97%)	95 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	650/738 (88%)	639 (98%)	11 (2%)	53	68
1	C	650/738 (88%)	638 (98%)	12 (2%)	51	68
2	B	663/730 (91%)	654 (99%)	9 (1%)	59	71
2	D	663/730 (91%)	652 (98%)	11 (2%)	53	68
All	All	2626/2936 (89%)	2583 (98%)	43 (2%)	54	70

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	99	VAL
1	A	175	THR
1	A	299	LEU
1	A	333	THR
1	A	389	VAL
1	A	430	VAL
1	A	433	THR
1	A	562	PHE
1	A	661	GLN
1	A	677	SER
2	B	105	THR
2	B	152	PHE

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Mol	Chain	Res	Type
2	B	213	GLU
2	B	241	THR
2	B	249	VAL
2	B	401	VAL
2	B	409	VAL
2	B	722	ARG
2	B	793	VAL
1	C	42	HIS
1	C	99	VAL
1	C	175	THR
1	C	299	LEU
1	C	333	THR
1	C	389	VAL
1	C	430	VAL
1	C	433	THR
1	C	562	PHE
1	C	661	GLN
1	C	677	SER
1	C	830	LEU
2	D	105	THR
2	D	152	PHE
2	D	213	GLU
2	D	241	THR
2	D	249	VAL
2	D	401	VAL
2	D	409	VAL
2	D	578	TYR
2	D	615	LEU
2	D	722	ARG
2	D	793	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	323	GLN
1	A	674	HIS
1	A	709	ASN
1	A	710	GLN
1	A	736	ASN
2	B	363	GLN
2	B	368	ASN

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Mol	Chain	Res	Type
2	B	556	GLN
2	B	559	GLN
2	B	686	GLN
2	B	724	ASN
2	B	782	ASN
1	C	68	ASN
1	C	674	HIS
2	D	59	GLN
2	D	70	ASN
2	D	363	GLN
2	D	368	ASN
2	D	404	HIS
2	D	556	GLN
2	D	650	ASN
2	D	674	ASN
2	D	686	GLN
2	D	724	ASN
2	D	782	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
4	6RM	C	902	-	27,28,28	0.60	0	31,41,41	0.80	3 (9%)
3	NAG	B	904	2	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	A	901	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	D	902	2	14,14,15	0.33	0	17,19,21	0.41	0
4	6RM	A	902	-	27,28,28	0.60	0	31,41,41	0.80	3 (9%)
3	NAG	D	904	2	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	B	905	2	14,14,15	0.89	1 (7%)	17,19,21	1.07	1 (5%)
3	NAG	D	906	2	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	B	901	2	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	D	901	2	14,14,15	0.27	0	17,19,21	0.45	0
3	NAG	B	903	2	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	B	906	2	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	B	902	2	14,14,15	0.33	0	17,19,21	0.40	0
3	NAG	C	901	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	D	905	2	14,14,15	0.89	1 (7%)	17,19,21	1.07	1 (5%)
3	NAG	D	903	2	14,14,15	0.26	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6RM	C	902	-	-	3/9/16/16	0/4/4/4
3	NAG	B	904	2	-	2/6/23/26	0/1/1/1
3	NAG	A	901	1	-	1/6/23/26	0/1/1/1
3	NAG	D	902	2	-	2/6/23/26	0/1/1/1
4	6RM	A	902	-	-	3/9/16/16	0/4/4/4
3	NAG	D	904	2	-	2/6/23/26	0/1/1/1
3	NAG	B	905	2	-	2/6/23/26	0/1/1/1
3	NAG	D	906	2	-	2/6/23/26	0/1/1/1
3	NAG	B	901	2	-	0/6/23/26	0/1/1/1
3	NAG	D	901	2	-	0/6/23/26	0/1/1/1
3	NAG	B	903	2	-	0/6/23/26	0/1/1/1
3	NAG	B	906	2	-	2/6/23/26	0/1/1/1
3	NAG	B	902	2	-	2/6/23/26	0/1/1/1
3	NAG	C	901	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	905	2	-	2/6/23/26	0/1/1/1
3	NAG	D	903	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	905	NAG	O5-C1	2.92	1.48	1.43
3	B	905	NAG	O5-C1	2.90	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	905	NAG	C1-O5-C5	4.16	117.76	112.19
3	D	905	NAG	C1-O5-C5	4.14	117.73	112.19
4	A	902	6RM	C7-O1-C8	2.41	121.95	117.63
4	C	902	6RM	C7-O1-C8	2.40	121.94	117.63
4	A	902	6RM	O1-C7-C5	2.06	114.20	109.19
4	C	902	6RM	C1-C2-N	2.05	114.81	112.57
4	A	902	6RM	C1-C2-N	2.05	114.80	112.57
4	C	902	6RM	O1-C7-C5	2.03	114.13	109.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	6RM	C14-C16-C17-O2
4	C	902	6RM	C14-C16-C17-O2
3	B	904	NAG	O5-C5-C6-O6
3	D	904	NAG	O5-C5-C6-O6
3	B	906	NAG	O5-C5-C6-O6
3	D	906	NAG	O5-C5-C6-O6
3	B	906	NAG	C4-C5-C6-O6
3	D	906	NAG	C4-C5-C6-O6
3	B	904	NAG	C4-C5-C6-O6
3	D	904	NAG	C4-C5-C6-O6
3	B	905	NAG	C4-C5-C6-O6
3	D	905	NAG	C4-C5-C6-O6
3	B	902	NAG	C4-C5-C6-O6
3	D	902	NAG	C4-C5-C6-O6
3	B	905	NAG	O5-C5-C6-O6
3	C	901	NAG	O5-C5-C6-O6

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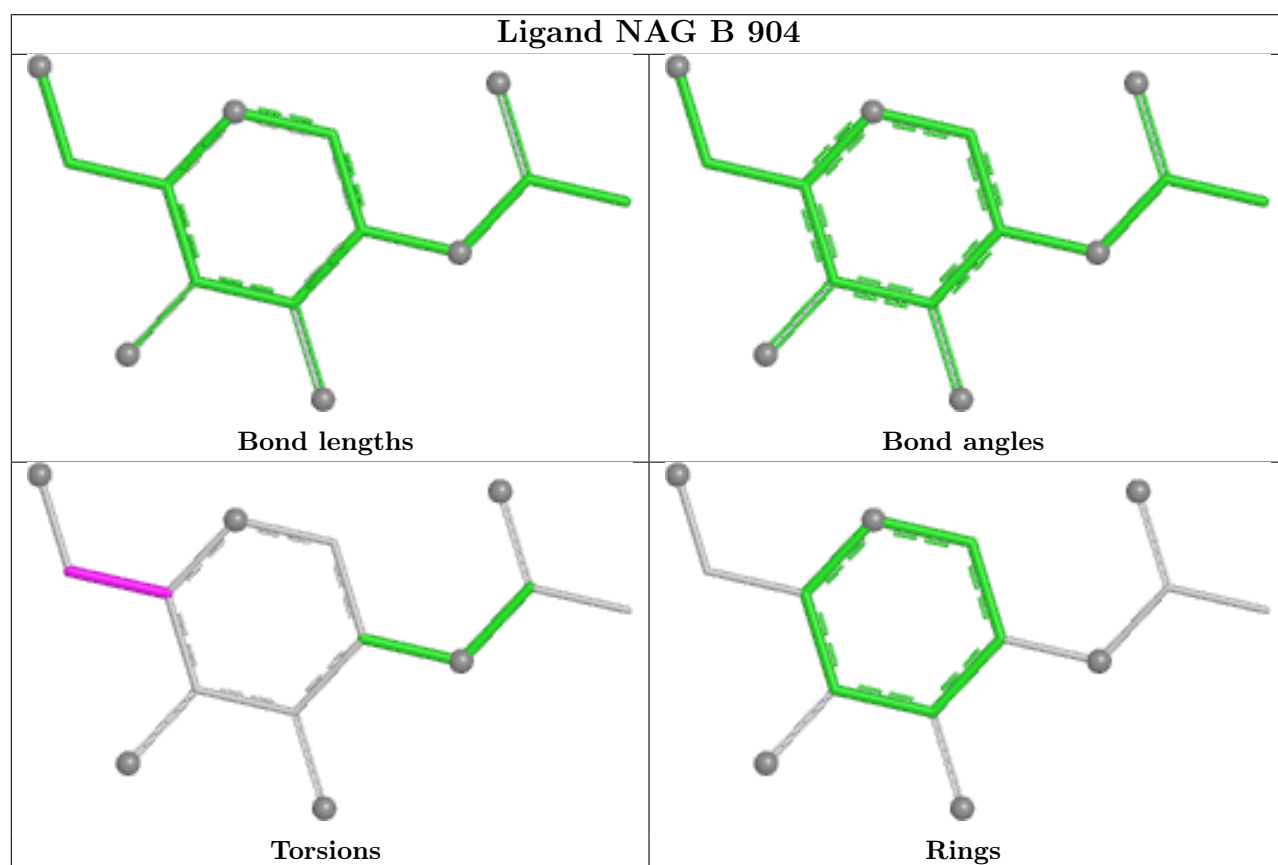
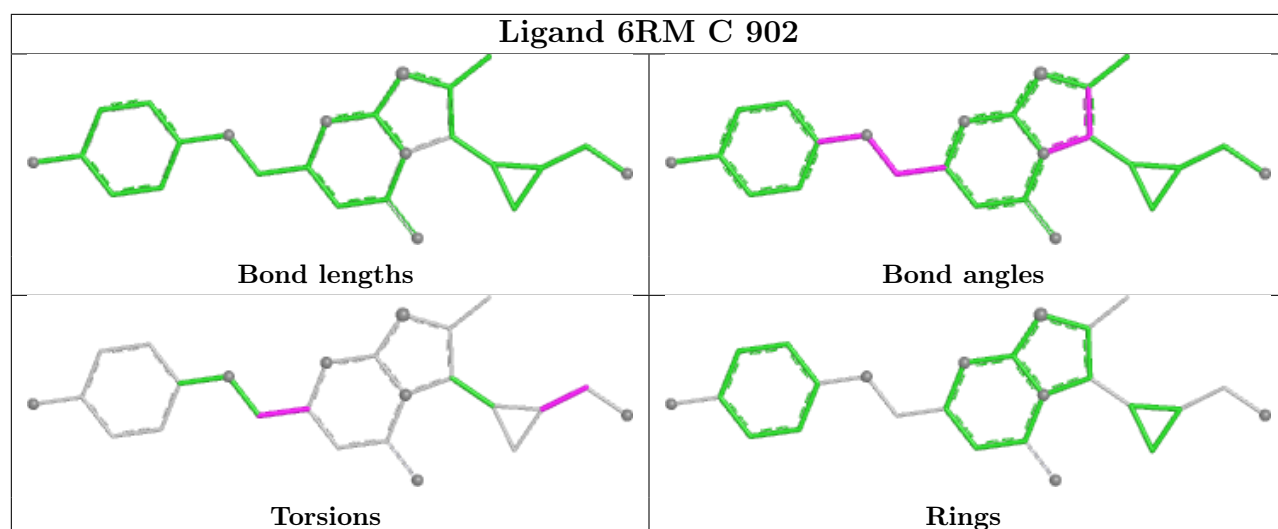
Mol	Chain	Res	Type	Atoms
3	A	901	NAG	O5-C5-C6-O6
3	D	905	NAG	O5-C5-C6-O6
4	A	902	6RM	C4-C5-C7-O1
4	C	902	6RM	C4-C5-C7-O1
3	D	902	NAG	O5-C5-C6-O6
3	B	902	NAG	O5-C5-C6-O6
4	A	902	6RM	C15-C16-C17-O2
4	C	902	6RM	C15-C16-C17-O2

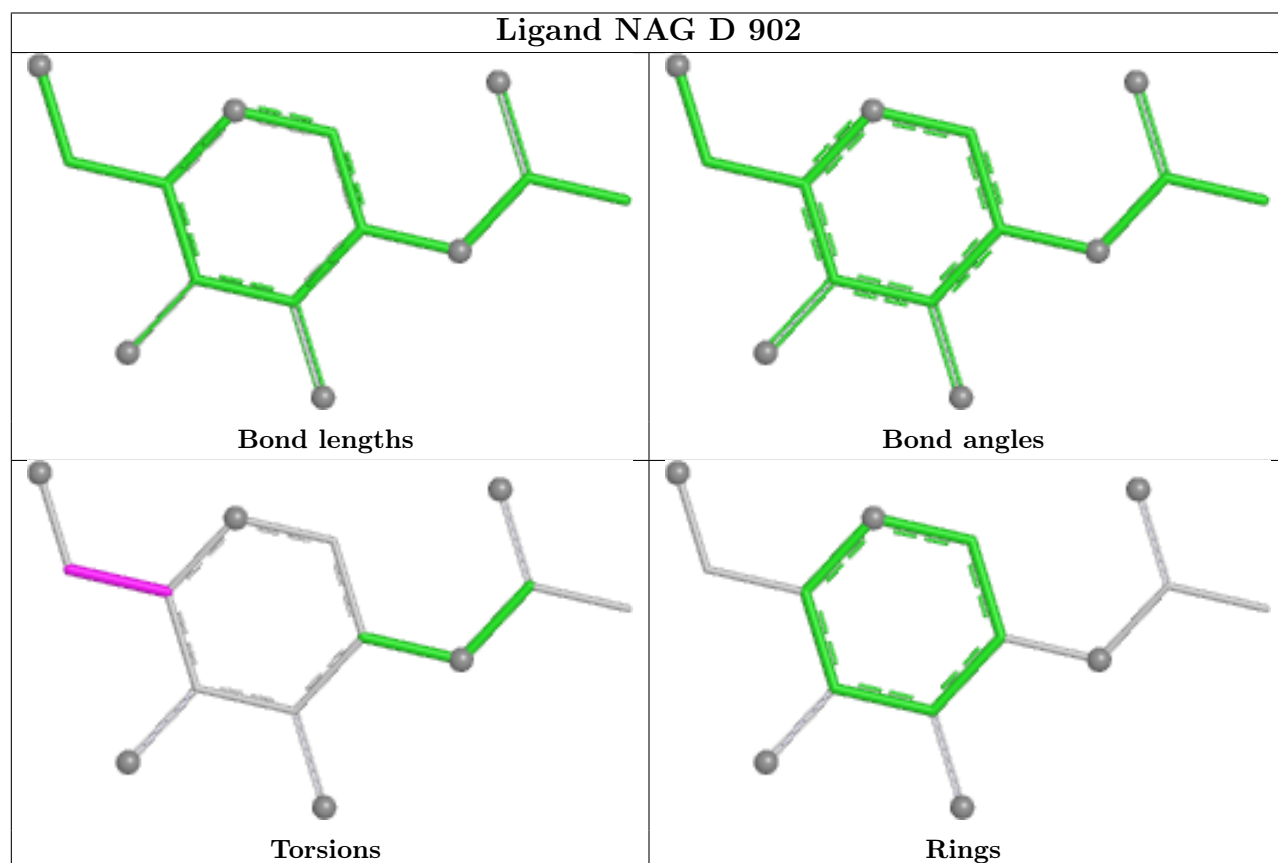
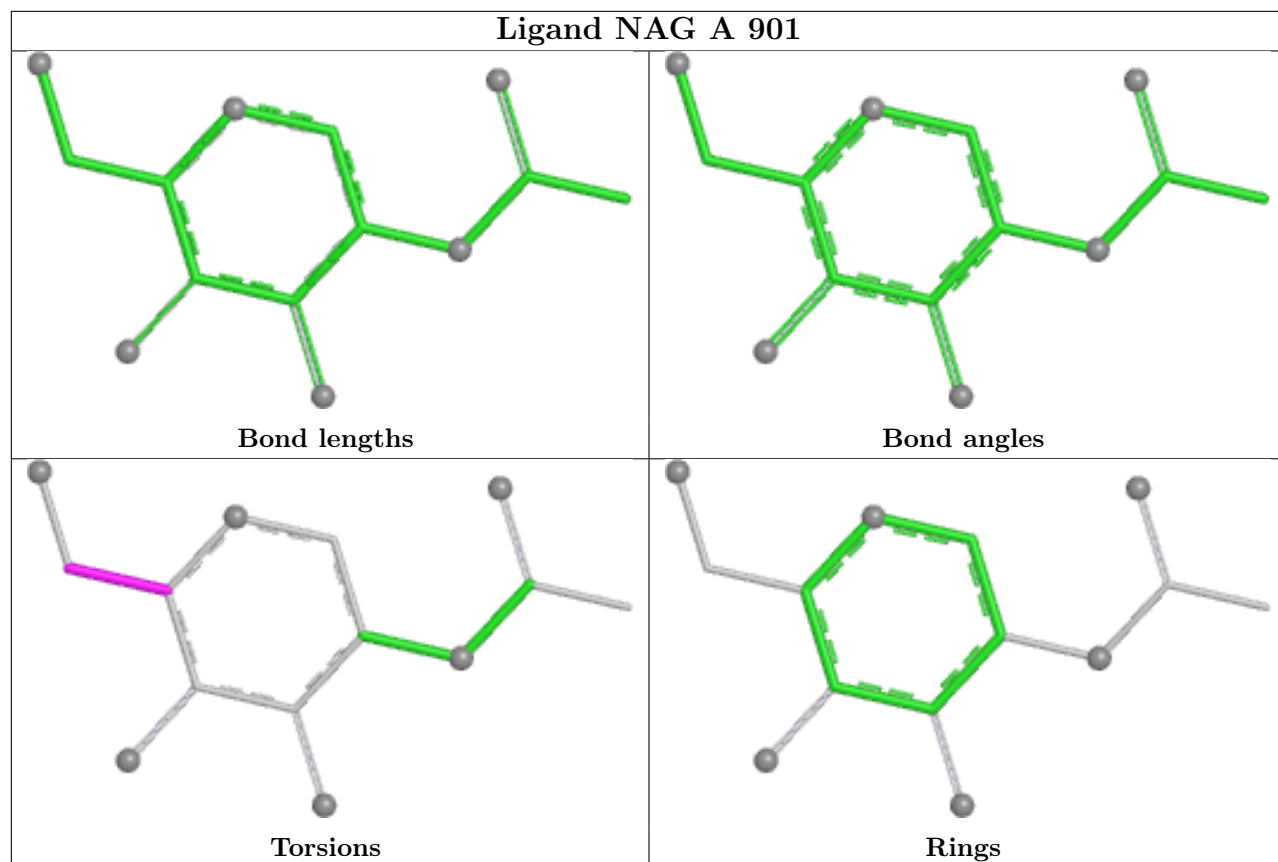
There are no ring outliers.

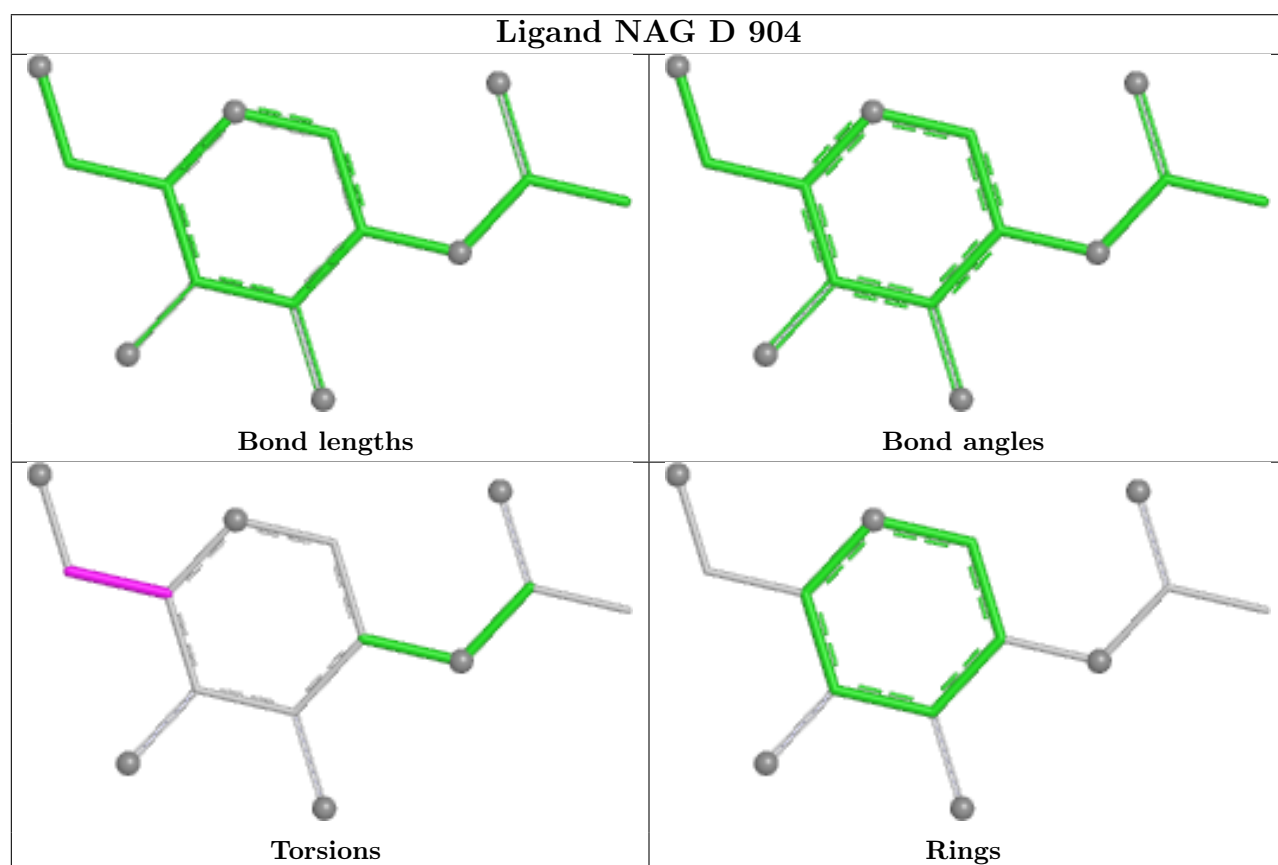
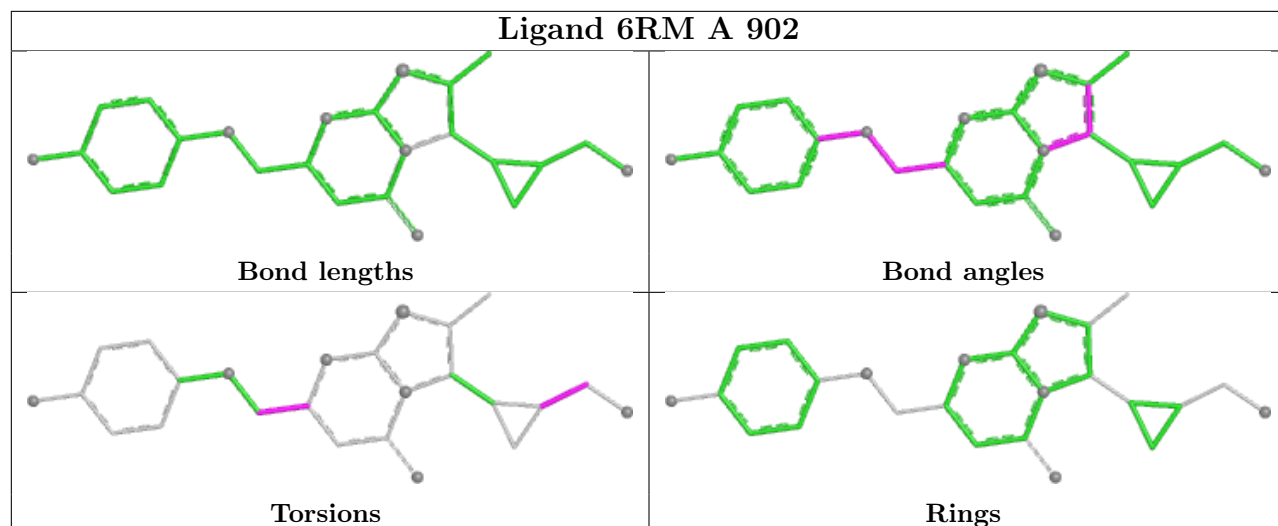
4 monomers are involved in 30 short contacts:

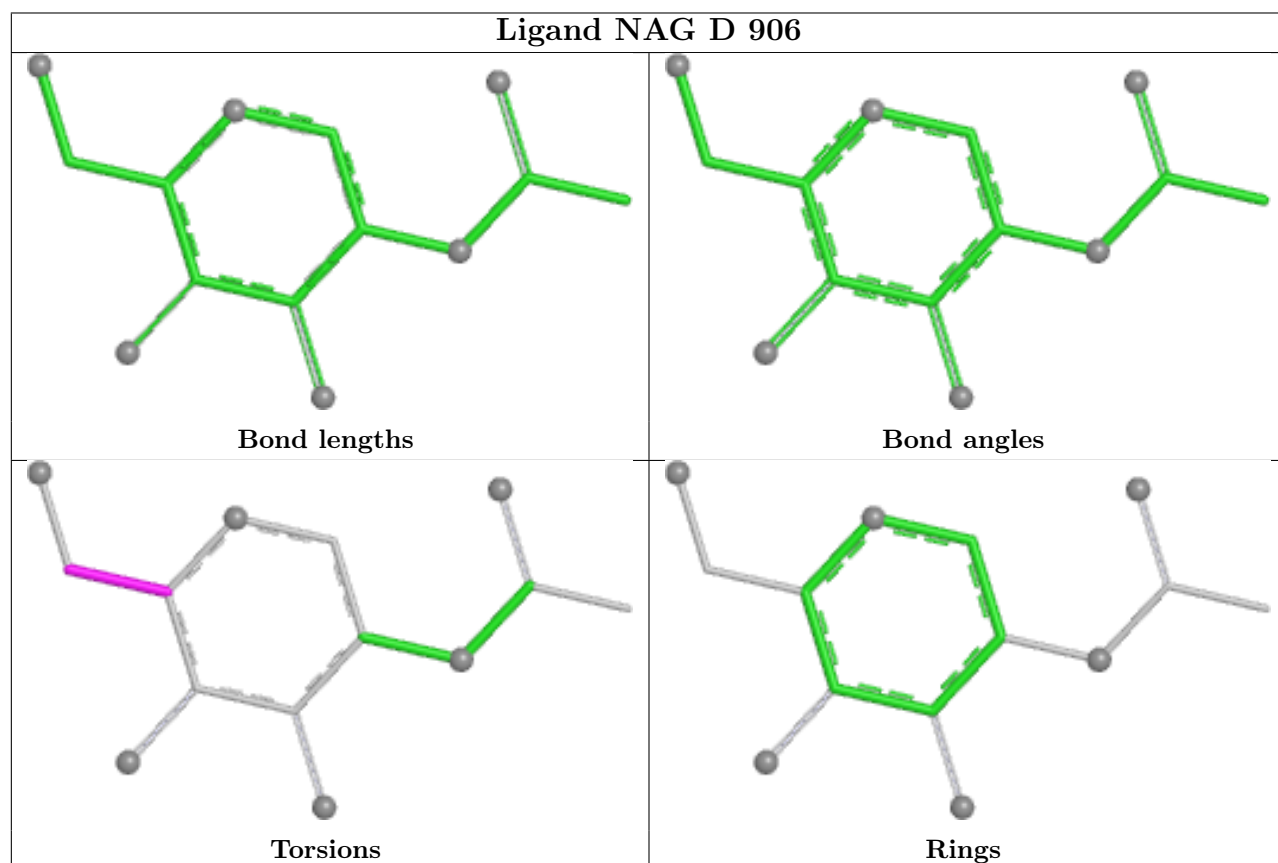
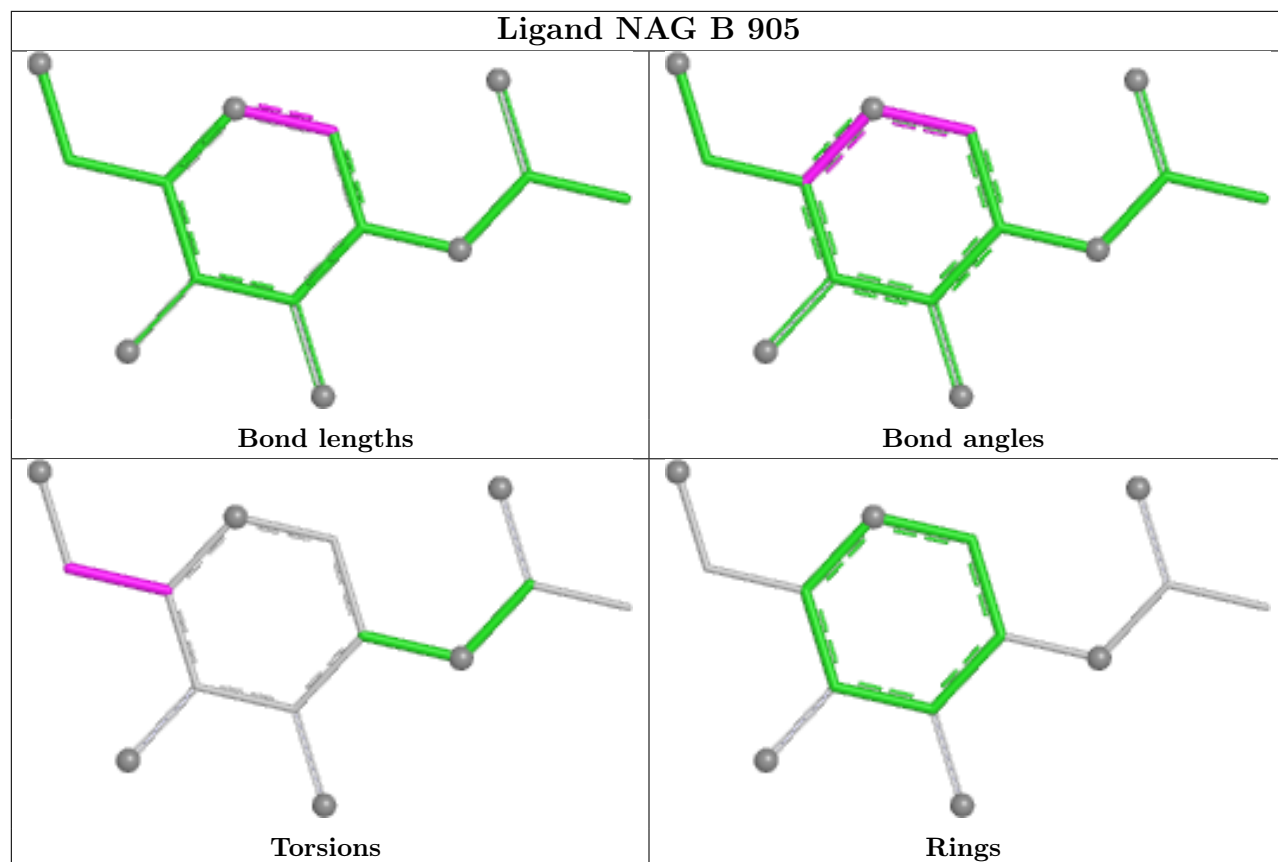
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	902	6RM	15	0
3	A	901	NAG	1	0
4	A	902	6RM	13	0
3	C	901	NAG	1	0

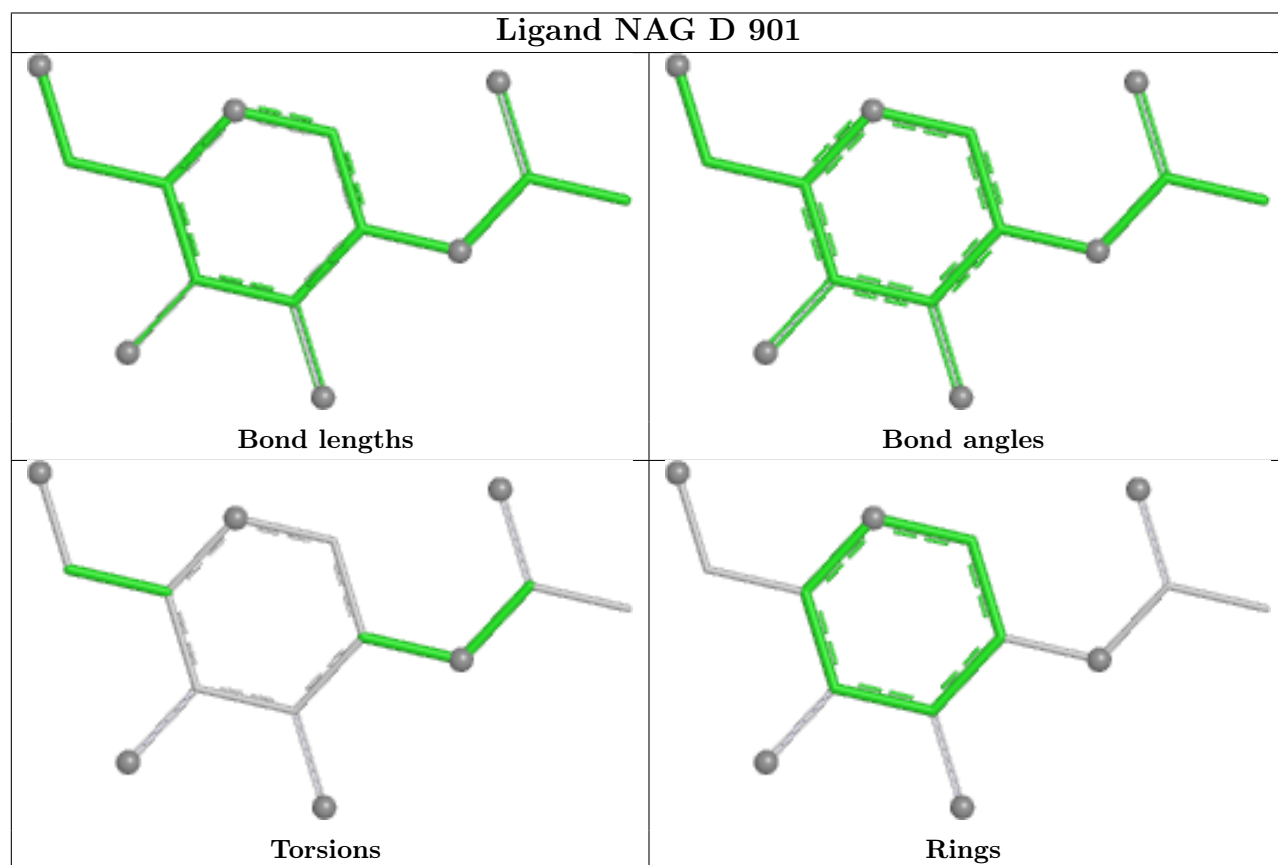
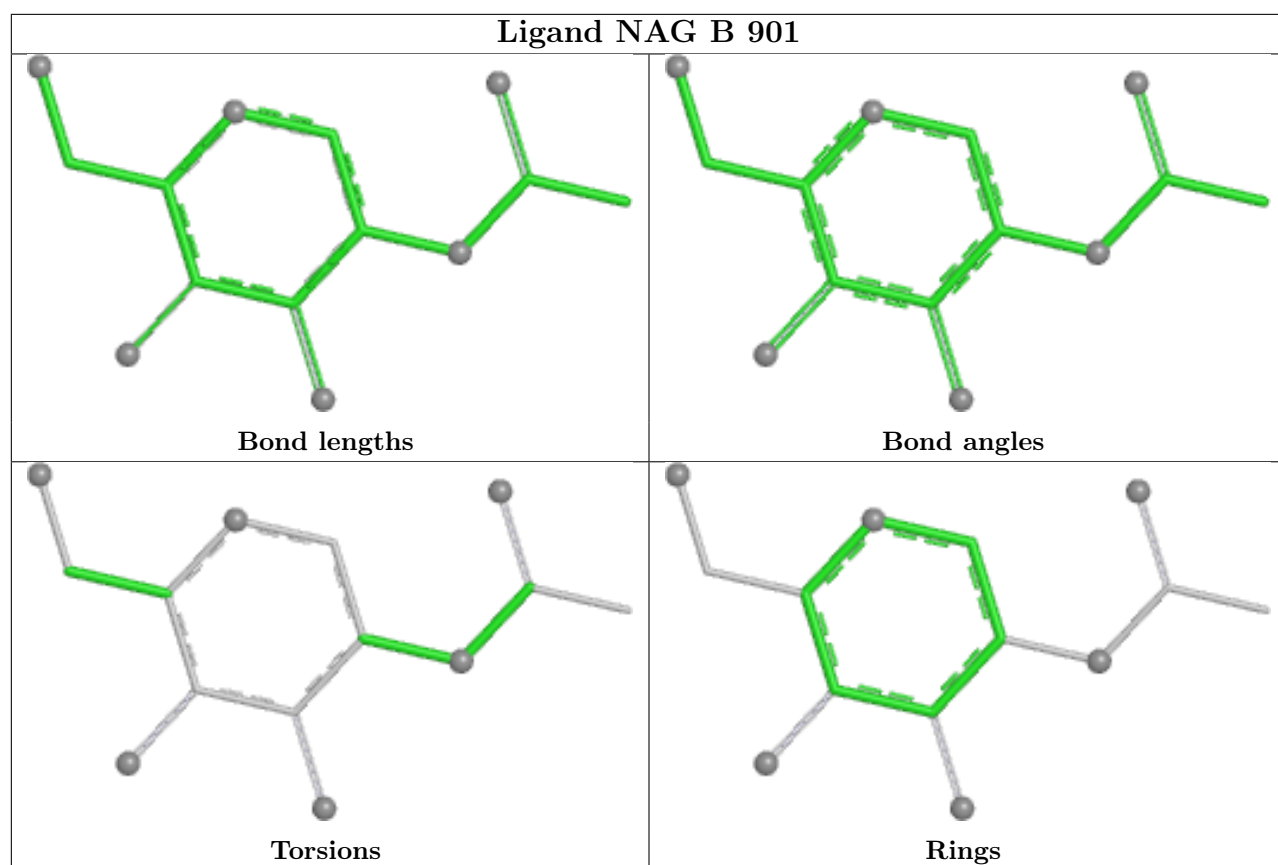
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

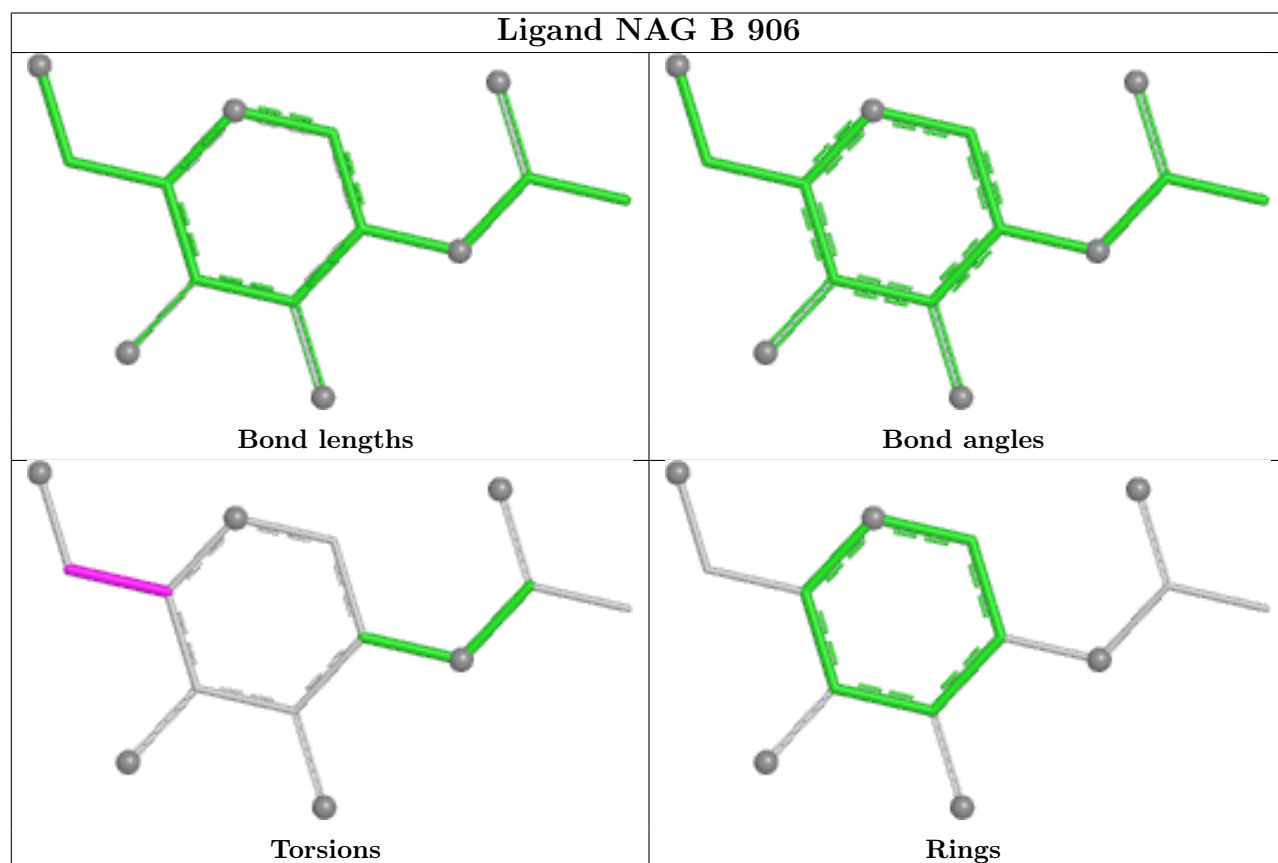
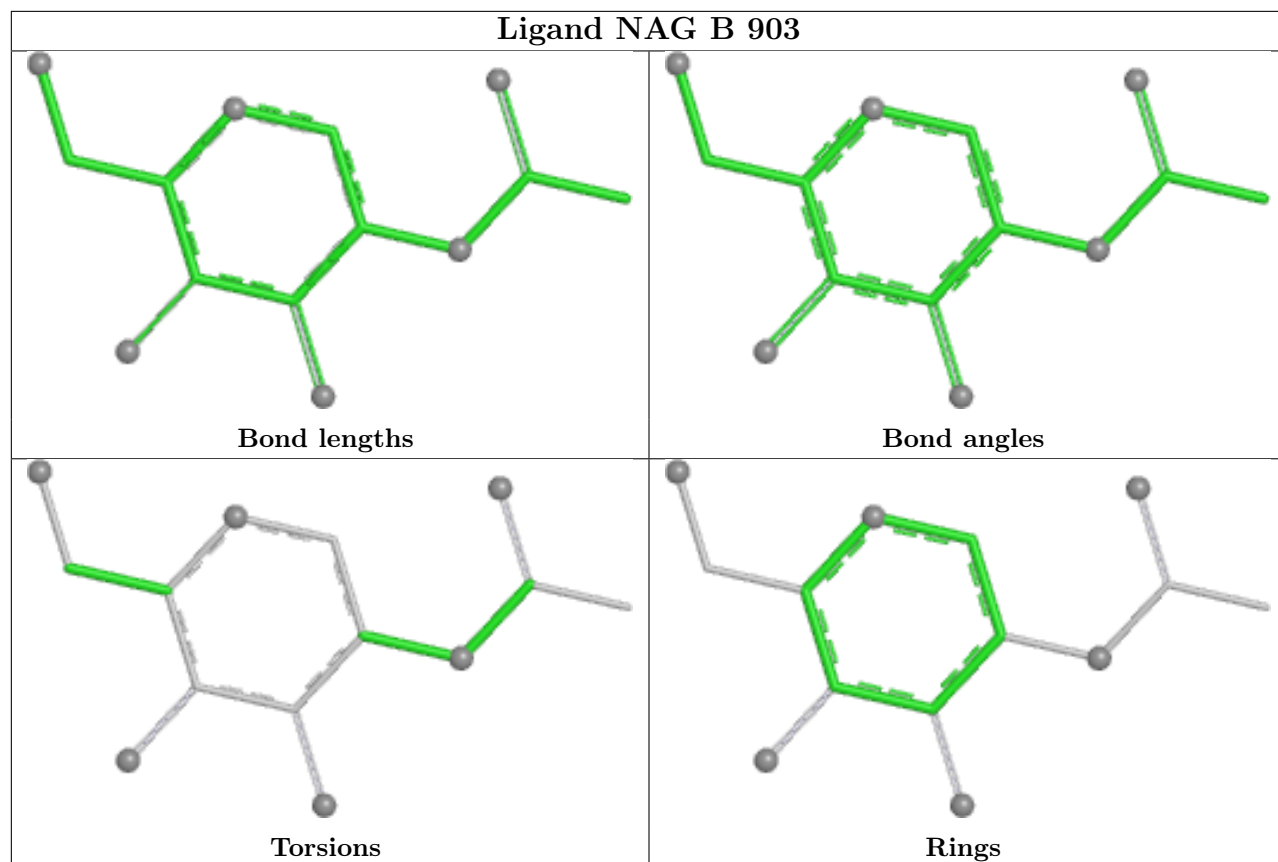


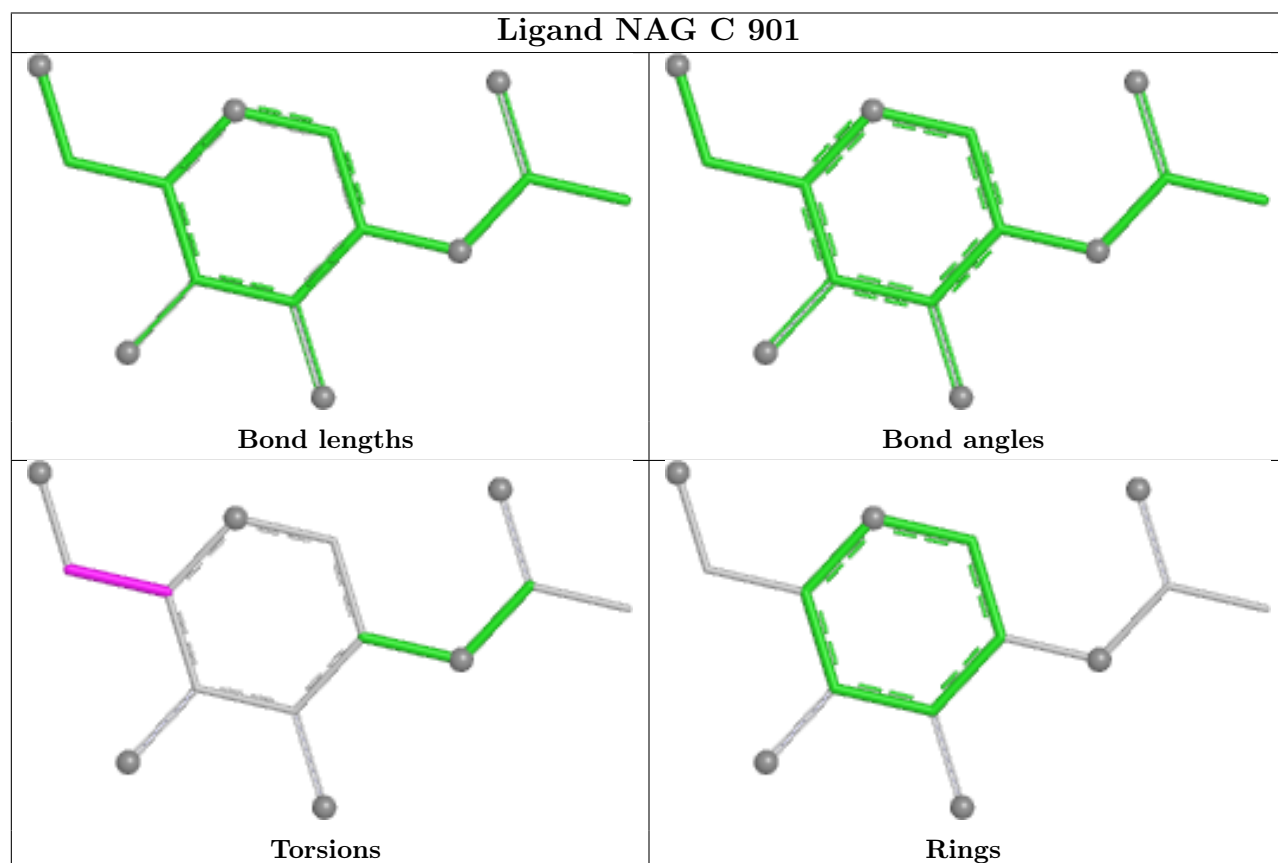
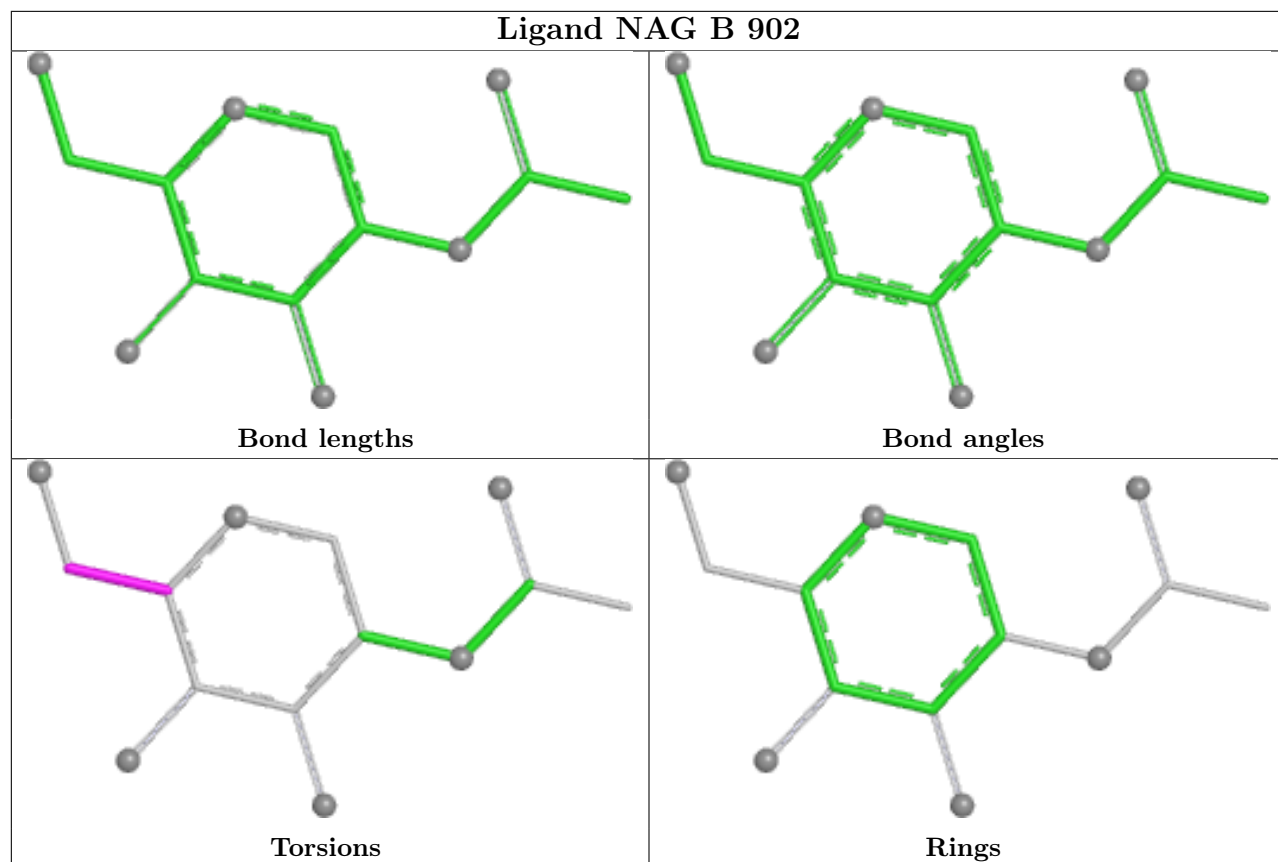


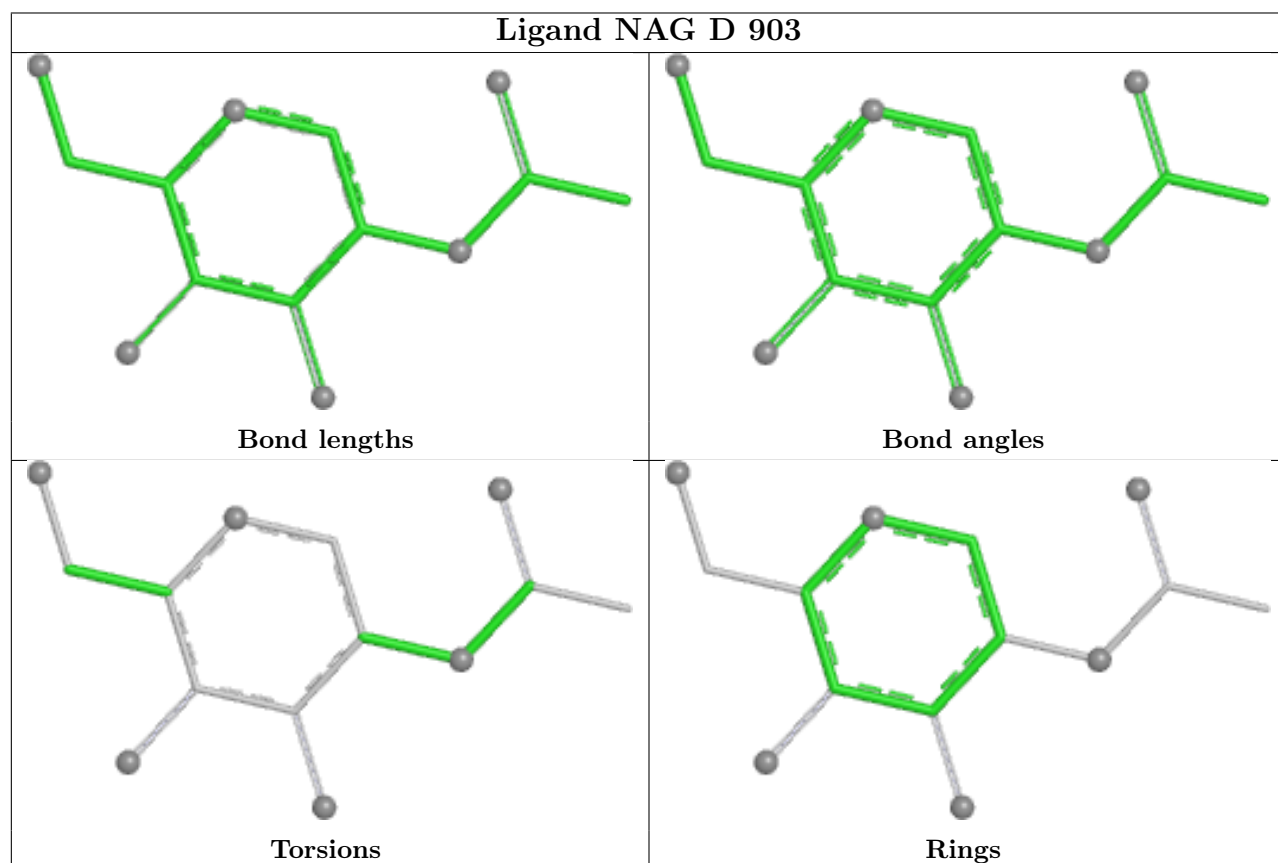
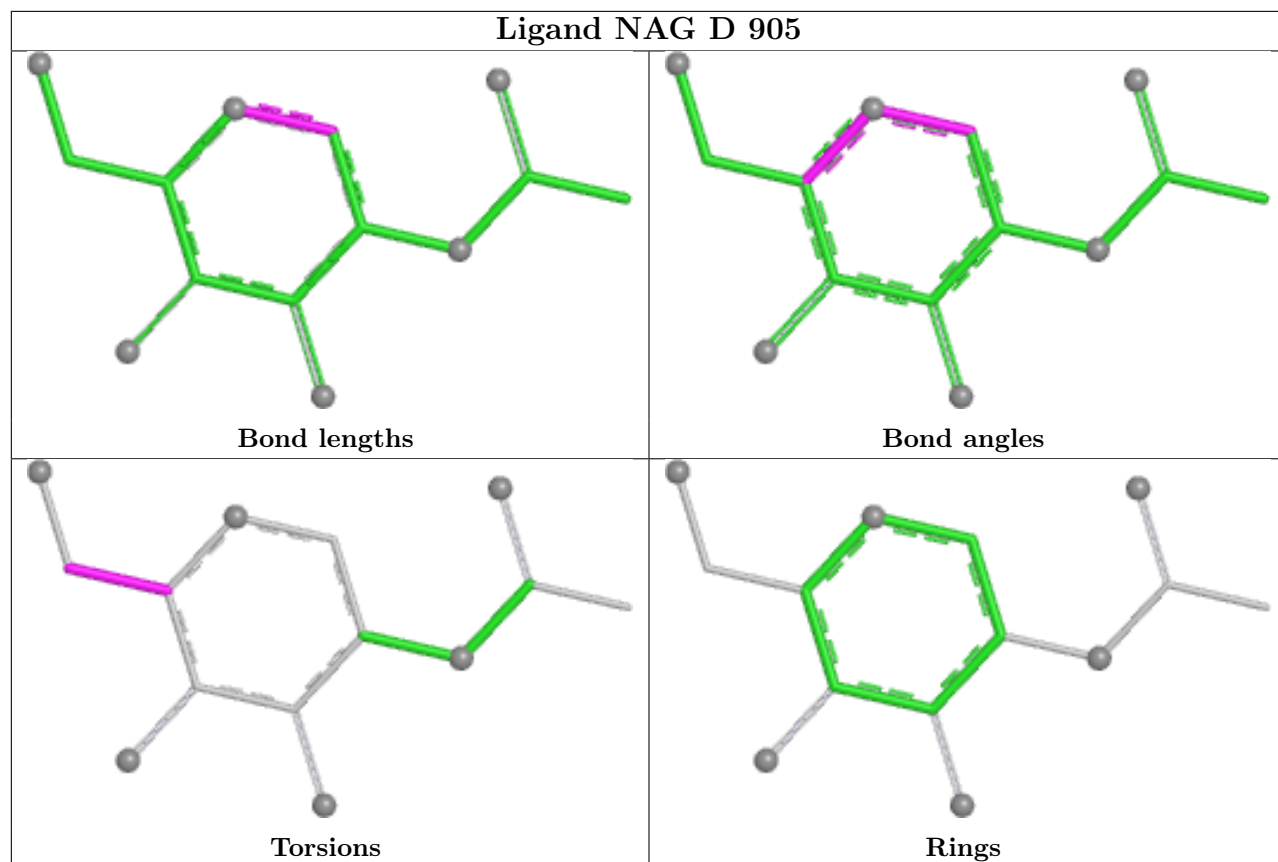












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

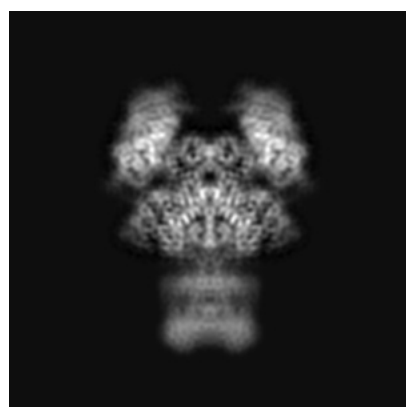
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31228. These allow visual inspection of the internal detail of the map and identification of artifacts.

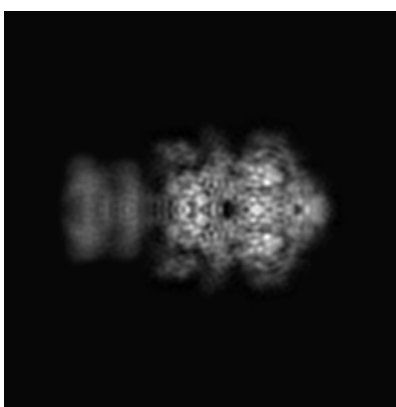
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

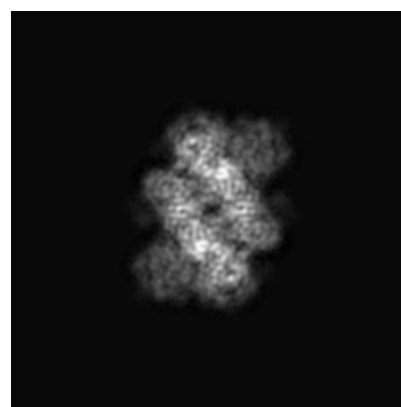
6.1.1 Primary map



X



Y

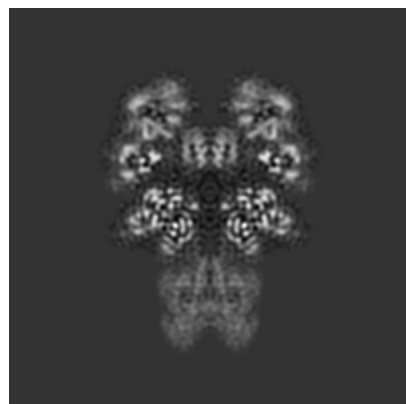


Z

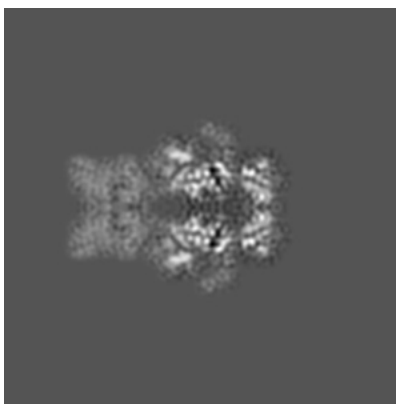
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

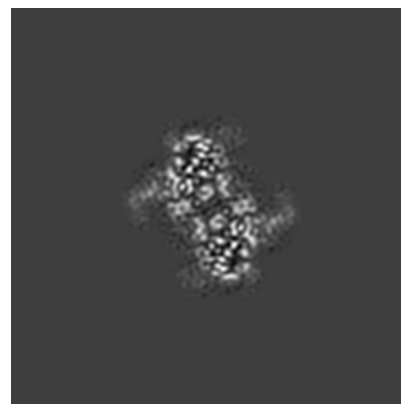
6.2.1 Primary map



X Index: 130



Y Index: 130

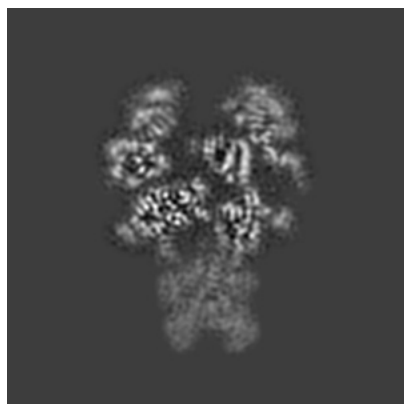


Z Index: 130

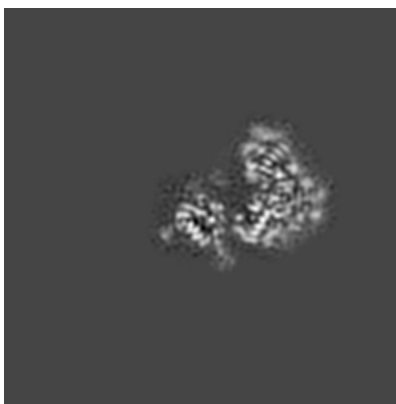
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 137



Y Index: 167

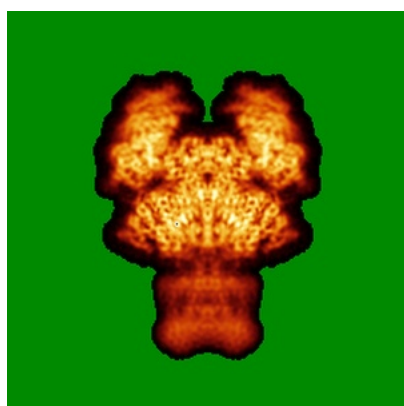


Z Index: 163

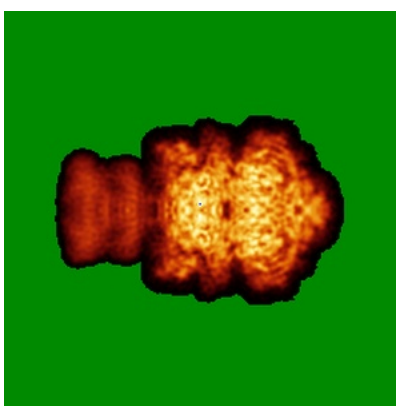
The images above show the largest variance slices of the map in three orthogonal directions.

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

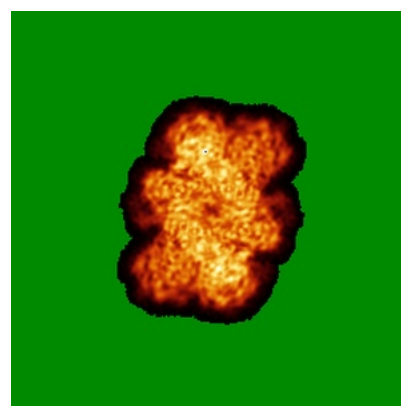
6.4.1 Primary map



X



Y

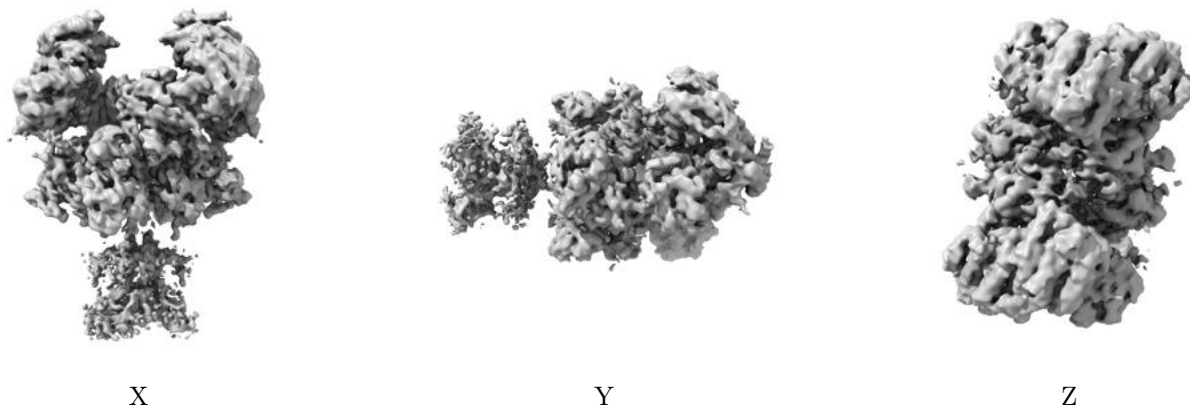


Z

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 0.0081. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

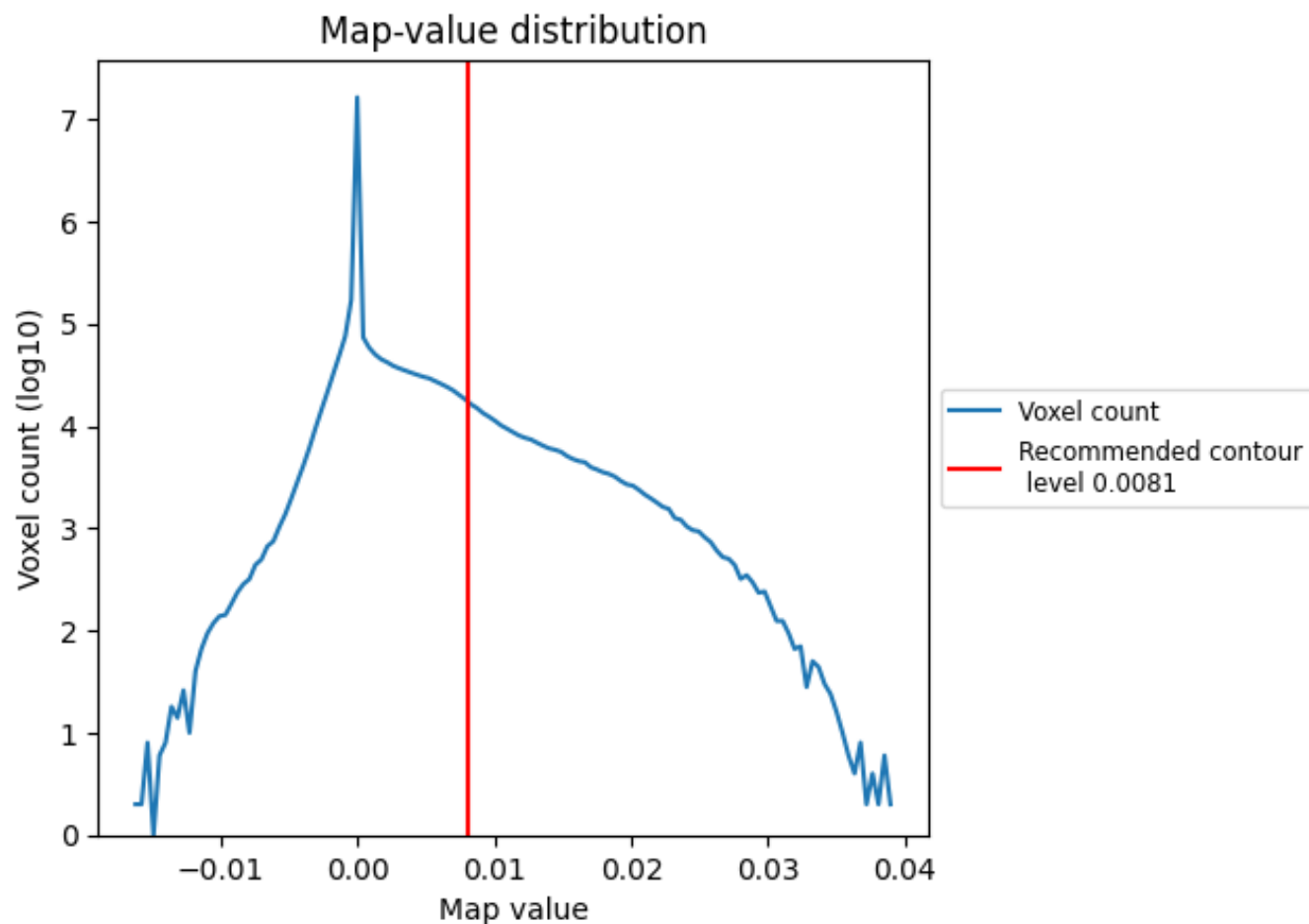
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

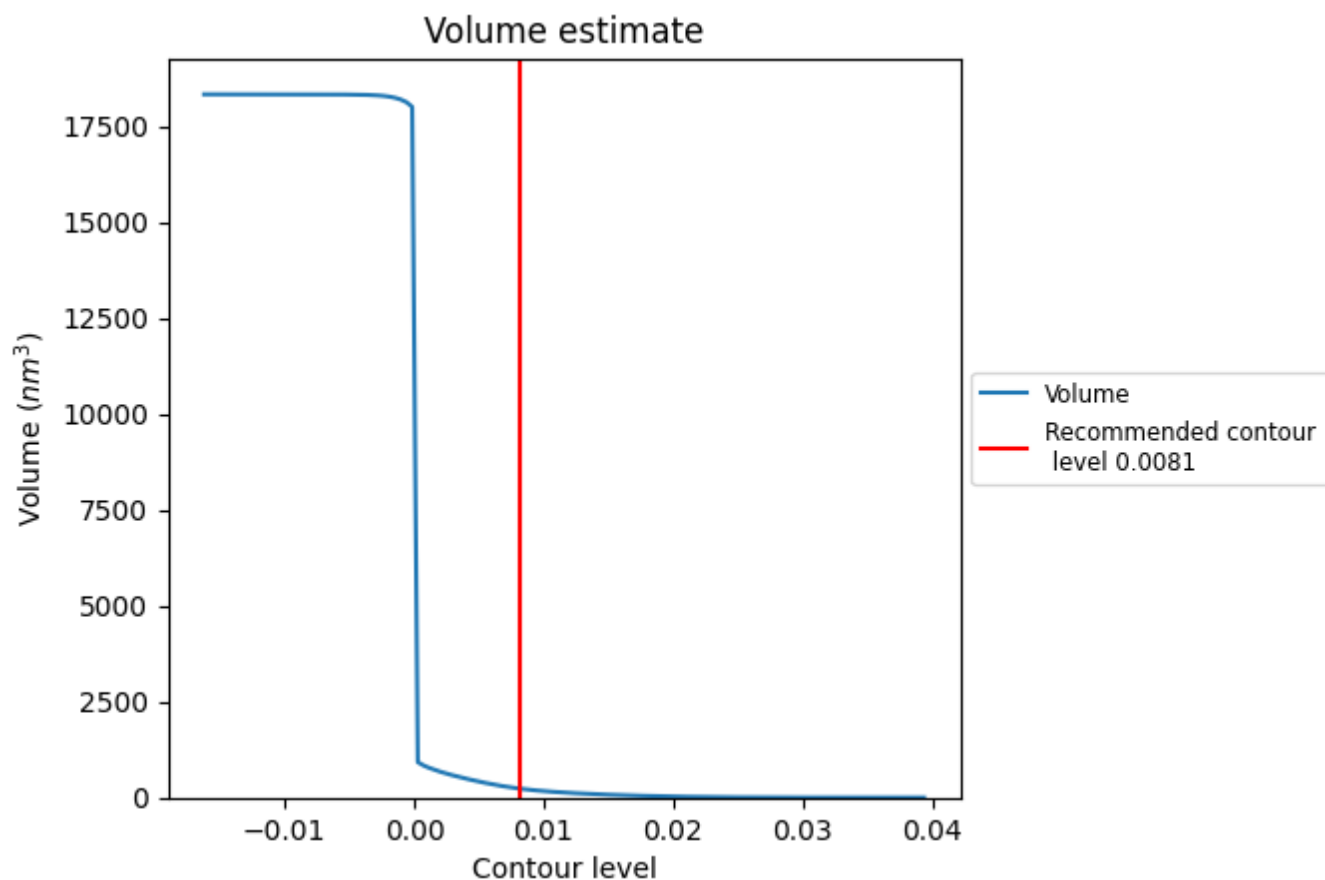
This section contains the results of statistical analysis of the map.

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.

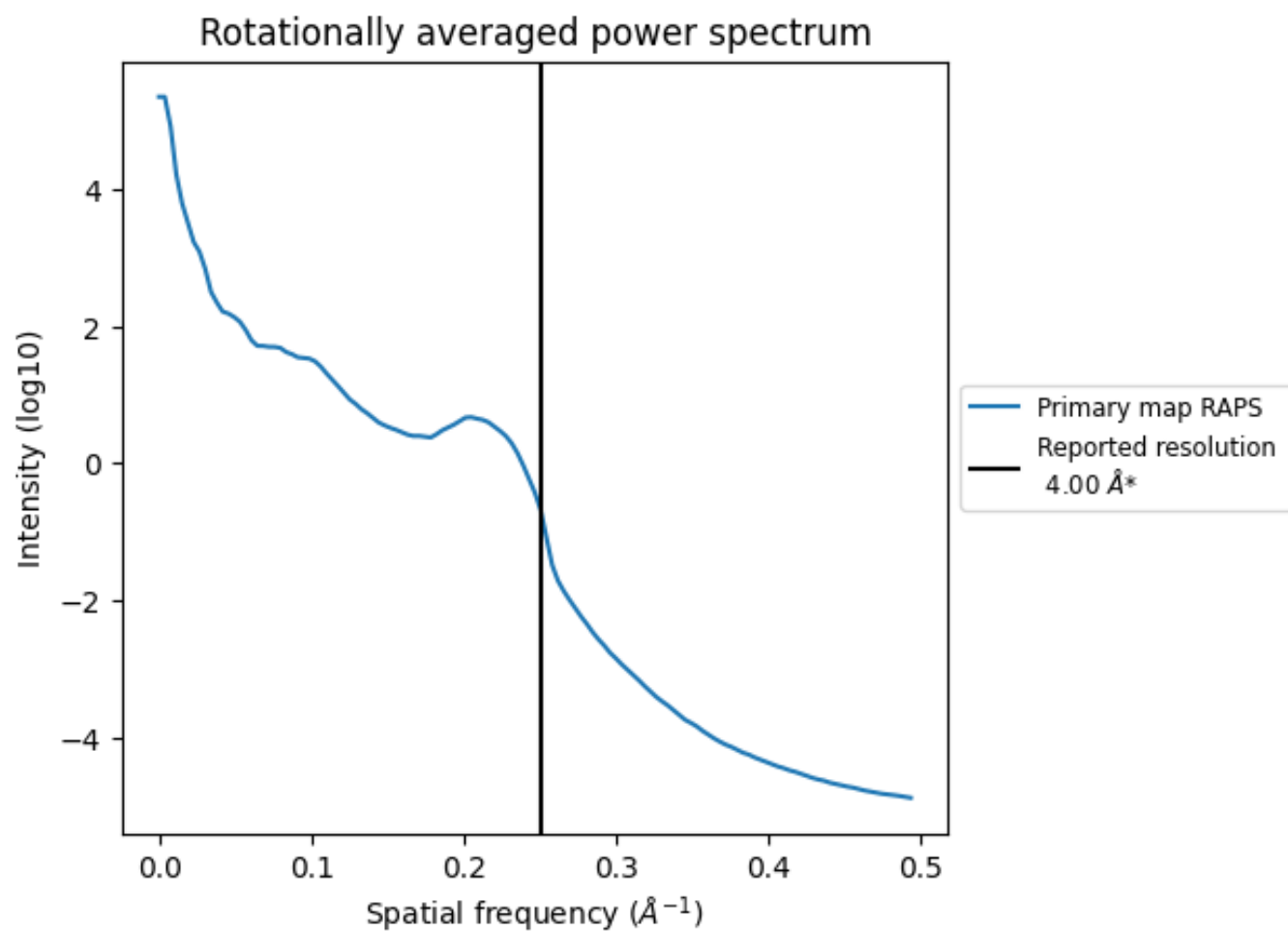
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 235 nm³; this corresponds to an approximate mass of 213 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 0.250 Å⁻¹

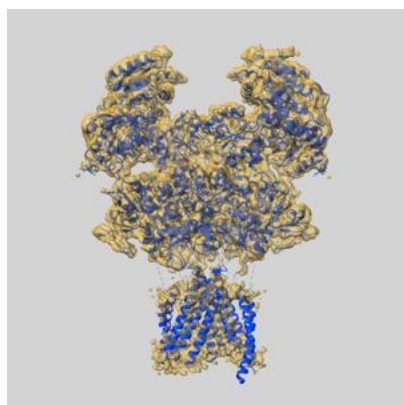
8 Fourier-Shell correlation

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

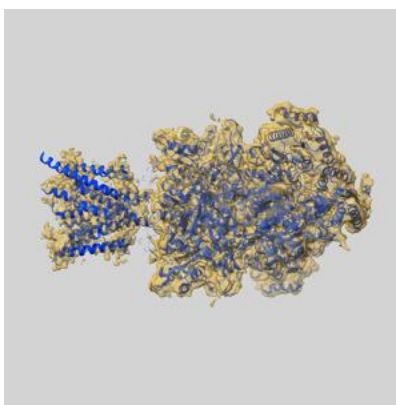
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31228 and PDB model 7EOR. Per-residue inclusion information can be found in section [3](#) on page [7](#).

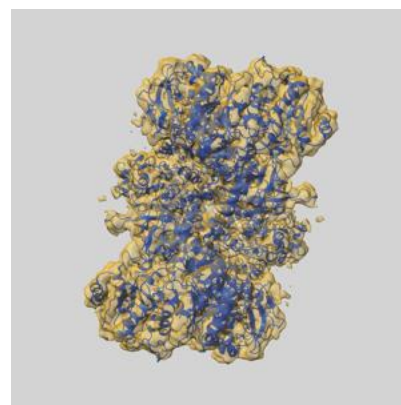
9.1 Map-model overlay [i](#)



X



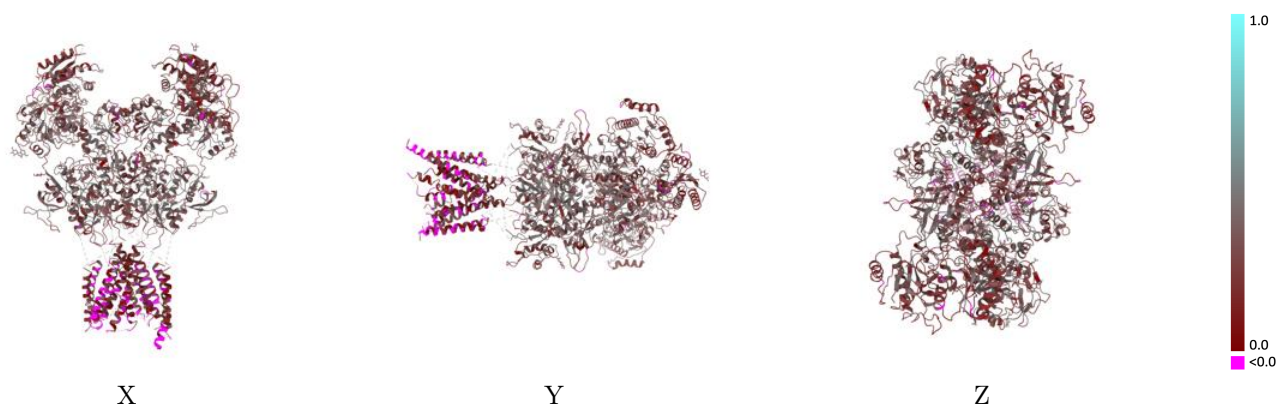
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0081 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](#)

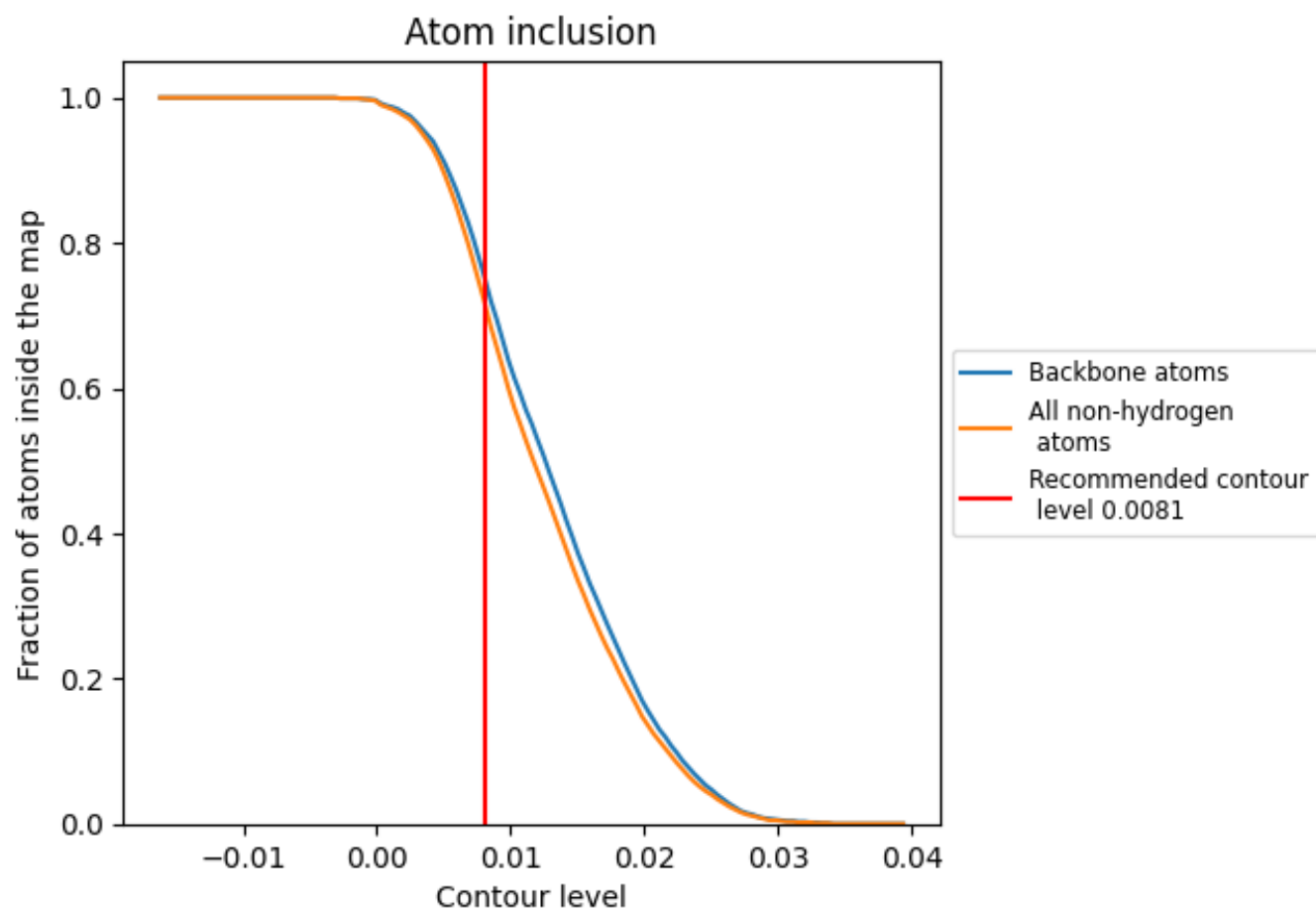


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.0081) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.2840
A	0.7160	0.2780
B	0.7260	0.2880
C	0.7170	0.2780
D	0.7280	0.2900

