



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 04:09 PM UTC

PDB ID : 7CUM / pdb_00007cum
EMDB ID : EMD-30472
Title : Cryo-EM structure of human GABA(B) receptor bound to the antagonist CGP54626
Authors : Kim, Y.; Jeong, E.; Jeong, J.; Kim, Y.; Cho, Y.
Deposited on : 2020-08-23
Resolution : 3.52 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

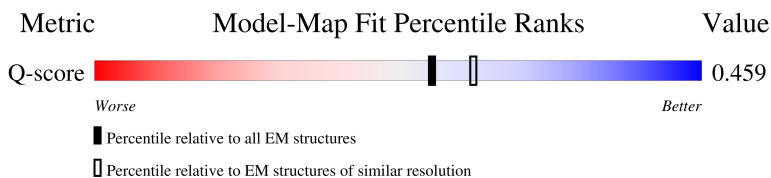
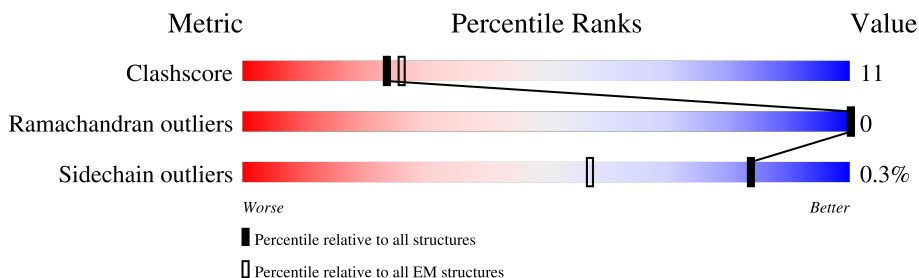
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 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	13017 (3.02 - 4.02)

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	771	9% 77% 11% 11%
2	B	822	12% 72% 10% 18%

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
3	2BV	A	1001	-	-	X	-
4	UNL	B	901	-	-	X	-
5	CLR	A	1004	-	-	X	-
5	CLR	B	912	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22336 atoms, of which 10974 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	683	Total	C	H	N	O	S	0	0
			10879	3521	5440	906	987	25		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	initiating methionine	UNP Q9UBS5
A	140	ARG	-	expression tag	UNP Q9UBS5
A	141	LEU	-	expression tag	UNP Q9UBS5
A	142	LEU	-	expression tag	UNP Q9UBS5
A	143	THR	-	expression tag	UNP Q9UBS5
A	144	ALA	-	expression tag	UNP Q9UBS5
A	145	LEU	-	expression tag	UNP Q9UBS5
A	146	PHE	-	expression tag	UNP Q9UBS5
A	147	ALA	-	expression tag	UNP Q9UBS5
A	148	TYR	-	expression tag	UNP Q9UBS5
A	149	PHE	-	expression tag	UNP Q9UBS5
A	150	ILE	-	expression tag	UNP Q9UBS5
A	151	VAL	-	expression tag	UNP Q9UBS5
A	152	ALA	-	expression tag	UNP Q9UBS5
A	153	LEU	-	expression tag	UNP Q9UBS5
A	154	ILE	-	expression tag	UNP Q9UBS5
A	155	LEU	-	expression tag	UNP Q9UBS5
A	156	ALA	-	expression tag	UNP Q9UBS5
A	157	PHE	-	expression tag	UNP Q9UBS5
A	158	SER	-	expression tag	UNP Q9UBS5
A	159	VAL	-	expression tag	UNP Q9UBS5
A	160	SER	-	expression tag	UNP Q9UBS5
A	161	ALA	-	expression tag	UNP Q9UBS5
A	162	LYS	-	expression tag	UNP Q9UBS5
A	163	SER	-	expression tag	UNP Q9UBS5
A	164	MET	-	expression tag	UNP Q9UBS5
A	901	SER	-	expression tag	UNP Q9UBS5
A	902	GLY	-	expression tag	UNP Q9UBS5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	903	ARG	-	expression tag	UNP Q9UBS5
A	904	LEU	-	expression tag	UNP Q9UBS5
A	905	GLU	-	expression tag	UNP Q9UBS5
A	906	VAL	-	expression tag	UNP Q9UBS5
A	907	LEU	-	expression tag	UNP Q9UBS5
A	908	PHE	-	expression tag	UNP Q9UBS5
A	909	GLN	-	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	675	Total	C	H	N	O	S	0	0
			10770	3469	5412	888	965	36		

There are 35 discrepancies between the modelled and reference sequences:

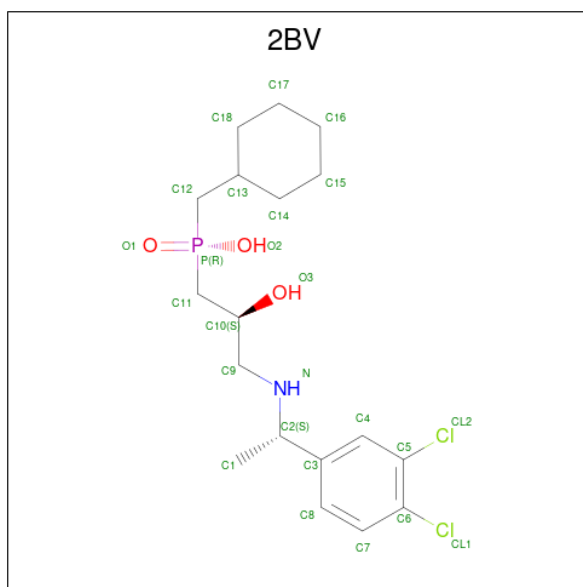
Chain	Residue	Modelled	Actual	Comment	Reference
B	788	SER	-	expression tag	UNP O75899
B	789	GLY	-	expression tag	UNP O75899
B	790	ARG	-	expression tag	UNP O75899
B	791	GLY	-	expression tag	UNP O75899
B	792	GLY	-	expression tag	UNP O75899
B	793	SER	-	expression tag	UNP O75899
B	794	GLU	-	expression tag	UNP O75899
B	795	ASN	-	expression tag	UNP O75899
B	796	LEU	-	expression tag	UNP O75899
B	797	TYR	-	expression tag	UNP O75899
B	798	PHE	-	expression tag	UNP O75899
B	799	GLN	-	expression tag	UNP O75899
B	800	GLY	-	expression tag	UNP O75899
B	801	GLY	-	expression tag	UNP O75899
B	802	SER	-	expression tag	UNP O75899
B	803	GLY	-	expression tag	UNP O75899
B	804	SER	-	expression tag	UNP O75899
B	805	GLY	-	expression tag	UNP O75899
B	806	GLY	-	expression tag	UNP O75899
B	807	ASP	-	expression tag	UNP O75899
B	808	TYR	-	expression tag	UNP O75899
B	809	LYS	-	expression tag	UNP O75899
B	810	ASP	-	expression tag	UNP O75899
B	811	ASP	-	expression tag	UNP O75899
B	812	ASP	-	expression tag	UNP O75899

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Chain	Residue	Modelled	Actual	Comment	Reference
B	813	ASP	-	expression tag	UNP O75899
B	814	LYS	-	expression tag	UNP O75899
B	815	ASP	-	expression tag	UNP O75899
B	816	TYR	-	expression tag	UNP O75899
B	817	LYS	-	expression tag	UNP O75899
B	818	ASP	-	expression tag	UNP O75899
B	819	ASP	-	expression tag	UNP O75899
B	820	ASP	-	expression tag	UNP O75899
B	821	ASP	-	expression tag	UNP O75899
B	822	LYS	-	expression tag	UNP O75899

- Molecule 3 is (R)-(cyclohexylmethyl)[(2S)-3-{[(1S)-1-(3,4-dichlorophenyl)ethyl]amino}-2-hydroxypropyl]phosphinic acid (CCD ID: 2BV) (formula: $C_{18}H_{28}Cl_2NO_3P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	Cl	N	O	P	0
			25	18	2	1	3	1	

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

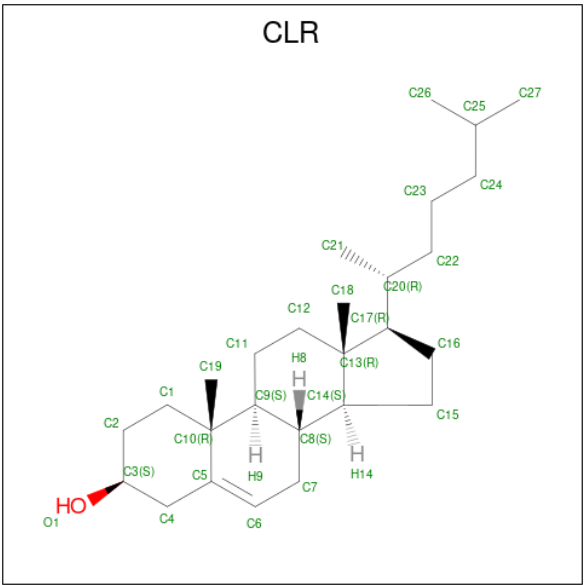
Mol	Chain	Residues	Atoms					AltConf	
4	A	1	Total	C	H	N	O	P	0
			108	37	61	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total	C	H	N	O	P	0
			106	35	61	1	8	1	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).

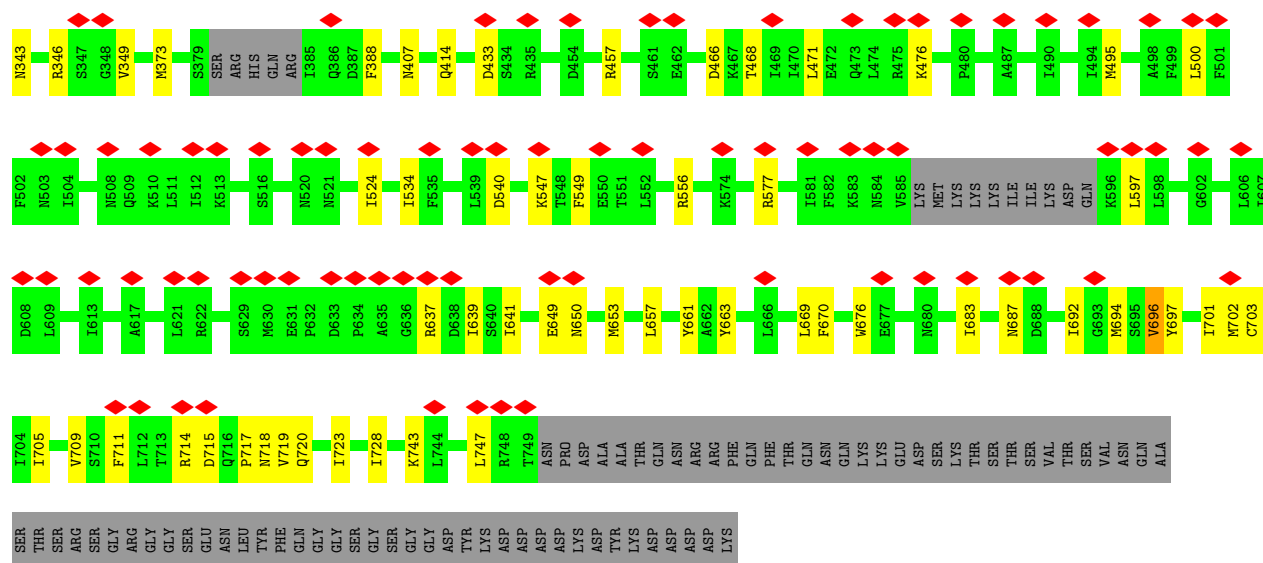


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27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

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	512675	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 ($e^-/\text{\AA}^2$)	50, 50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.052	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	250.70001, 250.70001, 250.70001	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2BV, UNL, CLR

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	0.33	1/5574 (0.0%)	0.57	5/7569 (0.1%)
2	B	0.28	0/5477	0.75	10/7420 (0.1%)
All	All	0.31	1/11051 (0.0%)	0.66	15/14989 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	840	ALA	C-N	10.71	1.47	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	717	PRO	N-CA-C	29.23	153.11	113.65
2	B	719	VAL	N-CA-C	17.30	128.52	110.36
2	B	718	ASN	CB-CA-C	13.06	132.72	110.79
2	B	696	VAL	CA-C-N	-10.10	106.90	120.54
2	B	696	VAL	C-N-CA	-10.10	106.90	120.54
2	B	717	PRO	CB-CA-C	-9.88	96.79	112.21
1	A	840	ALA	CA-C-N	-9.03	104.77	120.29
1	A	840	ALA	C-N-CA	-9.03	104.77	120.29
2	B	696	VAL	O-C-N	8.15	130.38	121.90
2	B	718	ASN	N-CA-C	-8.14	101.47	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	718	ASN	N-CA-CB	-7.70	98.74	110.13
2	B	719	VAL	N-CA-CB	-6.84	102.91	110.51
1	A	840	ALA	O-C-N	6.14	129.83	122.27
1	A	862	THR	N-CA-C	-5.64	105.67	113.18
1	A	750	ILE	N-CA-C	-5.30	108.34	113.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	683	ILE	Peptide

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	5439	5440	5442	89	0
2	B	5358	5412	5426	109	0
3	A	25	0	28	16	0
4	A	47	61	0	3	0
4	B	45	61	0	4	0
5	A	140	0	230	64	0
5	B	308	0	505	85	0
All	All	11362	10974	11631	251	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (251) 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:495:MET:CE	5:B:908:CLR:C26	1.78	1.61
5:A:1004:CLR:H262	5:B:912:CLR:C27	1.33	1.56
2:B:676:TRP:CZ2	5:B:912:CLR:H12	1.39	1.51
2:B:495:MET:HE3	5:B:908:CLR:C26	1.31	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:MET:HE2	5:B:908:CLR:C24	1.50	1.39
1:A:181:GLY:C	3:A:1001:2BV:H28	1.45	1.37
2:B:676:TRP:CH2	5:B:912:CLR:C1	2.09	1.35
2:B:495:MET:CE	5:B:908:CLR:C24	2.14	1.26
2:B:676:TRP:CH2	5:B:912:CLR:H11	1.67	1.26
2:B:676:TRP:CZ2	5:B:912:CLR:C1	2.18	1.24
5:A:1004:CLR:C26	5:B:912:CLR:H271	1.77	1.15
5:A:1004:CLR:C26	5:B:912:CLR:C27	2.28	1.12
1:A:666:ARG:HD3	4:A:1002:UNL:O25	1.49	1.11
5:A:1004:CLR:H213	5:B:912:CLR:H183	1.28	1.09
5:A:1004:CLR:H262	5:B:912:CLR:H272	1.32	1.08
2:B:495:MET:HE3	5:B:908:CLR:H263	1.28	1.07
1:A:792:LYS:NZ	5:A:1003:CLR:H3	1.68	1.07
5:A:1004:CLR:H262	5:B:912:CLR:H271	1.06	1.04
2:B:495:MET:CE	5:B:908:CLR:C25	2.33	1.04
1:A:181:GLY:C	3:A:1001:2BV:C16	2.31	1.03
1:A:779:LEU:HB3	5:A:1004:CLR:H261	1.41	1.03
2:B:495:MET:HE1	5:B:908:CLR:C26	1.84	1.03
2:B:94:LEU:O	2:B:97:TYR:O	1.75	1.03
5:B:911:CLR:H112	5:B:912:CLR:H71	1.40	1.02
1:A:824:MET:SD	5:A:1005:CLR:H9	2.00	1.01
1:A:841:ILE:HG12	4:A:1002:UNL:C08	1.94	0.97
2:B:495:MET:HE2	5:B:908:CLR:H242	0.98	0.97
2:B:669:LEU:HD21	5:B:912:CLR:H273	1.46	0.94
2:B:676:TRP:CA	2:B:697:TYR:OH	2.15	0.94
1:A:181:GLY:O	3:A:1001:2BV:H28	1.68	0.94
2:B:694:MET:SD	5:B:910:CLR:H71	2.07	0.94
2:B:701:ILE:HB	5:B:911:CLR:H263	1.50	0.93
1:A:713:THR:HG22	5:A:1004:CLR:H42	1.50	0.93
1:A:772:ILE:HA	5:A:1006:CLR:H231	1.49	0.93
1:A:792:LYS:HZ3	5:A:1003:CLR:H3	1.28	0.93
5:A:1004:CLR:H213	5:B:912:CLR:C18	2.00	0.92
1:A:181:GLY:O	3:A:1001:2BV:C16	2.18	0.89
1:A:824:MET:SD	5:A:1005:CLR:H112	2.12	0.89
2:B:495:MET:CE	5:B:908:CLR:H241	2.02	0.89
2:B:676:TRP:HZ2	5:B:912:CLR:H12	1.11	0.89
1:A:182:TRP:HB2	3:A:1001:2BV:H29	1.52	0.88
1:A:713:THR:CG2	5:A:1004:CLR:H42	2.04	0.88
5:A:1004:CLR:H122	5:B:912:CLR:H191	1.56	0.86
2:B:676:TRP:HH2	5:B:912:CLR:C1	1.87	0.85
1:A:810:TYR:CE2	5:A:1003:CLR:H71	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:MET:HE1	5:B:908:CLR:C25	2.05	0.84
5:A:1005:CLR:H72	5:A:1006:CLR:H151	1.58	0.84
2:B:495:MET:HE1	5:B:908:CLR:C24	2.05	0.83
1:A:824:MET:SD	5:A:1005:CLR:C11	2.67	0.83
2:B:676:TRP:HA	2:B:697:TYR:OH	1.76	0.83
1:A:779:LEU:HD13	5:B:912:CLR:H271	1.60	0.82
2:B:495:MET:CE	5:B:908:CLR:H263	1.90	0.82
1:A:792:LYS:HZ1	5:A:1003:CLR:H3	1.46	0.81
5:A:1006:CLR:H121	5:B:906:CLR:H152	1.63	0.80
1:A:779:LEU:CB	5:A:1004:CLR:H261	2.11	0.79
1:A:182:TRP:N	3:A:1001:2BV:H28	1.98	0.79
1:A:782:LEU:HB3	5:A:1007:CLR:H262	1.65	0.77
5:A:1004:CLR:H262	5:B:912:CLR:C25	2.12	0.77
1:A:666:ARG:CD	4:A:1002:UNL:O25	2.30	0.76
1:A:824:MET:SD	5:A:1005:CLR:C9	2.74	0.75
2:B:54:PRO:O	2:B:97:TYR:HB3	1.87	0.74
2:B:694:MET:HE1	5:B:910:CLR:H14	1.68	0.74
2:B:54:PRO:HD2	2:B:97:TYR:HD1	1.52	0.74
2:B:676:TRP:CH2	5:B:912:CLR:H12	1.87	0.72
5:B:911:CLR:C11	5:B:912:CLR:H71	2.17	0.71
1:A:182:TRP:HB2	3:A:1001:2BV:C15	2.21	0.71
1:A:662:VAL:O	1:A:666:ARG:HG2	1.91	0.70
5:A:1006:CLR:H9	5:B:905:CLR:C19	2.22	0.70
2:B:676:TRP:CB	2:B:697:TYR:OH	2.39	0.70
2:B:701:ILE:HD12	5:B:911:CLR:H25	1.74	0.70
2:B:54:PRO:HG2	2:B:97:TYR:CE1	2.27	0.69
2:B:663:TYR:CE1	5:B:907:CLR:H241	2.27	0.69
2:B:676:TRP:HH2	5:B:912:CLR:C2	2.05	0.68
2:B:676:TRP:CH2	5:B:912:CLR:C2	2.77	0.68
5:A:1006:CLR:C21	5:B:906:CLR:H162	2.24	0.67
2:B:96:PRO:HG3	2:B:373:MET:SD	2.35	0.67
1:A:662:VAL:O	1:A:666:ARG:CG	2.43	0.66
2:B:676:TRP:HB2	2:B:697:TYR:OH	1.95	0.66
5:A:1006:CLR:H9	5:B:905:CLR:H191	1.78	0.64
2:B:676:TRP:HH2	5:B:912:CLR:H21	1.62	0.64
1:A:182:TRP:CD1	3:A:1001:2BV:CL2	2.87	0.64
2:B:495:MET:HE1	5:B:908:CLR:H241	1.69	0.64
5:A:1004:CLR:H112	5:B:912:CLR:C19	2.28	0.64
2:B:676:TRP:N	2:B:697:TYR:OH	2.31	0.62
5:A:1004:CLR:H112	5:B:912:CLR:H192	1.82	0.61
2:B:676:TRP:HA	2:B:697:TYR:HH	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1005:CLR:H151	5:A:1006:CLR:H161	1.82	0.61
1:A:786:PHE:HD1	5:A:1007:CLR:C21	2.13	0.61
5:A:1004:CLR:H122	5:B:912:CLR:C19	2.30	0.61
2:B:701:ILE:CB	5:B:911:CLR:H263	2.29	0.60
5:A:1004:CLR:C26	5:B:912:CLR:H272	2.13	0.60
2:B:701:ILE:HD12	5:B:911:CLR:C26	2.32	0.60
1:A:786:PHE:CD1	5:A:1007:CLR:C21	2.84	0.59
5:A:1004:CLR:C12	5:B:912:CLR:C19	2.80	0.59
1:A:782:LEU:HD11	5:A:1005:CLR:H261	1.84	0.59
2:B:126:ASN:ND2	2:B:388:PHE:O	2.36	0.58
2:B:650:ASN:H	2:B:653:MET:HE3	1.69	0.58
2:B:212:ARG:NH1	2:B:216:THR:OG1	2.37	0.57
5:A:1005:CLR:C27	5:B:904:CLR:H221	2.34	0.57
2:B:54:PRO:CD	2:B:97:TYR:HD1	2.17	0.57
2:B:500:LEU:HB2	2:B:524:ILE:HG21	1.87	0.57
1:A:837:ALA:O	1:A:841:ILE:HG13	2.06	0.56
5:A:1005:CLR:H272	5:B:904:CLR:H221	1.87	0.56
5:A:1004:CLR:C12	5:B:912:CLR:H191	2.30	0.56
1:A:659:PHE:O	1:A:663:CYS:HB2	2.06	0.56
1:A:789:TYR:CE2	5:A:1007:CLR:H112	2.41	0.56
2:B:54:PRO:HG2	2:B:97:TYR:CD1	2.41	0.56
5:A:1006:CLR:C12	5:B:906:CLR:H152	2.34	0.55
1:A:214:ILE:HD12	1:A:239:LYS:HE3	1.88	0.55
2:B:154:LEU:HA	2:B:173:PHE:O	2.07	0.55
2:B:663:TYR:CD1	5:B:907:CLR:H241	2.40	0.55
2:B:54:PRO:HG2	2:B:97:TYR:HE1	1.71	0.55
2:B:495:MET:HE2	5:B:908:CLR:C25	2.13	0.55
2:B:701:ILE:HD12	5:B:911:CLR:C25	2.36	0.55
2:B:649:GLU:HB2	2:B:653:MET:HG3	1.88	0.55
5:A:1004:CLR:H241	5:B:912:CLR:H232	1.88	0.54
1:A:181:GLY:CA	3:A:1001:2BV:H28	2.31	0.54
2:B:407:ASN:OD1	2:B:414:GLN:NE2	2.40	0.54
5:B:902:CLR:H112	5:B:903:CLR:H6	1.89	0.54
1:A:713:THR:HG22	5:A:1004:CLR:C4	2.29	0.54
1:A:330:VAL:HG22	1:A:335:ILE:HB	1.89	0.54
2:B:95:ARG:N	2:B:96:PRO:HD2	2.23	0.54
1:A:532:SER:OG	1:A:533:ARG:N	2.40	0.54
2:B:471:LEU:HB3	2:B:641:ILE:HG22	1.89	0.53
2:B:158:ALA:O	2:B:174:ARG:NH1	2.38	0.53
5:A:1004:CLR:H273	5:B:912:CLR:H272	1.91	0.53
2:B:88:ILE:HG22	2:B:93:LEU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:OD1	1:A:204:ASP:N	2.42	0.52
1:A:355:LYS:NZ	1:A:382:ARG:O	2.42	0.52
1:A:497:ASP:OD1	1:A:497:ASP:N	2.43	0.52
1:A:395:TRP:CG	3:A:1001:2BV:H22	2.45	0.51
1:A:313:GLN:OE1	1:A:340:ARG:NH1	2.42	0.51
2:B:433:ASP:OD2	2:B:457:ARG:NH2	2.43	0.51
1:A:182:TRP:CB	3:A:1001:2BV:H29	2.33	0.51
1:A:378:VAL:HG13	1:A:383:LEU:HB3	1.93	0.51
1:A:307:LYS:HA	1:A:335:ILE:HG23	1.93	0.50
2:B:663:TYR:CD1	5:B:907:CLR:C24	2.95	0.50
2:B:709:VAL:HG11	2:B:723:ILE:HD13	1.94	0.50
1:A:181:GLY:O	3:A:1001:2BV:H9	2.09	0.50
2:B:54:PRO:CG	2:B:97:TYR:CD1	2.95	0.50
2:B:676:TRP:CA	2:B:697:TYR:HH	2.22	0.50
2:B:65:THR:OG1	2:B:67:GLU:OE1	2.30	0.49
1:A:231:GLU:O	1:A:235:ASN:ND2	2.45	0.49
1:A:738:ILE:HG12	1:A:759:GLU:HB3	1.93	0.49
2:B:702:MET:HA	2:B:705:ILE:HG22	1.93	0.49
1:A:355:LYS:HD3	1:A:383:LEU:HD13	1.95	0.49
2:B:466:ASP:N	2:B:466:ASP:OD1	2.43	0.49
1:A:366:PHE:O	1:A:396:TYR:OH	2.31	0.48
1:A:182:TRP:CD1	3:A:1001:2BV:C5	2.96	0.48
1:A:266:SER:OG	1:A:267:TYR:N	2.46	0.48
2:B:88:ILE:CG2	2:B:93:LEU:HB3	2.43	0.48
2:B:63:PRO:HB2	2:B:71:GLY:HA2	1.95	0.48
2:B:534:ILE:HD11	2:B:728:ILE:HG21	1.96	0.48
5:B:903:CLR:H9	5:B:904:CLR:H193	1.95	0.48
1:A:576:ASP:OD1	1:A:576:ASP:N	2.47	0.48
2:B:88:ILE:HG23	2:B:93:LEU:HD23	1.95	0.48
1:A:810:TYR:CE2	5:A:1003:CLR:C7	2.90	0.47
2:B:661:TYR:OH	4:B:901:UNL:C41	2.62	0.47
2:B:303:LEU:HB3	2:B:306:ASN:HD22	1.78	0.47
2:B:714:ARG:O	2:B:714:ARG:HG2	2.14	0.47
1:A:581:ILE:HB	1:A:754:ILE:HG22	1.97	0.47
1:A:662:VAL:O	1:A:666:ARG:HG3	2.13	0.47
5:A:1007:CLR:H272	2:B:670:PHE:CD1	2.50	0.47
1:A:782:LEU:CD1	5:A:1005:CLR:H261	2.44	0.47
5:A:1006:CLR:H213	5:B:906:CLR:H162	1.96	0.47
1:A:736:ARG:HH11	1:A:738:ILE:HD11	1.79	0.47
2:B:669:LEU:CD2	5:B:912:CLR:H273	2.31	0.47
2:B:696:VAL:O	2:B:697:TYR:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1004:CLR:H261	5:B:912:CLR:H271	1.85	0.47
2:B:92:SER:OG	2:B:95:ARG:HG2	2.15	0.47
2:B:577:ARG:HD2	2:B:597:LEU:HD21	1.97	0.47
2:B:657:LEU:HD21	2:B:711:PHE:HZ	1.80	0.46
5:B:904:CLR:H151	5:B:905:CLR:H161	1.98	0.46
5:A:1005:CLR:H6	5:A:1006:CLR:H72	1.97	0.46
1:A:346:ASP:OD1	1:A:346:ASP:N	2.49	0.46
2:B:68:VAL:HG23	2:B:71:GLY:H	1.80	0.46
2:B:54:PRO:CG	2:B:97:TYR:HD1	2.29	0.46
1:A:831:ASP:OD1	1:A:831:ASP:N	2.49	0.45
2:B:495:MET:HE1	5:B:908:CLR:C27	2.47	0.45
2:B:339:GLU:O	2:B:343:ASN:ND2	2.41	0.45
1:A:802:HIS:CD2	1:A:803:ARG:H	2.34	0.45
2:B:96:PRO:CG	2:B:373:MET:SD	3.04	0.45
1:A:776:TYR:N	5:A:1006:CLR:H263	2.31	0.45
5:A:1006:CLR:H12	5:B:905:CLR:H192	1.99	0.45
1:A:543:GLN:NE2	1:A:565:THR:O	2.46	0.45
1:A:810:TYR:CZ	5:A:1003:CLR:H71	2.51	0.45
1:A:399:ASN:OD1	1:A:399:ASN:N	2.50	0.45
2:B:687:ASN:OD1	2:B:687:ASN:N	2.50	0.45
1:A:566:ASP:OD1	1:A:566:ASP:N	2.40	0.44
5:A:1004:CLR:C11	5:B:912:CLR:C19	2.93	0.44
5:A:1005:CLR:H271	5:B:904:CLR:H241	1.99	0.44
2:B:637:ARG:HG3	2:B:639:ILE:HG12	1.98	0.44
2:B:343:ASN:HA	2:B:346:ARG:HG2	1.99	0.44
1:A:781:LEU:HD21	1:A:813:ALA:HA	1.99	0.44
1:A:447:VAL:O	1:A:451:THR:OG1	2.30	0.44
5:B:911:CLR:C21	5:B:912:CLR:H161	2.48	0.44
1:A:792:LYS:HZ1	5:A:1003:CLR:C3	2.24	0.44
2:B:556:ARG:HH12	4:B:901:UNL:C25	2.31	0.44
2:B:720:GLN:HA	2:B:723:ILE:HG22	2.00	0.43
1:A:411:THR:HB	1:A:414:GLU:HB2	2.00	0.43
1:A:811:ASN:O	1:A:815:LEU:HB2	2.19	0.43
2:B:692:ILE:HD13	2:B:692:ILE:HA	1.91	0.43
1:A:457:HIS:HB2	1:A:460:GLU:HG2	2.00	0.43
1:A:650:ASP:OD1	1:A:650:ASP:N	2.52	0.43
1:A:182:TRP:HD1	3:A:1001:2BV:CL2	2.38	0.43
2:B:346:ARG:NH1	2:B:349:VAL:O	2.52	0.43
1:A:782:LEU:CD1	5:A:1005:CLR:C26	2.97	0.43
1:A:554:ASP:OD2	1:A:557:LYS:NZ	2.52	0.42
2:B:476:LYS:HE3	2:B:476:LYS:HB2	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ALA:HA	1:A:374:VAL:HG12	2.00	0.42
2:B:547:LYS:HD3	2:B:547:LYS:HA	1.82	0.42
2:B:715:ASP:OD1	2:B:715:ASP:N	2.51	0.42
2:B:728:ILE:HD13	4:B:901:UNL:C49	2.49	0.42
1:A:181:GLY:CA	3:A:1001:2BV:C16	2.93	0.42
1:A:604:VAL:HA	1:A:607:VAL:HG12	2.02	0.42
2:B:88:ILE:HG23	2:B:93:LEU:CD2	2.49	0.42
2:B:540:ASP:HA	2:B:549:PHE:HE1	1.84	0.42
2:B:166:LYS:HD3	2:B:166:LYS:HA	1.82	0.42
2:B:373:MET:HE3	2:B:373:MET:HB2	1.88	0.42
2:B:249:ARG:HH22	2:B:468:THR:HB	1.84	0.42
5:B:904:CLR:H212	5:B:904:CLR:H121	2.02	0.42
5:B:905:CLR:H121	5:B:905:CLR:H212	2.02	0.42
5:B:910:CLR:H121	5:B:910:CLR:H212	2.02	0.41
1:A:243:MET:HE2	1:A:243:MET:HB3	1.90	0.41
5:A:1004:CLR:H121	5:A:1004:CLR:H212	2.02	0.41
5:B:908:CLR:H121	5:B:908:CLR:H212	2.02	0.41
5:B:907:CLR:H121	5:B:907:CLR:H212	2.02	0.41
1:A:562:TRP:CD1	1:A:564:LYS:H	2.39	0.41
1:A:824:MET:CE	5:A:1005:CLR:H122	2.49	0.41
2:B:701:ILE:CG1	5:B:911:CLR:H263	2.50	0.41
2:B:743:LYS:O	2:B:747:LEU:HB2	2.20	0.41
5:B:903:CLR:H121	5:B:903:CLR:H212	2.02	0.41
5:A:1003:CLR:H121	5:A:1003:CLR:H212	2.02	0.41
5:B:912:CLR:H121	5:B:912:CLR:H212	2.02	0.41
1:A:441:MET:SD	1:A:449:LYS:NZ	2.77	0.41
5:A:1005:CLR:C7	5:A:1006:CLR:H151	2.41	0.41
2:B:669:LEU:HD12	2:B:669:LEU:HA	1.83	0.41
5:B:909:CLR:H121	5:B:909:CLR:H212	2.02	0.41
1:A:182:TRP:NE1	3:A:1001:2BV:CL2	2.91	0.41
1:A:721:ASP:OD2	1:A:777:LYS:NZ	2.35	0.41
5:A:1007:CLR:H212	5:A:1007:CLR:H121	2.02	0.41
2:B:650:ASN:OD1	2:B:650:ASN:N	2.52	0.41
2:B:694:MET:CE	5:B:910:CLR:H71	2.51	0.41
2:B:703:CYS:SG	4:B:901:UNL:C07	3.09	0.41
5:A:1006:CLR:H121	5:A:1006:CLR:H212	2.02	0.41
5:B:902:CLR:H212	5:B:902:CLR:H121	2.03	0.41
2:B:54:PRO:HD2	2:B:97:TYR:CD1	2.42	0.40
5:B:906:CLR:H212	5:B:906:CLR:H121	2.02	0.40
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.93	0.40
1:A:854:VAL:O	1:A:858:ARG:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ILE:CG2	2:B:93:LEU:CB	2.99	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	677/771 (88%)	636 (94%)	41 (6%)	0	100	100
2	B	667/822 (81%)	612 (92%)	55 (8%)	0	100	100
All	All	1344/1593 (84%)	1248 (93%)	96 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	593/669 (89%)	589 (99%)	4 (1%)	76	78
2	B	589/713 (83%)	589 (100%)	0	100	100
All	All	1182/1382 (86%)	1178 (100%)	4 (0%)	84	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	VAL
1	A	428	VAL
1	A	666	ARG
1	A	794	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	A	482	ASN
1	A	613	ASN
1	A	631	ASN
1	A	657	ASN
1	A	757	GLN
1	A	830	GLN
2	B	326	GLN
2	B	503	ASN
2	B	506	ASN
2	B	652	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are unknown - leaving 17 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
5	CLR	B	902	-	31,31,31	0.83	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	B	909	-	31,31,31	0.84	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	A	1006	-	31,31,31	0.84	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	A	1003	-	31,31,31	0.83	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	A	1007	-	31,31,31	0.83	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	B	908	-	31,31,31	0.83	1 (3%)	48,48,48	1.26	5 (10%)
5	CLR	B	903	-	31,31,31	0.83	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	B	906	-	31,31,31	0.84	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	A	1004	-	31,31,31	0.83	1 (3%)	48,48,48	1.26	5 (10%)
5	CLR	B	907	-	31,31,31	0.83	1 (3%)	48,48,48	1.26	5 (10%)
5	CLR	B	905	-	31,31,31	0.84	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	B	910	-	31,31,31	0.84	1 (3%)	48,48,48	1.26	5 (10%)
5	CLR	B	912	-	31,31,31	0.83	1 (3%)	48,48,48	1.27	5 (10%)
3	2BV	A	1001	-	23,26,26	1.53	4 (17%)	26,36,36	1.51	6 (23%)
5	CLR	B	911	-	31,31,31	0.83	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	A	1005	-	31,31,31	0.84	1 (3%)	48,48,48	1.27	5 (10%)
5	CLR	B	904	-	31,31,31	0.82	1 (3%)	48,48,48	1.26	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLR	B	902	-	-	0/10/68/68	0/4/4/4
5	CLR	B	909	-	-	0/10/68/68	0/4/4/4
5	CLR	A	1006	-	-	0/10/68/68	0/4/4/4
5	CLR	A	1003	-	-	0/10/68/68	0/4/4/4
5	CLR	A	1007	-	-	0/10/68/68	0/4/4/4
5	CLR	B	908	-	-	0/10/68/68	0/4/4/4
5	CLR	B	903	-	-	0/10/68/68	0/4/4/4
5	CLR	B	906	-	-	0/10/68/68	0/4/4/4
5	CLR	A	1004	-	-	0/10/68/68	0/4/4/4
5	CLR	B	907	-	-	0/10/68/68	0/4/4/4
5	CLR	B	905	-	-	0/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLR	B	910	-	-	0/10/68/68	0/4/4/4
5	CLR	B	912	-	-	0/10/68/68	0/4/4/4
3	2BV	A	1001	-	-	1/19/27/27	0/2/2/2
5	CLR	B	911	-	-	0/10/68/68	0/4/4/4
5	CLR	A	1005	-	-	0/10/68/68	0/4/4/4
5	CLR	B	904	-	-	0/10/68/68	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	2BV	C5-C6	4.38	1.49	1.39
3	A	1001	2BV	P-C11	2.94	1.82	1.79
3	A	1001	2BV	C6-CL1	2.78	1.80	1.73
3	A	1001	2BV	P-C12	2.73	1.82	1.79
5	A	1005	CLR	C20-C17	2.43	1.58	1.54
5	B	909	CLR	C20-C17	2.42	1.58	1.54
5	B	905	CLR	C20-C17	2.42	1.58	1.54
5	A	1006	CLR	C20-C17	2.41	1.58	1.54
5	B	911	CLR	C20-C17	2.40	1.58	1.54
5	B	902	CLR	C20-C17	2.40	1.58	1.54
5	A	1003	CLR	C20-C17	2.39	1.58	1.54
5	B	906	CLR	C20-C17	2.39	1.58	1.54
5	B	908	CLR	C20-C17	2.39	1.58	1.54
5	A	1004	CLR	C20-C17	2.39	1.58	1.54
5	B	910	CLR	C20-C17	2.38	1.58	1.54
5	B	907	CLR	C20-C17	2.38	1.58	1.54
5	B	904	CLR	C20-C17	2.36	1.58	1.54
5	B	912	CLR	C20-C17	2.35	1.58	1.54
5	A	1007	CLR	C20-C17	2.35	1.58	1.54
5	B	903	CLR	C20-C17	2.35	1.58	1.54

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	902	CLR	C8-C7-C6	-3.21	108.32	112.76
5	B	904	CLR	C8-C7-C6	-3.21	108.32	112.76
5	B	903	CLR	C8-C7-C6	-3.20	108.33	112.76
5	A	1007	CLR	C8-C7-C6	-3.19	108.34	112.76
5	B	905	CLR	C8-C7-C6	-3.19	108.35	112.76
5	B	906	CLR	C8-C7-C6	-3.18	108.36	112.76
5	A	1005	CLR	C8-C7-C6	-3.18	108.36	112.76
5	A	1004	CLR	C8-C7-C6	-3.17	108.37	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	909	CLR	C8-C7-C6	-3.17	108.38	112.76
5	B	908	CLR	C8-C7-C6	-3.16	108.38	112.76
5	B	912	CLR	C8-C7-C6	-3.16	108.38	112.76
5	B	911	CLR	C8-C7-C6	-3.16	108.39	112.76
5	A	1006	CLR	C8-C7-C6	-3.15	108.40	112.76
5	A	1003	CLR	C8-C7-C6	-3.14	108.41	112.76
5	B	910	CLR	C8-C7-C6	-3.14	108.41	112.76
5	B	907	CLR	C8-C7-C6	-3.14	108.41	112.76
5	B	903	CLR	C10-C9-C8	-3.09	108.20	112.71
5	A	1006	CLR	C10-C9-C8	-3.09	108.20	112.71
5	A	1007	CLR	C10-C9-C8	-3.08	108.21	112.71
5	A	1005	CLR	C10-C9-C8	-3.07	108.22	112.71
5	B	912	CLR	C10-C9-C8	-3.07	108.23	112.71
5	B	906	CLR	C10-C9-C8	-3.07	108.23	112.71
5	B	905	CLR	C10-C9-C8	-3.07	108.23	112.71
5	B	904	CLR	C10-C9-C8	-3.06	108.24	112.71
5	B	902	CLR	C10-C9-C8	-3.06	108.24	112.71
5	A	1003	CLR	C10-C9-C8	-3.06	108.24	112.71
5	B	911	CLR	C10-C9-C8	-3.05	108.26	112.71
5	A	1004	CLR	C10-C9-C8	-3.04	108.27	112.71
5	B	908	CLR	C10-C9-C8	-3.03	108.28	112.71
5	B	909	CLR	C10-C9-C8	-3.03	108.28	112.71
5	B	907	CLR	C10-C9-C8	-3.02	108.30	112.71
5	B	910	CLR	C10-C9-C8	-3.01	108.31	112.71
3	A	1001	2BV	C1-C2-N	2.82	113.93	108.74
5	B	905	CLR	C13-C17-C20	-2.54	115.57	119.50
3	A	1001	2BV	C17-C18-C13	2.54	117.42	112.08
5	A	1005	CLR	C13-C17-C20	-2.53	115.59	119.50
5	B	902	CLR	C13-C17-C20	-2.53	115.59	119.50
5	B	906	CLR	C13-C17-C20	-2.52	115.60	119.50
5	A	1006	CLR	C13-C17-C20	-2.52	115.61	119.50
5	B	912	CLR	C13-C17-C20	-2.52	115.61	119.50
5	B	903	CLR	C13-C17-C20	-2.52	115.61	119.50
5	A	1007	CLR	C13-C17-C20	-2.51	115.61	119.50
3	A	1001	2BV	C7-C6-CL1	2.51	123.37	118.42
5	B	908	CLR	C13-C17-C20	-2.51	115.62	119.50
5	A	1004	CLR	C13-C17-C20	-2.50	115.64	119.50
5	B	911	CLR	C13-C17-C20	-2.50	115.64	119.50
5	A	1003	CLR	C13-C17-C20	-2.49	115.65	119.50
5	B	909	CLR	C13-C17-C20	-2.49	115.66	119.50
5	B	910	CLR	C13-C17-C20	-2.48	115.66	119.50
5	B	907	CLR	C13-C17-C20	-2.48	115.66	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	904	CLR	C13-C17-C20	-2.48	115.67	119.50
5	B	906	CLR	C23-C22-C20	-2.45	108.22	115.08
5	B	909	CLR	C23-C22-C20	-2.45	108.22	115.08
5	B	912	CLR	C11-C9-C8	2.44	115.19	111.78
5	A	1004	CLR	C23-C22-C20	-2.44	108.26	115.08
5	A	1005	CLR	C23-C22-C20	-2.44	108.26	115.08
5	A	1006	CLR	C11-C9-C8	2.44	115.18	111.78
5	B	908	CLR	C11-C9-C8	2.44	115.18	111.78
5	B	908	CLR	C23-C22-C20	-2.44	108.26	115.08
5	B	910	CLR	C23-C22-C20	-2.44	108.26	115.08
5	B	911	CLR	C23-C22-C20	-2.44	108.26	115.08
5	A	1003	CLR	C23-C22-C20	-2.44	108.26	115.08
5	B	903	CLR	C23-C22-C20	-2.43	108.27	115.08
5	B	905	CLR	C23-C22-C20	-2.43	108.27	115.08
5	B	912	CLR	C23-C22-C20	-2.43	108.27	115.08
5	B	906	CLR	C11-C9-C8	2.43	115.17	111.78
5	A	1006	CLR	C23-C22-C20	-2.43	108.27	115.08
5	B	905	CLR	C11-C9-C8	2.43	115.17	111.78
5	B	903	CLR	C11-C9-C8	2.43	115.16	111.78
5	A	1007	CLR	C23-C22-C20	-2.43	108.29	115.08
5	A	1005	CLR	C11-C9-C8	2.43	115.16	111.78
5	B	911	CLR	C11-C9-C8	2.42	115.16	111.78
5	B	904	CLR	C23-C22-C20	-2.42	108.31	115.08
5	B	902	CLR	C23-C22-C20	-2.42	108.31	115.08
5	B	907	CLR	C23-C22-C20	-2.42	108.31	115.08
5	A	1003	CLR	C11-C9-C8	2.42	115.15	111.78
5	A	1004	CLR	C11-C9-C8	2.42	115.15	111.78
5	B	909	CLR	C11-C9-C8	2.41	115.14	111.78
5	B	907	CLR	C11-C9-C8	2.41	115.14	111.78
5	A	1007	CLR	C11-C9-C8	2.40	115.13	111.78
5	B	904	CLR	C11-C9-C8	2.40	115.13	111.78
5	B	910	CLR	C11-C9-C8	2.40	115.13	111.78
5	B	902	CLR	C11-C9-C8	2.39	115.11	111.78
3	A	1001	2BV	C8-C3-C4	2.32	121.43	118.74
3	A	1001	2BV	C4-C5-CL2	2.08	121.85	118.45
3	A	1001	2BV	C16-C17-C18	2.02	115.56	111.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

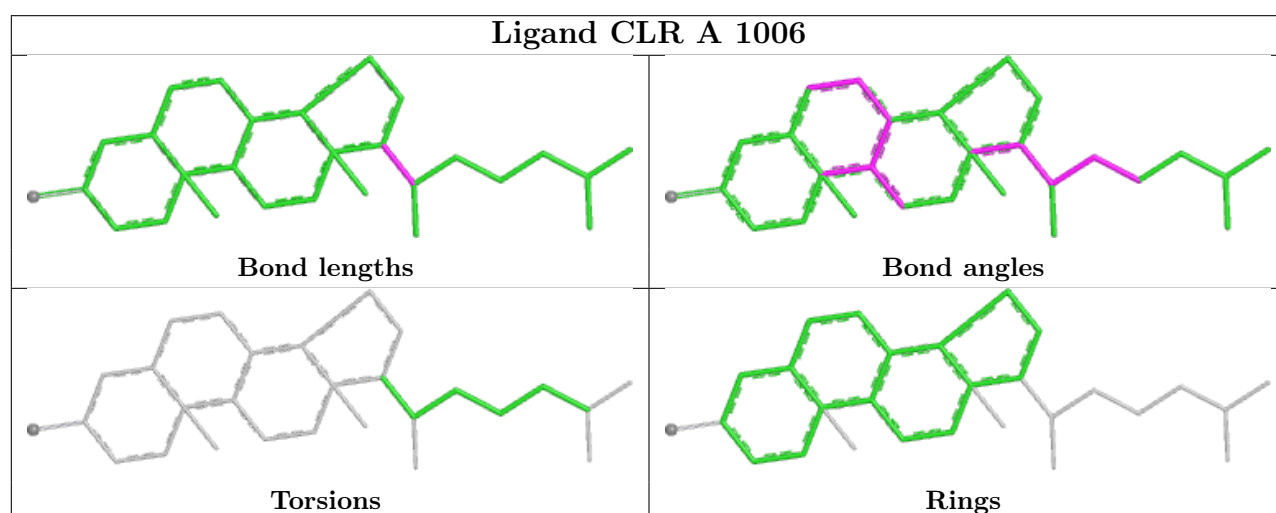
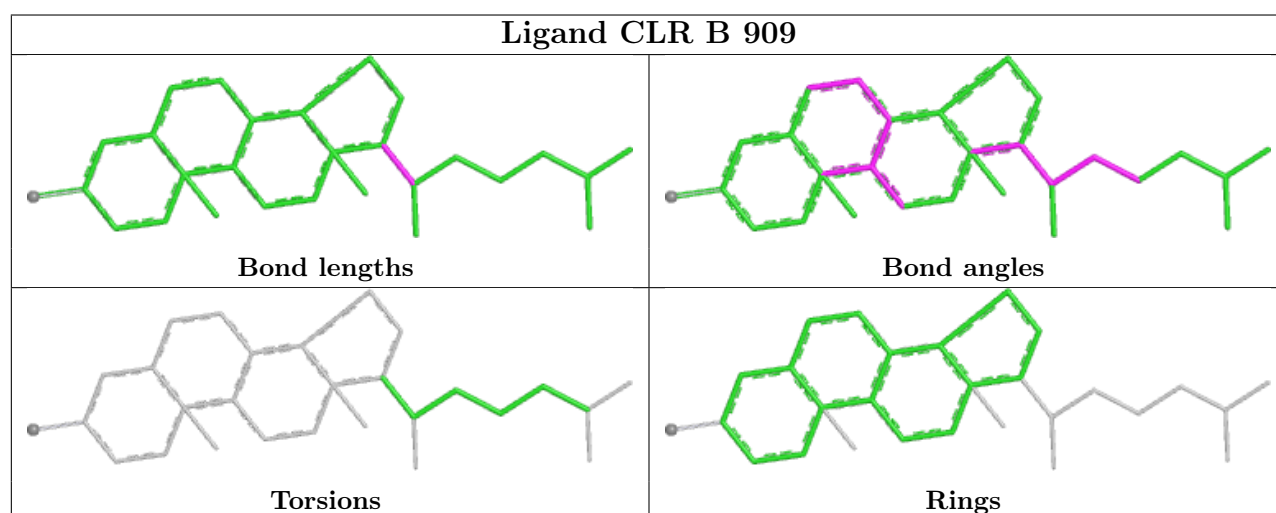
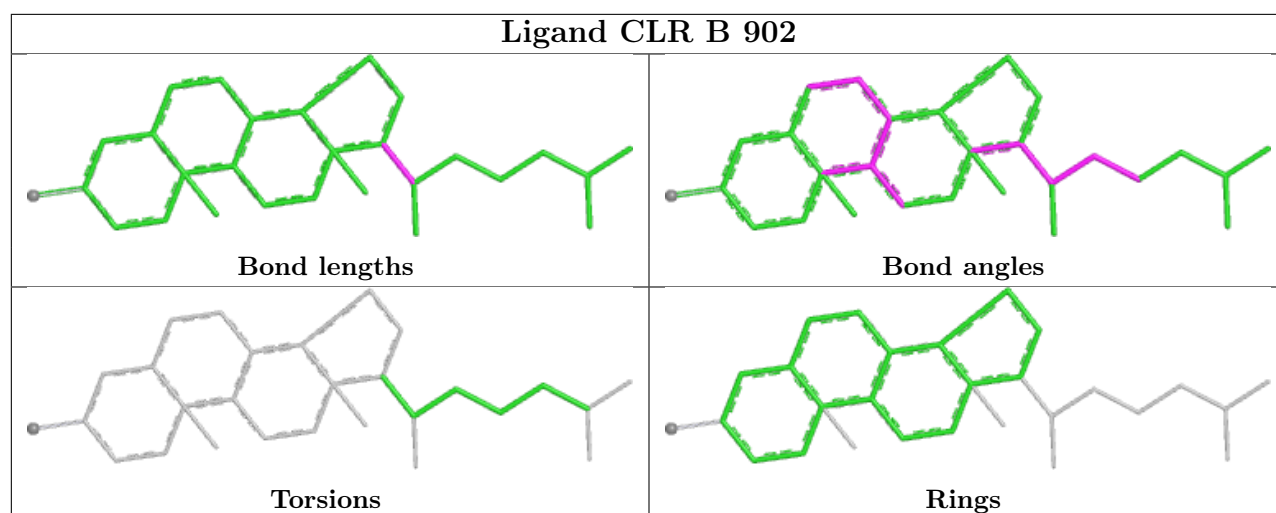
Mol	Chain	Res	Type	Atoms
3	A	1001	2BV	C10-C9-N-C2

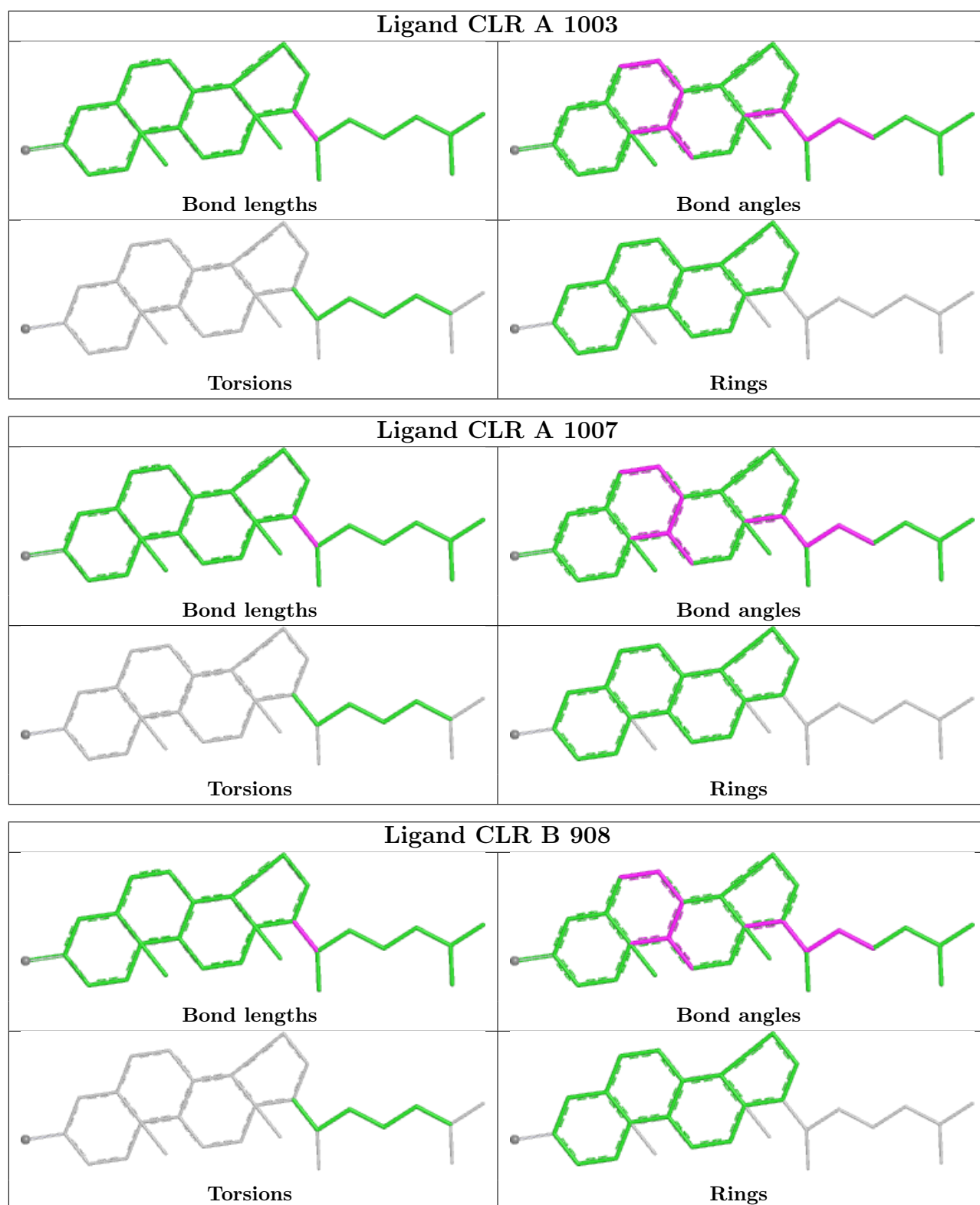
There are no ring outliers.

17 monomers are involved in 136 short contacts:

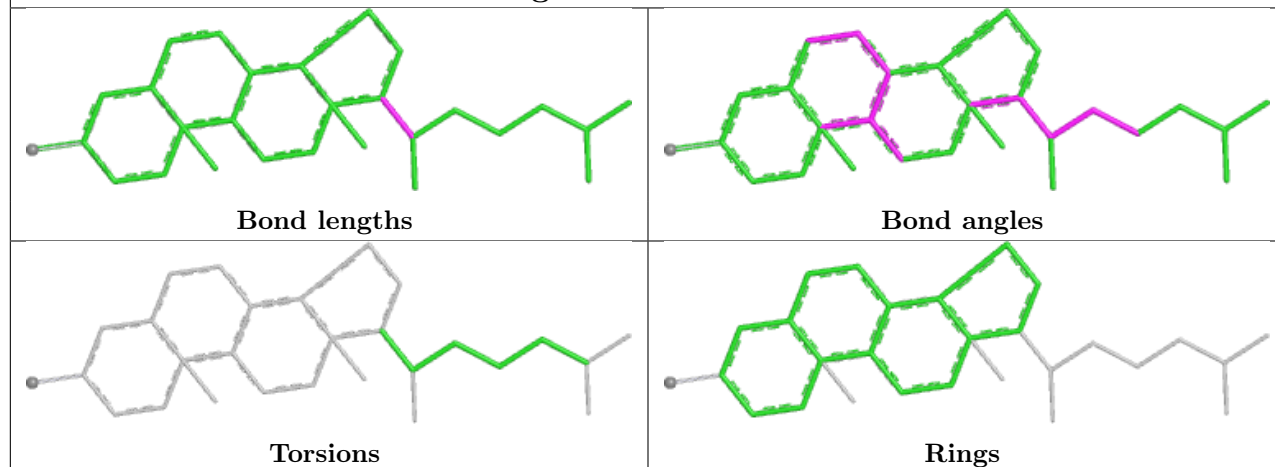
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	CLR	2	0
5	B	909	CLR	1	0
5	A	1006	CLR	14	0
5	A	1003	CLR	8	0
5	A	1007	CLR	6	0
5	B	908	CLR	16	0
5	B	903	CLR	3	0
5	B	906	CLR	5	0
5	A	1004	CLR	25	0
5	B	907	CLR	4	0
5	B	905	CLR	5	0
5	B	910	CLR	4	0
5	B	912	CLR	36	0
3	A	1001	2BV	16	0
5	B	911	CLR	9	0
5	A	1005	CLR	15	0
5	B	904	CLR	6	0

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

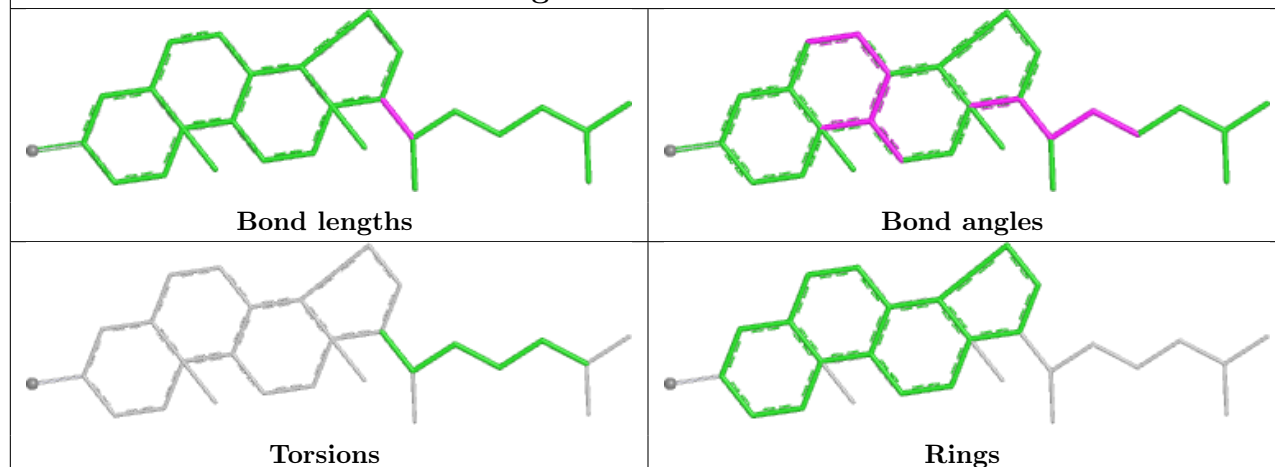




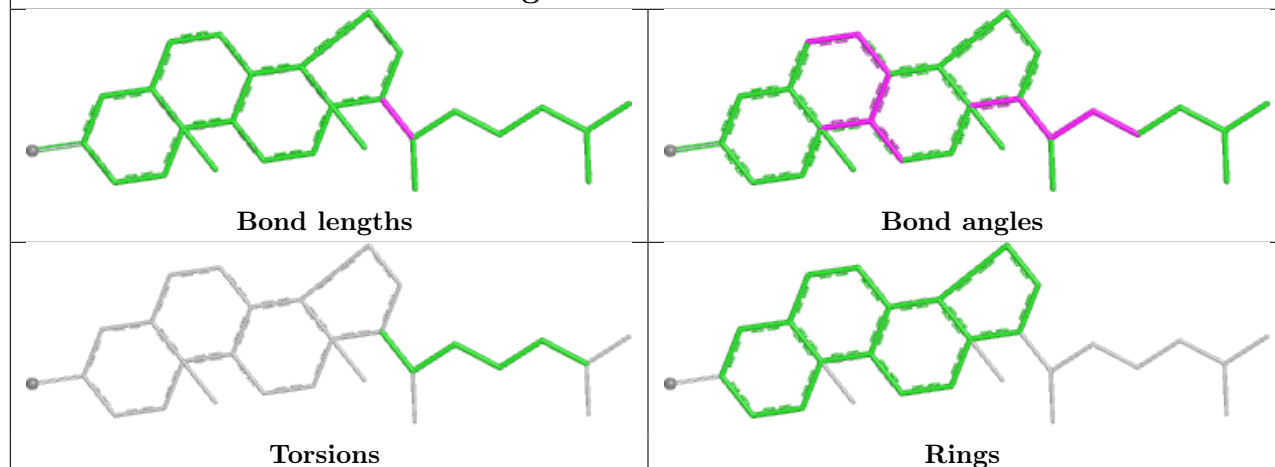
Ligand CLR B 903

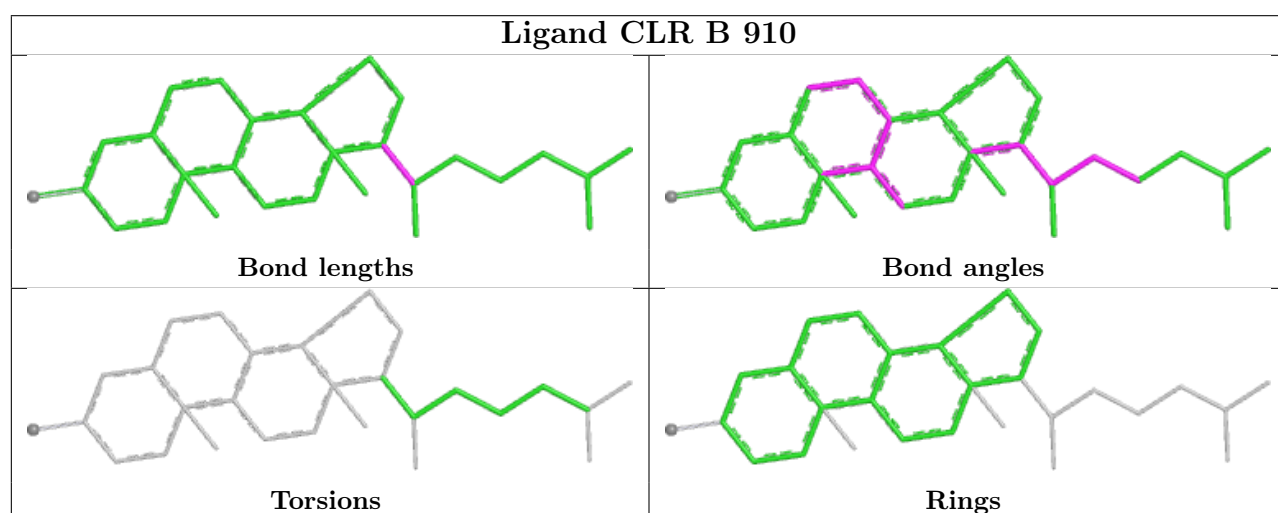
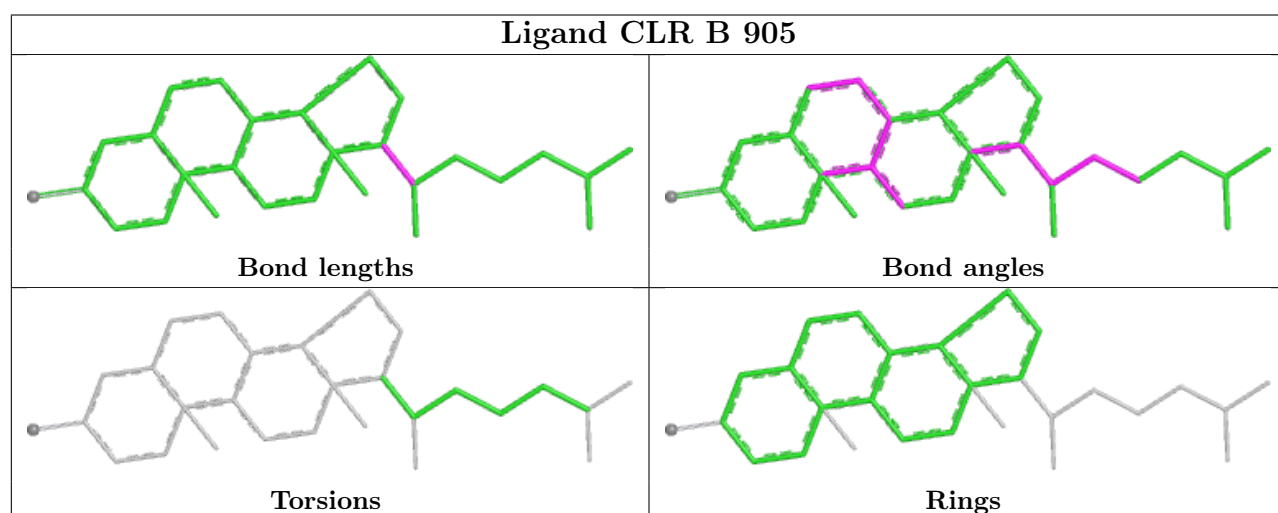
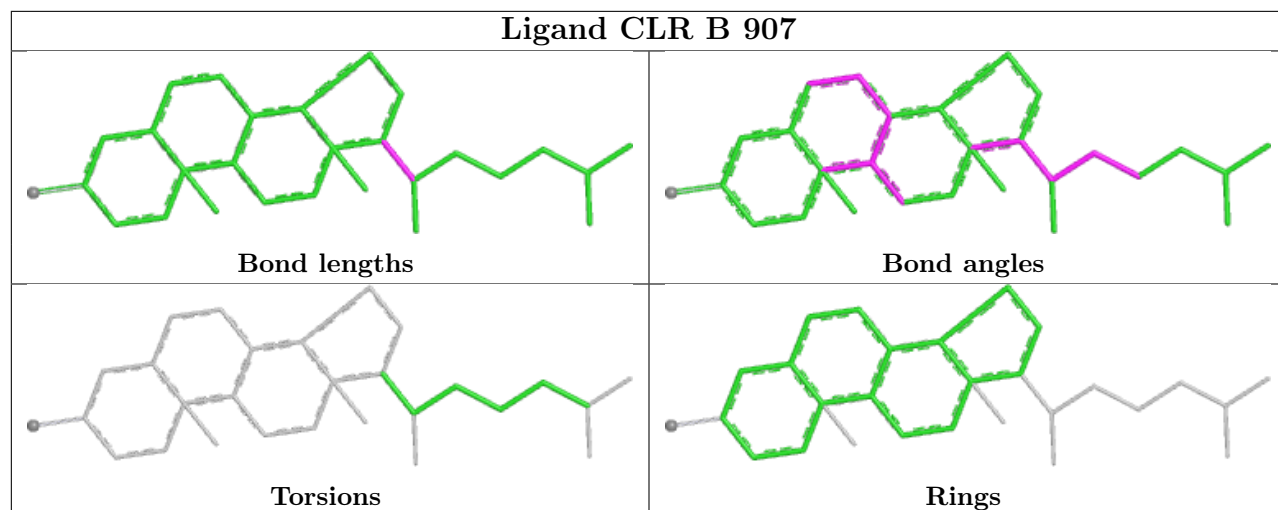


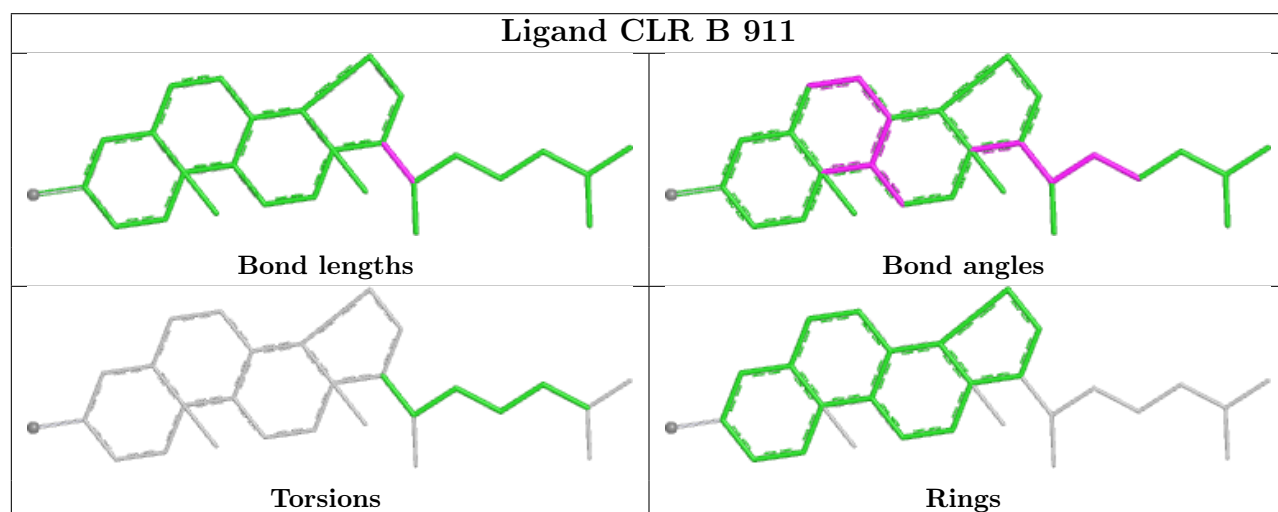
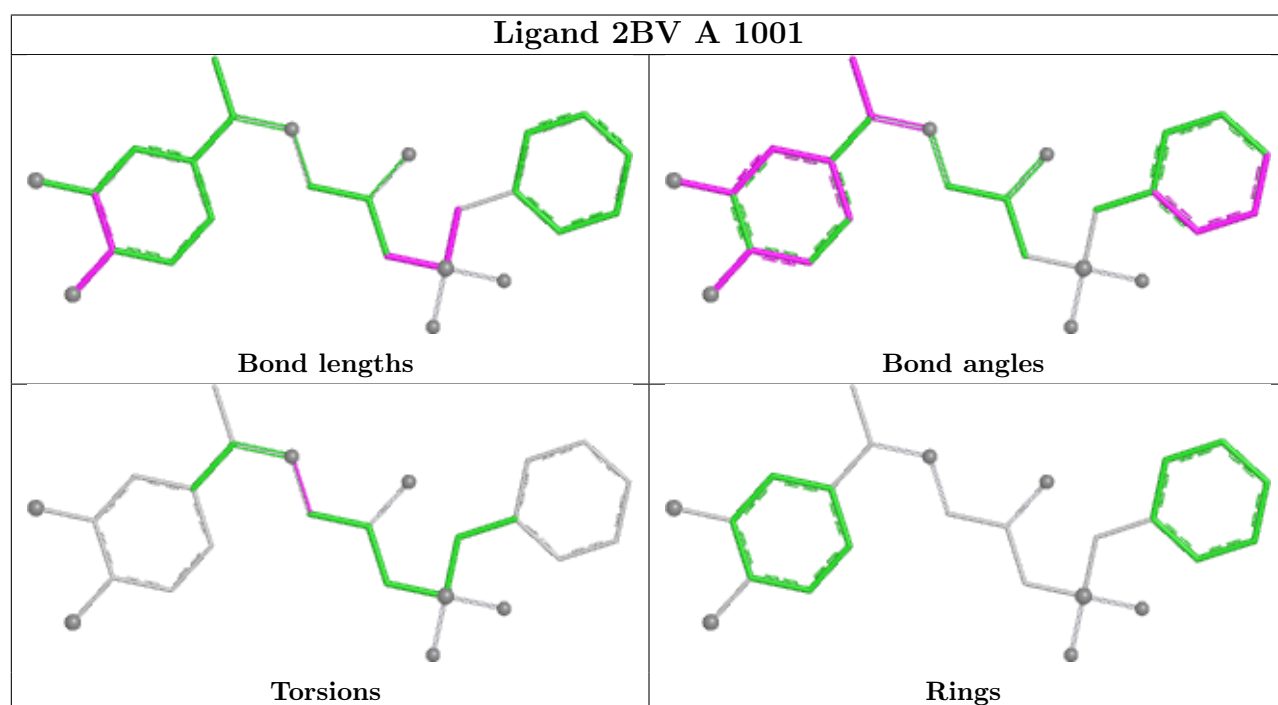
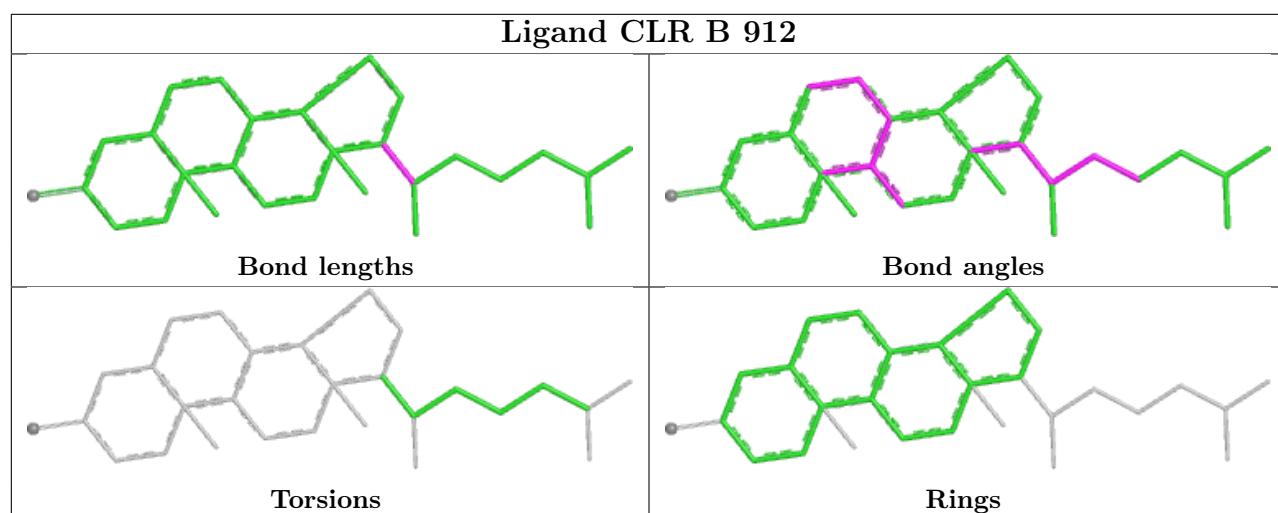
Ligand CLR B 906

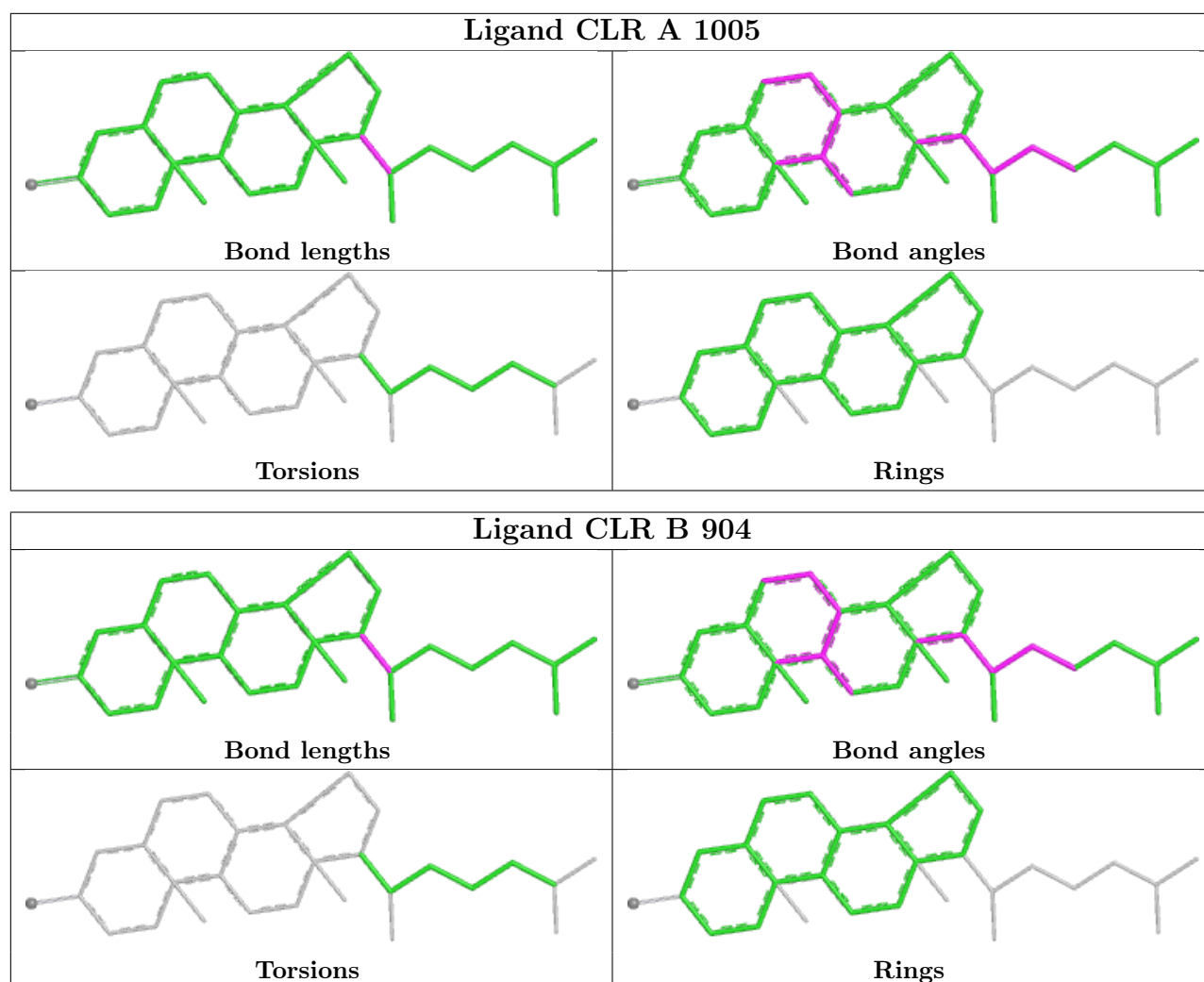


Ligand CLR A 1004









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.

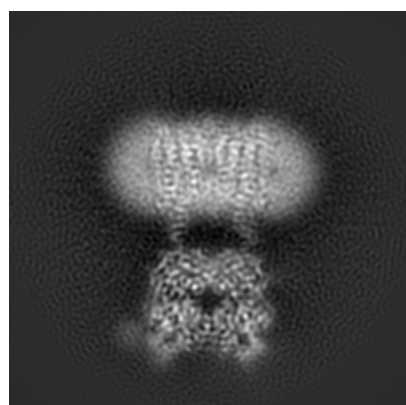
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30472. These allow visual inspection of the internal detail of the map and identification of artifacts.

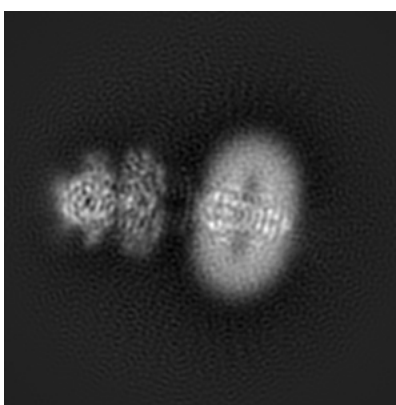
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

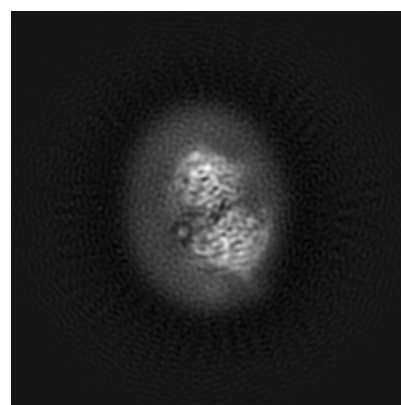
6.1.1 Primary map



X



Y

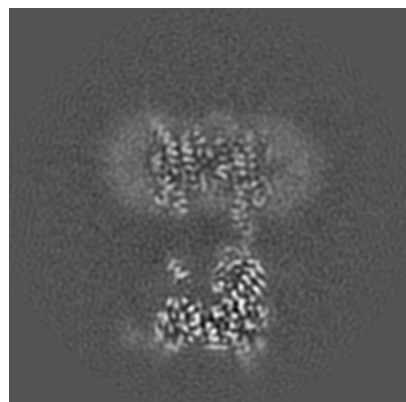


Z

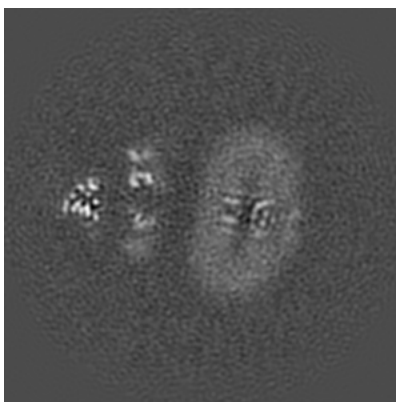
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

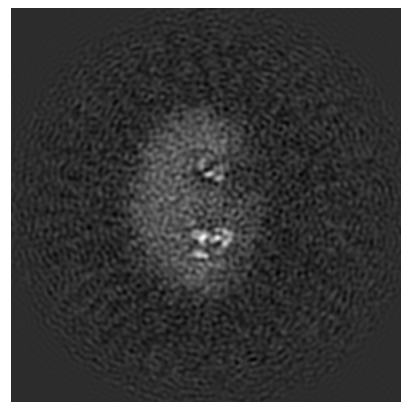
6.2.1 Primary map



X Index: 115



Y Index: 115

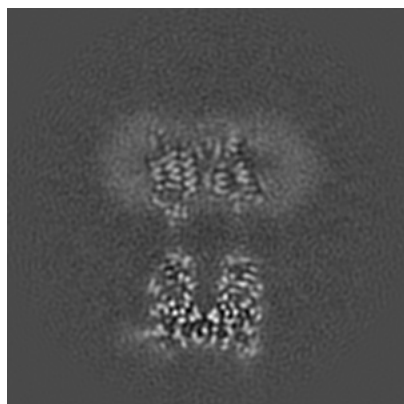


Z Index: 115

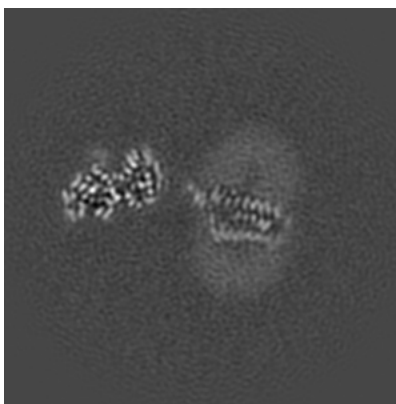
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

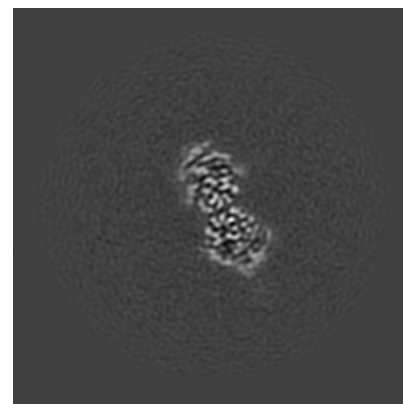
6.3.1 Primary map



X Index: 119



Y Index: 102

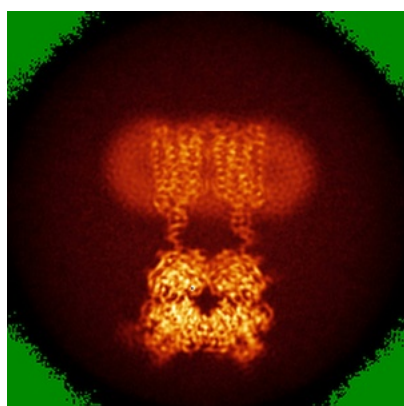


Z Index: 53

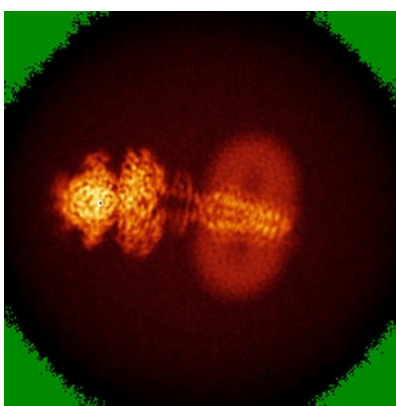
The images above show the largest variance slices of the map in three orthogonal directions.

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

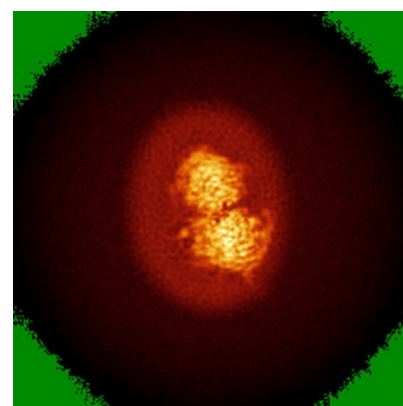
6.4.1 Primary map



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

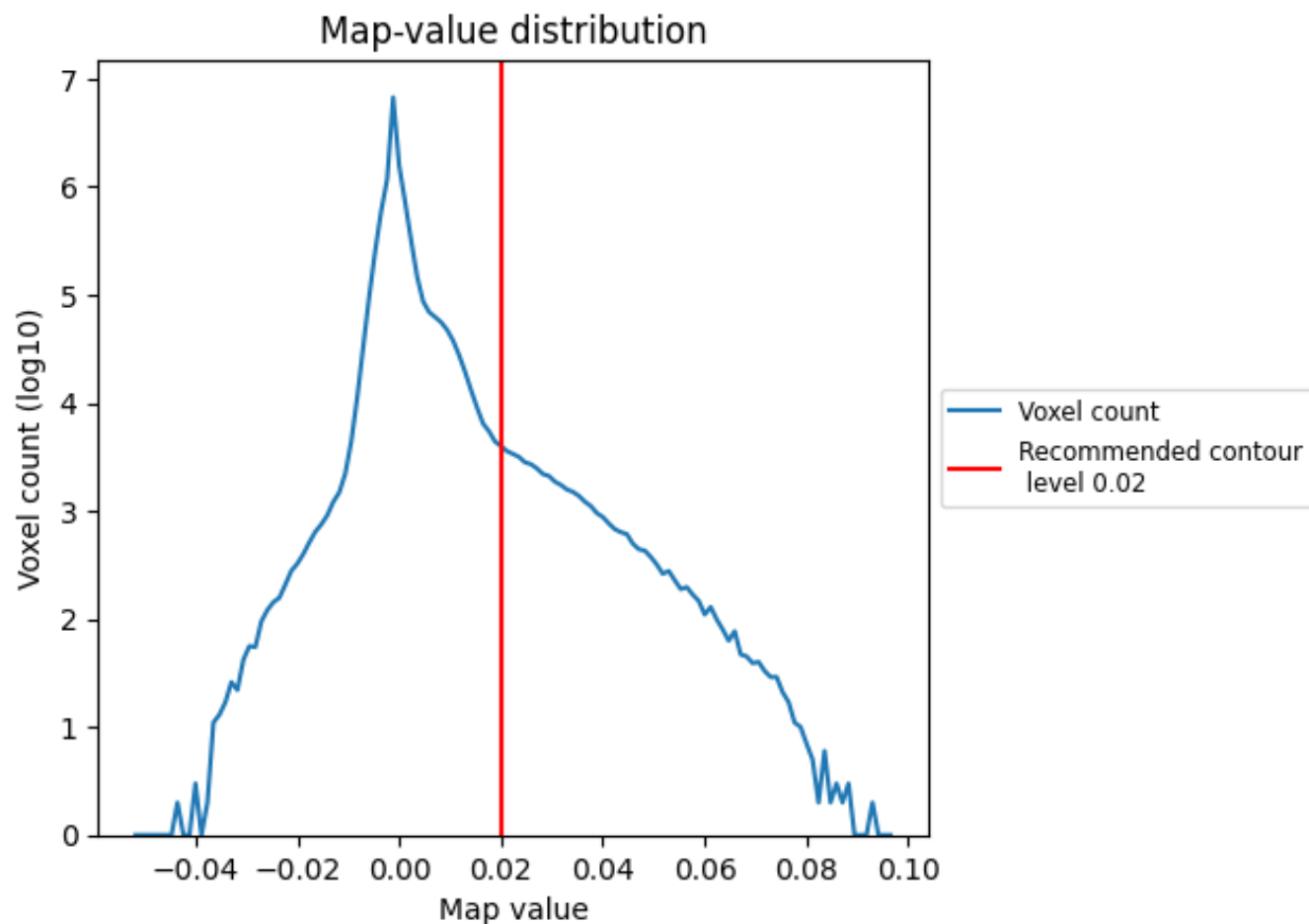
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

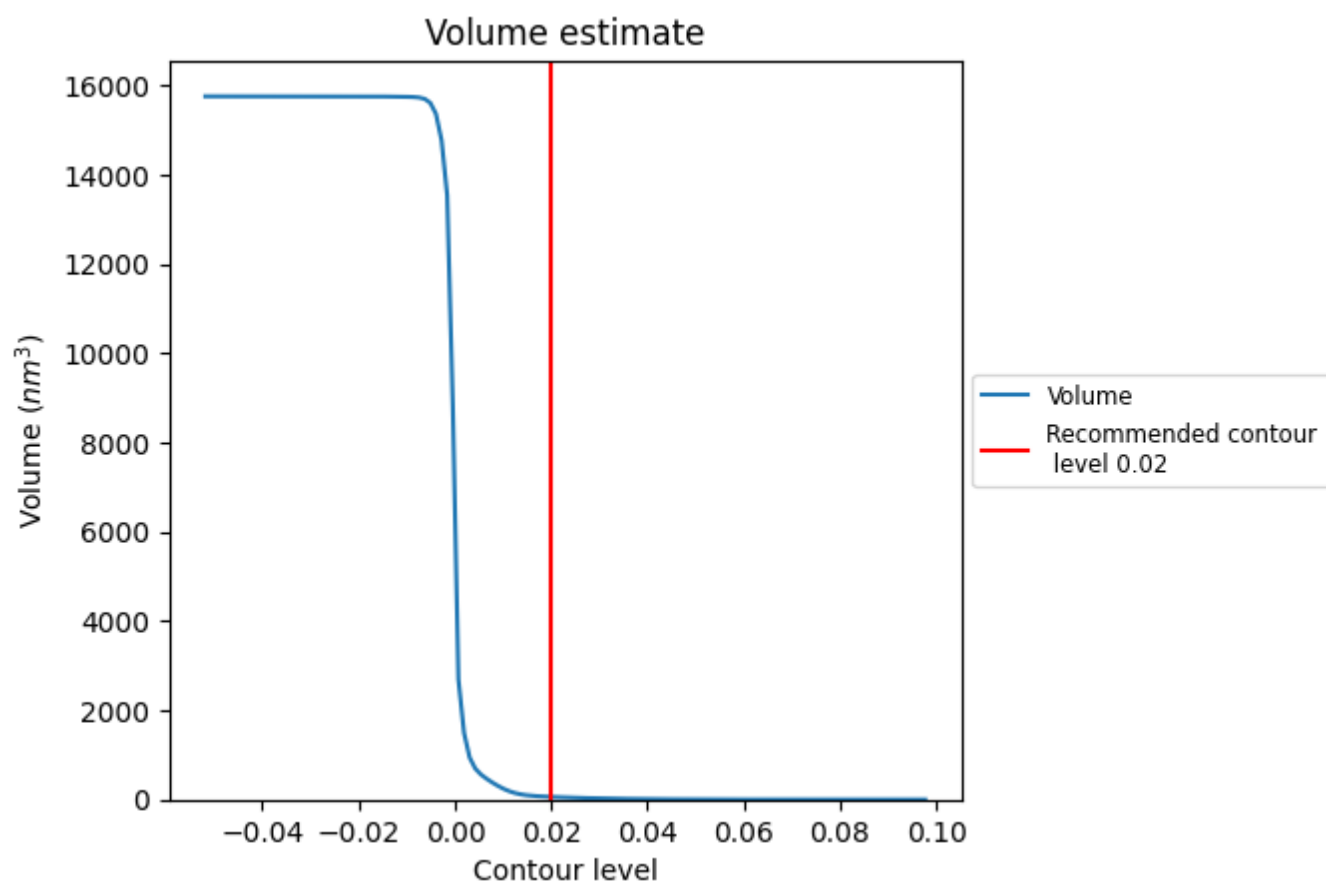
This section contains the results of statistical analysis of the map.

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.

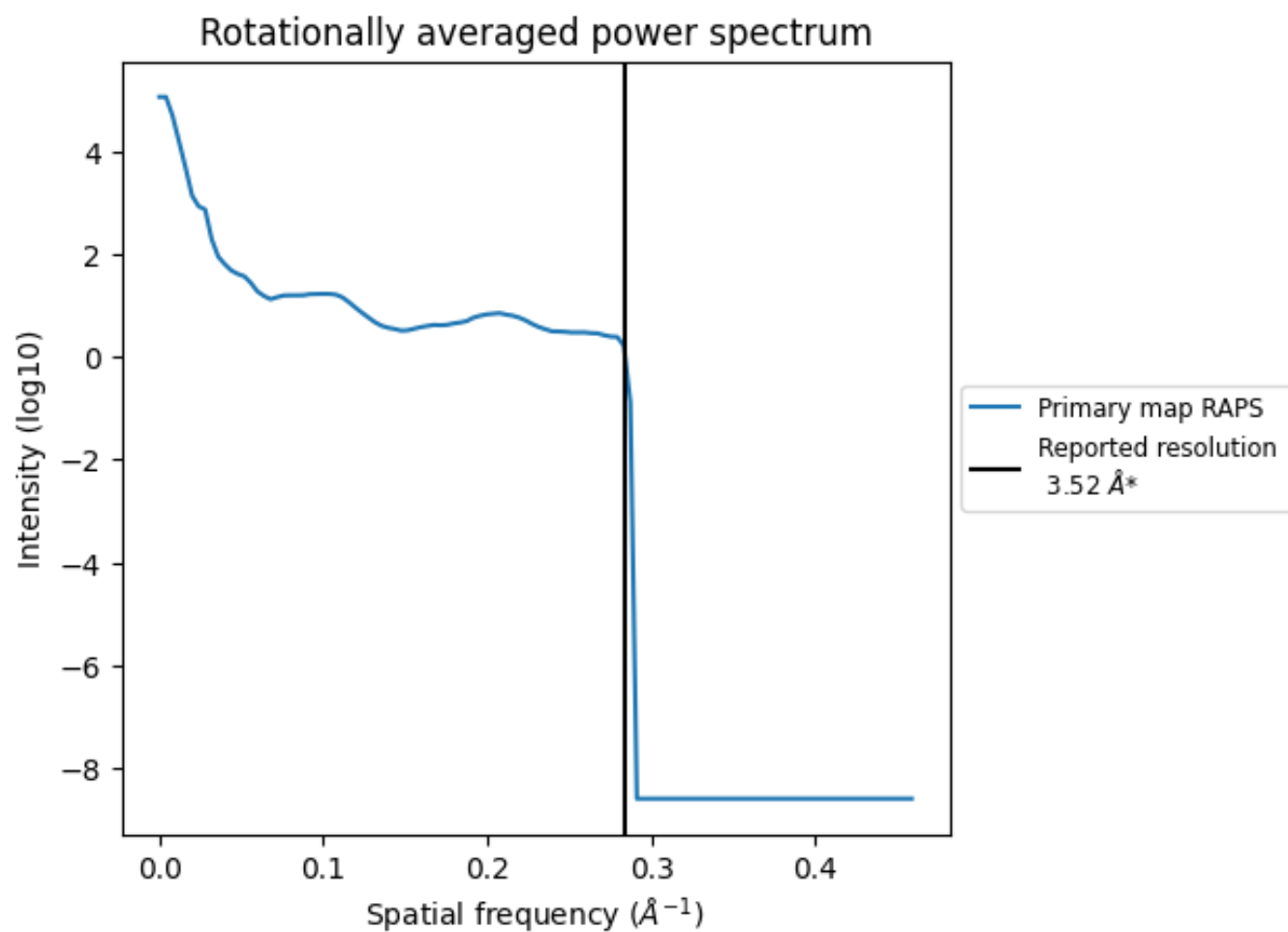
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm³; this corresponds to an approximate mass of 54 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 0.284 Å⁻¹

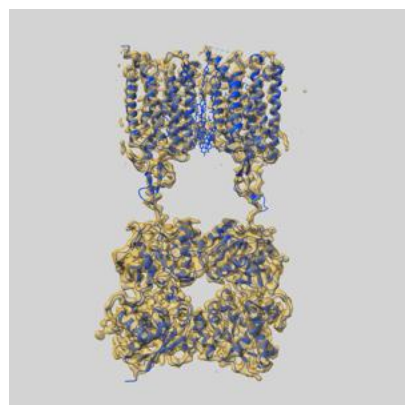
8 Fourier-Shell correlation

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

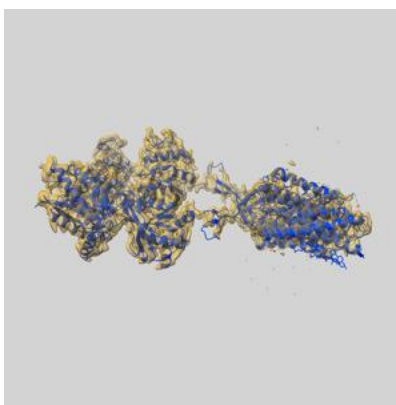
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30472 and PDB model 7CUM. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

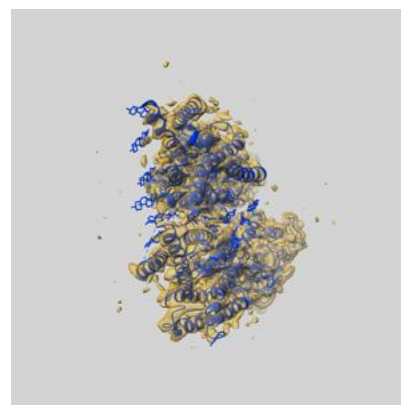
9.1 Map-model overlay [i](#)



X



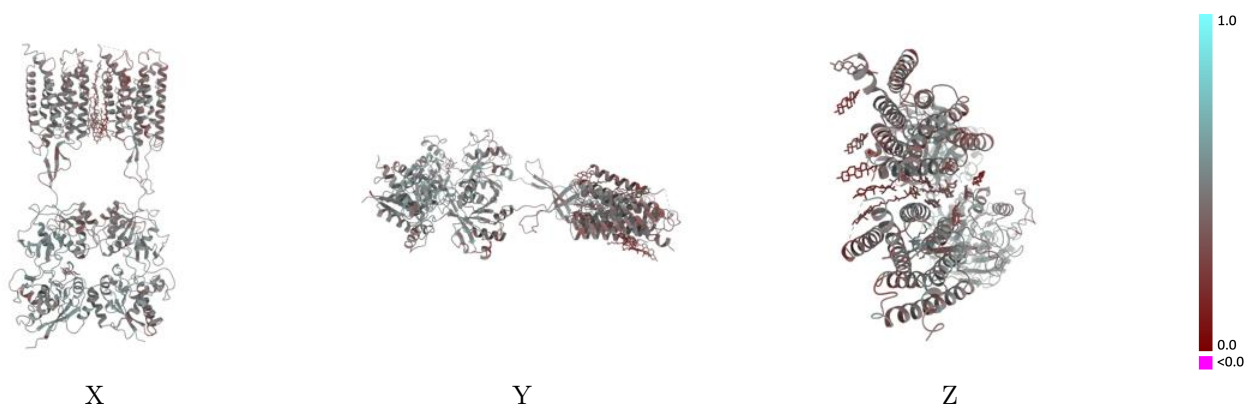
Y



Z

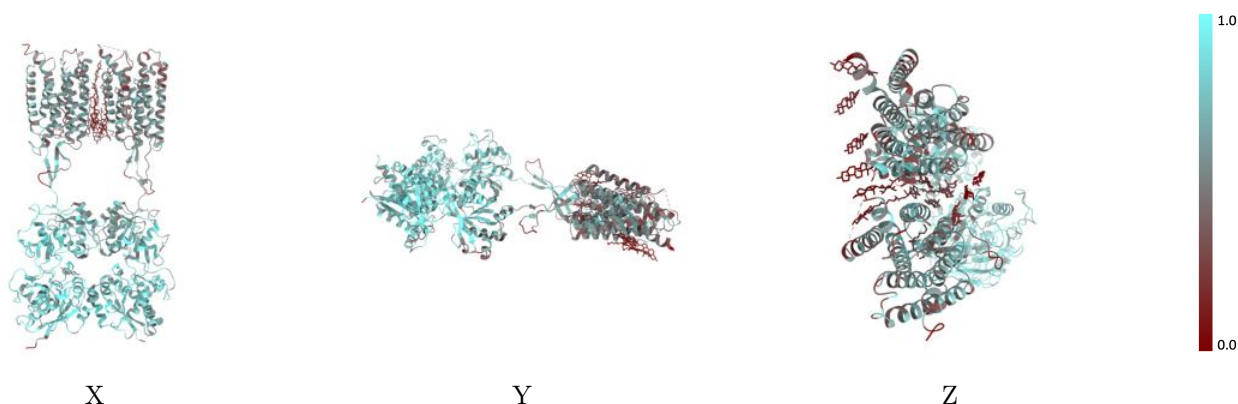
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



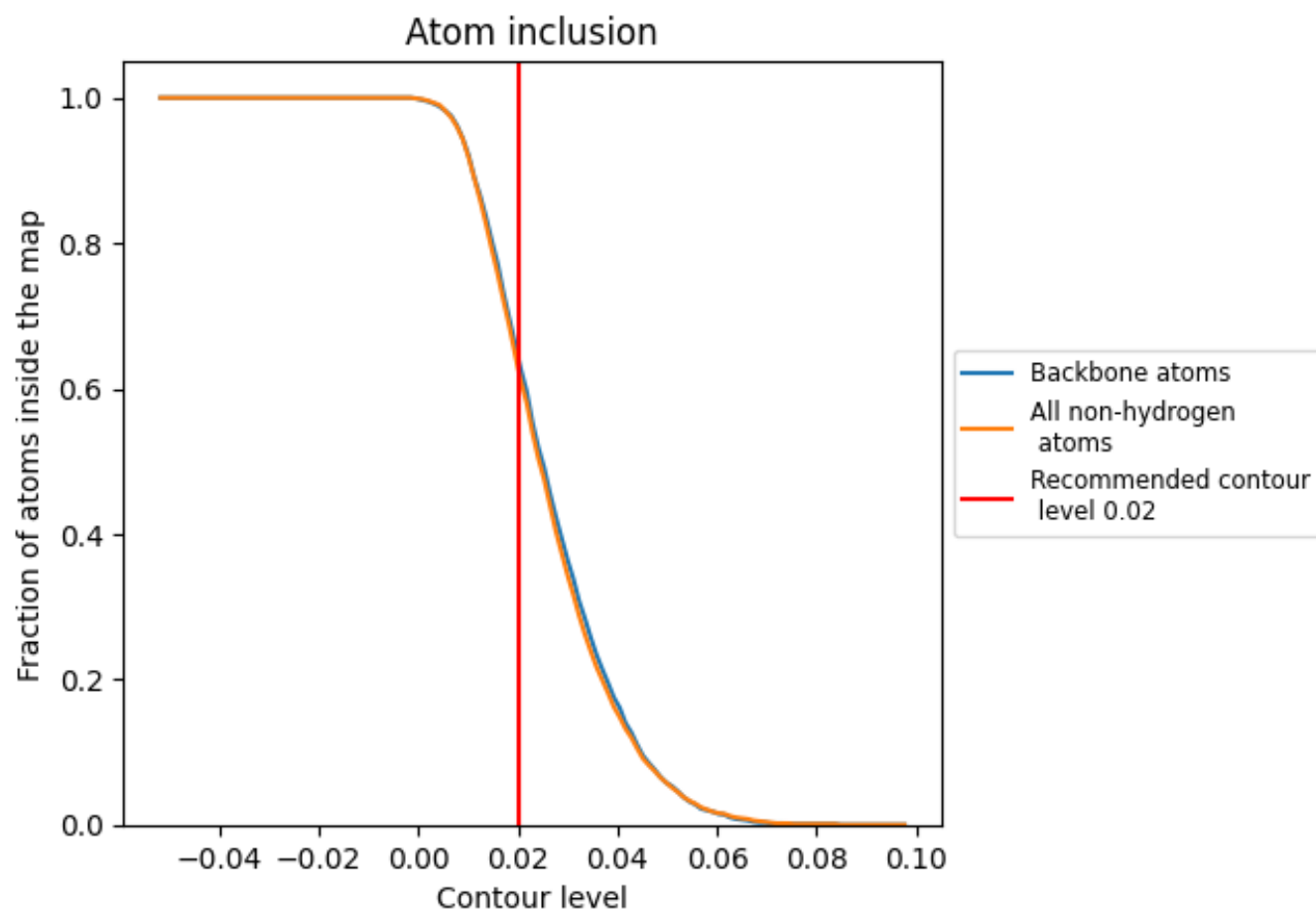
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 63% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6280	0.4590
A	0.6740	0.4720
B	0.6100	0.4460

