



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:44 AM UTC

PDB ID : 6WIV / pdb_00006wiv
EMDB ID : EMD-21685
Title : Structure of human GABA(B) receptor in an inactive state
Authors : Park, J.; Fu, Z.; Frangaj, A.; Liu, J.; Mosyak, L.; Shen, T.; Slavkovich, V.N.; Ray, K.M.; Taura, J.; Cao, B.; Geng, Y.; Zuo, H.; Kou, Y.; Grassucci, R.; Chen, S.; Liu, Z.; Lin, X.; Williams, J.P.; Rice, W.J.; Eng, E.T.; Huang, R.K.; Soni, R.K.; Kloss, B.; Yu, Z.; Javitch, J.A.; Hendrickson, W.A.; Slesinger, P.A.; Quick, M.; Graziano, J.; Yu, H.; Fiehn, O.; Clarke, O.B.; Frank, J.; Fan, Q.R.
Deposited on : 2020-04-10
Resolution : 3.30 Å(reported)
Based on initial model : 4MQE

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

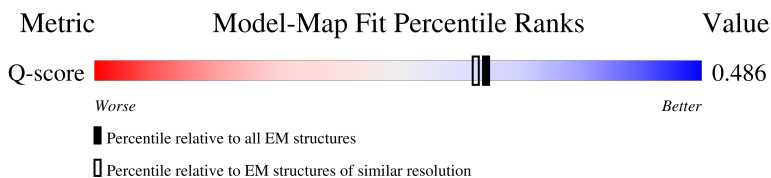
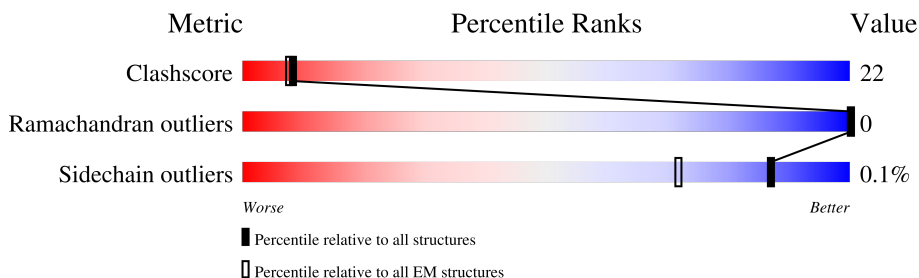
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	810	 50% 34% 16%
2	B	827	 45% 36% 19%

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11206 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 Gamma-aminobutyric acid type B receptor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	681	Total	C	N	O	S	0	0
			5427	3514	903	985	25		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	803	ASP	-	expression tag	UNP Q9UBS5
A	804	TYR	-	expression tag	UNP Q9UBS5
A	805	LYS	-	expression tag	UNP Q9UBS5
A	806	ASP	-	expression tag	UNP Q9UBS5
A	807	ASP	-	expression tag	UNP Q9UBS5
A	808	ASP	-	expression tag	UNP Q9UBS5
A	809	ASP	-	expression tag	UNP Q9UBS5
A	810	LYS	-	expression tag	UNP Q9UBS5

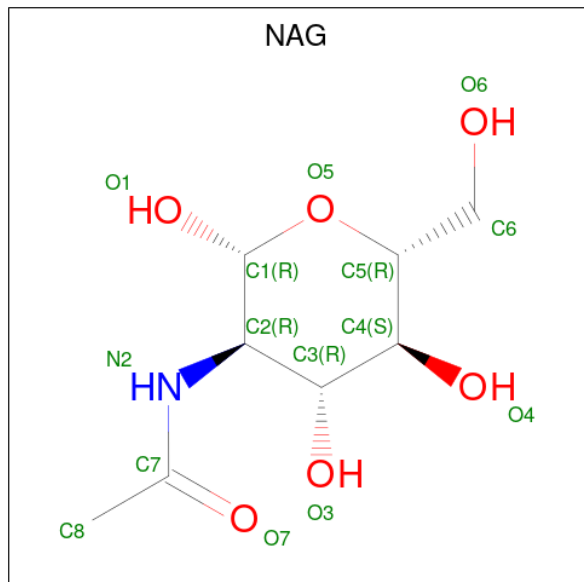
- Molecule 2 is a protein called Gamma-aminobutyric acid type B receptor subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	671	Total	C	N	O	S	0	0
			5333	3456	882	959	36		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	820	ASP	-	expression tag	UNP O75899
B	821	TYR	-	expression tag	UNP O75899
B	822	LYS	-	expression tag	UNP O75899
B	823	ASP	-	expression tag	UNP O75899
B	824	ASP	-	expression tag	UNP O75899
B	825	ASP	-	expression tag	UNP O75899
B	826	ASP	-	expression tag	UNP O75899
B	827	LYS	-	expression tag	UNP O75899

- 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).

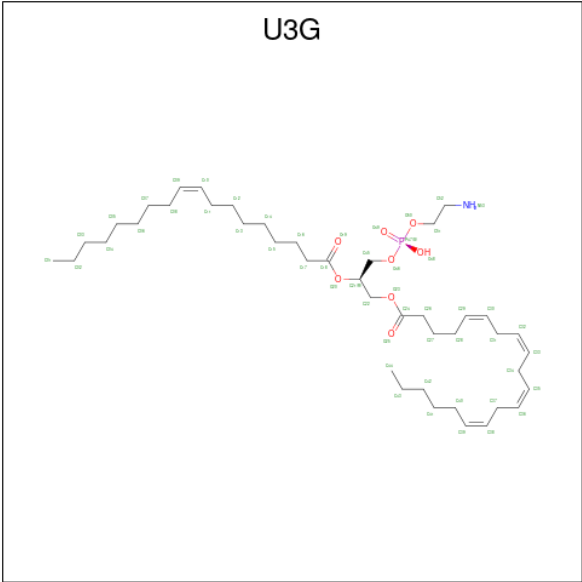


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

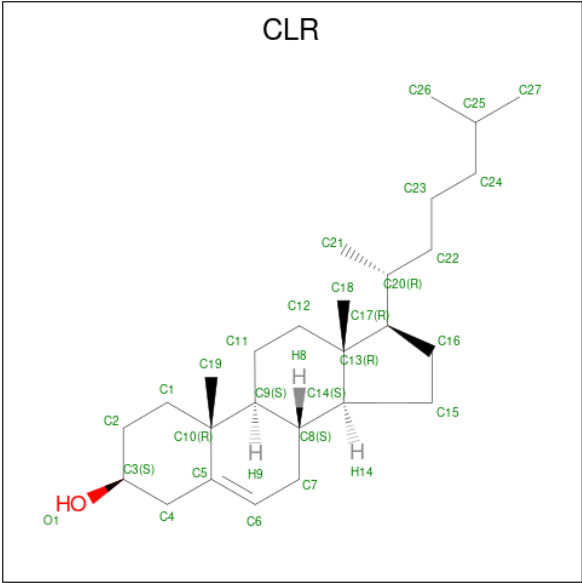
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	

- Molecule 5 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-{[(9Z)-octadec-9-enoyl]oxy}propyl (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoate (CCD ID: U3G) (formula: $C_{43}H_{76}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			53	43	1	8	1	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



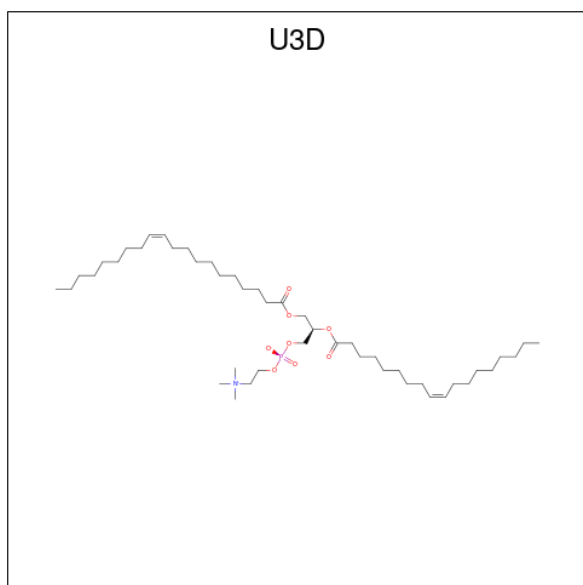
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	

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Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	

- Molecule 7 is [(2R)-3-[(Z)-icos-11-enoyl]oxy-2-[(Z)-octadec-9-enoyl]oxypropyl] 2-(trimethylazaniumyl)ethyl phosphate (CCD ID: U3D) (formula: C₄₆H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).

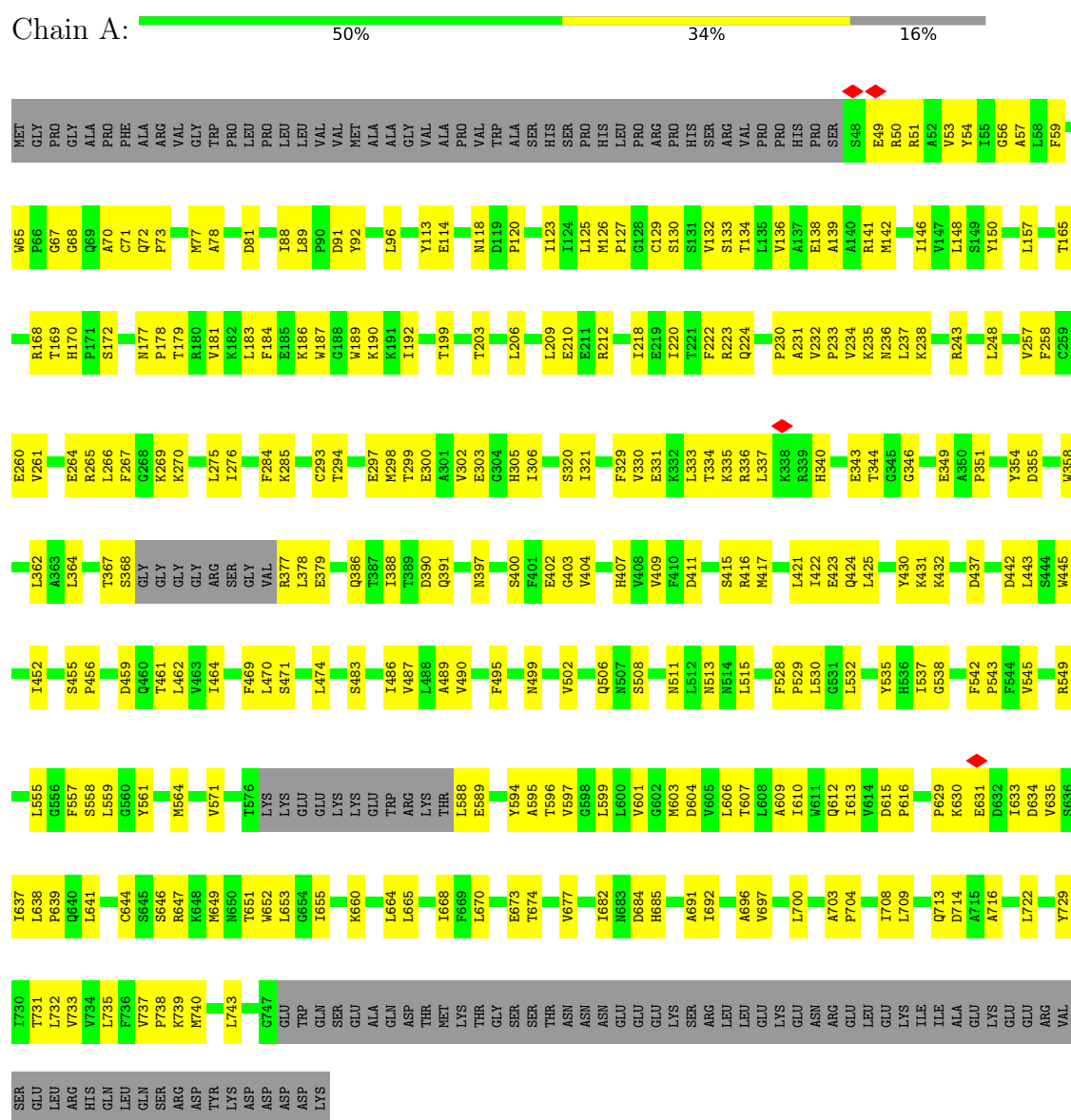


Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			56	46	1	8	1	

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: Gamma-aminobutyric acid type B receptor subunit 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	233737	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	85	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.170	Depositor
Minimum map value	-0.294	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U3D, NAG, CLR, U3G, CA

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	0/5562	0.40	0/7554
2	B	0.19	0/5452	0.40	0/7386
All	All	0.20	0/11014	0.40	0/14940

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

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	5427	0	5425	227	0
2	B	5333	0	5401	261	0
3	A	42	0	39	2	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
5	A	53	0	0	1	0
6	A	112	0	184	12	0
6	B	168	0	276	6	0
7	B	56	0	0	1	0
All	All	11206	0	11338	488	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 22.

All (488) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:628:TYR:HB2	2:B:643:PRO:HG2	1.45	0.97
2:B:526:GLY:HA3	2:B:567:ALA:HB2	1.48	0.96
1:A:146:ILE:HD13	1:A:165:THR:HB	1.48	0.94
2:B:198:VAL:HG12	2:B:250:ILE:HB	1.51	0.92
2:B:522:LEU:HD21	2:B:601:VAL:HG11	1.54	0.90
1:A:529:PRO:HB2	1:A:549:ARG:HG3	1.52	0.89
2:B:270:GLU:HB2	2:B:272:MET:HG3	1.55	0.87
1:A:664:LEU:HD23	1:A:696:ALA:HA	1.58	0.84
2:B:250:ILE:HD12	2:B:278:GLN:HB3	1.58	0.84
2:B:631:GLU:HG2	2:B:632:PRO:HD3	1.65	0.79
2:B:313:GLY:HA2	2:B:430:GLN:HE21	1.47	0.79
1:A:588:LEU:HD12	1:A:589:GLU:HG3	1.66	0.78
2:B:206:GLN:HE21	2:B:210:GLU:HG2	1.48	0.78
1:A:65:TRP:HZ2	1:A:349:GLU:HG3	1.48	0.77
1:A:134:THR:HG22	1:A:157:LEU:HD21	1.66	0.76
2:B:61:LEU:HD23	2:B:104:TYR:HB2	1.67	0.76
1:A:532:LEU:HD11	1:A:545:VAL:HG11	1.68	0.76
1:A:81:ASP:OD2	1:A:354:TYR:OH	2.04	0.75
2:B:566:THR:HG22	2:B:605:LEU:HD21	1.68	0.75
1:A:557:PHE:HZ	1:A:664:LEU:HD11	1.52	0.74
2:B:578:VAL:HG23	2:B:686:LEU:HD12	1.69	0.74
1:A:703:ALA:HB3	1:A:704:PRO:HD3	1.70	0.74
2:B:240:VAL:HG12	2:B:270:GLU:HG3	1.70	0.74
1:A:733:VAL:HG13	1:A:737:VAL:HG21	1.70	0.73
2:B:56:LEU:HD22	2:B:128:LEU:HD11	1.72	0.72
2:B:709:VAL:HG11	2:B:723:ILE:HG21	1.71	0.72
2:B:704:ILE:HG13	6:B:908:CLR:H261	1.72	0.72
2:B:290:TRP:HB3	2:B:311:MET:HE1	1.72	0.72
2:B:619:ASP:O	2:B:650:ASN:ND2	2.22	0.71
2:B:503:ASN:ND2	2:B:521:ASN:OD1	2.24	0.71
1:A:141:ARG:NH2	2:B:109:ASP:OD1	2.23	0.71
2:B:65:THR:HG22	2:B:67:GLU:H	1.55	0.69
2:B:407:ASN:OD1	2:B:414:GLN:NE2	2.24	0.69
2:B:191:LYS:HE2	2:B:224:ILE:HD11	1.72	0.69
1:A:248:LEU:HA	1:A:276:ILE:HD11	1.74	0.69
1:A:261:VAL:HG13	1:A:266:LEU:HB2	1.75	0.69
1:A:571:VAL:HG12	1:A:674:THR:HG21	1.74	0.68
2:B:699:VAL:HG23	2:B:735:THR:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:TYR:O	2:B:534:ILE:HG22	1.94	0.68
2:B:556:ARG:HA	2:B:559:ILE:HG22	1.76	0.67
2:B:514:MET:HE2	2:B:514:MET:HA	1.75	0.66
1:A:50:ARG:HA	1:A:91:ASP:O	1.95	0.66
1:A:528:PHE:HB2	1:A:529:PRO:HD3	1.77	0.66
1:A:388:ILE:HD11	3:A:902:NAG:H82	1.77	0.66
1:A:682:ILE:HG22	1:A:685:HIS:HB3	1.78	0.66
1:A:190:LYS:HA	1:A:218:ILE:HG23	1.76	0.66
1:A:713:GLN:OE1	1:A:713:GLN:N	2.28	0.66
1:A:206:LEU:O	1:A:210:GLU:HG2	1.96	0.66
2:B:304:ARG:HH11	2:B:308:LEU:HD12	1.61	0.65
1:A:92:TYR:OH	1:A:379:GLU:OE1	2.11	0.65
2:B:639:ILE:HG22	2:B:641:ILE:HD11	1.79	0.65
1:A:53:VAL:HG11	1:A:378:LEU:HD21	1.79	0.65
2:B:520:ASN:O	2:B:524:ILE:HD12	1.97	0.65
1:A:486:ILE:O	1:A:490:VAL:HG23	1.97	0.64
2:B:486:SER:O	2:B:490:ILE:HG13	1.97	0.64
2:B:89:ARG:NH2	2:B:99:LEU:O	2.30	0.64
2:B:58:ILE:HD11	2:B:99:LEU:HD11	1.80	0.64
2:B:154:LEU:HD11	2:B:175:THR:HG23	1.80	0.63
2:B:143:ALA:HA	2:B:146:LEU:HD12	1.81	0.63
1:A:130:SER:O	1:A:134:THR:HG23	1.99	0.63
1:A:508:SER:OG	1:A:684:ASP:OD1	2.13	0.63
1:A:596:THR:HA	6:A:909:CLR:H72	1.79	0.63
1:A:499:ASN:O	1:A:502:VAL:HG12	1.99	0.63
1:A:483:SER:O	1:A:487:VAL:HG23	1.99	0.63
2:B:485:LEU:HD13	2:B:725:ALA:HB3	1.81	0.63
1:A:68:GLY:HA2	1:A:71:CYS:HB2	1.80	0.62
1:A:113:TYR:HB2	2:B:118:TYR:CE1	2.34	0.62
1:A:423:GLU:HG2	1:A:432:LYS:HA	1.80	0.62
2:B:649:GLU:HB2	2:B:653:MET:HE2	1.82	0.62
1:A:232:VAL:HG12	1:A:233:PRO:HD3	1.81	0.62
2:B:259:MET:O	2:B:263:VAL:HG23	1.99	0.62
2:B:87:GLN:OE1	2:B:359:TYR:OH	2.14	0.62
2:B:236:PRO:O	2:B:240:VAL:HG23	2.00	0.62
2:B:731:CYS:O	2:B:735:THR:HG23	2.00	0.61
2:B:465:LYS:NZ	2:B:468:THR:HA	2.15	0.61
1:A:729:TYR:O	1:A:733:VAL:HG23	1.99	0.61
1:A:542:PHE:HE2	1:A:644:CYS:HB3	1.66	0.61
1:A:329:PHE:HE2	1:A:351:PRO:HG3	1.65	0.61
2:B:364:VAL:O	2:B:368:THR:OG1	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:VAL:CG1	1:A:674:THR:HG21	2.31	0.60
2:B:143:ALA:HA	2:B:146:LEU:CD1	2.31	0.60
1:A:638:LEU:HD12	1:A:639:PRO:HD2	1.83	0.60
2:B:465:LYS:HE2	2:B:469:ILE:H	1.66	0.60
2:B:479:LEU:HB3	2:B:480:PRO:HD3	1.84	0.60
1:A:386:GLN:HG2	1:A:390:ASP:OD1	2.01	0.60
2:B:64:LEU:HD11	2:B:103:LEU:HG	1.83	0.60
1:A:421:LEU:HD11	1:A:432:LYS:HB3	1.82	0.60
1:A:558:SER:HB2	1:A:604:ASP:OD1	2.01	0.60
2:B:574:LYS:HD3	2:B:692:ILE:HD13	1.84	0.60
2:B:550:GLU:OE2	2:B:622:ARG:HG2	2.02	0.59
1:A:330:VAL:O	1:A:334:THR:HG23	2.02	0.59
2:B:596:LYS:O	2:B:600:ILE:HG13	2.01	0.59
2:B:650:ASN:H	2:B:653:MET:HB2	1.66	0.59
2:B:655:ILE:O	2:B:659:ILE:HG23	2.02	0.59
1:A:737:VAL:HB	1:A:738:PRO:HD3	1.85	0.59
2:B:626:GLU:OE1	2:B:627:LYS:N	2.35	0.59
1:A:588:LEU:CD1	1:A:589:GLU:HG3	2.33	0.59
1:A:437:ASP:HB3	1:A:442:ASP:OD1	2.03	0.58
2:B:536:LEU:CD1	2:B:552:LEU:HD12	2.33	0.58
1:A:187:TRP:CD1	1:A:456:PRO:HG3	2.37	0.58
2:B:477:ILE:N	2:B:540:ASP:OD1	2.36	0.58
1:A:555:LEU:O	1:A:559:LEU:HG	2.04	0.58
2:B:685:ALA:O	2:B:686:LEU:HD23	2.03	0.58
2:B:562:VAL:HA	2:B:565:THR:HG22	1.86	0.58
1:A:284:PHE:CE2	1:A:285:LYS:HE3	2.39	0.58
1:A:258:PHE:CD1	1:A:302:VAL:HG12	2.39	0.58
2:B:439:VAL:HB	2:B:456:ILE:CG2	2.34	0.58
2:B:566:THR:CG2	2:B:605:LEU:HD21	2.33	0.58
2:B:85:ILE:HD13	2:B:362:ILE:HG21	1.86	0.57
1:A:513:ASN:HD22	1:A:735:LEU:HD23	1.69	0.57
2:B:63:PRO:O	2:B:74:GLY:HA3	2.03	0.57
2:B:741:VAL:O	2:B:744:LEU:HG	2.05	0.57
1:A:258:PHE:CZ	1:A:275:LEU:HD11	2.40	0.57
2:B:470:ILE:HG22	2:B:640:SER:OG	2.04	0.57
2:B:534:ILE:HD11	2:B:725:ALA:CA	2.34	0.57
1:A:430:TYR:O	1:A:431:LYS:HD3	2.05	0.57
1:A:615:ASP:OD2	1:A:647:ARG:HG2	2.04	0.57
1:A:231:ALA:O	1:A:235:LYS:HG3	2.05	0.57
2:B:394:THR:O	2:B:398:ILE:HG13	2.04	0.57
2:B:536:LEU:HD11	2:B:552:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:534:ILE:HD11	2:B:725:ALA:HA	1.87	0.57
2:B:603:GLY:O	2:B:607:ILE:HG13	2.05	0.57
1:A:557:PHE:CZ	1:A:664:LEU:HD11	2.38	0.56
2:B:215:LEU:O	2:B:219:LEU:HG	2.05	0.56
2:B:240:VAL:HG21	2:B:266:CYS:HB3	1.87	0.56
2:B:465:LYS:HZ1	2:B:468:THR:HA	1.68	0.56
2:B:709:VAL:CG1	2:B:723:ILE:HG21	2.35	0.56
2:B:204:ASP:OD1	2:B:231:SER:HB3	2.04	0.56
1:A:57:ALA:CB	1:A:96:LEU:HD11	2.35	0.56
2:B:175:THR:O	2:B:422:ARG:NH1	2.37	0.56
1:A:320:SER:HB2	1:A:403:GLY:HA2	1.87	0.56
1:A:529:PRO:O	1:A:549:ARG:HD2	2.06	0.56
2:B:412:THR:OG1	2:B:422:ARG:NH2	2.36	0.56
2:B:520:ASN:HB3	2:B:740:PHE:CZ	2.41	0.56
1:A:537:ILE:HG22	1:A:538:GLY:O	2.05	0.56
1:A:513:ASN:ND2	1:A:735:LEU:HD23	2.19	0.56
2:B:95:ARG:HG3	2:B:96:PRO:HA	1.88	0.56
1:A:651:THR:HA	6:A:906:CLR:C19	2.35	0.56
2:B:564:TYR:CE2	2:B:664:LYS:HD3	2.40	0.56
1:A:474:LEU:HD13	1:A:714:ASP:OD1	2.06	0.56
1:A:609:ALA:O	1:A:613:ILE:HG12	2.05	0.55
2:B:304:ARG:NH1	2:B:308:LEU:HD12	2.21	0.55
1:A:150:TYR:O	1:A:170:HIS:HB2	2.06	0.55
1:A:298:MET:O	1:A:302:VAL:HG22	2.06	0.55
1:A:731:THR:HG21	5:A:905:U3G:C01	2.36	0.55
2:B:328:LYS:HZ2	2:B:334:THR:H	1.54	0.55
2:B:81:VAL:O	2:B:85:ILE:HG12	2.05	0.55
2:B:117:PHE:CZ	2:B:121:ILE:HD11	2.41	0.55
2:B:519:MET:HB2	2:B:574:LYS:HE2	1.87	0.55
2:B:678:THR:O	2:B:681:VAL:HG12	2.07	0.55
1:A:230:PRO:C	1:A:233:PRO:HD2	2.32	0.55
1:A:542:PHE:CE2	1:A:644:CYS:HB3	2.41	0.55
1:A:65:TRP:CH2	1:A:67:GLY:HA3	2.42	0.55
2:B:578:VAL:CG2	2:B:686:LEU:HD12	2.36	0.55
2:B:161:PRO:HB3	2:B:180:ASN:ND2	2.21	0.55
2:B:627:LYS:HG2	2:B:644:LEU:HD13	1.89	0.55
1:A:67:GLY:HA2	1:A:346:GLY:HA3	1.89	0.55
1:A:340:HIS:HB2	1:A:343:GLU:OE1	2.06	0.54
1:A:532:LEU:HD13	1:A:537:ILE:HG12	1.88	0.54
1:A:615:ASP:CG	1:A:646:SER:HB2	2.31	0.54
2:B:346:ARG:NH1	2:B:351:PRO:HD3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:HG22	1:A:297:GLU:CD	2.31	0.54
1:A:561:TYR:OH	1:A:664:LEU:HA	2.08	0.54
2:B:571:MET:HE1	2:B:699:VAL:HG21	1.89	0.54
2:B:490:ILE:HG12	2:B:535:PHE:HZ	1.73	0.54
2:B:579:HIS:HB2	2:B:678:THR:HG21	1.90	0.54
2:B:715:ASP:OD2	2:B:716:GLN:HG3	2.07	0.54
1:A:123:ILE:HD11	1:A:364:LEU:HD11	1.89	0.54
2:B:524:ILE:HG13	2:B:736:LEU:HD11	1.89	0.54
2:B:512:ILE:HD13	2:B:743:LYS:HD3	1.90	0.54
1:A:532:LEU:HD11	1:A:545:VAL:CG1	2.37	0.54
1:A:57:ALA:HB2	1:A:96:LEU:HD11	1.90	0.53
1:A:192:ILE:HD13	1:A:218:ILE:HG21	1.89	0.53
2:B:609:LEU:O	2:B:613:ILE:HG22	2.08	0.53
1:A:564:MET:HE2	1:A:692:ILE:HG13	1.91	0.53
2:B:228:ASP:OD1	2:B:246:ASN:ND2	2.40	0.53
2:B:236:PRO:CB	2:B:263:VAL:HG22	2.38	0.53
2:B:244:LYS:HD2	2:B:270:GLU:HB3	1.90	0.53
2:B:314:TYR:CE1	2:B:431:PHE:HB2	2.44	0.53
1:A:599:LEU:O	1:A:603:MET:HG3	2.07	0.53
1:A:649:MET:HG2	1:A:653:LEU:HD23	1.90	0.53
1:A:230:PRO:O	1:A:233:PRO:HD2	2.09	0.53
1:A:595:ALA:O	1:A:599:LEU:HD23	2.09	0.53
2:B:55:PRO:HB3	2:B:98:PHE:CZ	2.43	0.53
2:B:425:THR:O	2:B:426:ILE:HD13	2.08	0.53
1:A:230:PRO:O	1:A:234:VAL:HG13	2.08	0.53
1:A:248:LEU:HD23	1:A:276:ILE:HD11	1.90	0.53
1:A:615:ASP:OD2	1:A:646:SER:HB2	2.09	0.53
2:B:240:VAL:CG1	2:B:270:GLU:HG3	2.38	0.53
2:B:557:THR:OG1	7:B:902:U3D:O21	2.27	0.53
1:A:270:LYS:HE2	1:A:634:ASP:CG	2.33	0.52
2:B:477:ILE:HB	2:B:540:ASP:HB2	1.91	0.52
2:B:516:SER:OG	2:B:519:MET:HG2	2.09	0.52
2:B:577:ARG:HG3	2:B:597:LEU:HD21	1.90	0.52
1:A:532:LEU:HD13	1:A:537:ILE:CG1	2.40	0.52
2:B:574:LYS:HD3	2:B:692:ILE:CD1	2.39	0.52
2:B:701:ILE:HG22	2:B:702:MET:HE2	1.91	0.52
2:B:548:THR:O	2:B:552:LEU:HD23	2.09	0.52
1:A:53:VAL:HG13	1:A:123:ILE:HG21	1.91	0.52
1:A:665:LEU:HD22	6:A:907:CLR:H25	1.91	0.52
2:B:607:ILE:O	2:B:611:ILE:HG13	2.10	0.52
2:B:240:VAL:HG21	2:B:266:CYS:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PHE:CE2	1:A:300:GLU:HG2	2.45	0.51
2:B:91:GLU:HB2	2:B:93:LEU:CD1	2.41	0.51
2:B:533:SER:OG	2:B:560:LEU:HB2	2.09	0.51
2:B:701:ILE:O	2:B:705:ILE:HG12	2.10	0.51
2:B:500:LEU:HB2	2:B:524:ILE:HG21	1.92	0.51
2:B:474:LEU:HD23	2:B:475:ARG:O	2.11	0.51
2:B:480:PRO:O	2:B:484:ILE:HG22	2.10	0.51
1:A:231:ALA:O	1:A:234:VAL:HG22	2.11	0.51
1:A:238:LYS:NZ	1:A:264:GLU:O	2.25	0.51
2:B:737:CYS:SG	2:B:741:VAL:HG21	2.51	0.51
1:A:402:GLU:OE2	1:A:407:HIS:ND1	2.41	0.51
1:A:177:ASN:OD1	1:A:209:LEU:HD13	2.11	0.51
1:A:223:ARG:O	1:A:224:GLN:NE2	2.40	0.51
1:A:610:ILE:HG22	1:A:652:TRP:HH2	1.75	0.50
2:B:485:LEU:HD13	2:B:725:ALA:CB	2.41	0.50
1:A:49:GLU:HG3	1:A:51:ARG:CZ	2.40	0.50
1:A:123:ILE:CD1	1:A:364:LEU:HD11	2.40	0.50
1:A:142:MET:HE2	1:A:142:MET:HA	1.92	0.50
2:B:493:MET:HE2	2:B:531:TYR:CB	2.41	0.50
1:A:78:ALA:HB2	1:A:354:TYR:CD1	2.46	0.50
1:A:303:GLU:HA	1:A:425:LEU:HD23	1.94	0.50
2:B:58:ILE:CD1	2:B:99:LEU:HD11	2.41	0.50
2:B:668:MET:HE3	2:B:700:GLY:HA2	1.92	0.50
1:A:53:VAL:CG1	1:A:123:ILE:HD13	2.42	0.50
2:B:204:ASP:OD2	2:B:233:SER:OG	2.23	0.50
2:B:546:GLU:OE1	2:B:623:ARG:NE	2.45	0.50
1:A:530:LEU:HD23	1:A:530:LEU:O	2.12	0.50
2:B:545:SER:OG	2:B:546:GLU:N	2.43	0.50
2:B:439:VAL:HB	2:B:456:ILE:HG22	1.94	0.50
2:B:551:THR:O	2:B:555:VAL:HG23	2.12	0.50
1:A:70:ALA:HB2	1:A:344:THR:CG2	2.41	0.50
1:A:127:PRO:HG3	1:A:136:VAL:HG21	1.94	0.50
1:A:179:THR:CG2	1:A:422:ILE:HD11	2.42	0.49
1:A:192:ILE:O	1:A:220:ILE:HA	2.12	0.49
1:A:443:LEU:HD21	1:A:445:TRP:CE3	2.47	0.49
1:A:511:ASN:ND2	1:A:594:TYR:OH	2.31	0.49
1:A:606:LEU:O	1:A:610:ILE:HG12	2.12	0.49
2:B:522:LEU:CD2	2:B:601:VAL:HG11	2.34	0.49
2:B:623:ARG:NH1	2:B:646:GLU:OE2	2.45	0.49
2:B:649:GLU:HB2	2:B:653:MET:CE	2.41	0.49
2:B:65:THR:O	2:B:68:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ASN:ND2	2:B:388:PHE:O	2.45	0.49
1:A:269:LYS:HA	1:A:452:ILE:HD12	1.94	0.49
2:B:142:ILE:O	2:B:146:LEU:HG	2.12	0.49
2:B:493:MET:HE2	2:B:531:TYR:HB3	1.93	0.49
1:A:299:THR:O	1:A:303:GLU:HB2	2.13	0.49
2:B:321:PRO:O	2:B:322:LEU:HD23	2.12	0.49
2:B:470:ILE:HG22	2:B:640:SER:HG	1.78	0.49
2:B:605:LEU:O	2:B:609:LEU:HD13	2.12	0.49
1:A:302:VAL:HG23	1:A:425:LEU:CD2	2.43	0.49
1:A:329:PHE:CE2	1:A:351:PRO:HG3	2.46	0.49
2:B:573:ALA:HB1	2:B:597:LEU:HD23	1.94	0.49
2:B:524:ILE:HD11	2:B:740:PHE:CE2	2.48	0.49
2:B:532:ALA:O	2:B:536:LEU:HD23	2.12	0.49
2:B:534:ILE:HA	2:B:537:PHE:CE1	2.47	0.49
2:B:474:LEU:HD11	2:B:646:GLU:OE1	2.13	0.49
1:A:629:PRO:HG3	1:A:637:ILE:CD1	2.43	0.49
2:B:346:ARG:HD2	2:B:346:ARG:O	2.13	0.49
2:B:568:PHE:CE1	2:B:696:VAL:HG23	2.48	0.49
1:A:537:ILE:HG13	1:A:545:VAL:HG21	1.94	0.48
1:A:655:ILE:HG22	6:A:906:CLR:H183	1.95	0.48
2:B:250:ILE:CD1	2:B:278:GLN:HB3	2.38	0.48
2:B:465:LYS:HE3	2:B:638:ASP:CG	2.38	0.48
1:A:355:ASP:OD1	1:A:404:VAL:HG22	2.13	0.48
2:B:693:GLY:O	2:B:696:VAL:HG12	2.13	0.48
1:A:129:CYS:O	1:A:133:SER:HB2	2.12	0.48
2:B:129:MET:HG3	2:B:152:VAL:HG13	1.93	0.48
1:A:169:THR:O	1:A:416:ARG:HD3	2.14	0.48
1:A:333:LEU:HG	1:A:337:LEU:HD13	1.96	0.48
1:A:134:THR:HG22	1:A:157:LEU:CD2	2.39	0.48
1:A:641:LEU:HD11	1:A:713:GLN:HB3	1.95	0.48
2:B:243:LEU:O	2:B:248:VAL:HG22	2.14	0.48
2:B:247:ASP:OD1	2:B:249:ARG:NH2	2.44	0.48
2:B:255:PHE:CE2	2:B:260:ALA:HA	2.49	0.48
2:B:466:ASP:OD1	2:B:466:ASP:N	2.46	0.48
1:A:704:PRO:O	1:A:708:ILE:HG12	2.13	0.48
2:B:449:LEU:HG	2:B:451:ILE:HD11	1.94	0.48
2:B:639:ILE:CG2	2:B:641:ILE:HD11	2.43	0.48
1:A:132:VAL:O	1:A:136:VAL:HG13	2.14	0.48
2:B:334:THR:HG23	2:B:337:GLN:H	1.78	0.48
1:A:178:PRO:HG3	1:A:212:ARG:CZ	2.43	0.48
1:A:199:THR:O	1:A:203:THR:OG1	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLU:OE2	2:B:579:HIS:NE2	2.29	0.48
2:B:663:TYR:HA	6:B:903:CLR:H271	1.96	0.48
2:B:523:ILE:HD11	2:B:571:MET:HG3	1.96	0.48
2:B:62:MET:SD	2:B:103:LEU:HD11	2.54	0.47
2:B:290:TRP:CD1	2:B:291:GLU:HG3	2.49	0.47
1:A:417:MET:HA	1:A:417:MET:HE2	1.95	0.47
2:B:154:LEU:HD11	2:B:175:THR:CG2	2.43	0.47
1:A:222:PHE:HD2	1:A:237:LEU:HD23	1.80	0.47
1:A:377:ARG:N	1:A:379:GLU:OE1	2.47	0.47
1:A:397:ASN:OD1	3:A:903:NAG:N2	2.47	0.47
2:B:62:MET:CG	2:B:103:LEU:HD11	2.45	0.47
2:B:183:ASN:HB2	2:B:184:PRO:HD3	1.97	0.47
1:A:179:THR:HG23	1:A:422:ILE:HD11	1.97	0.47
1:A:400:SER:OG	1:A:409:VAL:HG12	2.15	0.47
1:A:469:PHE:CD1	1:A:535:TYR:HB2	2.49	0.47
1:A:649:MET:O	1:A:653:LEU:HG	2.15	0.47
2:B:95:ARG:CG	2:B:96:PRO:HA	2.45	0.47
2:B:114:LEU:HG	2:B:118:TYR:CE2	2.49	0.47
2:B:136:PRO:HA	2:B:139:THR:HG22	1.96	0.47
2:B:470:ILE:O	2:B:470:ILE:HG13	2.14	0.47
6:A:907:CLR:H261	2:B:666:LEU:HD13	1.96	0.47
6:A:909:CLR:H183	6:A:909:CLR:H212	1.97	0.47
2:B:61:LEU:CD1	2:B:142:ILE:HD13	2.45	0.47
1:A:72:GLN:HB3	1:A:73:PRO:HD3	1.97	0.47
1:A:411:ASP:OD1	1:A:415:SER:N	2.48	0.47
1:A:571:VAL:HG23	1:A:682:ILE:HD12	1.97	0.47
2:B:129:MET:HG3	2:B:152:VAL:O	2.15	0.47
2:B:371:ARG:O	2:B:375:THR:HG23	2.15	0.47
1:A:651:THR:HA	6:A:906:CLR:H192	1.97	0.46
2:B:602:GLY:O	2:B:606:LEU:HD23	2.15	0.46
1:A:603:MET:O	1:A:607:THR:HG23	2.14	0.46
2:B:60:GLY:HA2	2:B:131:PHE:O	2.15	0.46
1:A:232:VAL:CG1	1:A:233:PRO:HD3	2.43	0.46
2:B:631:GLU:HG2	2:B:632:PRO:CD	2.40	0.46
1:A:735:LEU:O	1:A:739:LYS:HE2	2.15	0.46
2:B:700:GLY:O	2:B:704:ILE:HG12	2.16	0.46
1:A:56:GLY:O	1:A:125:LEU:HA	2.16	0.46
2:B:699:VAL:CG2	2:B:735:THR:HG21	2.43	0.46
1:A:358:TRP:O	1:A:362:LEU:HG	2.16	0.46
1:A:630:LYS:HG3	1:A:631:GLU:H	1.79	0.46
1:A:697:VAL:HG22	6:A:908:CLR:H161	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:PHE:CZ	1:A:740:MET:HA	2.51	0.46
2:B:289:TRP:CZ2	2:B:311:MET:HE3	2.51	0.46
2:B:360:ASP:O	2:B:364:VAL:HG23	2.15	0.46
1:A:59:PHE:HE2	1:A:96:LEU:HD21	1.81	0.46
2:B:238:THR:O	2:B:241:LYS:HG2	2.15	0.46
1:A:65:TRP:CZ3	1:A:67:GLY:HA3	2.52	0.45
1:A:459:ASP:OD1	1:A:459:ASP:N	2.50	0.45
1:A:660:LYS:O	1:A:664:LEU:HD13	2.17	0.45
1:A:77:MET:HE2	1:A:336:ARG:HD3	1.99	0.45
1:A:114:GLU:O	1:A:118:ASN:HB2	2.16	0.45
1:A:668:ILE:HD11	1:A:696:ALA:HB3	1.99	0.45
2:B:429:THR:HG22	2:B:438:LYS:HA	1.97	0.45
2:B:303:LEU:HB2	2:B:306:ASN:HD22	1.82	0.45
2:B:650:ASN:N	2:B:653:MET:HB2	2.31	0.45
2:B:134:VAL:HG22	2:B:157:ALA:HB3	1.98	0.45
6:B:904:CLR:H183	6:B:904:CLR:H212	1.98	0.45
2:B:228:ASP:CG	2:B:243:LEU:HD23	2.41	0.45
2:B:275:SER:N	2:B:459:GLN:OE1	2.50	0.45
2:B:325:LYS:HD3	2:B:327:ILE:HD11	1.99	0.45
1:A:183:LEU:HD11	1:A:422:ILE:HG21	1.97	0.45
2:B:520:ASN:HB3	2:B:740:PHE:HZ	1.81	0.45
2:B:729:ILE:O	2:B:733:THR:HG22	2.17	0.45
1:A:275:LEU:HD12	1:A:305:HIS:CE1	2.51	0.44
2:B:166:LYS:HA	2:B:166:LYS:HD3	1.74	0.44
6:B:903:CLR:H183	6:B:903:CLR:H212	1.98	0.44
2:B:84:ALA:HB2	2:B:359:TYR:CD1	2.52	0.44
2:B:449:LEU:HG	2:B:451:ILE:CD1	2.47	0.44
2:B:320:GLU:OE1	2:B:427:LYS:HB2	2.18	0.44
1:A:377:ARG:NH2	1:A:391:GLN:HE22	2.15	0.44
1:A:127:PRO:HG3	1:A:136:VAL:CG2	2.47	0.44
6:A:907:CLR:H183	6:A:907:CLR:H212	2.00	0.44
2:B:214:ASP:O	2:B:218:VAL:HG23	2.18	0.44
1:A:53:VAL:HG21	1:A:378:LEU:HD21	1.98	0.44
1:A:321:ILE:HG12	1:A:402:GLU:O	2.17	0.44
1:A:511:ASN:O	1:A:515:LEU:HG	2.18	0.44
1:A:629:PRO:HG3	1:A:637:ILE:HD12	1.99	0.44
2:B:743:LYS:O	2:B:747:LEU:HD23	2.18	0.44
6:B:907:CLR:H121	6:B:907:CLR:H212	1.99	0.44
1:A:222:PHE:CZ	1:A:236:ASN:HB3	2.52	0.44
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.90	0.44
1:A:294:THR:HG22	1:A:297:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:ALA:HB1	2:B:597:LEU:CD2	2.48	0.44
2:B:627:LYS:HG2	2:B:644:LEU:CD1	2.48	0.44
2:B:701:ILE:HG22	2:B:702:MET:CE	2.48	0.44
1:A:722:LEU:HA	1:A:722:LEU:HD23	1.67	0.43
2:B:503:ASN:HB2	2:B:740:PHE:HE1	1.83	0.43
2:B:536:LEU:HB3	2:B:556:ARG:HB2	2.00	0.43
1:A:532:LEU:CD1	1:A:545:VAL:HG11	2.43	0.43
1:A:674:THR:CG2	1:A:677:VAL:HB	2.48	0.43
2:B:100:ASP:OD2	2:B:102:ARG:NH1	2.51	0.43
2:B:163:LEU:HD13	2:B:172:PHE:CE2	2.52	0.43
1:A:270:LYS:HE2	1:A:634:ASP:OD2	2.18	0.43
1:A:400:SER:HA	1:A:409:VAL:HG12	1.99	0.43
1:A:502:VAL:O	1:A:506:GLN:HB2	2.17	0.43
1:A:612:GLN:O	1:A:616:PRO:HG3	2.18	0.43
2:B:615:TRP:HE1	2:B:650:ASN:HD22	1.66	0.43
1:A:222:PHE:CD2	1:A:237:LEU:HD23	2.53	0.43
1:A:260:GLU:O	1:A:264:GLU:HG2	2.18	0.43
1:A:455:SER:HB2	1:A:456:PRO:HD2	2.00	0.43
1:A:470:LEU:HD12	1:A:471:SER:H	1.84	0.43
2:B:230:GLU:OE2	2:B:242:LYS:HB3	2.18	0.43
2:B:472:GLU:O	2:B:472:GLU:HG3	2.18	0.43
1:A:126:MET:HE2	1:A:126:MET:HB3	1.94	0.43
2:B:442:TYR:CZ	2:B:444:ALA:HA	2.54	0.43
2:B:449:LEU:CD2	2:B:451:ILE:HD11	2.49	0.43
1:A:186:LYS:O	1:A:186:LYS:HG3	2.18	0.43
2:B:152:VAL:HG23	2:B:171:TYR:O	2.19	0.43
2:B:163:LEU:HD13	2:B:172:PHE:CZ	2.53	0.43
2:B:473:GLN:HG2	2:B:641:ILE:HG21	1.99	0.43
2:B:534:ILE:CD1	2:B:729:ILE:HG13	2.49	0.43
1:A:70:ALA:HB2	1:A:344:THR:HG21	1.99	0.43
2:B:132:GLY:HA2	2:B:156:PHE:CE2	2.54	0.43
2:B:228:ASP:OD2	2:B:230:GLU:HG2	2.19	0.43
2:B:288:SER:HA	2:B:290:TRP:CH2	2.53	0.43
2:B:473:GLN:HG2	2:B:641:ILE:CG2	2.49	0.43
2:B:534:ILE:HD11	2:B:725:ALA:HB1	2.01	0.43
1:A:367:THR:OG1	1:A:368:SER:N	2.52	0.43
2:B:93:LEU:HB3	2:B:370:GLN:NE2	2.33	0.43
2:B:456:ILE:O	2:B:456:ILE:HG13	2.18	0.43
2:B:639:ILE:HG22	2:B:641:ILE:CD1	2.48	0.43
1:A:177:ASN:HB2	1:A:178:PRO:HD3	2.00	0.43
2:B:465:LYS:HG2	2:B:638:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:VAL:O	1:A:601:VAL:HG23	2.19	0.42
1:A:571:VAL:CG2	1:A:682:ILE:HD12	2.49	0.42
2:B:56:LEU:HD22	2:B:128:LEU:CD1	2.45	0.42
1:A:168:ARG:NH2	1:A:172:SER:HB2	2.34	0.42
1:A:635:VAL:O	1:A:635:VAL:HG23	2.20	0.42
1:A:139:ALA:CB	2:B:114:LEU:HD23	2.50	0.42
1:A:142:MET:HG2	2:B:111:ALA:HB1	2.01	0.42
1:A:294:THR:HG22	1:A:297:GLU:CG	2.49	0.42
1:A:630:LYS:HA	1:A:630:LYS:HD2	1.81	0.42
2:B:146:LEU:HD11	2:B:153:GLN:HB2	2.02	0.42
2:B:325:LYS:HB3	2:B:327:ILE:HG13	2.02	0.42
1:A:123:ILE:HG21	1:A:378:LEU:HD11	2.02	0.42
1:A:138:GLU:OE2	2:B:110:ASN:ND2	2.52	0.42
1:A:709:LEU:O	1:A:716:ALA:HB2	2.20	0.42
1:A:88:ILE:HG23	1:A:89:LEU:H	1.84	0.42
1:A:489:ALA:HB2	1:A:732:LEU:HD11	2.02	0.42
2:B:313:GLY:HA2	2:B:430:GLN:NE2	2.26	0.42
2:B:333:LYS:HD3	2:B:341:GLU:OE2	2.20	0.42
2:B:524:ILE:HD11	2:B:740:PHE:CZ	2.55	0.42
1:A:54:TYR:CZ	1:A:120:PRO:HG3	2.55	0.42
6:A:906:CLR:H121	6:A:906:CLR:H212	2.02	0.42
2:B:735:THR:O	2:B:739:VAL:HG23	2.20	0.42
1:A:224:GLN:HB3	1:A:233:PRO:HB3	2.02	0.42
1:A:230:PRO:CB	1:A:257:VAL:HG22	2.50	0.42
1:A:243:ARG:HH21	1:A:461:THR:CG2	2.33	0.42
1:A:364:LEU:O	1:A:368:SER:N	2.52	0.42
2:B:290:TRP:HB3	2:B:311:MET:CE	2.46	0.42
2:B:387:ASP:OD1	2:B:387:ASP:N	2.50	0.42
2:B:679:ARG:H	2:B:679:ARG:HG3	1.74	0.42
1:A:615:ASP:CG	1:A:647:ARG:HG2	2.45	0.41
2:B:77:VAL:HG12	2:B:355:HIS:HA	2.02	0.41
2:B:412:THR:CB	2:B:422:ARG:HH22	2.32	0.41
2:B:475:ARG:HD2	2:B:717:PRO:HG3	2.02	0.41
1:A:306:ILE:HD13	1:A:424:GLN:HG3	2.00	0.41
2:B:307:LEU:HD12	2:B:307:LEU:HA	1.86	0.41
2:B:702:MET:CB	2:B:731:CYS:HB2	2.51	0.41
6:B:906:CLR:H121	6:B:906:CLR:H212	2.01	0.41
2:B:202:THR:HG22	2:B:203:GLN:O	2.21	0.41
1:A:123:ILE:HD12	1:A:364:LEU:HD21	2.02	0.41
1:A:462:LEU:CD1	1:A:464:ILE:HG13	2.50	0.41
1:A:696:ALA:O	1:A:700:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:PHE:CE1	2:B:311:MET:HA	2.55	0.41
1:A:65:TRP:CZ2	1:A:349:GLU:HG3	2.40	0.41
1:A:633:ILE:O	1:A:635:VAL:N	2.54	0.41
1:A:651:THR:HA	6:A:906:CLR:H193	2.02	0.41
2:B:257:GLN:NE2	2:B:286:GLU:OE1	2.53	0.41
2:B:702:MET:HE2	2:B:702:MET:HA	2.03	0.41
2:B:136:PRO:HA	2:B:139:THR:CG2	2.51	0.41
2:B:334:THR:HG22	2:B:337:GLN:CD	2.46	0.41
2:B:652:HIS:O	2:B:655:ILE:HG22	2.21	0.41
1:A:674:THR:HG22	1:A:674:THR:O	2.21	0.41
2:B:61:LEU:HD13	2:B:142:ILE:HD13	2.03	0.41
2:B:534:ILE:HD11	2:B:725:ALA:CB	2.51	0.41
1:A:53:VAL:HG21	1:A:378:LEU:CD2	2.51	0.41
1:A:181:VAL:HA	1:A:184:PHE:CD2	2.56	0.41
1:A:189:TRP:HA	1:A:459:ASP:HB3	2.03	0.41
1:A:564:MET:HE1	1:A:691:ALA:HB3	2.02	0.41
2:B:58:ILE:O	2:B:101:LEU:HD12	2.20	0.41
2:B:130:VAL:O	2:B:153:GLN:HA	2.21	0.41
2:B:136:PRO:HB3	2:B:160:THR:HG21	2.03	0.41
2:B:281:ILE:HD12	2:B:285:TYR:HE2	1.85	0.41
1:A:126:MET:HA	1:A:148:LEU:O	2.21	0.41
1:A:261:VAL:O	1:A:265:ARG:N	2.53	0.41
2:B:167:LYS:HD3	2:B:167:LYS:HA	1.92	0.41
1:A:542:PHE:N	1:A:543:PRO:HD2	2.35	0.40
2:B:287:PRO:O	2:B:288:SER:OG	2.36	0.40
1:A:599:LEU:HG	6:A:909:CLR:H71	2.03	0.40
2:B:230:GLU:HG3	2:B:243:LEU:HG	2.03	0.40
2:B:365:ILE:O	2:B:368:THR:HB	2.21	0.40
2:B:442:TYR:CE2	2:B:444:ALA:HB2	2.56	0.40
1:A:331:GLU:OE2	1:A:335:LYS:HG2	2.21	0.40
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.89	0.40
1:A:682:ILE:CG2	1:A:685:HIS:HB3	2.48	0.40
1:A:743:LEU:HA	1:A:743:LEU:HD23	1.77	0.40
2:B:249:ARG:C	2:B:250:ILE:HD13	2.46	0.40
1:A:138:GLU:CD	2:B:110:ASN:HD22	2.30	0.40
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.78	0.40
2:B:621:LEU:H	2:B:621:LEU:HD12	1.87	0.40
1:A:178:PRO:HG3	1:A:212:ARG:NH1	2.37	0.40
2:B:268:TYR:CZ	2:B:306:ASN:HB3	2.57	0.40
2:B:477:ILE:HG12	2:B:540:ASP:OD1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	675/810 (83%)	653 (97%)	22 (3%)	0	100	100
2	B	663/827 (80%)	643 (97%)	20 (3%)	0	100	100
All	All	1338/1637 (82%)	1296 (97%)	42 (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	592/703 (84%)	591 (100%)	1 (0%)	87	88
2	B	586/725 (81%)	586 (100%)	0	100	100
All	All	1178/1428 (82%)	1177 (100%)	1 (0%)	87	90

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

Mol	Chain	Res	Type
1	A	293	CYS

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

Mol	Chain	Res	Type
1	A	240	GLN
1	A	292	ASN

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Mol	Chain	Res	Type
1	A	391	GLN
1	A	499	ASN
1	A	509	GLN
1	A	513	ASN
1	A	514	ASN
1	A	547	GLN
1	A	618	HIS
2	B	150	ASN
2	B	206	GLN
2	B	278	GLN
2	B	306	ASN
2	B	370	GLN
2	B	430	GLN
2	B	432	GLN
2	B	453	ASN
2	B	503	ASN
2	B	508	ASN
2	B	616	GLN
2	B	647	HIS
2	B	652	HIS
2	B	698	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](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CLR	B	904	-	31,31,31	0.74	0	48,48,48	1.05	3 (6%)
6	CLR	B	903	-	31,31,31	0.72	0	48,48,48	1.15	4 (8%)
6	CLR	A	907	-	31,31,31	0.78	0	48,48,48	1.11	3 (6%)
6	CLR	B	908	-	31,31,31	0.84	0	48,48,48	1.09	4 (8%)
3	NAG	A	903	1	14,14,15	0.38	0	17,19,21	0.48	0
3	NAG	A	901	1	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	A	902	1	14,14,15	0.21	0	17,19,21	0.51	0
5	U3G	A	905	-	52,52,52	1.16	3 (5%)	55,57,57	0.82	2 (3%)
6	CLR	A	906	-	31,31,31	0.83	1 (3%)	48,48,48	1.27	5 (10%)
6	CLR	A	908	-	31,31,31	0.68	0	48,48,48	1.04	3 (6%)
6	CLR	A	909	-	31,31,31	0.74	1 (3%)	48,48,48	1.08	1 (2%)
6	CLR	B	906	-	31,31,31	0.84	1 (3%)	48,48,48	1.22	5 (10%)
6	CLR	B	907	-	31,31,31	0.82	1 (3%)	48,48,48	1.24	4 (8%)
7	U3D	B	902	-	55,55,55	1.41	8 (14%)	61,63,63	0.88	3 (4%)
3	NAG	B	901	2	14,14,15	0.17	0	17,19,21	0.40	0
6	CLR	B	905	-	31,31,31	0.68	0	48,48,48	1.06	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	B	904	-	-	1/10/68/68	0/4/4/4
6	CLR	B	903	-	-	1/10/68/68	0/4/4/4
6	CLR	A	907	-	-	3/10/68/68	0/4/4/4
6	CLR	B	908	-	-	3/10/68/68	0/4/4/4
3	NAG	A	903	1	-	2/6/23/26	0/1/1/1
3	NAG	A	901	1	-	2/6/23/26	0/1/1/1
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1
5	U3G	A	905	-	-	22/56/56/56	-
6	CLR	A	906	-	-	0/10/68/68	0/4/4/4
6	CLR	A	908	-	-	3/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	A	909	-	-	0/10/68/68	0/4/4/4
6	CLR	B	906	-	-	0/10/68/68	0/4/4/4
6	CLR	B	907	-	-	2/10/68/68	0/4/4/4
7	U3D	B	902	-	-	27/59/59/59	-
3	NAG	B	901	2	-	4/6/23/26	0/1/1/1
6	CLR	B	905	-	-	0/10/68/68	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	902	U3D	O37-C38	3.93	1.45	1.34
7	B	902	U3D	O22-C20	3.50	1.43	1.33
5	A	905	U3G	O23-C24	3.25	1.42	1.33
5	A	905	U3G	O20-C21	-3.02	1.39	1.46
7	B	902	U3D	C40-C38	2.91	1.59	1.50
5	A	905	U3G	O20-C18	2.84	1.42	1.34
7	B	902	U3D	C41-C40	2.65	1.61	1.52
7	B	902	U3D	O37-C24	-2.52	1.40	1.46
6	A	906	CLR	C20-C17	2.38	1.58	1.54
6	B	907	CLR	C18-C13	2.27	1.58	1.54
7	B	902	U3D	P27-O30	2.17	1.67	1.59
6	B	906	CLR	C20-C17	2.11	1.58	1.54
7	B	902	U3D	C32-C31	2.08	1.57	1.51
7	B	902	U3D	P27-O26	2.05	1.67	1.59
6	A	909	CLR	C10-C9	2.01	1.59	1.56

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	902	U3D	O37-C38-C40	4.10	120.34	111.48
5	A	905	U3G	O20-C18-C17	3.33	118.68	111.48
6	A	906	CLR	C8-C7-C6	-3.19	108.35	112.76
6	B	907	CLR	C8-C7-C6	-3.15	108.39	112.76
6	A	906	CLR	C10-C9-C8	-3.06	108.24	112.71
6	B	903	CLR	C7-C8-C9	3.01	113.20	109.72
6	A	907	CLR	C4-C5-C6	-2.90	116.64	120.57
6	B	907	CLR	C10-C9-C8	-2.82	108.59	112.71
6	B	903	CLR	C14-C8-C9	-2.74	105.50	109.09
6	B	906	CLR	C10-C9-C8	-2.64	108.85	112.71
7	B	902	U3D	O22-C20-C19	2.63	119.85	111.83
6	A	909	CLR	C8-C7-C6	-2.60	109.17	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	905	U3G	O23-C24-C26	2.59	119.74	111.83
6	B	908	CLR	C8-C7-C6	-2.54	109.25	112.76
6	A	906	CLR	C13-C17-C20	-2.50	115.63	119.50
6	B	906	CLR	C8-C7-C6	-2.48	109.33	112.76
6	B	906	CLR	C13-C17-C20	-2.47	115.68	119.50
6	B	906	CLR	C23-C22-C20	-2.44	108.25	115.08
6	A	906	CLR	C11-C9-C8	2.42	115.16	111.78
6	A	906	CLR	C23-C22-C20	-2.42	108.32	115.08
6	B	903	CLR	C4-C5-C6	-2.41	117.30	120.57
6	B	905	CLR	C4-C5-C6	-2.37	117.36	120.57
6	B	905	CLR	C2-C3-C4	-2.35	106.99	110.29
6	B	904	CLR	C21-C20-C22	-2.34	106.71	110.34
6	A	908	CLR	C8-C7-C6	-2.34	109.52	112.76
6	B	907	CLR	C23-C22-C20	-2.33	108.56	115.08
6	A	907	CLR	C10-C9-C8	-2.30	109.35	112.71
6	B	904	CLR	C10-C9-C8	-2.27	109.40	112.71
6	B	908	CLR	C4-C5-C6	-2.24	117.53	120.57
6	B	903	CLR	C11-C9-C8	-2.23	108.66	111.78
6	A	908	CLR	C10-C9-C8	-2.22	109.46	112.71
6	A	907	CLR	C7-C8-C14	-2.21	107.80	110.93
6	B	906	CLR	C11-C9-C8	2.21	114.87	111.78
6	B	904	CLR	C8-C7-C6	-2.16	109.77	112.76
6	B	907	CLR	C4-C5-C6	-2.14	117.67	120.57
7	B	902	U3D	C24-O37-C38	-2.11	112.74	117.80
6	A	908	CLR	C2-C3-C4	-2.10	107.33	110.29
6	B	908	CLR	C10-C9-C8	-2.09	109.66	112.71
6	B	908	CLR	C13-C17-C20	-2.04	116.35	119.50

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	905	U3G	C45-O46-P47-O49
7	B	902	U3D	C25-O26-P27-O29
7	B	902	U3D	C31-O30-P27-O26
7	B	902	U3D	C31-O30-P27-O28
5	A	905	U3G	O25-C24-O23-C22
5	A	905	U3G	C26-C24-O23-C22
3	B	901	NAG	O5-C5-C6-O6
7	B	902	U3D	C19-C20-O22-C23
3	A	901	NAG	C4-C5-C6-O6
3	B	901	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	901	NAG	O5-C5-C6-O6
6	A	907	CLR	C17-C20-C22-C23
6	B	908	CLR	C17-C20-C22-C23
7	B	902	U3D	O21-C20-O22-C23
6	B	908	CLR	C21-C20-C22-C23
3	A	903	NAG	C4-C5-C6-O6
6	A	908	CLR	C17-C20-C22-C23
6	A	907	CLR	C21-C20-C22-C23
3	B	901	NAG	C8-C7-N2-C2
3	B	901	NAG	O7-C7-N2-C2
6	A	907	CLR	C22-C23-C24-C25
6	A	908	CLR	C21-C20-C22-C23
6	B	908	CLR	C22-C23-C24-C25
3	A	903	NAG	O5-C5-C6-O6
6	B	907	CLR	C17-C20-C22-C23
5	A	905	U3G	C14-C15-C16-C17
6	B	907	CLR	C21-C20-C22-C23
5	A	905	U3G	C24-C26-C27-C28
5	A	905	U3G	C39-C40-C41-C42
7	B	902	U3D	C13-C14-C15-C16
7	B	902	U3D	C51-C52-C53-C54
5	A	905	U3G	C11-C12-C13-C14
7	B	902	U3D	C40-C38-O37-C24
5	A	905	U3G	C41-C42-C43-C44
5	A	905	U3G	C26-C27-C28-C29
7	B	902	U3D	C42-C43-C44-C45
5	A	905	U3G	C04-C05-C06-C07
7	B	902	U3D	C11-C12-C13-C14
7	B	902	U3D	O39-C38-O37-C24
7	B	902	U3D	C50-C51-C52-C53
7	B	902	U3D	C04-C05-C06-C07
5	A	905	U3G	O20-C21-C22-O23
7	B	902	U3D	C48-C49-C50-C51
3	A	902	NAG	C4-C5-C6-O6
7	B	902	U3D	C41-C42-C43-C44
7	B	902	U3D	O22-C23-C24-O37
5	A	905	U3G	C32-C33-C34-C35
5	A	905	U3G	C33-C34-C35-C36
3	A	902	NAG	O5-C5-C6-O6
5	A	905	U3G	C15-C16-C17-C18
7	B	902	U3D	C15-C16-C17-C18
7	B	902	U3D	O30-C31-C32-N33

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Mol	Chain	Res	Type	Atoms
6	B	903	CLR	C20-C22-C23-C24
5	A	905	U3G	C05-C06-C07-C08
5	A	905	U3G	C45-C21-C22-O23
6	B	904	CLR	C16-C17-C20-C22
7	B	902	U3D	C45-C46-C47-C48
6	A	908	CLR	C22-C23-C24-C25
7	B	902	U3D	C43-C44-C45-C46
7	B	902	U3D	C09-C10-C11-C12
5	A	905	U3G	C29-C30-C31-C32
5	A	905	U3G	C35-C36-C37-C38
7	B	902	U3D	C40-C41-C42-C43
5	A	905	U3G	C09-C10-C11-C12
7	B	902	U3D	C07-C08-C09-C10
7	B	902	U3D	O22-C23-C24-C25
5	A	905	U3G	C38-C39-C40-C41
7	B	902	U3D	C18-C19-C20-O22
5	A	905	U3G	C16-C17-C18-O20
7	B	902	U3D	C18-C19-C20-O21
7	B	902	U3D	C14-C15-C16-C17
5	A	905	U3G	O23-C24-C26-C27

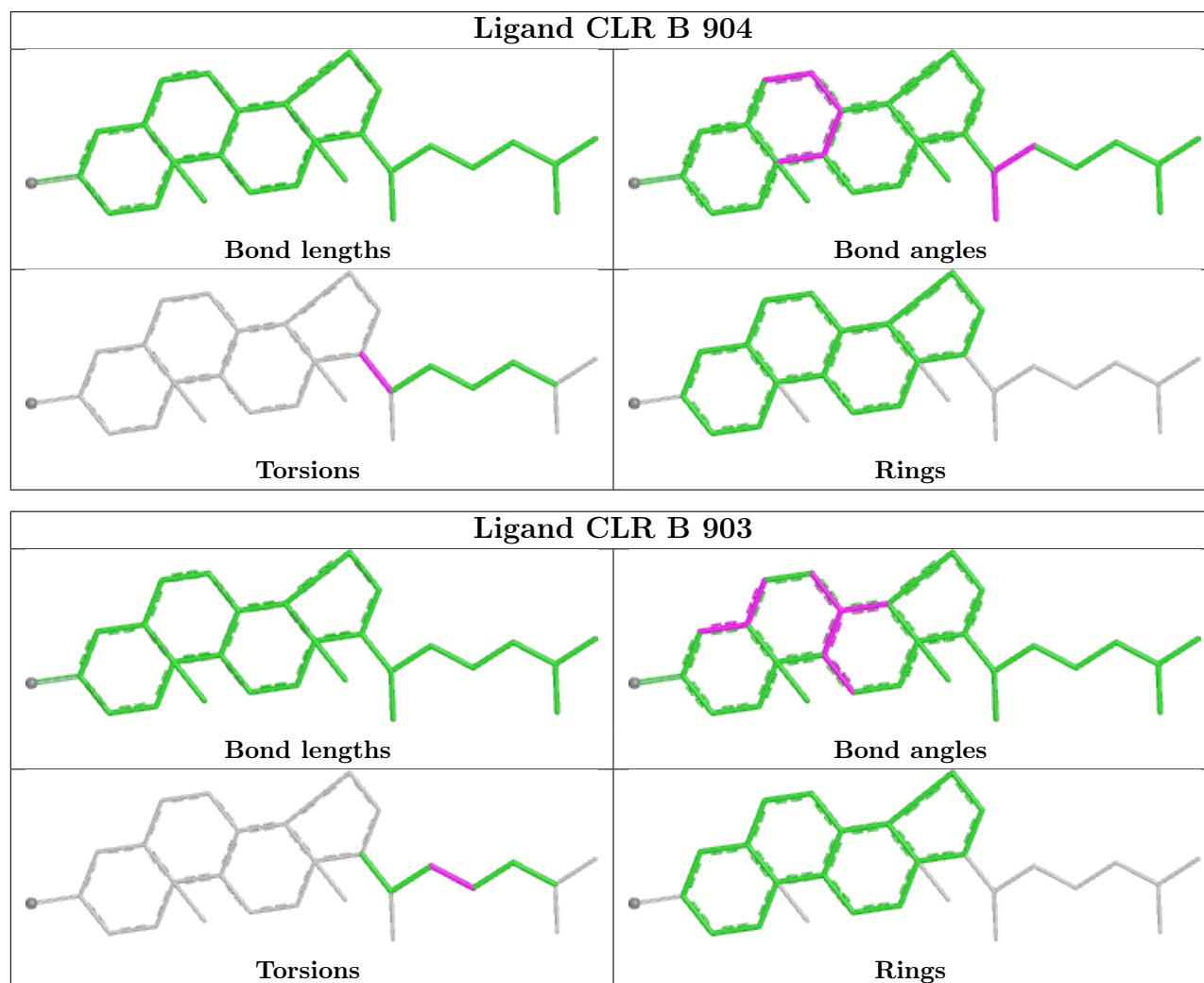
There are no ring outliers.

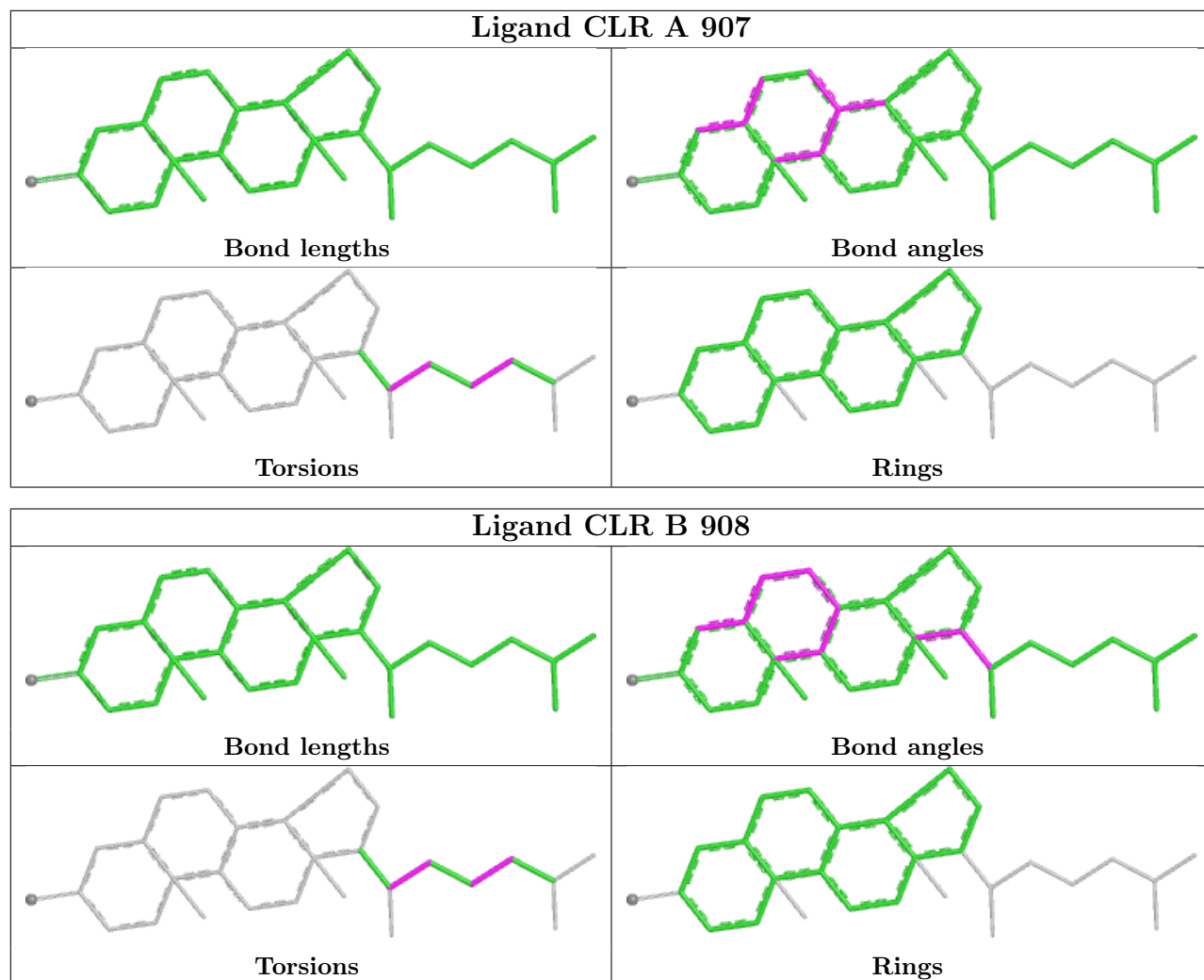
13 monomers are involved in 22 short contacts:

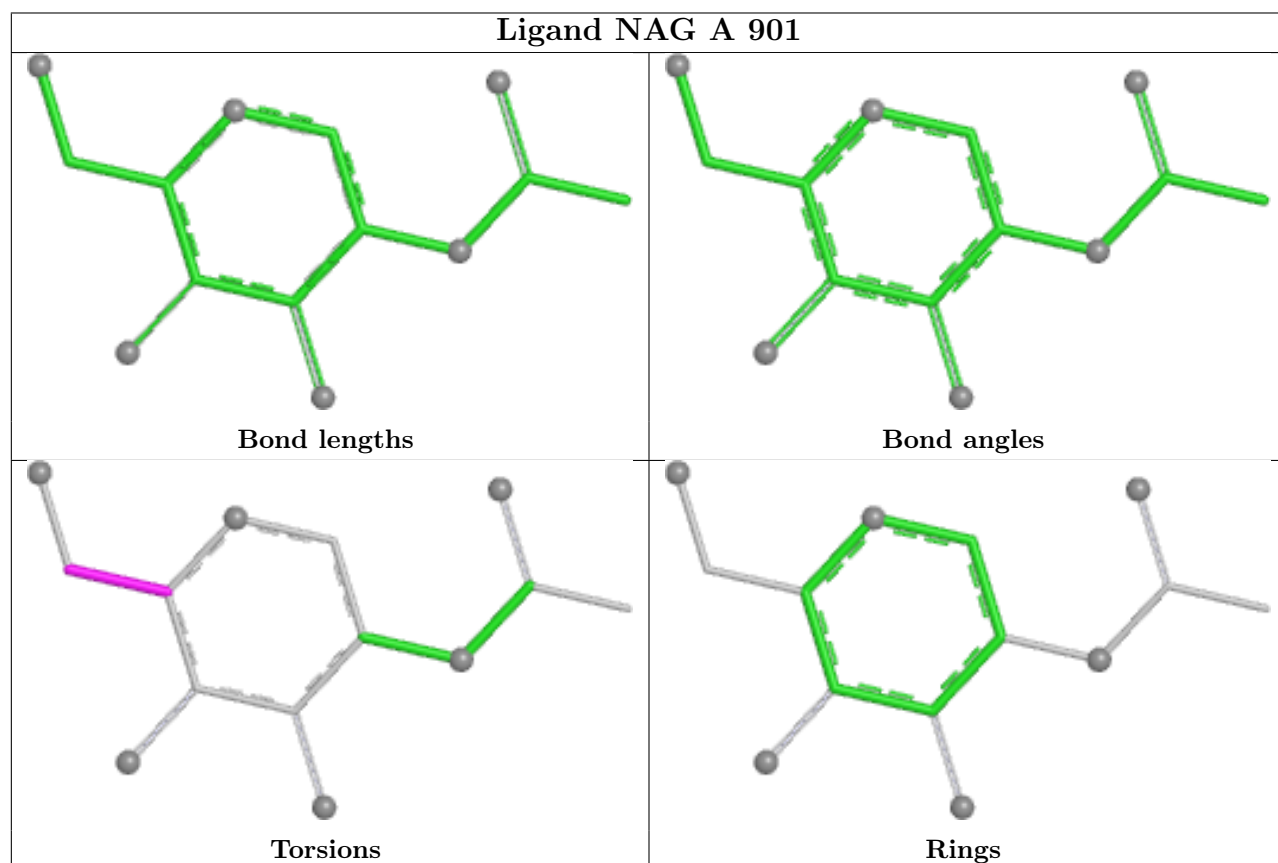
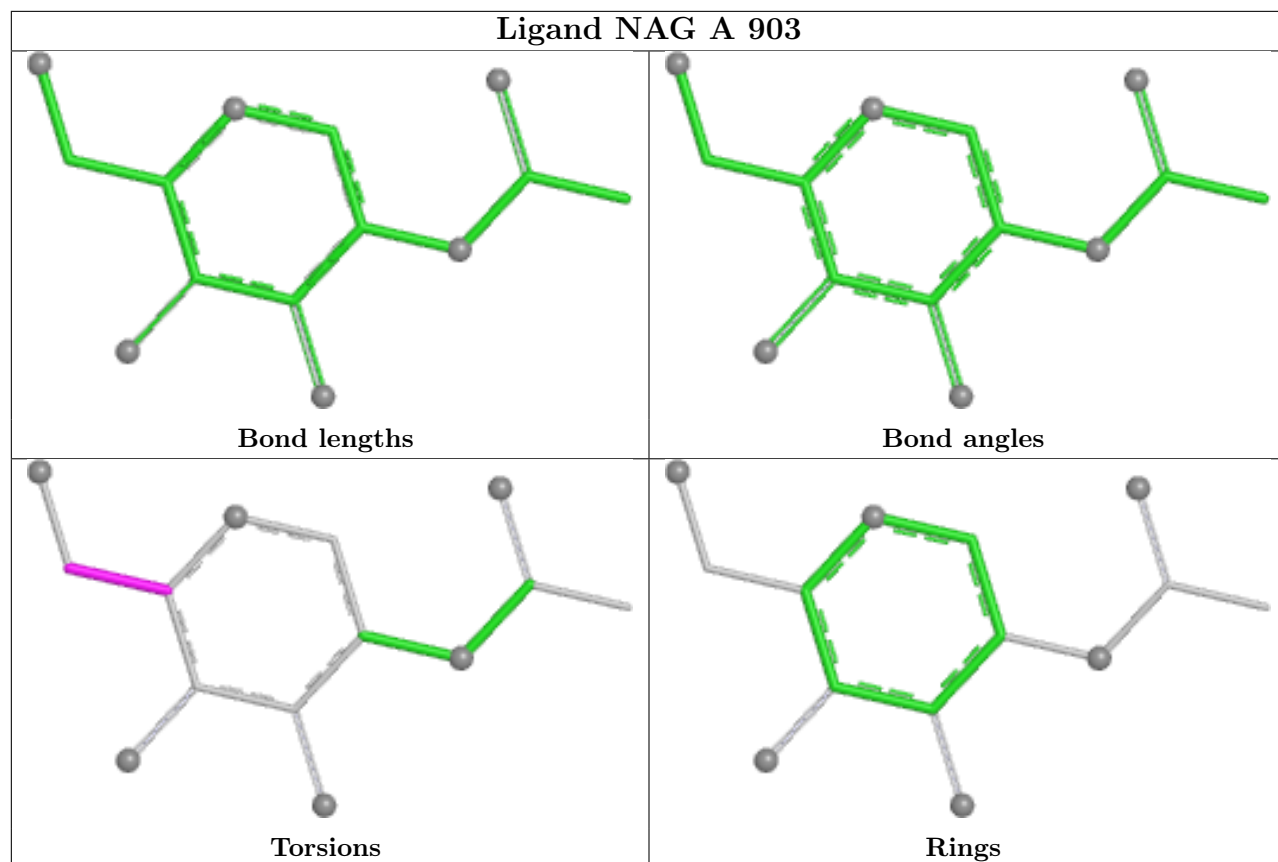
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	904	CLR	1	0
6	B	903	CLR	2	0
6	A	907	CLR	3	0
6	B	908	CLR	1	0
3	A	903	NAG	1	0
3	A	902	NAG	1	0
5	A	905	U3G	1	0
6	A	906	CLR	5	0
6	A	908	CLR	1	0
6	A	909	CLR	3	0
6	B	906	CLR	1	0
6	B	907	CLR	1	0
7	B	902	U3D	1	0

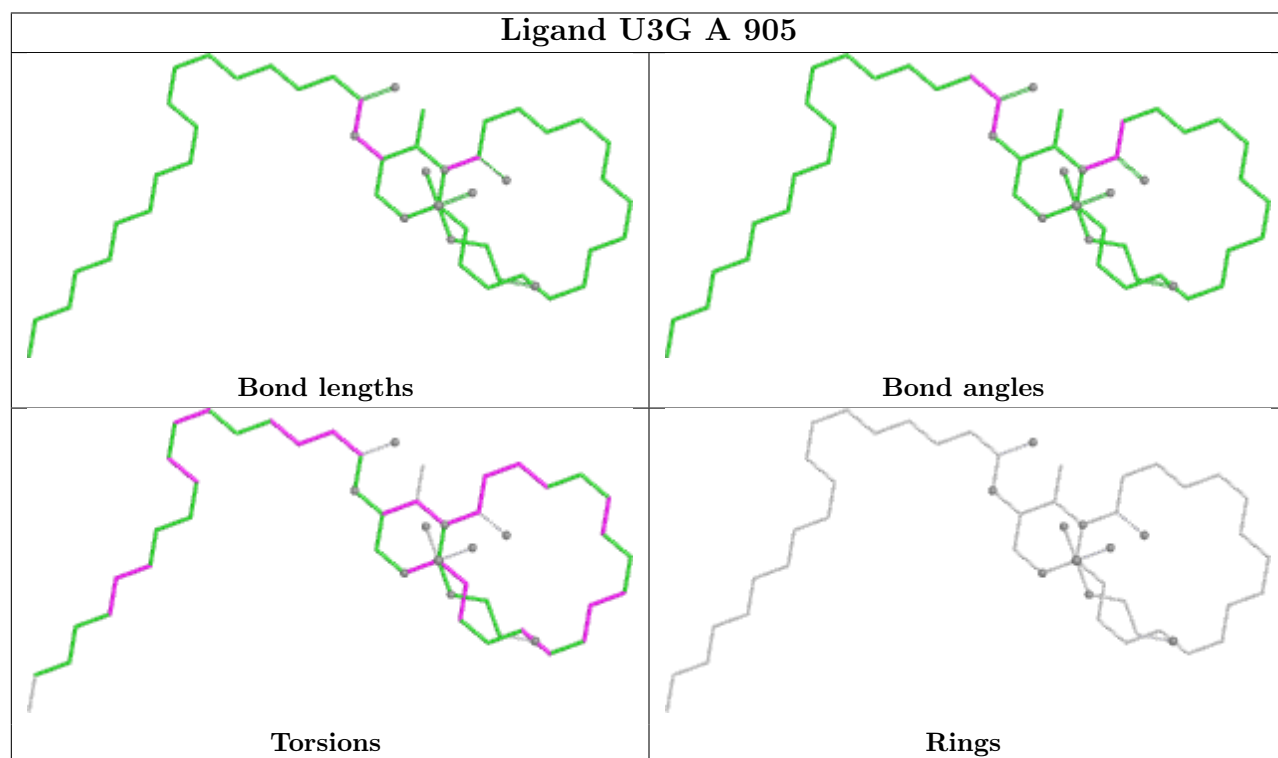
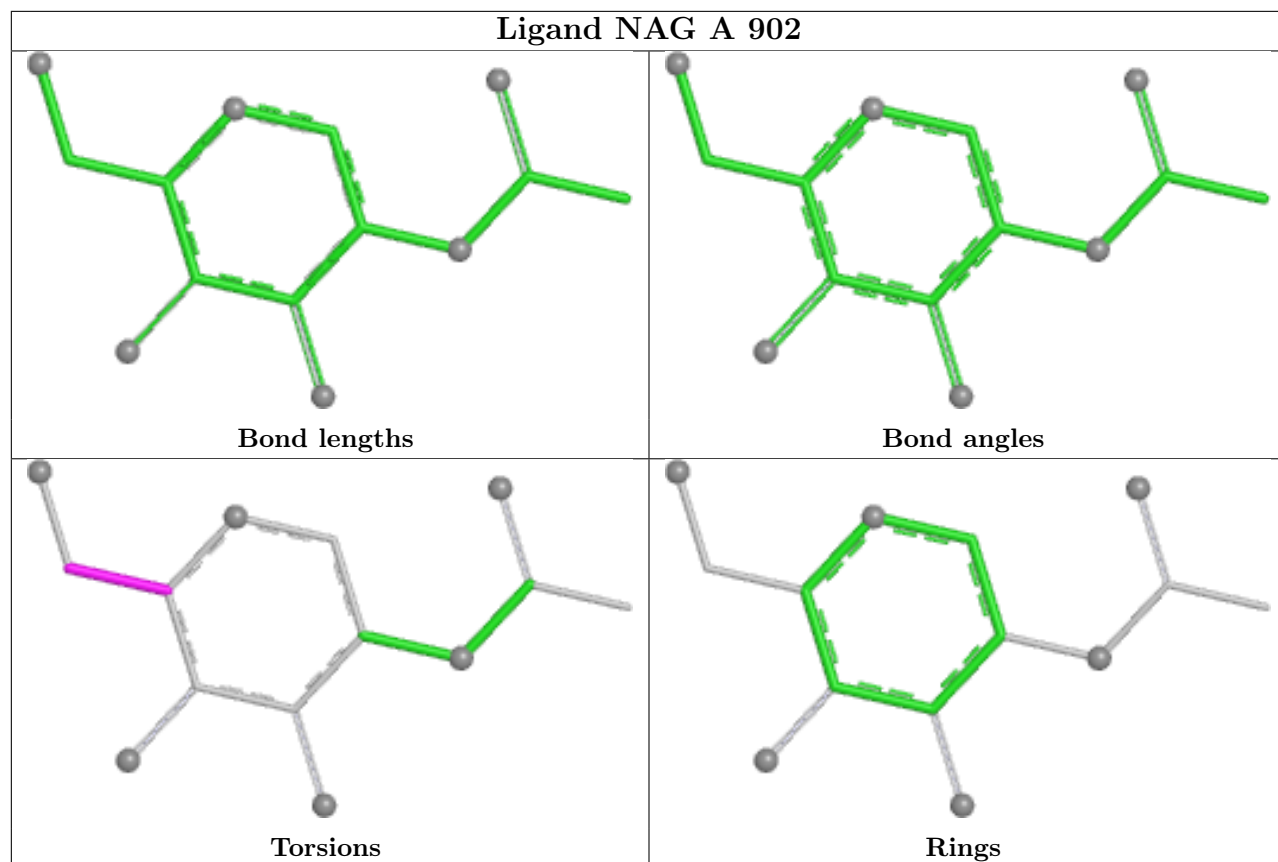
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

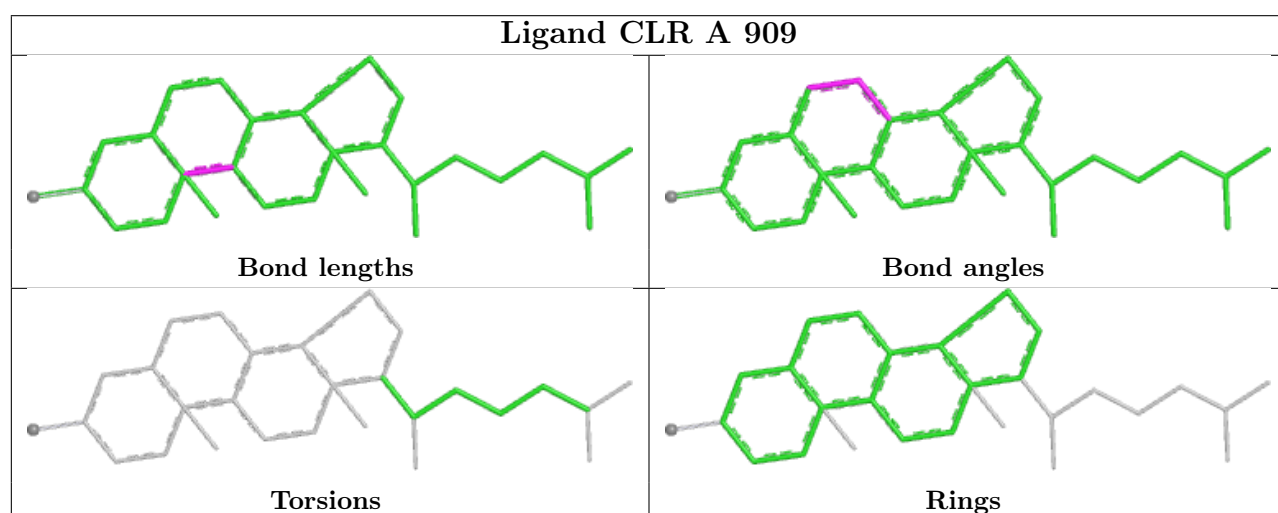
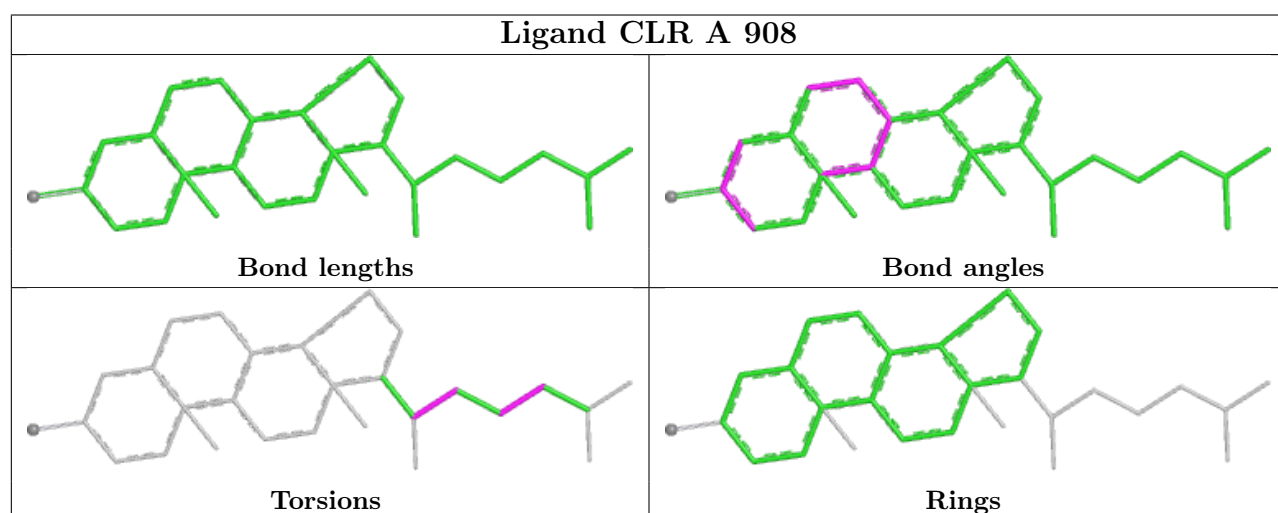
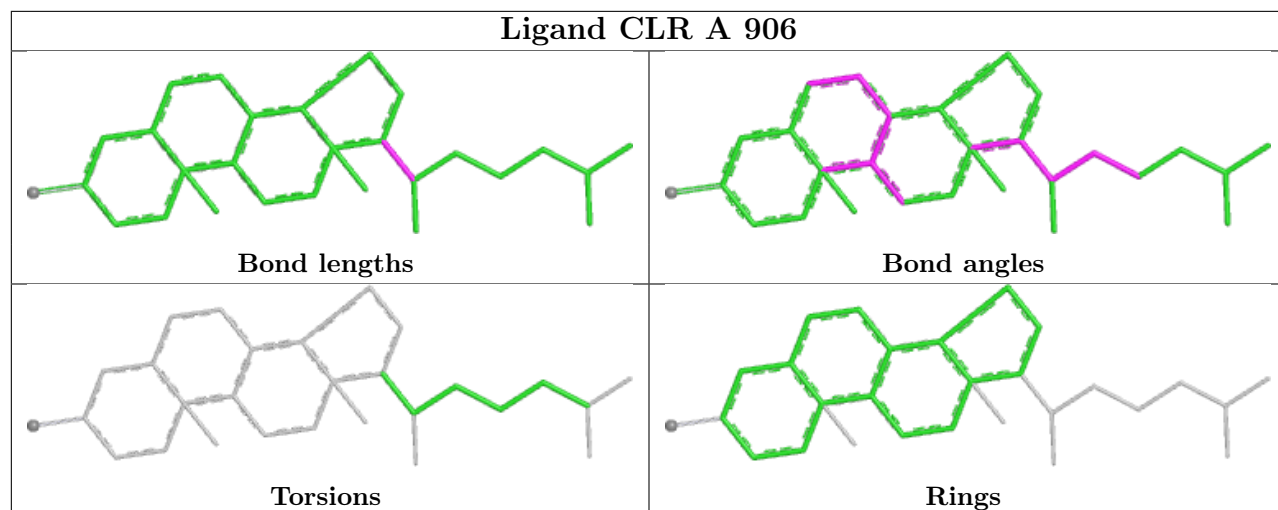
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

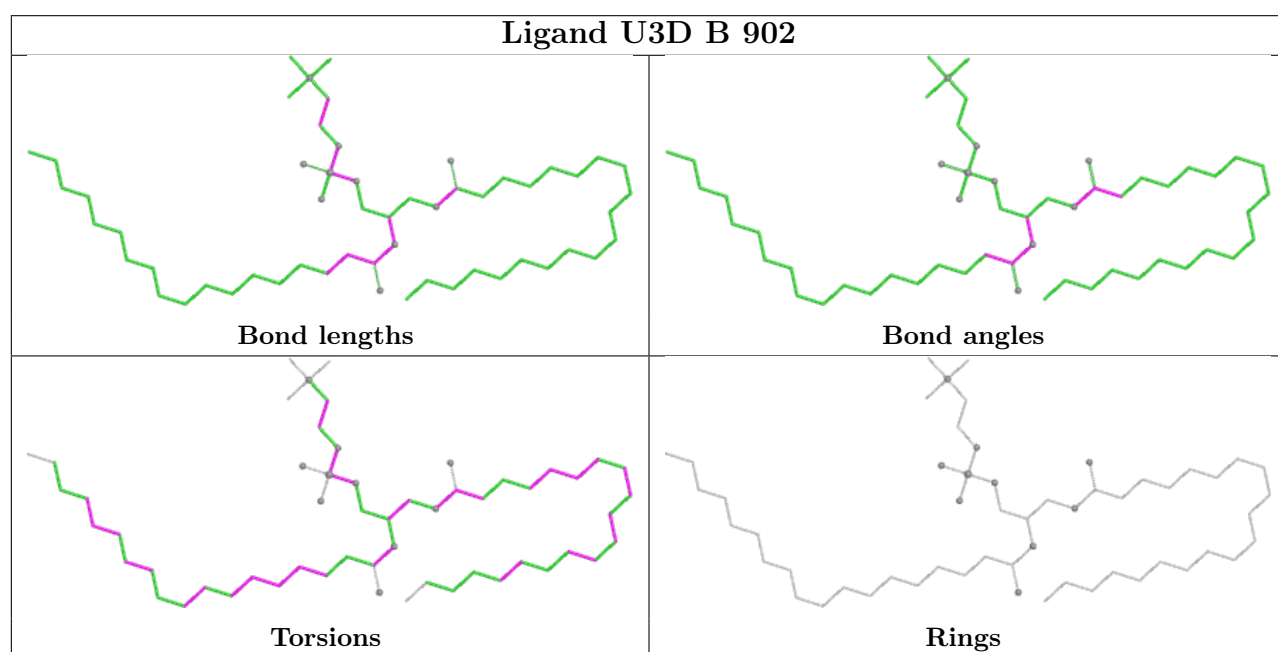
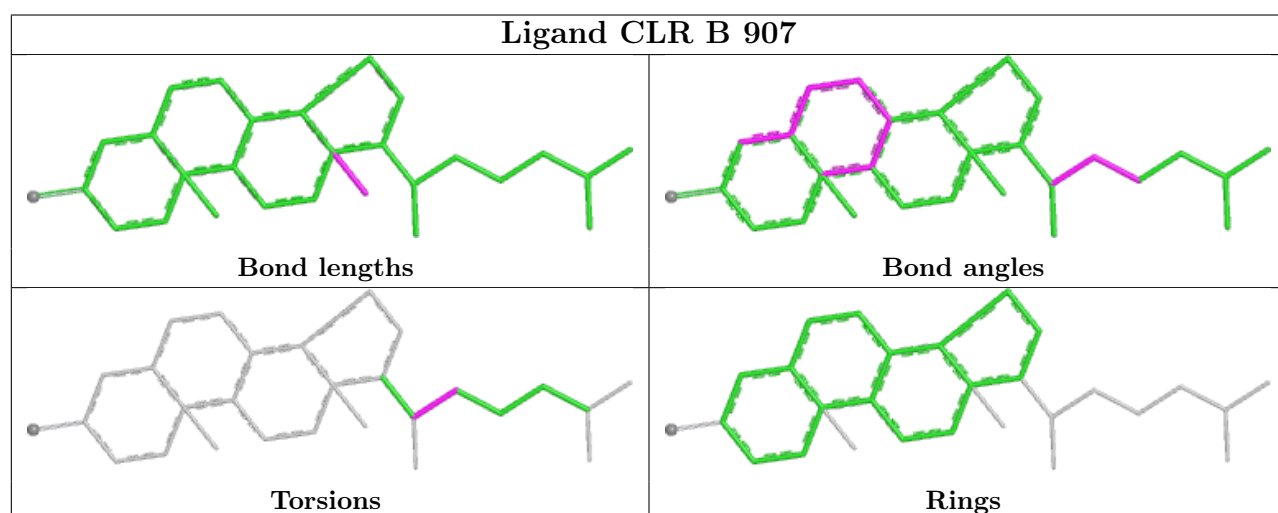
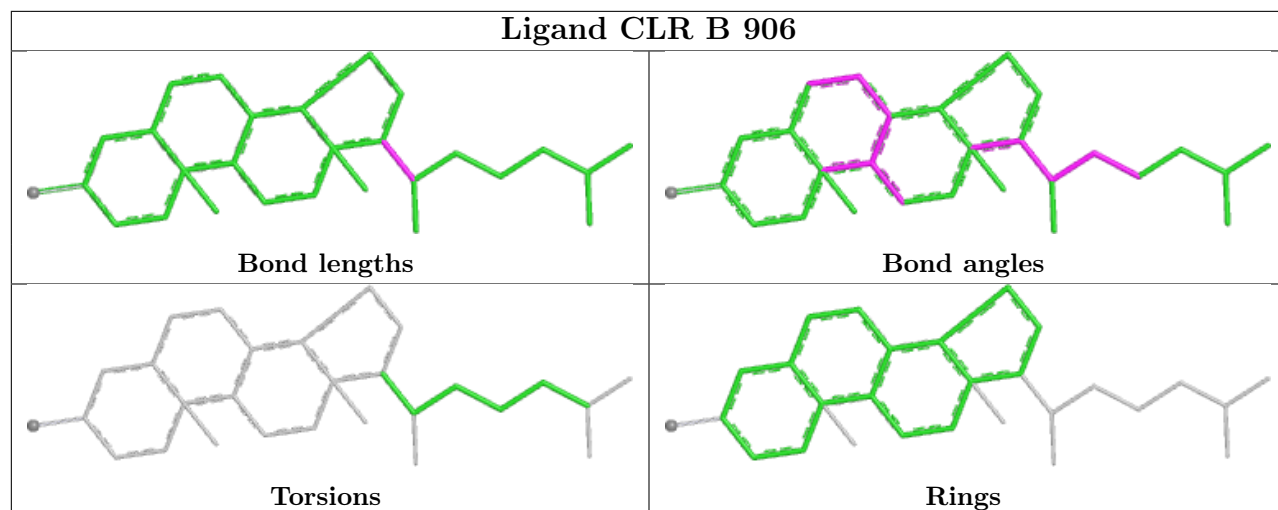


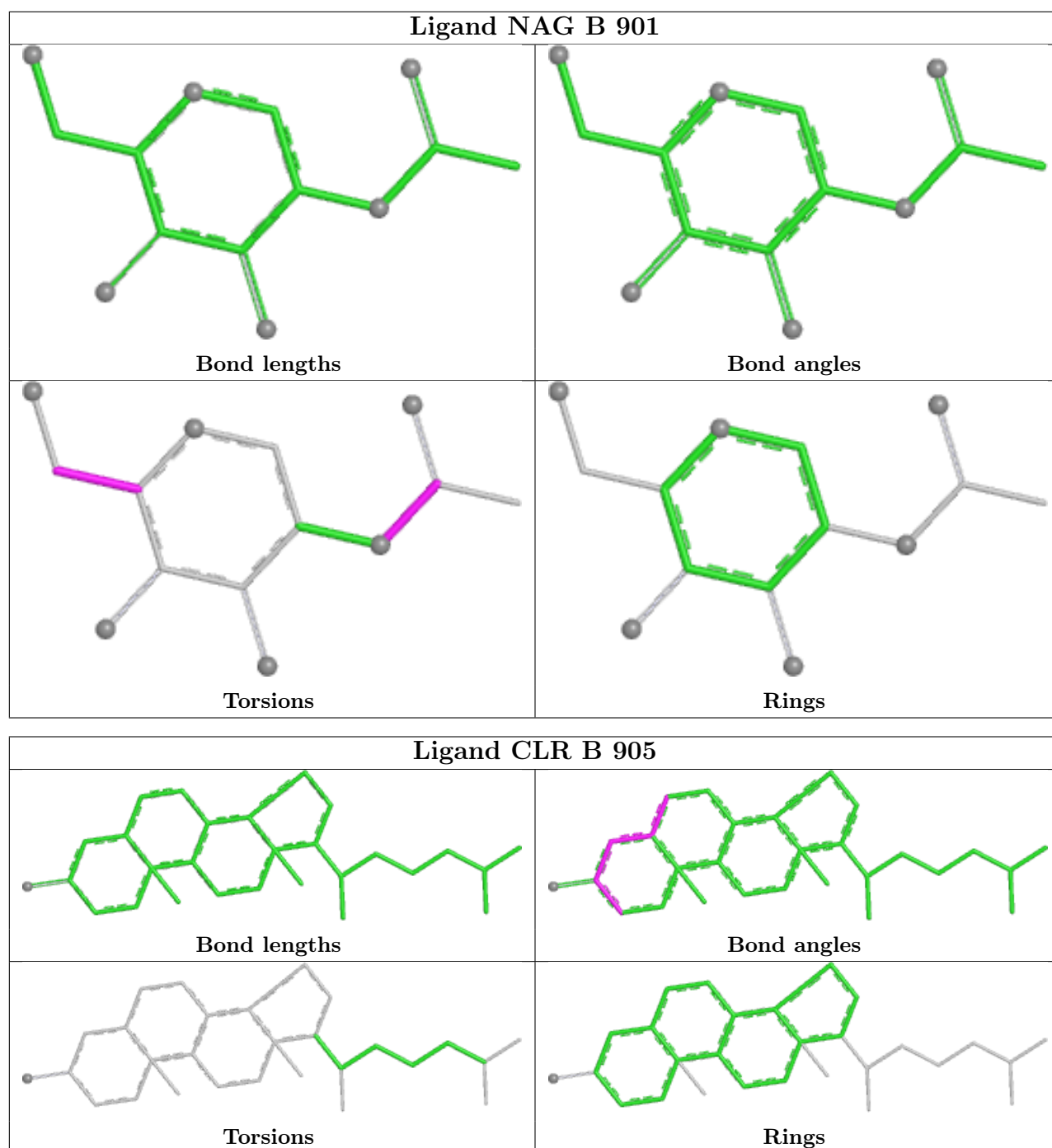












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

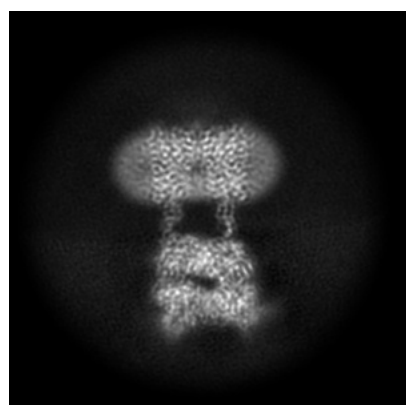
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21685. These allow visual inspection of the internal detail of the map and identification of artifacts.

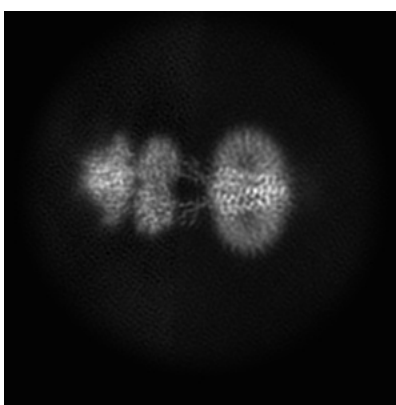
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

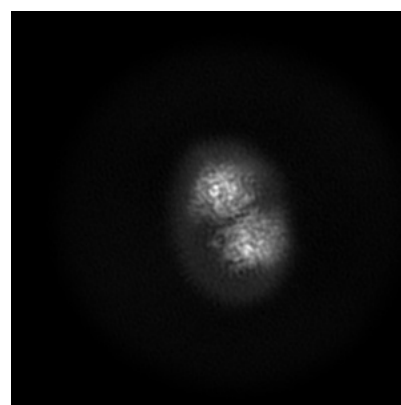
6.1.1 Primary map



X



Y

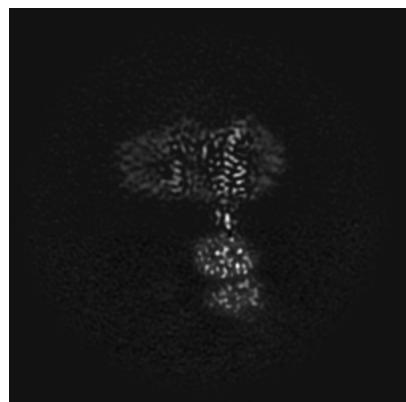


Z

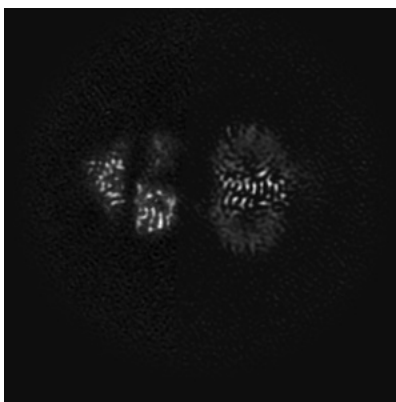
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

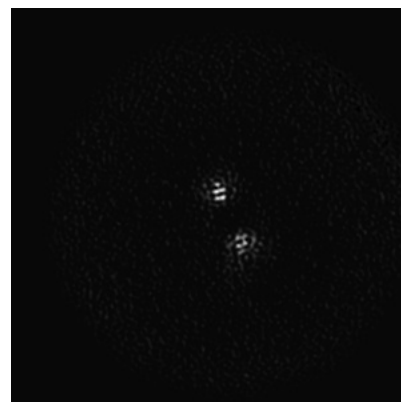
6.2.1 Primary map



X Index: 128



Y Index: 128

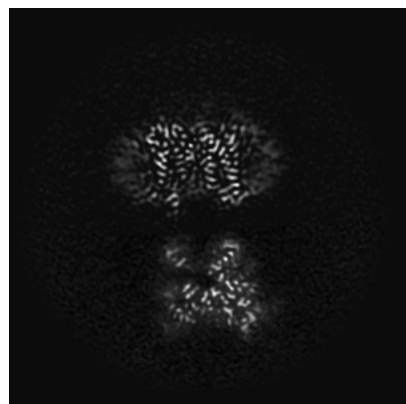


Z Index: 128

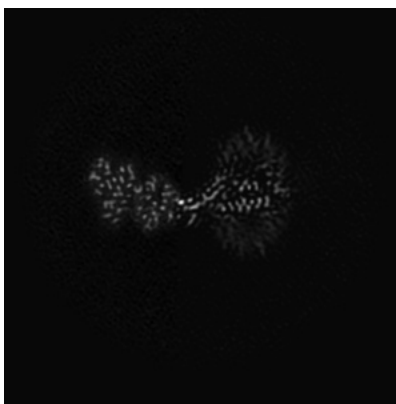
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

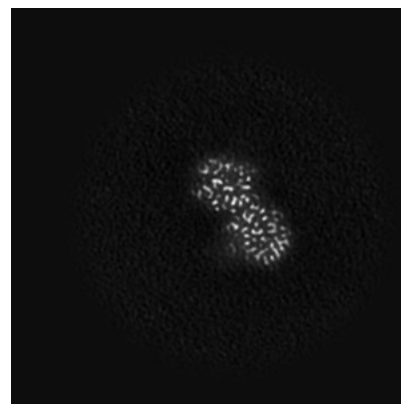
6.3.1 Primary map



X Index: 142



Y Index: 139

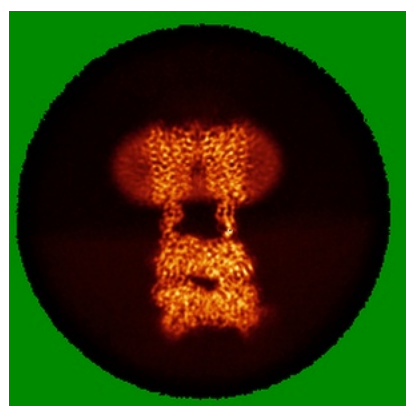


Z Index: 73

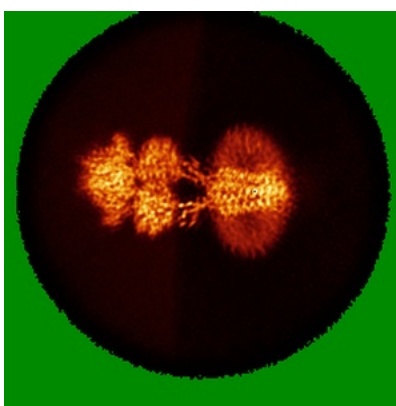
The images above show the largest variance slices of the map in three orthogonal directions.

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

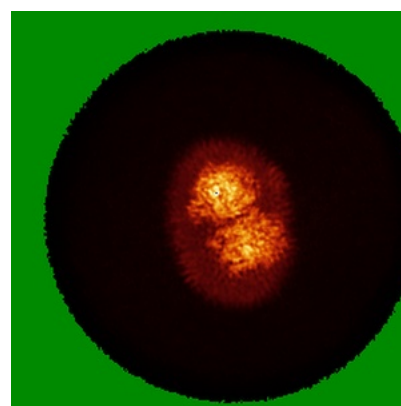
6.4.1 Primary map



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

This section was not generated.

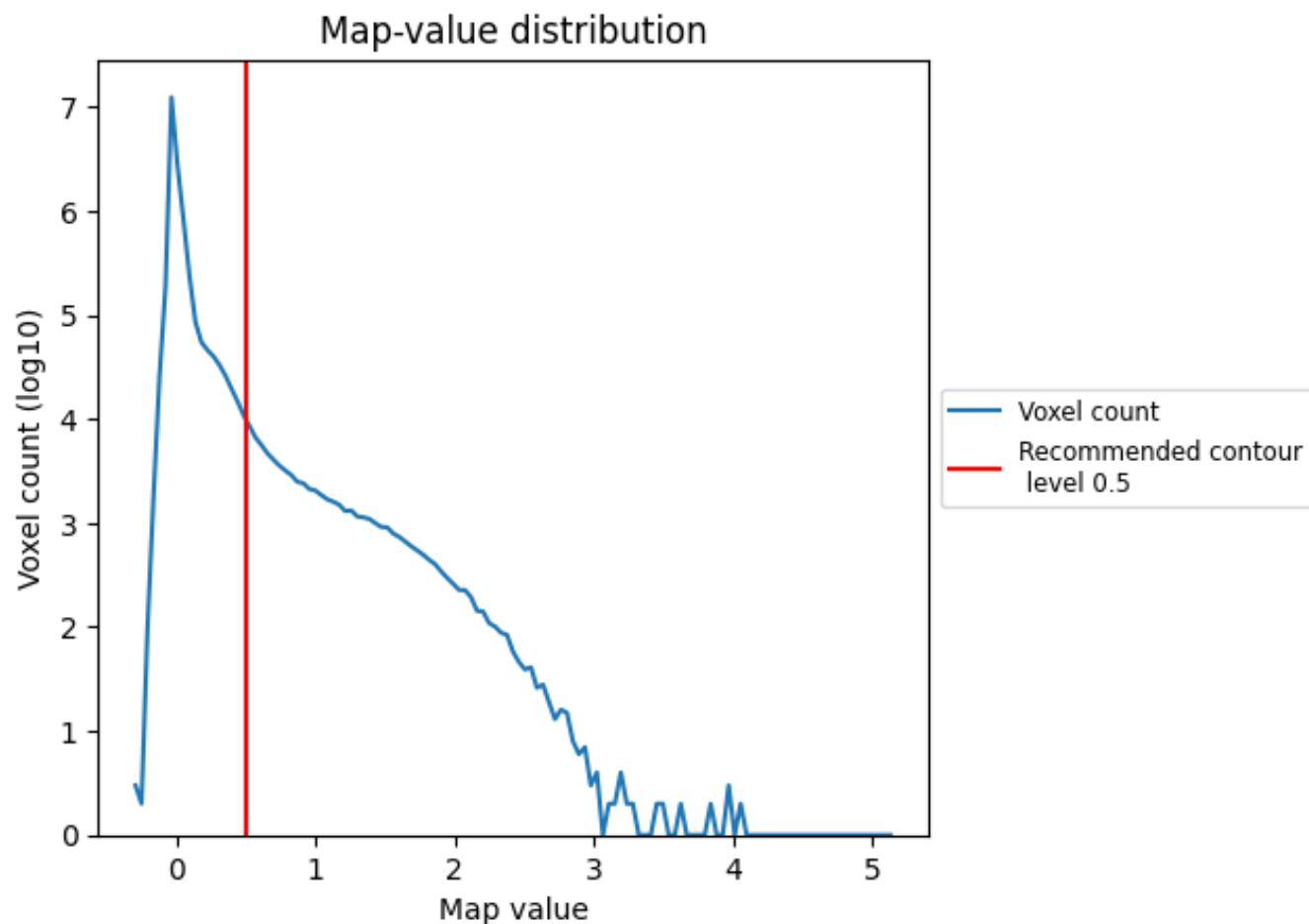
6.6 Mask visualisation

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

7 Map analysis [i](#)

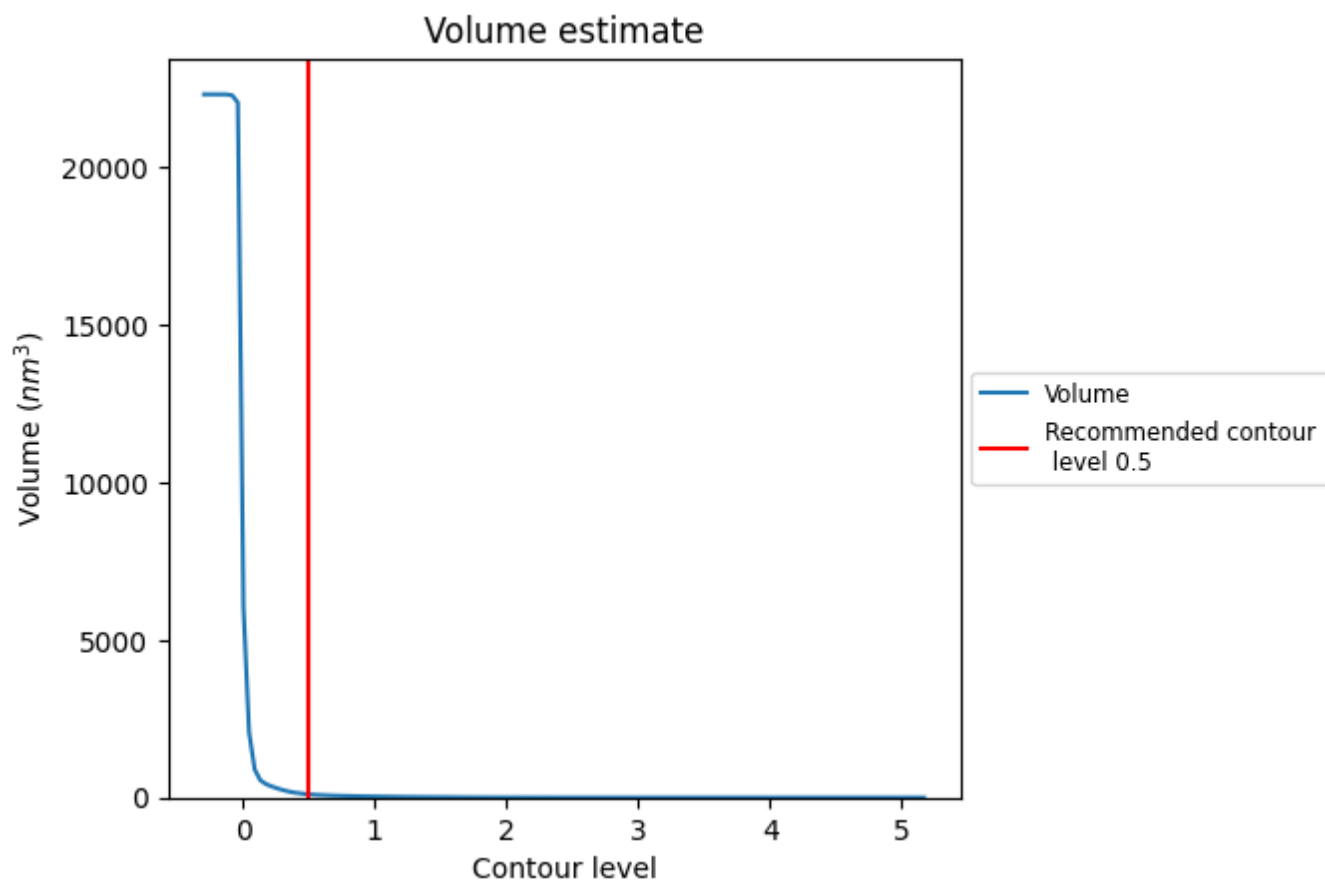
This section contains the results of statistical analysis of the map.

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.

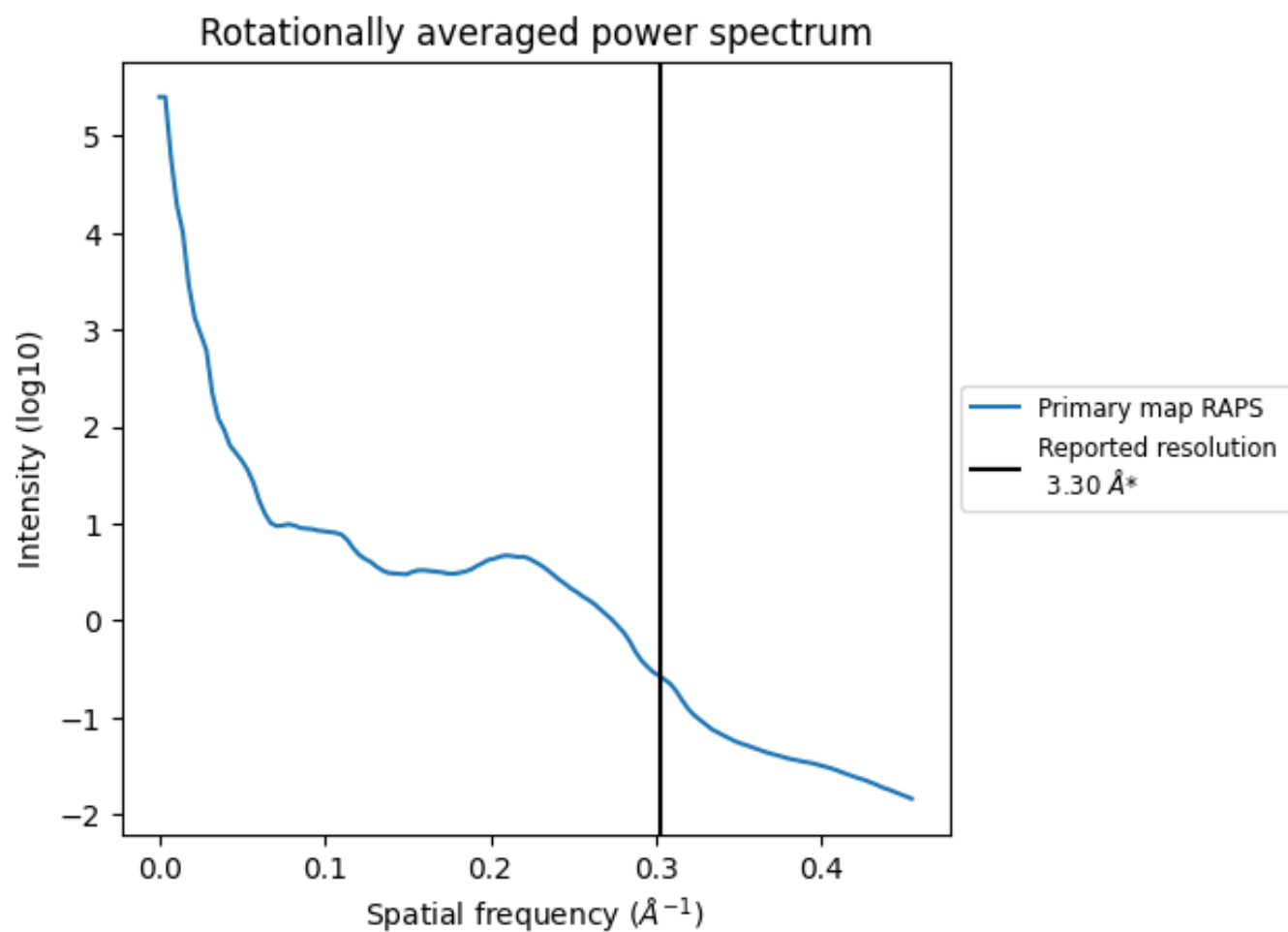
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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 0.303 Å⁻¹

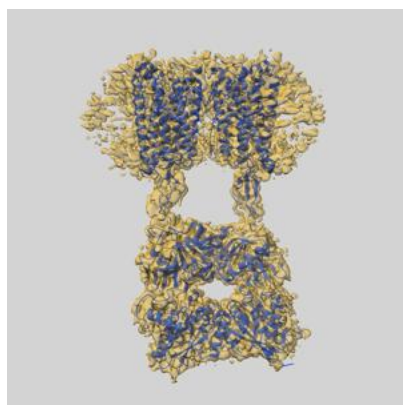
8 Fourier-Shell correlation ⓘ

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

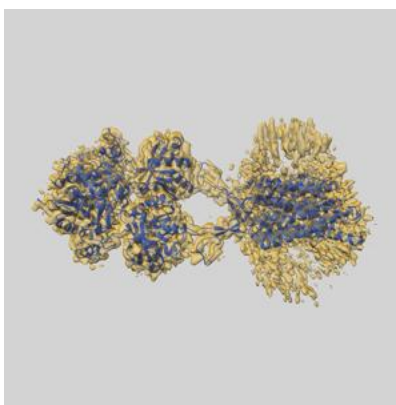
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21685 and PDB model 6WIV. Per-residue inclusion information can be found in section [3](#) on page [7](#).

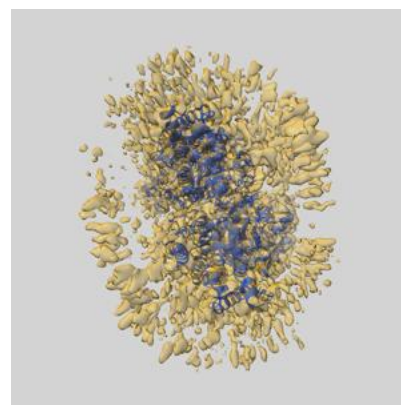
9.1 Map-model overlay [i](#)



X



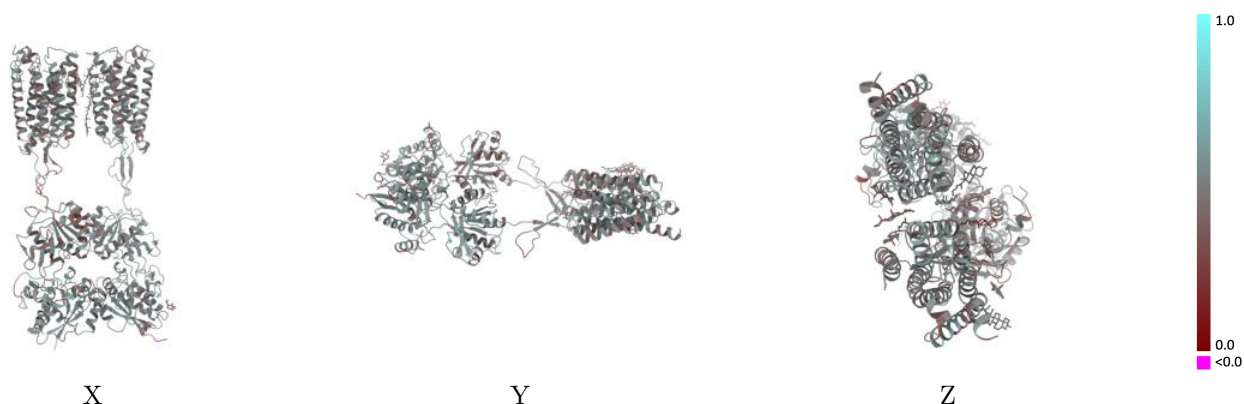
Y



Z

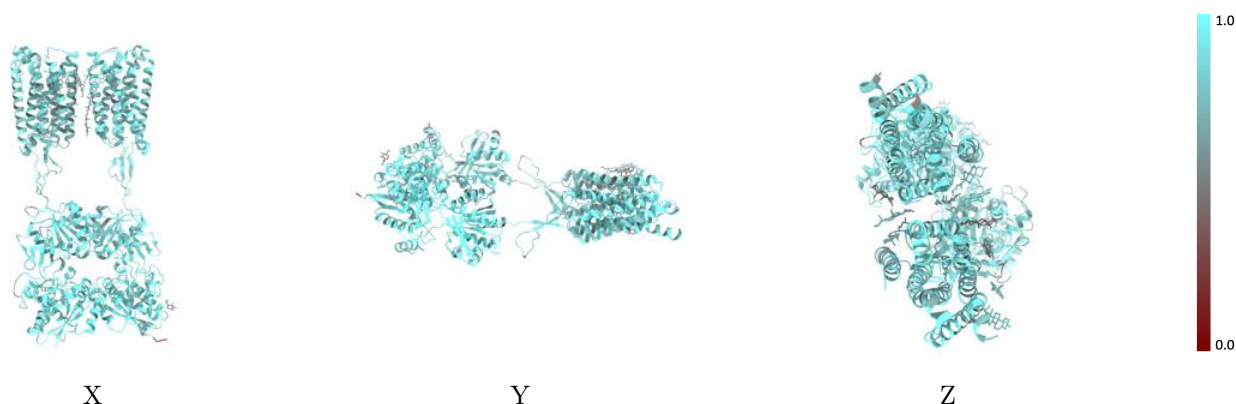
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



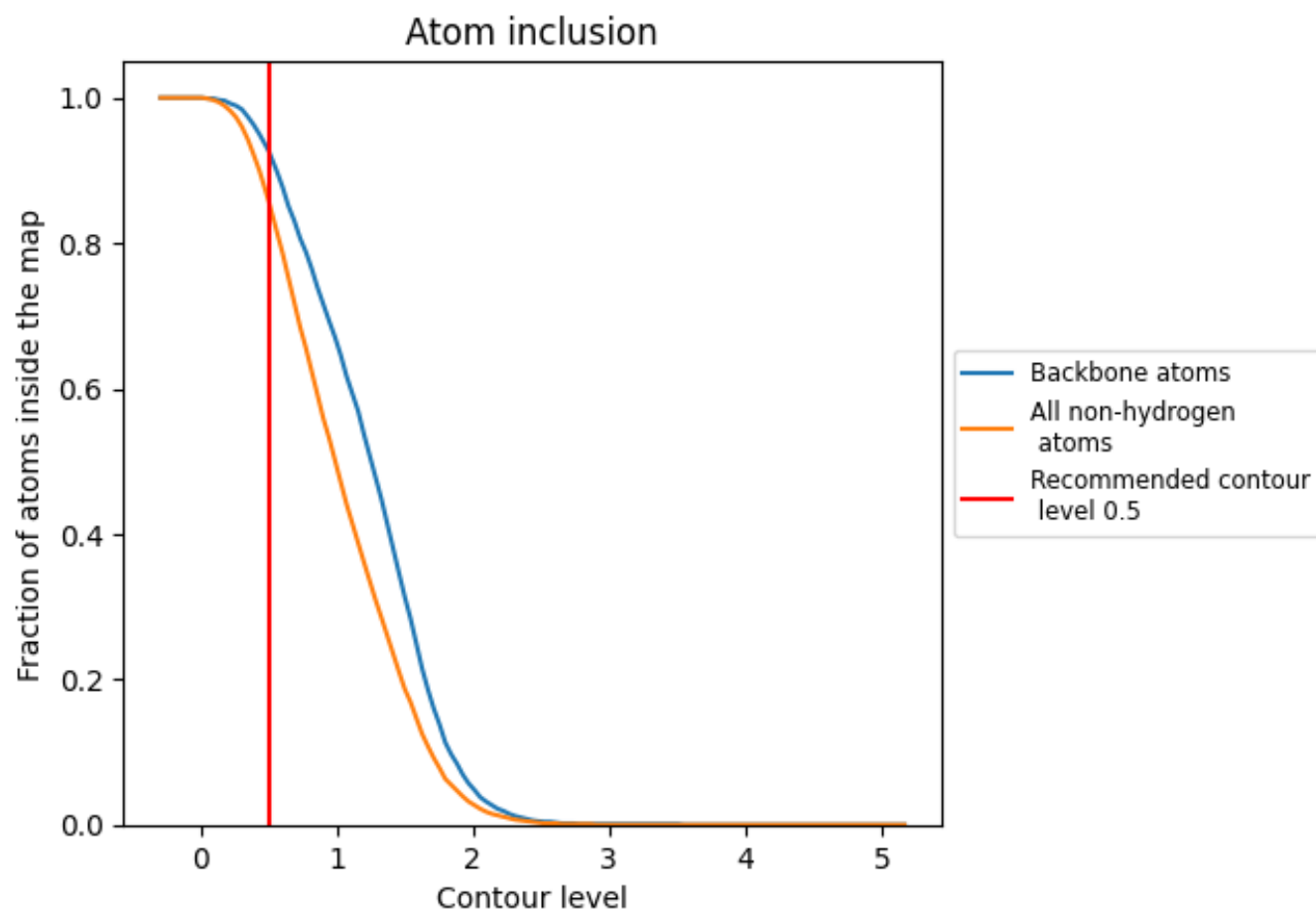
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8580	0.4860
A	0.8730	0.4960
B	0.8420	0.4750

