Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 04:51 PM JST

PDB ID	:	7CA3
EMDB ID	:	EMD-30323
Title	:	Cryo-EM structure of human GABA(B) receptor bound to the positive allosteric modulator rac-BHFF
Authors	:	Kim, Y.; Jeong, E.; Jeong, J.; Kim, Y.; Cho, Y.
Deposited on	:	2020-06-08
Resolution	:	4.50 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 (i) 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 (1)) were used in the production of this report:

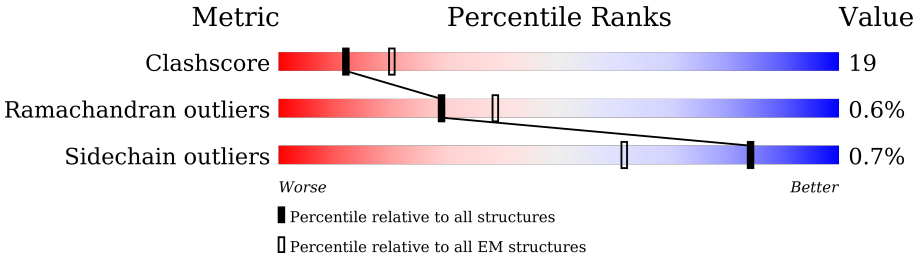
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	16% 59% 27% • 13%
2	B	822	23% 52% 30% • 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19862 atoms, of which 9307 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
			Total	C	H	N	O	S		
1	A	669	9628	3328	4491	857	928	24	0	0

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
			Total	C	H	N	O	S		
2	B	681	10127	3435	4816	887	955	34	0	0

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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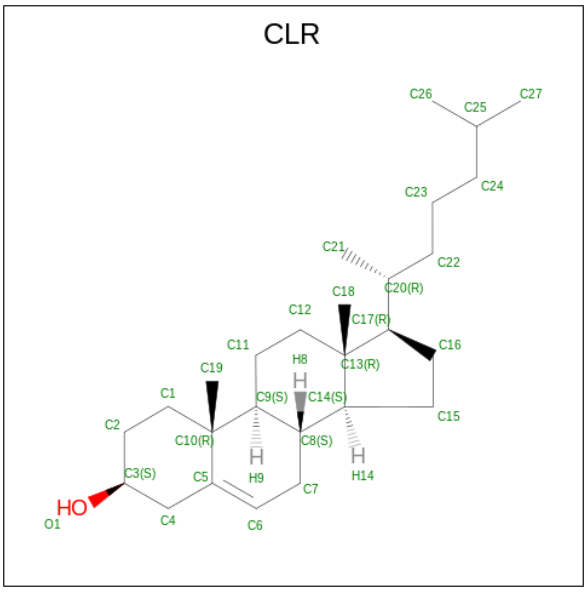
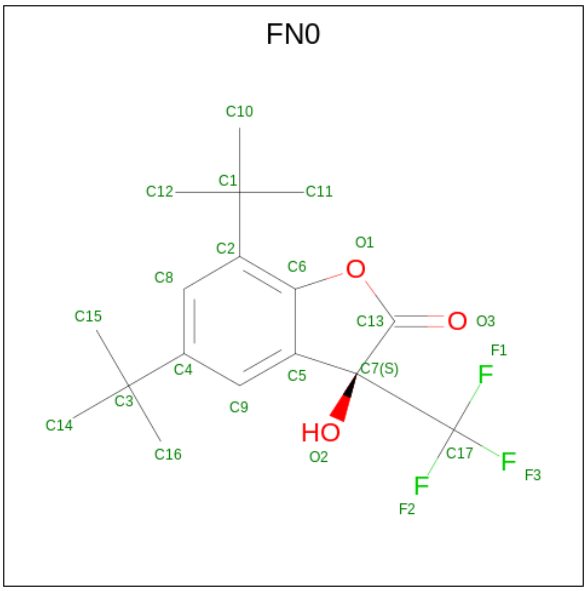
Chain	Residue	Modelled	Actual	Comment	Reference
B	813	ASP	-	expression tag	UNP O75899
B	814	LYS	-	expression tag	UNP O75899
B	815	ASP	-	expression tag	UNP O75899
B	816	TYR	-	expression tag	UNP O75899
B	817	LYS	-	expression tag	UNP O75899
B	818	ASP	-	expression tag	UNP O75899
B	819	ASP	-	expression tag	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 CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	56	54	2	0
			Total	C	O	
3	A	1	56	54	2	0
			Total	C	O	
3	B	1	28	27	1	0

- Molecule 4 is (3S)-5,7-ditert-butyl-3-oxidanyl-3-(trifluoromethyl)-1-benzofuran-2-one (three-letter code: FN0) (formula: $C_{17}H_{21}F_3O_3$) (labeled as "Ligand of Interest" by depositor).



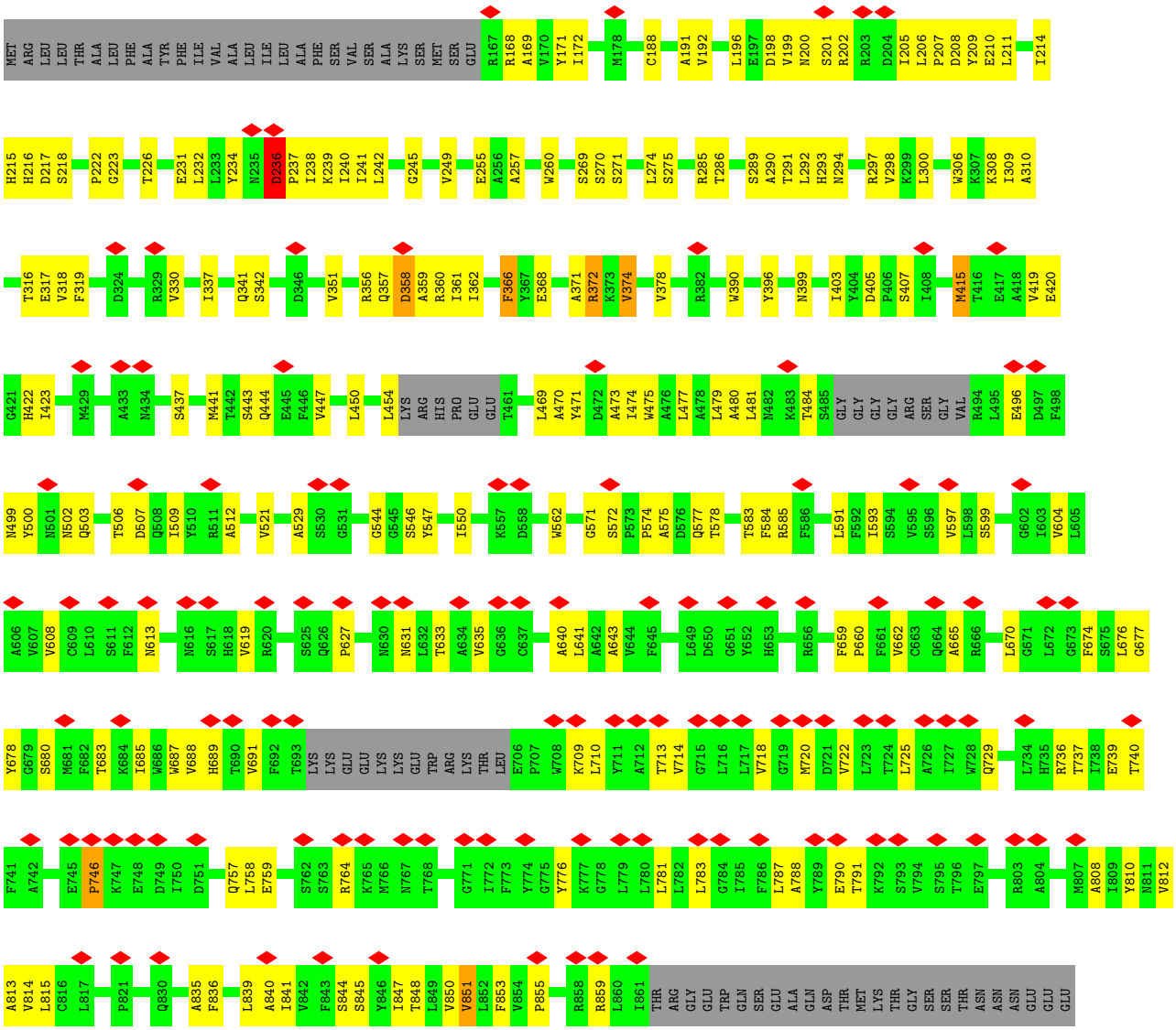
Mol	Chain	Residues	Atoms				AltConf
			Total	C	F	O	
4	B	1	23	17	3	3	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

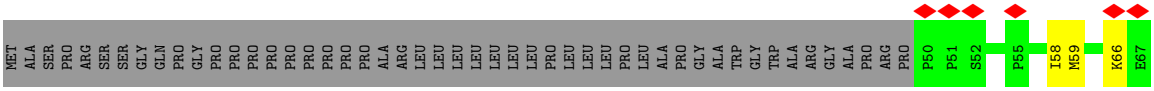
- Molecule 1: Gamma-aminobutyric acid type B receptor subunit 1

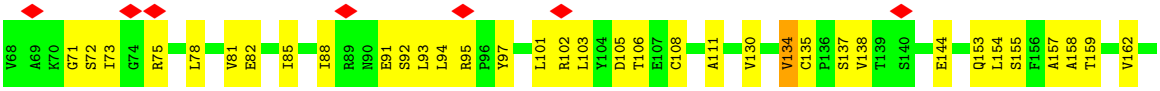
Chain A: 16% 59% 27% • 13%

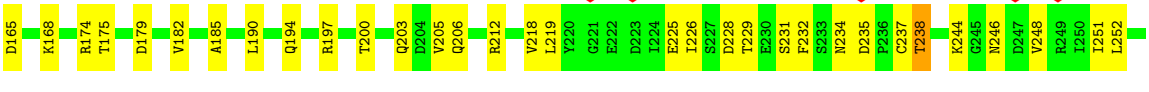


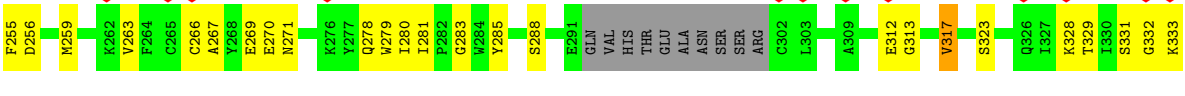
- Molecule 2: Gamma-aminobutyric acid type B receptor subunit 2

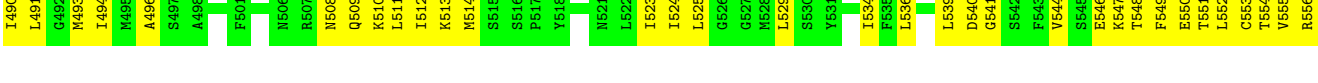
Chain B:

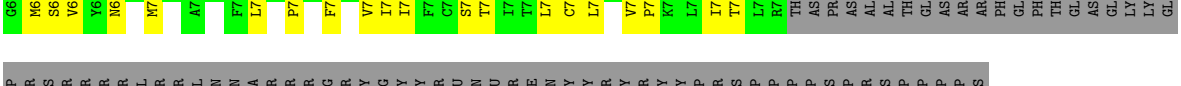












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	294926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	41.05, 41.05, 41.05	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), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.029	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, FN0

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	0.79	4/5262 (0.1%)	0.71	6/7161 (0.1%)
2	B	0.76	3/5427 (0.1%)	0.75	14/7357 (0.2%)
All	All	0.77	7/10689 (0.1%)	0.73	20/14518 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	654	THR	C-N	6.18	1.48	1.34
1	A	374	VAL	CB-CG2	-6.03	1.40	1.52
2	B	317	VAL	CB-CG2	-5.89	1.40	1.52
2	B	137	SER	C-N	5.49	1.46	1.34
1	A	351	VAL	CB-CG2	-5.14	1.42	1.52
1	A	249	VAL	CB-CG1	-5.09	1.42	1.52
1	A	366	PHE	CD1-CE1	-5.07	1.29	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	851	VAL	CB-CA-C	7.01	124.72	111.40
2	B	634	PRO	N-CA-CB	6.62	111.24	103.30
2	B	398	ILE	CG1-CB-CG2	6.51	125.72	111.40
2	B	620	PRO	N-CA-CB	6.42	111.00	103.30
2	B	609	LEU	CB-CG-CD2	6.34	121.78	111.00
2	B	632	PRO	N-CA-CB	6.32	110.89	103.30
2	B	385	ILE	C-N-CA	6.26	137.35	121.70
1	A	234	TYR	CB-CA-C	6.02	122.44	110.40
2	B	654	THR	C-N-CA	-5.86	107.06	121.70
1	A	746	PRO	N-CA-CB	5.85	110.32	103.30
1	A	358	ASP	CB-CG-OD1	5.52	123.26	118.30
2	B	597	LEU	CB-CG-CD2	5.48	120.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	654	THR	O-C-N	5.23	131.06	122.70
2	B	238	THR	N-CA-C	-5.18	97.01	111.00
1	A	236	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	597	LEU	CB-CG-CD1	5.12	119.71	111.00
2	B	738	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	372	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	B	643	PRO	N-CA-CB	5.06	109.37	103.30
2	B	609	LEU	CB-CG-CD1	5.04	119.56	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5137	4491	4973	172	0
2	B	5311	4816	5289	228	0
3	A	56	0	92	15	0
3	B	28	0	46	9	0
4	B	23	0	0	4	0
All	All	10555	9307	10400	406	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 19.

All (406) 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:108:CYS:SG	2:B:135:CYS:HB2	1.56	1.43
1:A:232:LEU:O	1:A:236:ASP:CB	1.75	1.34
2:B:108:CYS:SG	2:B:135:CYS:CB	2.21	1.29
2:B:135:CYS:SG	2:B:138:VAL:HG12	1.73	1.28
2:B:478:SER:CB	2:B:481:LEU:HB2	1.65	1.26
2:B:135:CYS:SG	2:B:138:VAL:CG1	2.29	1.21
1:A:232:LEU:O	1:A:236:ASP:HB3	1.41	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LEU:HD12	3:A:1002:CLR:H112	1.22	1.14
1:A:232:LEU:O	1:A:236:ASP:HB2	1.42	1.13
2:B:353:LYS:HG3	2:B:354:PHE:CE1	1.97	0.98
1:A:171:TYR:HD2	1:A:237:PRO:CG	1.76	0.98
1:A:171:TYR:CD2	1:A:237:PRO:CG	2.49	0.96
2:B:135:CYS:HG	2:B:138:VAL:HG12	0.80	0.96
2:B:478:SER:CB	2:B:481:LEU:CB	2.43	0.95
2:B:508:ASN:HA	2:B:512:ILE:HD13	1.49	0.94
2:B:108:CYS:HG	2:B:135:CYS:CB	1.79	0.93
1:A:171:TYR:CE2	1:A:237:PRO:HG3	2.05	0.91
1:A:206:LEU:HD13	1:A:209:TYR:HB2	1.51	0.91
2:B:477:ILE:HD11	2:B:721:PHE:HB3	1.50	0.90
1:A:232:LEU:C	1:A:236:ASP:HB2	1.92	0.89
2:B:477:ILE:HD12	2:B:717:PRO:O	1.72	0.89
2:B:135:CYS:SG	2:B:138:VAL:HG11	2.12	0.88
2:B:353:LYS:CG	2:B:354:PHE:CE1	2.58	0.87
2:B:237:CYS:HB3	2:B:266:CYS:SG	2.15	0.86
2:B:135:CYS:HG	2:B:138:VAL:CG1	1.72	0.86
1:A:171:TYR:HD2	1:A:237:PRO:HG2	1.38	0.85
1:A:171:TYR:CD2	1:A:237:PRO:HG3	2.12	0.83
1:A:591:LEU:HD12	3:A:1002:CLR:C11	2.05	0.83
1:A:788:ALA:HB1	4:B:902:FN0:C16	2.09	0.82
2:B:353:LYS:HG3	2:B:354:PHE:CD1	2.15	0.81
2:B:158:ALA:O	2:B:174:ARG:NH1	2.14	0.81
2:B:553:CYS:HA	2:B:556:ARG:HB2	1.64	0.80
1:A:237:PRO:N	1:A:239:LYS:NZ	2.29	0.79
2:B:108:CYS:SG	2:B:135:CYS:HB3	2.23	0.79
2:B:108:CYS:HG	2:B:135:CYS:HB2	1.41	0.79
2:B:553:CYS:HA	2:B:556:ARG:HD3	1.66	0.78
2:B:486:SER:O	2:B:489:THR:OG1	2.02	0.78
2:B:66:LYS:NZ	2:B:71:GLY:O	2.16	0.76
2:B:546:GLU:HG2	2:B:548:THR:H	1.50	0.76
2:B:283:GLY:N	2:B:317:VAL:O	2.18	0.76
1:A:223:GLY:N	2:B:144:GLU:OE2	2.18	0.75
2:B:546:GLU:HG2	2:B:548:THR:HG23	1.68	0.75
1:A:366:PHE:O	1:A:396:TYR:OH	2.05	0.74
2:B:477:ILE:HD11	2:B:721:PHE:CB	2.17	0.74
2:B:478:SER:CB	2:B:481:LEU:CG	2.66	0.74
1:A:850:VAL:HG13	1:A:851:VAL:HG23	1.68	0.73
1:A:841:ILE:O	1:A:844:SER:OG	2.03	0.73
2:B:476:LYS:O	2:B:476:LYS:HG2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:ASN:OD1	2:B:414:GLN:NE2	2.21	0.73
1:A:739:GLU:O	1:A:758:LEU:N	2.19	0.72
1:A:285:ARG:NH1	1:A:289:SER:OG	2.23	0.72
2:B:244:LYS:NZ	2:B:270:GLU:O	2.22	0.72
2:B:267:ALA:O	2:B:271:ASN:N	2.22	0.72
2:B:471:LEU:N	2:B:640:SER:O	2.23	0.72
2:B:165:ASP:OD1	2:B:168:LYS:N	2.22	0.72
1:A:172:ILE:O	1:A:214:ILE:N	2.23	0.71
2:B:203:GLN:NE2	2:B:256:ASP:OD1	2.23	0.71
1:A:759:GLU:OE2	1:A:759:GLU:N	2.23	0.71
2:B:92:SER:O	2:B:95:ARG:NH1	2.22	0.71
2:B:478:SER:CB	2:B:481:LEU:HG	2.21	0.71
2:B:547:LYS:HA	2:B:623:ARG:HH11	1.56	0.71
2:B:692:ILE:O	2:B:695:SER:OG	2.08	0.71
1:A:443:SER:OG	1:A:444:GLN:NE2	2.24	0.71
2:B:688:ASP:HB2	2:B:691:TYR:CD1	2.25	0.70
1:A:168:ARG:NH1	1:A:496:GLU:OE1	2.24	0.70
2:B:153:GLN:NE2	2:B:154:LEU:O	2.24	0.70
2:B:683:ILE:HD12	2:B:683:ILE:H	1.57	0.70
1:A:399:ASN:ND2	1:A:403:ILE:HD11	2.07	0.70
2:B:97:TYR:OH	2:B:382:HIS:O	2.10	0.69
1:A:368:GLU:OE2	1:A:372:ARG:NE	2.25	0.69
2:B:237:CYS:CB	2:B:266:CYS:SG	2.81	0.69
1:A:683:THR:HG21	1:A:714:VAL:HG22	1.73	0.69
1:A:171:TYR:HE2	1:A:237:PRO:HG3	1.56	0.69
1:A:627:PRO:O	1:A:631:ASN:ND2	2.26	0.69
2:B:452:ILE:HD12	2:B:455:THR:HG21	1.74	0.69
2:B:694:MET:CE	4:B:902:FN0:C14	2.71	0.69
2:B:255:PHE:O	2:B:285:TYR:OH	2.10	0.68
2:B:331:SER:O	2:B:333:LYS:NZ	2.24	0.68
2:B:334:THR:OG1	2:B:337:GLN:NE2	2.26	0.68
1:A:215:HIS:O	1:A:216:HIS:ND1	2.27	0.68
1:A:168:ARG:N	1:A:208:ASP:O	2.27	0.67
2:B:392:ASP:OD1	2:B:395:LEU:N	2.28	0.67
1:A:670:LEU:O	1:A:674:PHE:N	2.27	0.67
2:B:82:GLU:HA	2:B:85:ILE:HD12	1.77	0.67
2:B:553:CYS:SG	2:B:556:ARG:NH2	2.69	0.66
2:B:452:ILE:CD1	2:B:455:THR:HG21	2.25	0.66
1:A:309:ILE:HD12	1:A:361:ILE:HG21	1.77	0.66
2:B:237:CYS:CB	2:B:266:CYS:HG	2.09	0.66
1:A:659:PHE:HD2	1:A:736:ARG:HD2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1001:CLR:H71	3:B:901:CLR:H22	1.77	0.66
1:A:198:ASP:O	1:A:201:SER:OG	2.14	0.66
2:B:59:MET:HB3	2:B:130:VAL:HG22	1.78	0.66
2:B:91:GLU:OE1	2:B:93:LEU:N	2.29	0.66
2:B:101:LEU:HD21	2:B:103:LEU:HD21	1.77	0.65
2:B:280:ILE:O	2:B:281:ILE:HD13	1.95	0.65
2:B:185:ALA:HB2	2:B:442:TYR:CD2	2.31	0.65
2:B:613:ILE:HD12	2:B:616:GLN:HB2	1.79	0.65
1:A:270:SER:OG	1:A:290:ALA:N	2.29	0.65
2:B:681:VAL:HG12	2:B:683:ILE:HG13	1.77	0.65
2:B:175:THR:O	2:B:422:ARG:NH1	2.28	0.65
2:B:471:LEU:O	2:B:641:ILE:HA	1.98	0.64
2:B:555:VAL:O	2:B:559:ILE:HG22	1.97	0.64
1:A:844:SER:OG	1:A:845:SER:N	2.30	0.63
1:A:318:VAL:HG13	1:A:319:PHE:CD1	2.33	0.63
1:A:593:ILE:O	1:A:597:VAL:HG23	1.98	0.63
1:A:844:SER:O	1:A:848:THR:N	2.32	0.63
2:B:362:ILE:HA	2:B:365:ILE:HD12	1.81	0.63
2:B:609:LEU:HA	2:B:612:LEU:HD12	1.81	0.63
2:B:742:PRO:O	2:B:746:THR:HG23	1.98	0.62
2:B:694:MET:HE1	4:B:902:FN0:C14	2.30	0.62
2:B:729:ILE:O	2:B:733:THR:OG1	2.14	0.62
2:B:548:THR:HB	2:B:551:THR:HG21	1.81	0.62
1:A:294:ASN:O	1:A:297:ARG:N	2.33	0.62
2:B:686:LEU:HD12	2:B:687:ASN:HB2	1.82	0.62
2:B:392:ASP:HB3	2:B:395:LEU:HD12	1.81	0.61
1:A:810:TYR:OH	2:B:698:ASN:ND2	2.33	0.61
1:A:687:TRP:O	1:A:691:VAL:N	2.26	0.61
2:B:674:LEU:O	2:B:678:THR:HG23	2.01	0.61
2:B:681:VAL:CG1	2:B:683:ILE:HG13	2.30	0.61
2:B:228:ASP:OD2	2:B:246:ASN:ND2	2.34	0.61
2:B:200:THR:OG1	2:B:212:ARG:NE	2.33	0.61
3:A:1001:CLR:H71	3:B:901:CLR:C19	2.31	0.61
2:B:365:ILE:O	2:B:369:LEU:HD23	2.01	0.61
2:B:689:SER:HA	2:B:692:ILE:HD12	1.82	0.61
1:A:306:TRP:NE1	1:A:574:PRO:O	2.34	0.60
2:B:395:LEU:HA	2:B:398:ILE:HD12	1.82	0.60
2:B:101:LEU:HD12	2:B:102:ARG:N	2.16	0.60
1:A:240:ILE:HG13	1:A:241:ILE:HG22	1.84	0.60
2:B:353:LYS:HE2	2:B:354:PHE:CZ	2.37	0.59
2:B:487:ALA:HA	2:B:490:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:574:LYS:O	2:B:578:VAL:HG23	2.02	0.59
2:B:579:HIS:O	2:B:583:LYS:N	2.36	0.59
3:A:1001:CLR:H71	3:B:901:CLR:H192	1.84	0.59
2:B:94:LEU:O	2:B:97:TYR:N	2.35	0.59
1:A:502:ASN:OD1	1:A:503:GLN:N	2.36	0.59
2:B:509:GLN:O	2:B:512:ILE:HG12	2.03	0.59
2:B:536:LEU:HB3	2:B:556:ARG:HG2	1.84	0.59
1:A:685:ILE:O	1:A:688:VAL:HG22	2.03	0.59
2:B:442:TYR:CE2	2:B:444:ALA:HB2	2.38	0.59
1:A:787:LEU:O	1:A:791:THR:HG22	2.03	0.59
1:A:368:GLU:O	1:A:371:ALA:N	2.36	0.58
1:A:471:TYR:HD2	1:A:521:VAL:HG21	1.69	0.58
1:A:659:PHE:CD2	1:A:736:ARG:HD2	2.37	0.58
1:A:855:PRO:O	1:A:859:ARG:N	2.35	0.58
1:A:169:ALA:HA	1:A:210:GLU:H	1.68	0.58
2:B:524:ILE:HG22	2:B:736:LEU:HD21	1.85	0.58
1:A:443:SER:O	1:A:447:VAL:HG23	2.04	0.58
2:B:509:GLN:HB3	2:B:511:LEU:CD2	2.34	0.58
2:B:654:THR:HG23	2:B:654:THR:O	2.04	0.58
1:A:840:ALA:O	1:A:844:SER:N	2.37	0.57
2:B:452:ILE:O	2:B:455:THR:OG1	2.22	0.57
2:B:622:ARG:HH12	2:B:650:ASN:HA	1.69	0.57
1:A:725:LEU:O	1:A:729:GLN:N	2.38	0.57
1:A:781:LEU:HD13	1:A:813:ALA:HB1	1.85	0.57
1:A:238:ILE:HG23	1:A:238:ILE:O	2.04	0.57
2:B:134:VAL:HA	2:B:157:ALA:HB3	1.85	0.57
1:A:171:TYR:CD2	1:A:237:PRO:CB	2.88	0.57
1:A:676:LEU:HD11	1:A:718:VAL:HG13	1.85	0.57
2:B:105:ASP:OD1	2:B:106:THR:N	2.38	0.57
1:A:718:VAL:O	1:A:722:VAL:HG23	2.05	0.57
2:B:323:SER:OG	2:B:411:VAL:O	2.15	0.57
2:B:428:PHE:O	2:B:439:VAL:HG22	2.05	0.56
1:A:206:LEU:CD1	1:A:209:TYR:HB2	2.29	0.56
1:A:437:SER:OG	1:A:441:MET:N	2.37	0.56
2:B:269:GLU:N	2:B:269:GLU:OE1	2.38	0.56
2:B:329:THR:HG23	2:B:333:LYS:O	2.05	0.56
2:B:489:THR:HG21	2:B:534:ILE:HG21	1.87	0.56
2:B:190:LEU:O	2:B:194:GLN:N	2.38	0.56
2:B:477:ILE:CD1	2:B:721:PHE:CB	2.83	0.56
2:B:553:CYS:CA	2:B:556:ARG:HD3	2.36	0.56
1:A:599:SER:HA	1:A:641:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:LEU:HD12	2:B:552:LEU:H	1.70	0.56
3:A:1001:CLR:C7	3:B:901:CLR:C19	2.84	0.56
1:A:847:ILE:HA	1:A:850:VAL:HG11	1.88	0.55
2:B:552:LEU:O	2:B:556:ARG:N	2.38	0.55
1:A:308:LYS:O	1:A:309:ILE:HD13	2.06	0.55
2:B:354:PHE:CD1	2:B:354:PHE:N	2.75	0.55
2:B:469:ILE:O	2:B:640:SER:N	2.30	0.55
2:B:694:MET:HE3	4:B:902:FN0:C14	2.37	0.55
2:B:278:GLN:NE2	2:B:313:GLY:O	2.38	0.55
1:A:286:THR:CG2	1:A:469:LEU:HD12	2.37	0.55
2:B:550:GLU:O	2:B:621:LEU:HD22	2.06	0.55
2:B:453:ASN:O	2:B:455:THR:HG23	2.07	0.55
2:B:621:LEU:C	2:B:622:ARG:HD3	2.28	0.55
1:A:739:GLU:N	1:A:758:LEU:O	2.22	0.54
1:A:257:ALA:O	1:A:260:TRP:N	2.39	0.54
1:A:471:TYR:CD2	1:A:521:VAL:HG21	2.43	0.54
2:B:607:ILE:HG21	2:B:663:TYR:CZ	2.43	0.54
1:A:207:PRO:HG2	1:A:208:ASP:OD2	2.07	0.54
2:B:511:LEU:HA	2:B:514:MET:SD	2.48	0.54
1:A:710:LEU:O	1:A:714:VAL:HG23	2.07	0.54
2:B:101:LEU:HD12	2:B:102:ARG:H	1.73	0.54
2:B:509:GLN:OE1	2:B:510:LYS:HG2	2.08	0.54
1:A:550:ILE:HD11	1:A:562:TRP:CZ2	2.43	0.53
2:B:482:TYR:O	2:B:486:SER:OG	2.18	0.53
1:A:206:LEU:HD13	1:A:209:TYR:CD2	2.44	0.53
3:A:1001:CLR:H151	3:B:901:CLR:H193	1.91	0.53
1:A:503:GLN:O	1:A:506:THR:OG1	2.27	0.53
1:A:237:PRO:CD	1:A:239:LYS:NZ	2.71	0.53
1:A:499:ASN:OD1	1:A:500:TYR:N	2.41	0.53
2:B:540:ASP:HA	2:B:544:VAL:HG21	1.89	0.53
1:A:583:THR:OG1	1:A:584:PHE:N	2.42	0.53
2:B:523:ILE:CG1	2:B:570:ALA:HB3	2.39	0.53
2:B:93:LEU:HD21	2:B:370:GLN:CD	2.29	0.52
1:A:199:VAL:O	1:A:205:ILE:HG13	2.09	0.52
2:B:621:LEU:O	2:B:622:ARG:HD3	2.08	0.52
1:A:192:VAL:HG12	1:A:470:ALA:HB1	1.91	0.52
1:A:475:TRP:O	1:A:479:LEU:HD23	2.10	0.52
2:B:523:ILE:HG13	2:B:570:ALA:HB3	1.91	0.52
1:A:171:TYR:CE2	1:A:237:PRO:CG	2.80	0.52
1:A:341:GLN:O	1:A:342:SER:OG	2.20	0.52
2:B:154:LEU:HD11	2:B:175:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:691:TYR:CE2	2:B:742:PRO:HG2	2.45	0.52
1:A:300:LEU:H	1:A:300:LEU:HD12	1.75	0.52
2:B:449:LEU:HD12	2:B:450:GLU:H	1.75	0.52
2:B:476:LYS:HB2	2:B:541:GLY:HA3	1.91	0.52
1:A:687:TRP:HA	1:A:691:VAL:HG23	1.92	0.52
3:A:1001:CLR:C7	3:B:901:CLR:H192	2.40	0.51
2:B:605:LEU:O	2:B:609:LEU:HG	2.11	0.51
2:B:259:MET:O	2:B:263:VAL:HG23	2.10	0.51
2:B:742:PRO:HA	2:B:745:ILE:HD12	1.92	0.51
1:A:309:ILE:HG22	1:A:310:ALA:N	2.26	0.51
2:B:88:ILE:O	2:B:92:SER:N	2.39	0.51
2:B:411:VAL:HG23	2:B:412:THR:HG23	1.92	0.51
1:A:808:ALA:O	1:A:812:VAL:HG23	2.10	0.51
2:B:412:THR:OG1	2:B:422:ARG:NH2	2.44	0.51
2:B:553:CYS:HA	2:B:556:ARG:CD	2.40	0.51
2:B:558:TRP:O	2:B:561:THR:OG1	2.29	0.51
1:A:199:VAL:HB	1:A:205:ILE:HG21	1.93	0.50
1:A:709:LYS:O	1:A:713:THR:OG1	2.21	0.50
2:B:197:ARG:HH22	2:B:248:VAL:HG12	1.75	0.50
2:B:491:LEU:O	2:B:494:ILE:HG22	2.11	0.50
2:B:548:THR:HB	2:B:551:THR:CG2	2.42	0.50
2:B:174:ARG:NH2	2:B:421:GLU:OE1	2.44	0.50
1:A:232:LEU:CA	1:A:236:ASP:HB2	2.41	0.50
1:A:422:HIS:O	1:A:423:ILE:HD13	2.11	0.50
2:B:554:THR:HG22	2:B:621:LEU:HD11	1.93	0.50
2:B:553:CYS:HA	2:B:556:ARG:CB	2.39	0.50
1:A:631:ASN:O	1:A:635:VAL:HG23	2.12	0.49
2:B:614:CYS:SG	2:B:615:TRP:N	2.85	0.49
1:A:217:ASP:OD1	1:A:218:SER:N	2.45	0.49
1:A:356:ARG:NH2	2:B:226:ILE:O	2.45	0.49
1:A:450:LEU:O	1:A:454:LEU:N	2.45	0.49
1:A:546:SER:OG	1:A:547:TYR:N	2.44	0.49
1:A:232:LEU:HA	1:A:236:ASP:CG	2.33	0.49
1:A:740:THR:HA	1:A:757:GLN:HA	1.93	0.49
1:A:836:PHE:CE1	3:A:1001:CLR:H213	2.47	0.49
2:B:328:LYS:NZ	2:B:332:GLY:O	2.45	0.49
1:A:662:VAL:O	1:A:665:ALA:HB3	2.13	0.49
2:B:251:ILE:HD13	2:B:279:TRP:CZ3	2.46	0.49
2:B:513:LYS:HE3	2:B:513:LYS:HA	1.95	0.49
2:B:550:GLU:OE2	2:B:623:ARG:N	2.43	0.49
2:B:255:PHE:CE2	2:B:263:VAL:HG21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:ASP:CB	2:B:395:LEU:HD12	2.42	0.49
1:A:196:LEU:O	1:A:199:VAL:HG22	2.13	0.49
1:A:237:PRO:CD	1:A:239:LYS:HZ2	2.26	0.49
1:A:271:SER:HB2	1:A:274:LEU:HD23	1.95	0.49
1:A:286:THR:HG23	1:A:469:LEU:HD12	1.95	0.49
1:A:290:ALA:HB1	1:A:293:HIS:HD1	1.78	0.49
1:A:374:VAL:O	1:A:378:VAL:HG23	2.13	0.49
1:A:481:LEU:HA	1:A:484:THR:HG22	1.95	0.49
1:A:168:ARG:O	1:A:210:GLU:HG2	2.12	0.48
2:B:441:GLU:O	2:B:449:LEU:HD12	2.13	0.48
1:A:604:VAL:O	1:A:608:VAL:HG23	2.13	0.48
2:B:692:ILE:O	2:B:696:VAL:HG23	2.13	0.48
2:B:508:ASN:HA	2:B:512:ILE:CD1	2.33	0.48
1:A:237:PRO:CG	1:A:239:LYS:NZ	2.77	0.48
2:B:154:LEU:HD12	2:B:155:SER:N	2.29	0.48
1:A:232:LEU:HD21	1:A:242:LEU:HD21	1.94	0.48
1:A:640:ALA:O	1:A:643:ALA:HB3	2.13	0.48
3:A:1001:CLR:C7	3:B:901:CLR:H193	2.42	0.48
2:B:154:LEU:HD12	2:B:155:SER:H	1.79	0.48
2:B:552:LEU:O	2:B:556:ARG:HG3	2.13	0.48
2:B:432:GLN:NE2	2:B:455:THR:O	2.43	0.48
2:B:508:ASN:N	2:B:512:ILE:HG21	2.28	0.48
2:B:683:ILE:O	2:B:685:ALA:N	2.47	0.48
2:B:58:ILE:HG22	2:B:101:LEU:HD13	1.95	0.48
1:A:403:ILE:HD12	1:A:403:ILE:N	2.29	0.47
2:B:477:ILE:CD1	2:B:721:PHE:HB2	2.44	0.47
2:B:702:MET:HB3	2:B:727:VAL:HG23	1.95	0.47
2:B:737:CYS:O	2:B:741:VAL:HG23	2.14	0.47
2:B:691:TYR:HE2	2:B:742:PRO:HG2	1.78	0.47
1:A:231:GLU:O	1:A:236:ASP:HB2	2.14	0.47
1:A:509:ILE:O	1:A:512:ALA:HB3	2.14	0.47
1:A:477:LEU:O	1:A:480:ALA:HB3	2.15	0.47
1:A:676:LEU:HD11	1:A:718:VAL:CG1	2.45	0.47
1:A:677:GLY:O	1:A:680:SER:OG	2.22	0.47
1:A:757:GLN:O	1:A:758:LEU:HD22	2.14	0.47
2:B:392:ASP:OD1	2:B:394:THR:OG1	2.24	0.47
1:A:659:PHE:O	1:A:662:VAL:HG22	2.15	0.47
2:B:477:ILE:CD1	2:B:721:PHE:HB3	2.34	0.47
1:A:585:ARG:CB	1:A:758:LEU:HD21	2.45	0.47
2:B:355:HIS:O	2:B:358:ALA:HB3	2.15	0.47
1:A:362:ILE:HG21	1:A:390:TRP:CE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:LEU:CD2	2:B:280:ILE:HD12	2.45	0.46
2:B:508:ASN:CA	2:B:512:ILE:HD13	2.31	0.46
1:A:737:THR:O	1:A:759:GLU:HA	2.15	0.46
1:A:202:ARG:HB2	1:A:205:ILE:CG1	2.46	0.46
1:A:473:ALA:HB3	1:A:474:ILE:HD12	1.97	0.46
1:A:678:TYR:OH	1:A:781:LEU:N	2.49	0.46
1:A:783:LEU:O	1:A:787:LEU:HD23	2.15	0.46
1:A:360:ARG:NH2	1:A:578:THR:HB	2.30	0.46
2:B:609:LEU:HG	2:B:609:LEU:H	1.75	0.46
1:A:290:ALA:O	1:A:293:HIS:ND1	2.47	0.46
1:A:291:THR:HG23	1:A:292:LEU:HD22	1.97	0.46
2:B:218:VAL:HG13	2:B:219:LEU:HD23	1.98	0.46
1:A:571:GLY:O	1:A:572:SER:OG	2.33	0.46
1:A:591:LEU:HD12	3:A:1002:CLR:C12	2.45	0.46
2:B:312:GLU:OE2	2:B:433:ASP:N	2.49	0.46
1:A:720:MET:SD	1:A:776:TYR:OH	2.70	0.46
2:B:72:SER:OG	2:B:73:ILE:N	2.49	0.46
2:B:228:ASP:C	2:B:229:THR:HG1	2.17	0.45
1:A:192:VAL:HG12	1:A:470:ALA:CB	2.45	0.45
2:B:440:GLY:HA3	2:B:451:ILE:HD13	1.99	0.45
2:B:512:ILE:HG13	2:B:513:LYS:N	2.32	0.45
2:B:539:LEU:H	2:B:539:LEU:HD23	1.80	0.45
1:A:222:PRO:O	1:A:226:THR:OG1	2.30	0.45
2:B:378:ALA:HB1	2:B:382:HIS:CE1	2.51	0.45
2:B:549:PHE:HA	2:B:552:LEU:CD1	2.47	0.45
2:B:686:LEU:CD1	2:B:687:ASN:HB2	2.46	0.45
1:A:232:LEU:HD12	1:A:236:ASP:OD2	2.17	0.45
1:A:633:THR:OG1	1:A:680:SER:OG	2.17	0.45
2:B:91:GLU:O	2:B:92:SER:OG	2.35	0.45
1:A:362:ILE:HD13	1:A:390:TRP:CZ3	2.52	0.45
1:A:689:HIS:ND1	1:A:790:GLU:OE2	2.50	0.45
1:A:309:ILE:HB	1:A:337:ILE:HD13	1.99	0.45
1:A:357:GLN:O	1:A:359:ALA:N	2.50	0.44
2:B:480:PRO:O	2:B:483:SER:OG	2.23	0.44
1:A:206:LEU:HA	1:A:206:LEU:HD23	1.65	0.44
2:B:546:GLU:CG	2:B:548:THR:H	2.27	0.44
1:A:206:LEU:HD13	1:A:209:TYR:HD2	1.82	0.44
2:B:557:THR:O	2:B:561:THR:HG23	2.16	0.44
3:A:1001:CLR:H72	3:B:901:CLR:C19	2.48	0.44
2:B:346:ARG:NH1	2:B:349:VAL:O	2.51	0.44
1:A:245:GLY:O	1:A:269:SER:OG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:OE2	1:A:544:GLY:N	2.43	0.44
1:A:835:ALA:HB1	3:A:1001:CLR:H212	1.98	0.44
2:B:157:ALA:O	2:B:159:THR:N	2.50	0.44
2:B:179:ASP:O	2:B:182:VAL:HG22	2.18	0.44
1:A:211:LEU:HD13	1:A:211:LEU:HA	1.69	0.44
2:B:428:PHE:C	2:B:439:VAL:HG22	2.37	0.44
1:A:168:ARG:O	1:A:210:GLU:N	2.51	0.43
2:B:231:SER:OG	2:B:232:PHE:N	2.51	0.43
2:B:594:ASP:OD1	2:B:595:GLN:N	2.51	0.43
1:A:171:TYR:CD2	1:A:237:PRO:HG2	2.28	0.43
2:B:205:VAL:HG12	2:B:206:GLN:N	2.33	0.43
2:B:225:GLU:OE1	2:B:225:GLU:N	2.38	0.43
1:A:290:ALA:HB1	1:A:293:HIS:ND1	2.33	0.43
1:A:415:MET:O	1:A:419:VAL:HG22	2.19	0.43
1:A:316:THR:HG22	1:A:317:GLU:N	2.32	0.43
2:B:234:ASN:OD1	2:B:235:ASP:N	2.52	0.43
2:B:485:LEU:O	2:B:489:THR:HG23	2.17	0.43
2:B:609:LEU:HA	2:B:612:LEU:HB2	2.00	0.43
1:A:275:SER:OG	1:A:529:ALA:O	2.29	0.43
2:B:548:THR:O	2:B:551:THR:OG1	2.21	0.43
2:B:727:VAL:HG13	2:B:728:ILE:N	2.33	0.43
1:A:575:ALA:O	1:A:577:GLN:N	2.52	0.43
2:B:548:THR:O	2:B:552:LEU:HD12	2.19	0.43
2:B:78:LEU:O	2:B:81:VAL:N	2.48	0.42
2:B:474:LEU:HD23	2:B:474:LEU:O	2.19	0.42
2:B:509:GLN:HB3	2:B:511:LEU:HD23	2.01	0.42
2:B:509:GLN:H	2:B:512:ILE:HG12	1.83	0.42
2:B:573:ALA:HB1	2:B:597:LEU:CD1	2.49	0.42
2:B:66:LYS:HZ1	2:B:75:ARG:CB	2.32	0.42
2:B:732:SER:OG	2:B:733:THR:N	2.52	0.42
2:B:101:LEU:CD2	2:B:103:LEU:HD21	2.47	0.42
1:A:613:ASN:OD1	1:A:853:PHE:CD1	2.73	0.42
1:A:764:ARG:H	1:A:764:ARG:HG2	1.62	0.42
2:B:411:VAL:CG2	2:B:412:THR:HG23	2.49	0.42
1:A:255:GLU:O	2:B:111:ALA:HB2	2.19	0.42
1:A:405:ASP:OD1	1:A:407:SER:N	2.43	0.42
2:B:493:MET:O	2:B:496:ALA:HB3	2.20	0.42
2:B:649:GLU:C	2:B:651:THR:H	2.22	0.42
1:A:236:ASP:CG	1:A:237:PRO:HD2	2.40	0.42
1:A:298:VAL:HG12	1:A:330:VAL:HG12	2.02	0.42
1:A:206:LEU:HD13	1:A:209:TYR:CB	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:VAL:HG13	1:A:815:LEU:HD22	2.02	0.42
2:B:525:LEU:O	2:B:529:LEU:HD23	2.19	0.42
1:A:200:ASN:HD22	1:A:210:GLU:HB3	1.84	0.41
1:A:300:LEU:HD12	1:A:300:LEU:N	2.35	0.41
1:A:171:TYR:CD2	1:A:237:PRO:HB2	2.55	0.41
1:A:474:ILE:HD12	1:A:474:ILE:H	1.85	0.41
2:B:352:SER:OG	2:B:353:LYS:N	2.53	0.41
1:A:659:PHE:N	1:A:660:PRO:HD2	2.36	0.41
2:B:288:SER:OG	2:B:288:SER:O	2.39	0.41
2:B:353:LYS:CD	2:B:354:PHE:CE1	3.03	0.41
3:B:901:CLR:H212	3:B:901:CLR:H121	2.02	0.41
1:A:507:ASP:N	1:A:507:ASP:OD1	2.52	0.41
2:B:403:MET:O	2:B:406:THR:HG22	2.21	0.41
2:B:449:LEU:HD12	2:B:450:GLU:N	2.35	0.41
2:B:536:LEU:O	2:B:539:LEU:HD22	2.20	0.41
2:B:162:VAL:HG11	2:B:206:GLN:NE2	2.36	0.41
2:B:364:VAL:O	2:B:368:THR:HG22	2.20	0.41
3:A:1002:CLR:H121	3:A:1002:CLR:H212	2.02	0.40
2:B:436:GLU:OE1	2:B:436:GLU:N	2.53	0.40
2:B:553:CYS:HB2	2:B:621:LEU:HD23	2.03	0.40
1:A:188:CYS:HA	1:A:191:ALA:HB3	2.04	0.40
2:B:546:GLU:OE2	2:B:546:GLU:N	2.50	0.40
2:B:691:TYR:HE2	2:B:742:PRO:CG	2.33	0.40
1:A:839:LEU:HD23	3:A:1001:CLR:H272	2.03	0.40
2:B:523:ILE:HD11	2:B:570:ALA:HB3	2.04	0.40
2:B:544:VAL:O	2:B:544:VAL:HG23	2.20	0.40
2:B:620:PRO:C	2:B:621:LEU:HD12	2.42	0.40
1:A:286:THR:OG1	1:A:469:LEU:HD12	2.21	0.40
1:A:736:ARG:O	1:A:736:ARG:HG3	2.22	0.40
2:B:360:ASP:O	2:B:364:VAL:HG23	2.21	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	661/771 (86%)	557 (84%)	101 (15%)	3 (0%)	29	68
2	B	675/822 (82%)	568 (84%)	102 (15%)	5 (1%)	22	62
All	All	1336/1593 (84%)	1125 (84%)	203 (15%)	8 (1%)	29	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	620	PRO
2	B	634	PRO
1	A	619	VAL
2	B	238	THR
2	B	619	ASP
1	A	358	ASP
2	B	631	GLU
1	A	746	PRO

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	526/669 (79%)	524 (100%)	2 (0%)	91	94
2	B	563/713 (79%)	557 (99%)	6 (1%)	73	85
All	All	1089/1382 (79%)	1081 (99%)	8 (1%)	84	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	ASP
1	A	415	MET
2	B	134	VAL
2	B	354	PHE
2	B	476	LYS

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Mol	Chain	Res	Type
2	B	477	ILE
2	B	653	MET
2	B	712	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	A	444	GLN
1	A	501	ASN
1	A	613	ASN
1	A	630	ASN
1	A	664	GLN
1	A	811	ASN
2	B	87	GLN
2	B	110	ASN
2	B	246	ASN
2	B	326	GLN
2	B	337	GLN
2	B	383	GLN
2	B	407	ASN
2	B	414	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CLR	B	901	-	31,31,31	0.81	1 (3%)	48,48,48	1.23	5 (10%)
4	FN0	B	902	-	23,24,24	1.04	2 (8%)	35,42,42	2.06	5 (14%)
3	CLR	A	1002	-	31,31,31	0.81	1 (3%)	48,48,48	1.23	5 (10%)
3	CLR	A	1001	-	31,31,31	0.81	1 (3%)	48,48,48	1.23	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
3	CLR	B	901	-	-	0/10/68/68	0/4/4/4
4	FN0	B	902	-	-	9/21/37/37	0/2/2/2
3	CLR	A	1002	-	-	0/10/68/68	0/4/4/4
3	CLR	A	1001	-	-	0/10/68/68	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	FN0	O3-C13	2.44	1.26	1.20
3	A	1001	CLR	C20-C17	2.34	1.58	1.54
3	B	901	CLR	C20-C17	2.32	1.58	1.54
3	A	1002	CLR	C20-C17	2.31	1.58	1.54
4	B	902	FN0	C6-C2	-2.05	1.37	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	902	FN0	C5-C7-C13	-7.78	98.07	101.75
4	B	902	FN0	C17-C7-C5	5.69	121.99	112.72
4	B	902	FN0	C4-C9-C5	-3.25	118.75	123.80
3	A	1001	CLR	C8-C7-C6	-3.05	108.35	112.73
3	A	1002	CLR	C8-C7-C6	-3.02	108.39	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	901	CLR	C8-C7-C6	-3.01	108.40	112.73
3	B	901	CLR	C10-C9-C8	-2.99	108.26	112.73
3	A	1002	CLR	C10-C9-C8	-2.98	108.27	112.73
3	A	1001	CLR	C10-C9-C8	-2.98	108.27	112.73
4	B	902	FN0	C8-C2-C6	-2.71	113.23	117.11
4	B	902	FN0	C7-C5-C6	-2.49	107.82	108.88
3	A	1001	CLR	C13-C17-C20	-2.48	115.60	119.49
3	A	1002	CLR	C13-C17-C20	-2.46	115.63	119.49
3	B	901	CLR	C13-C17-C20	-2.44	115.66	119.49
3	A	1002	CLR	C11-C9-C8	2.37	115.16	111.75
3	B	901	CLR	C11-C9-C8	2.36	115.15	111.75
3	B	901	CLR	C23-C22-C20	-2.35	108.27	115.03
3	A	1001	CLR	C11-C9-C8	2.34	115.13	111.75
3	A	1002	CLR	C23-C22-C20	-2.34	108.30	115.03
3	A	1001	CLR	C23-C22-C20	-2.34	108.31	115.03

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	902	FN0	F1-C17-C7-C5
4	B	902	FN0	F2-C17-C7-C5
4	B	902	FN0	F3-C17-C7-C5
4	B	902	FN0	C10-C1-C2-C6
4	B	902	FN0	C11-C1-C2-C6
4	B	902	FN0	C12-C1-C2-C6
4	B	902	FN0	C10-C1-C2-C8
4	B	902	FN0	C12-C1-C2-C8
4	B	902	FN0	C11-C1-C2-C8

There are no ring outliers.

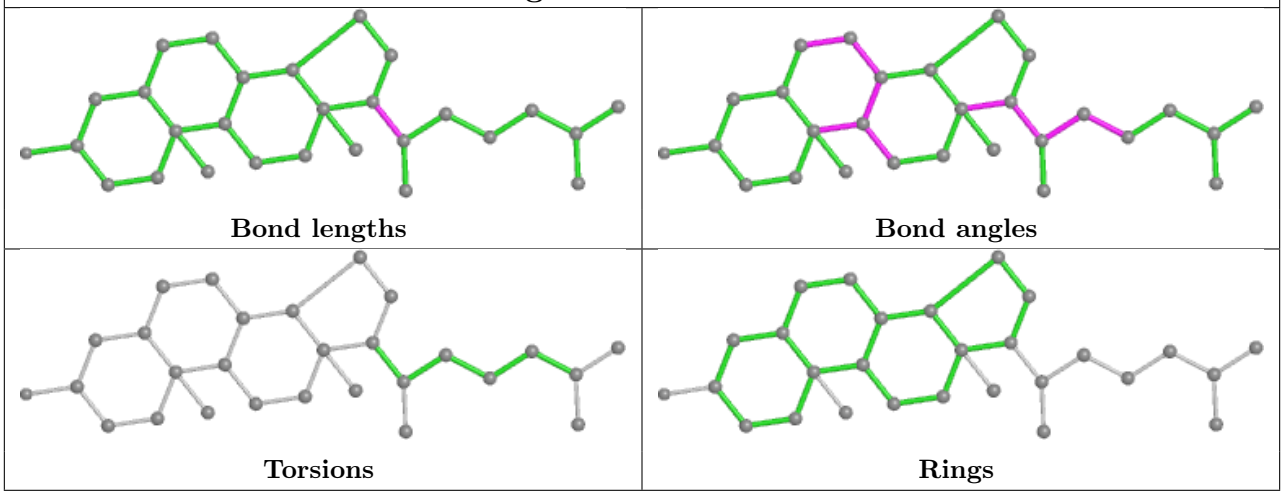
4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	CLR	9	0
4	B	902	FN0	4	0
3	A	1002	CLR	4	0
3	A	1001	CLR	11	0

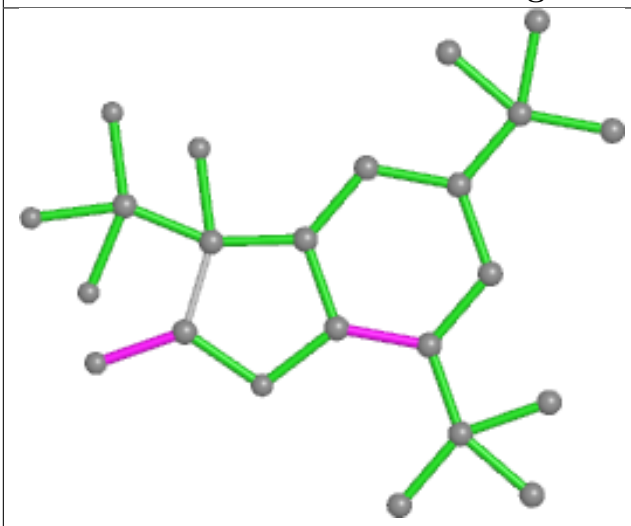
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

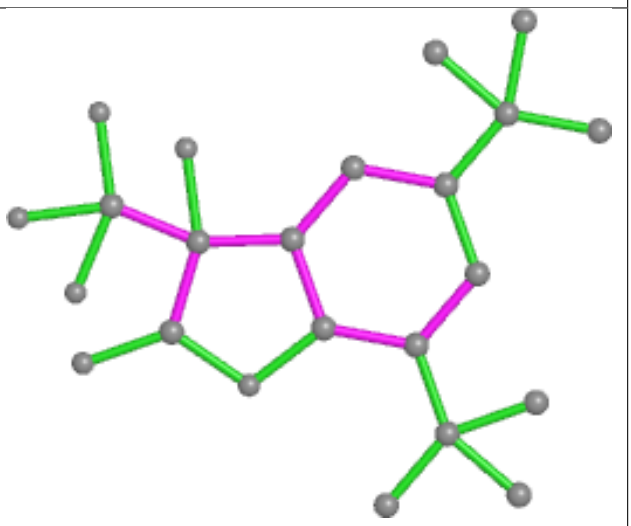
Ligand CLR B 901



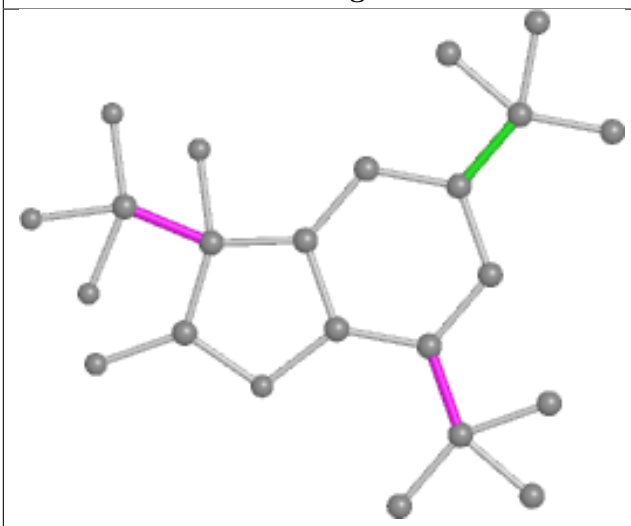
Ligand FN0 B 902



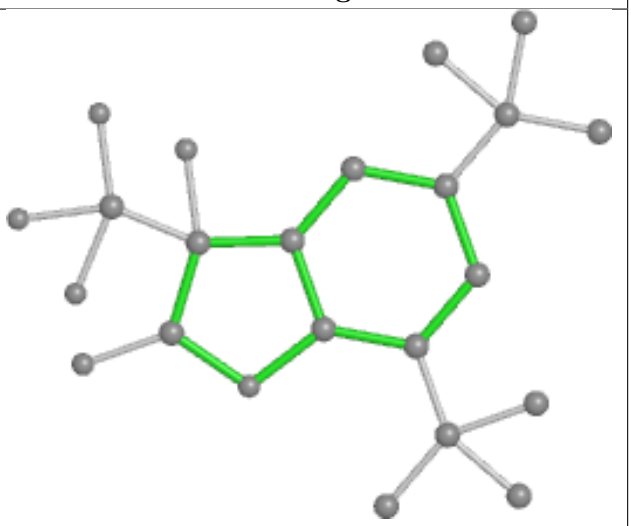
Bond lengths



Bond angles

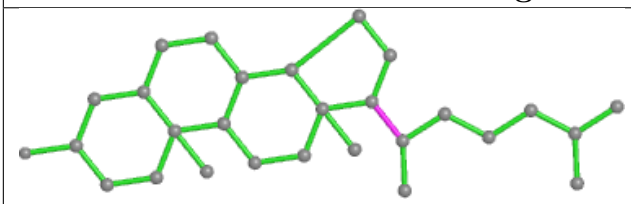


Torsions

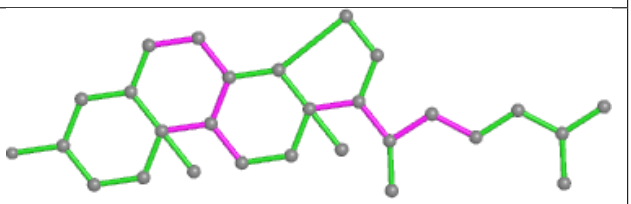


Rings

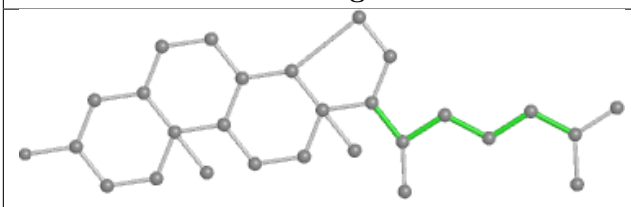
Ligand CLR A 1002



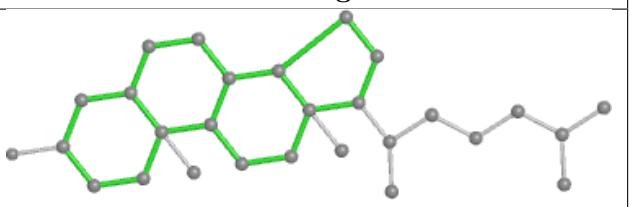
Bond lengths



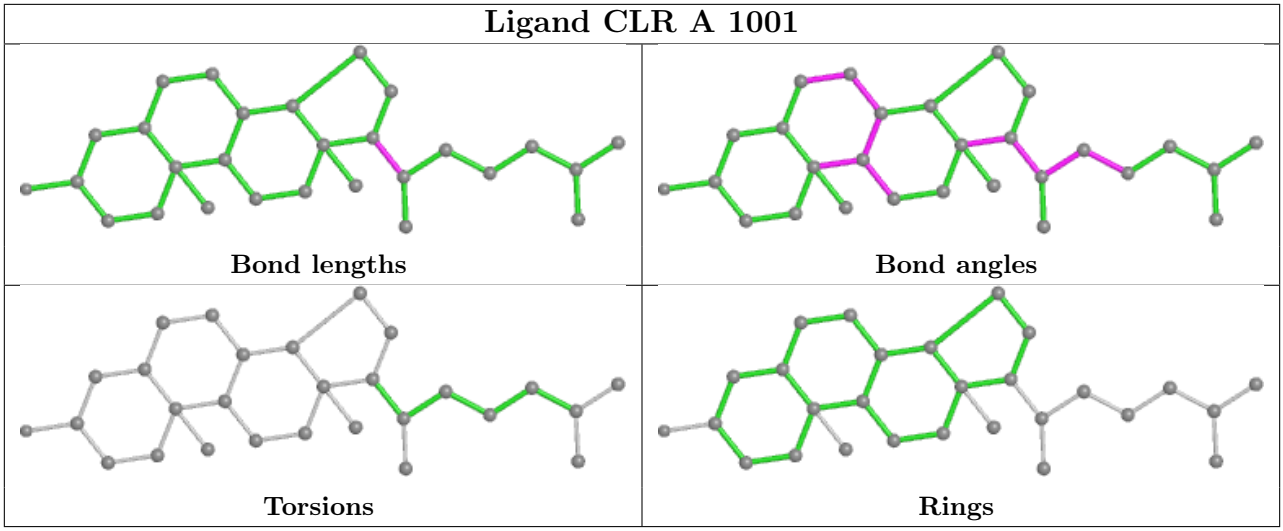
Bond angles



Torsions



Rings



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.

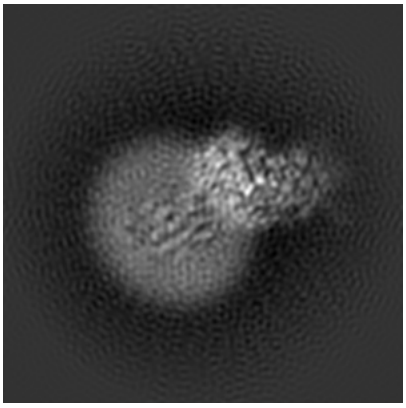
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30323. These allow visual inspection of the internal detail of the map and identification of artifacts.

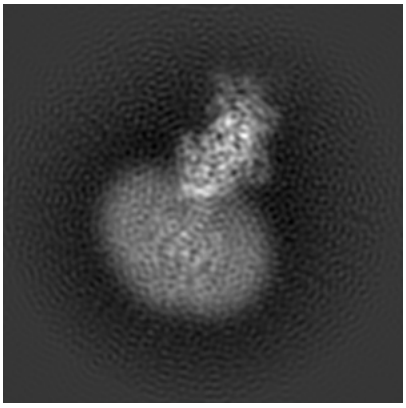
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

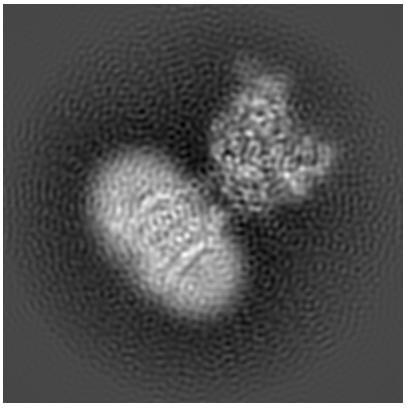
6.1.1 Primary map



X



Y

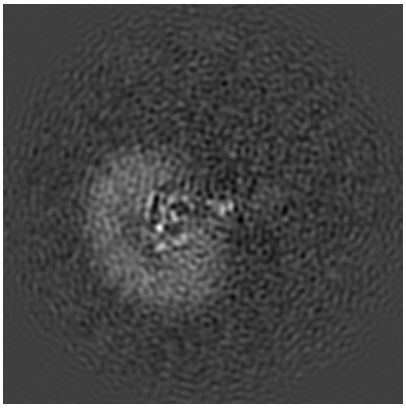


Z

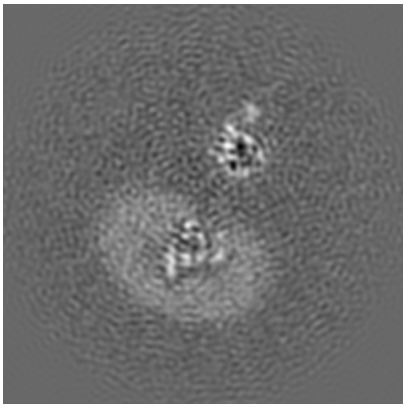
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

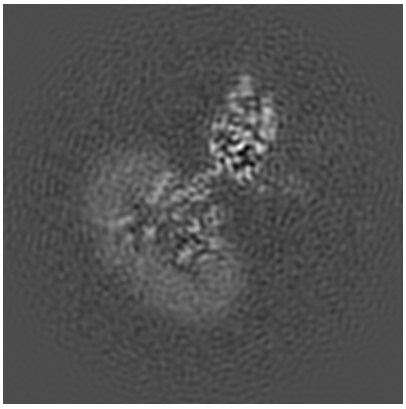
6.2.1 Primary map



X Index: 150



Y Index: 150

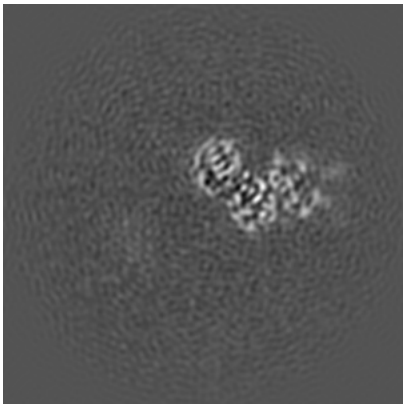


Z Index: 150

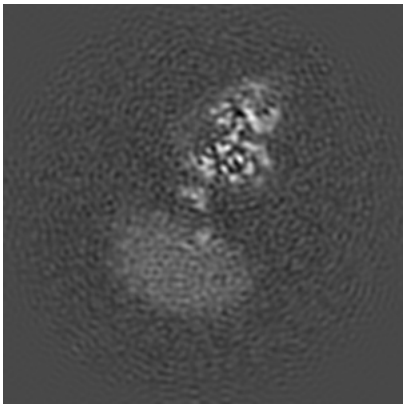
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

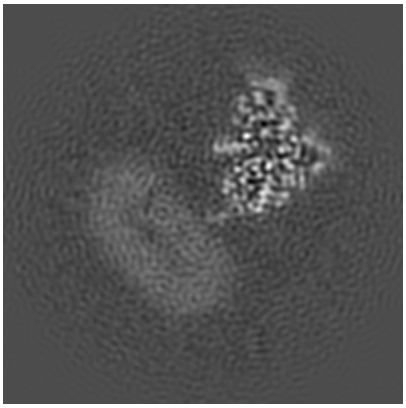
6.3.1 Primary map



X Index: 185



Y Index: 171



Z Index: 169

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

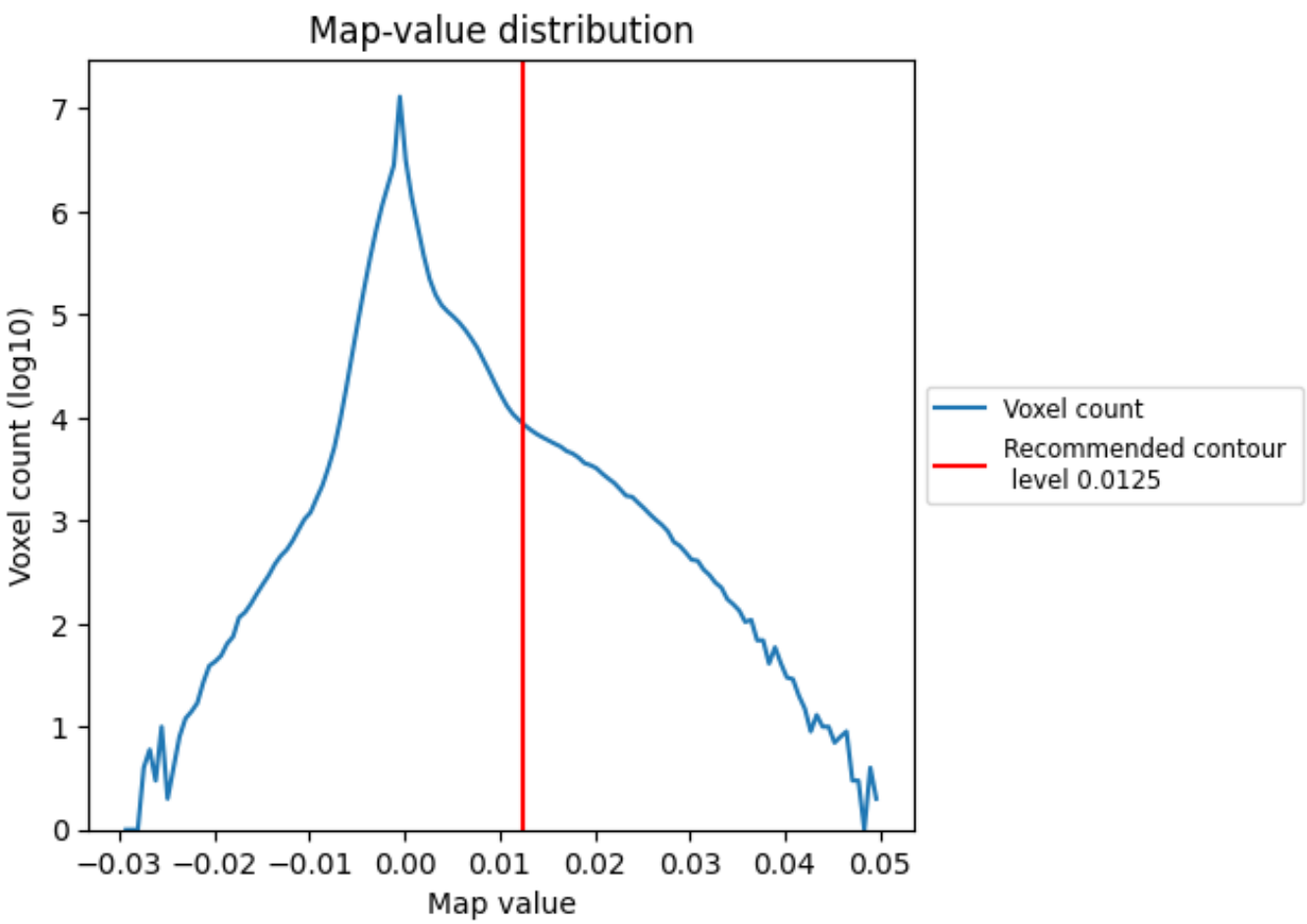
6.5 Mask visualisation (i)

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

7 Map analysis (i)

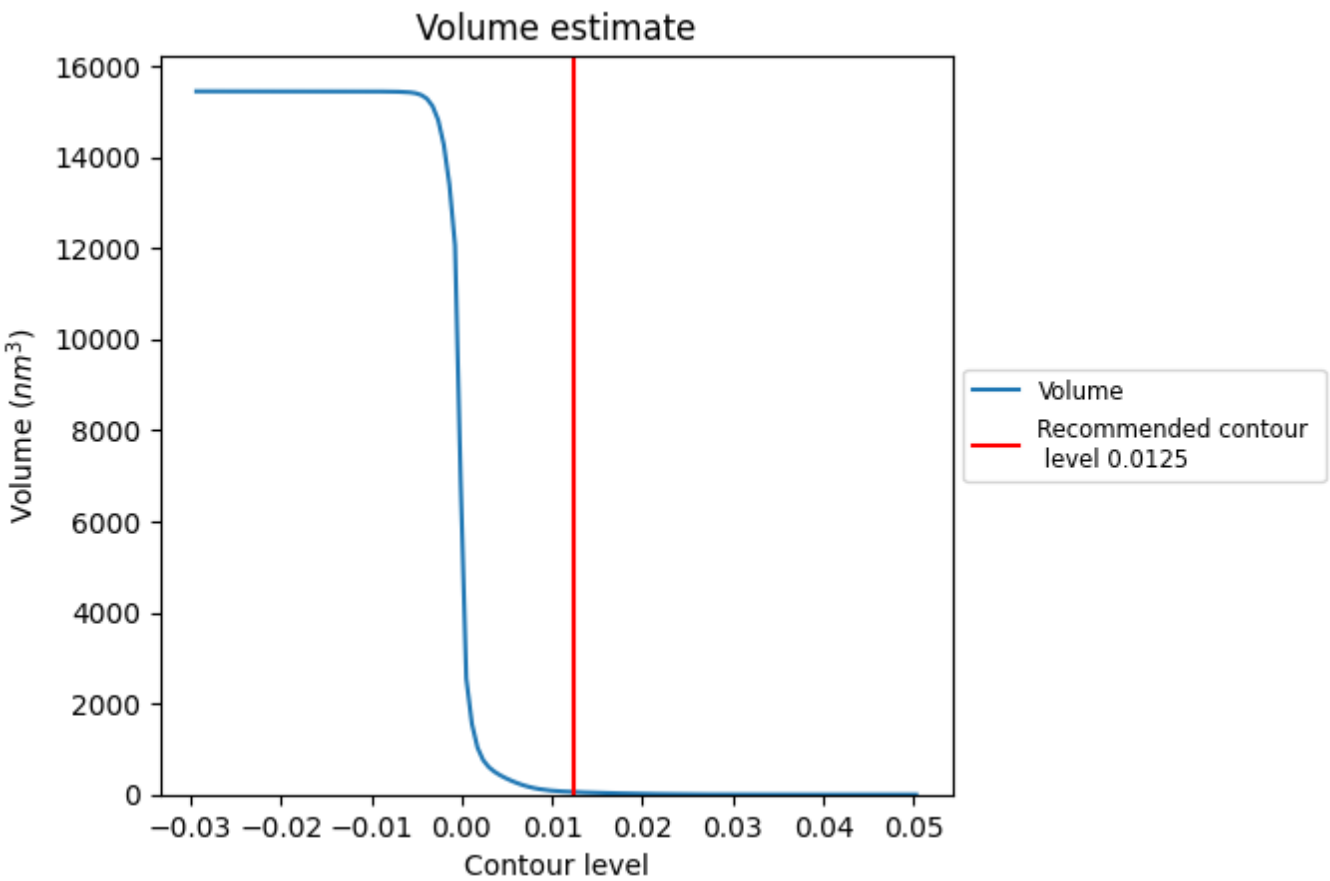
This section contains the results of statistical analysis of the map.

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.

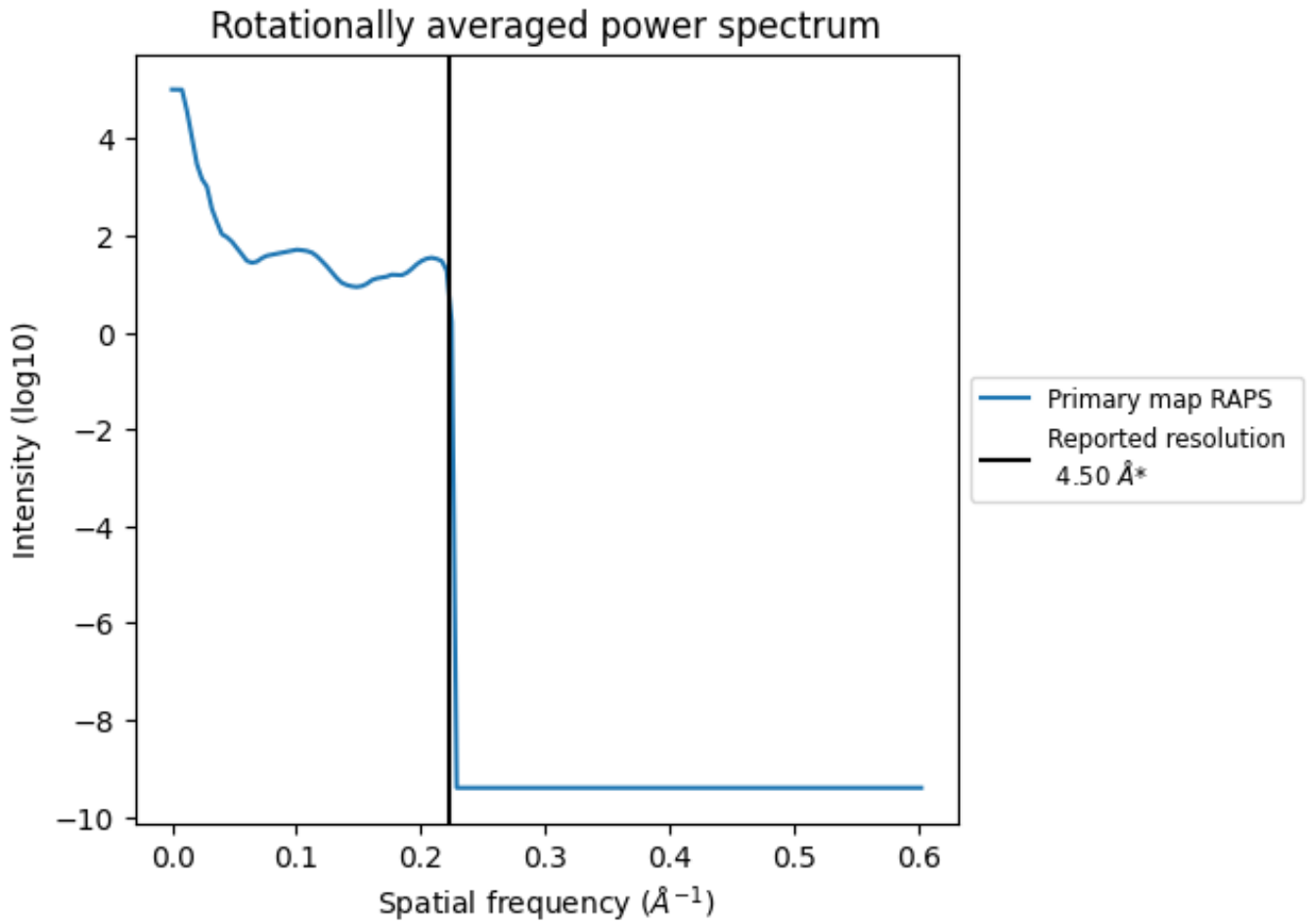
7.2 Volume estimate (i)



The volume at the recommended contour level is 55 nm^3; this corresponds to an approximate mass of 50 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 (i)



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

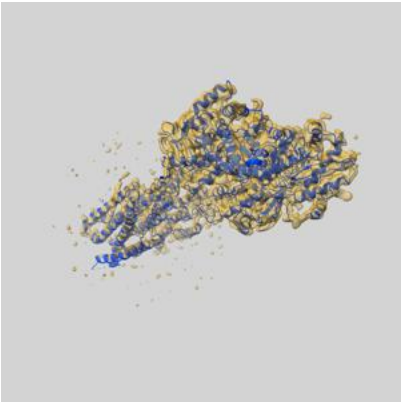
8 Fourier-Shell correlation (i)

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

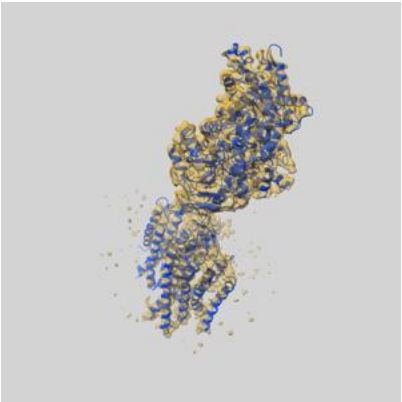
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30323 and PDB model 7CA3. Per-residue inclusion information can be found in section 3 on page 7.

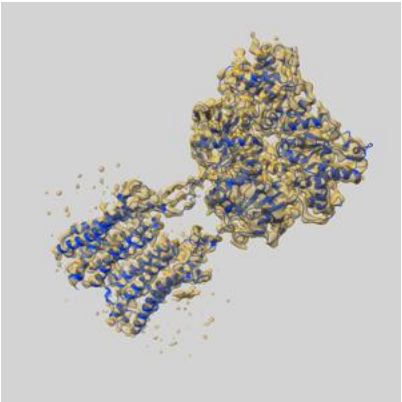
9.1 Map-model overlay (i)



X



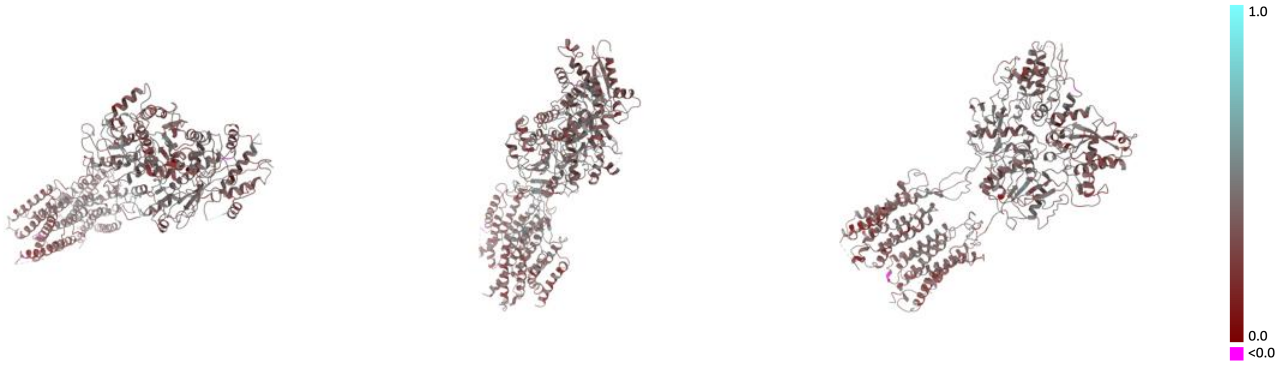
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0125 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.

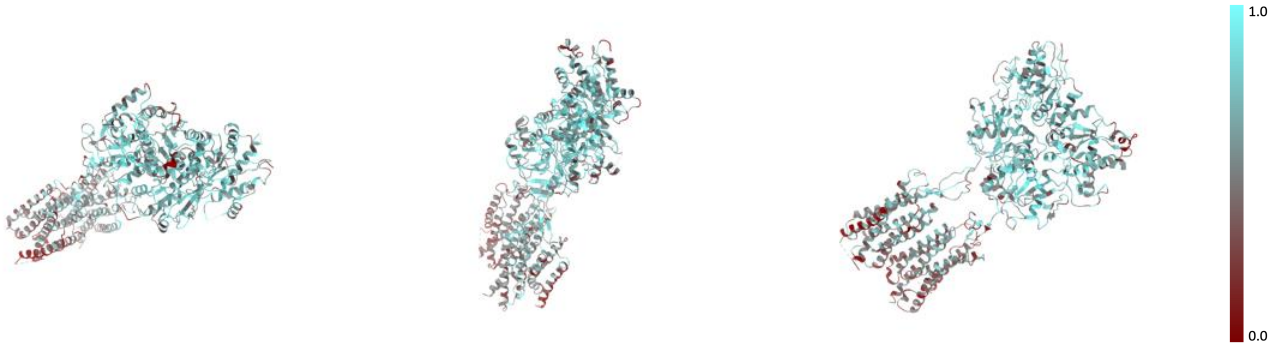
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

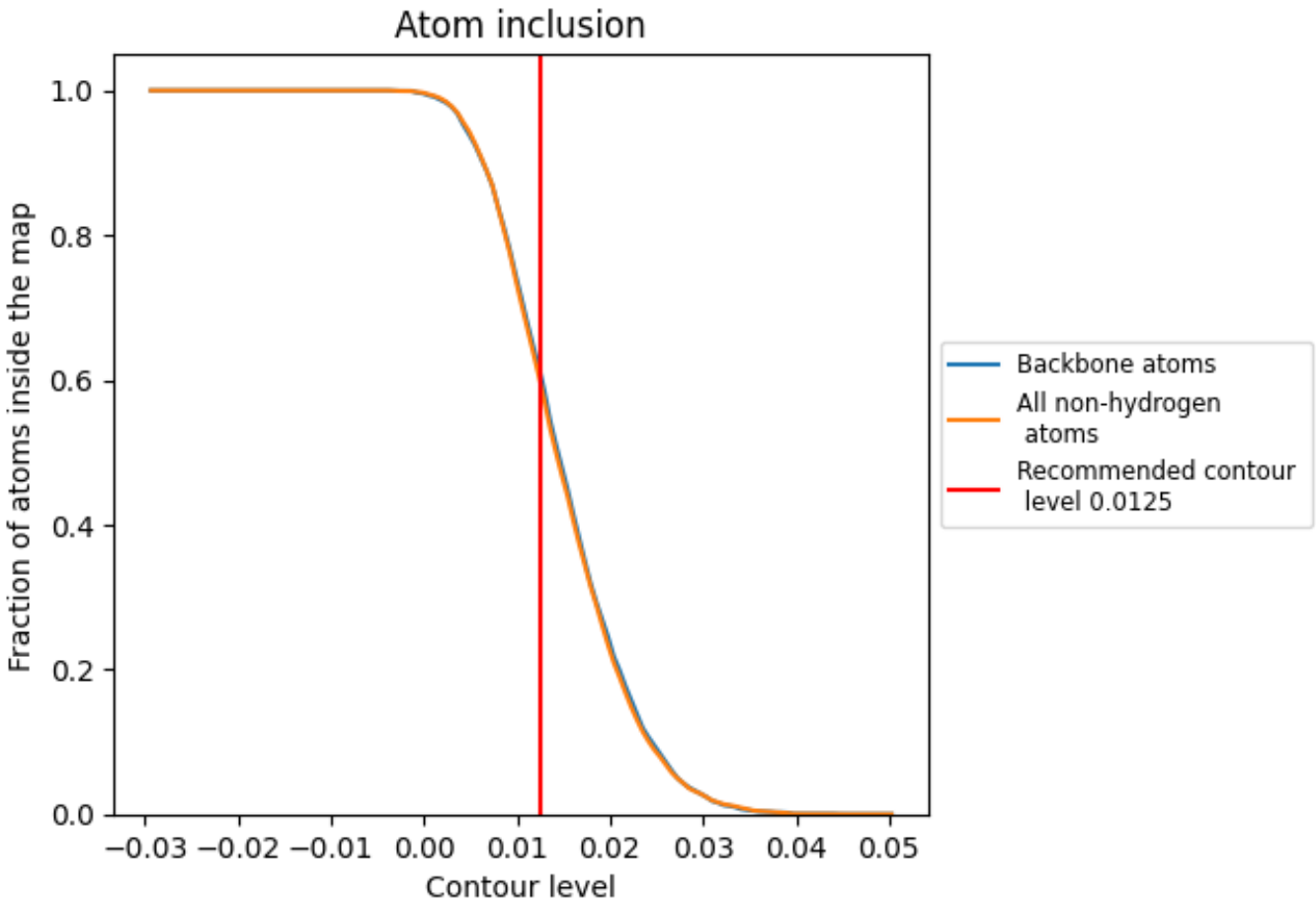
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0125).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5974	0.3760
A	0.6171	0.3860
B	0.5631	0.3660