Full wwPDB EM Validation Report

Feb 22, 2025 – 11:10 AM EST

PDB ID	:	8Z8Z
EMDB ID	:	EMD-39851
Title	:	Cryo-EM structure of LYCHOS
Authors	:	Xiong, Q.; Zhu, Z.; Li, T.; Zhou, Z.; Chao, Y.; Qu, Q.; Li, D.
Deposited on	:	2024-04-22
Resolution	:	2.11 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:

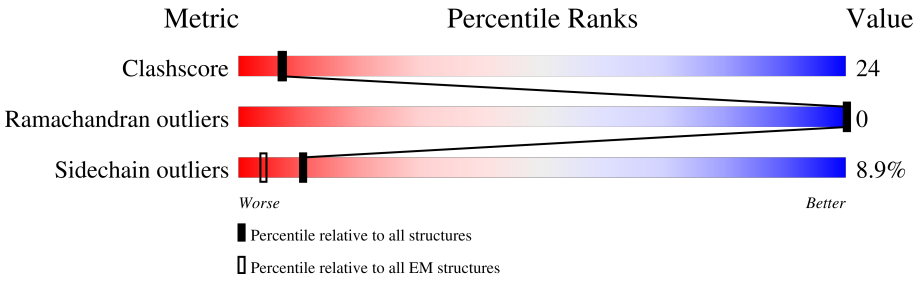
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.11 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1144	8% 30% 19% · 49%
1	B	1144	8% 30% 18% · 49%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9410 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

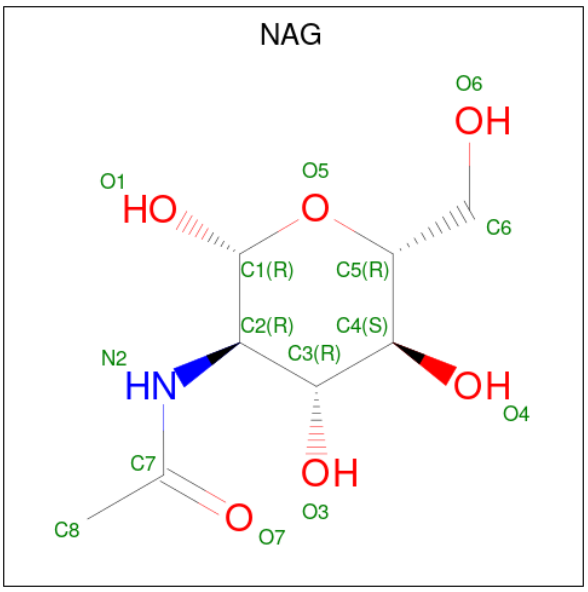
- Molecule 1 is a protein called Lysosomal cholesterol signaling protein,Fluorescent Protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	579	Total 4409	C 2952	N 680	O 750	S 27	0	0
1	B	579	Total 4409	C 2952	N 680	O 750	S 27	0	0

There are 6 discrepancies between the modelled and reference sequences:

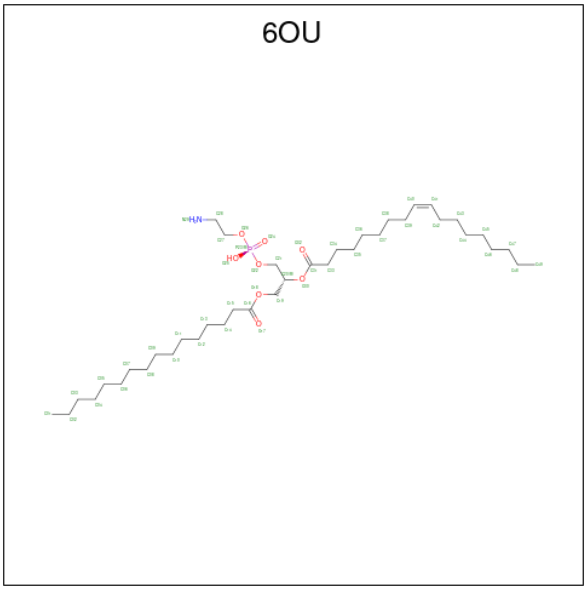
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q7Z3F1
A	-1	GLY	-	expression tag	UNP Q7Z3F1
A	0	SER	-	expression tag	UNP Q7Z3F1
B	-2	MET	-	initiating methionine	UNP Q7Z3F1
B	-1	GLY	-	expression tag	UNP Q7Z3F1
B	0	SER	-	expression tag	UNP Q7Z3F1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



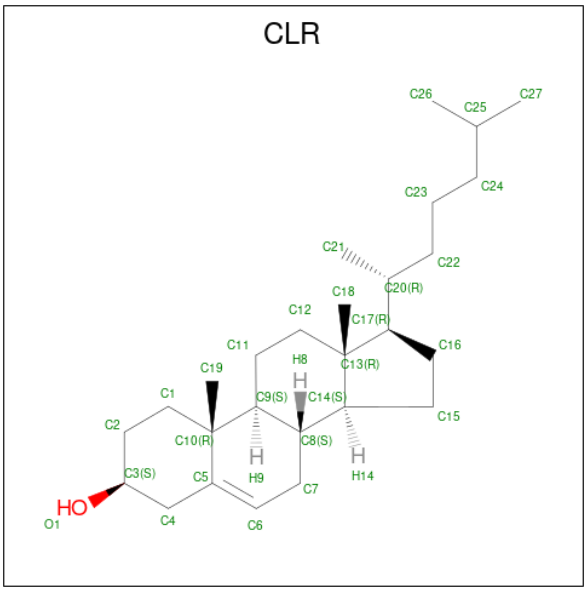
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$).



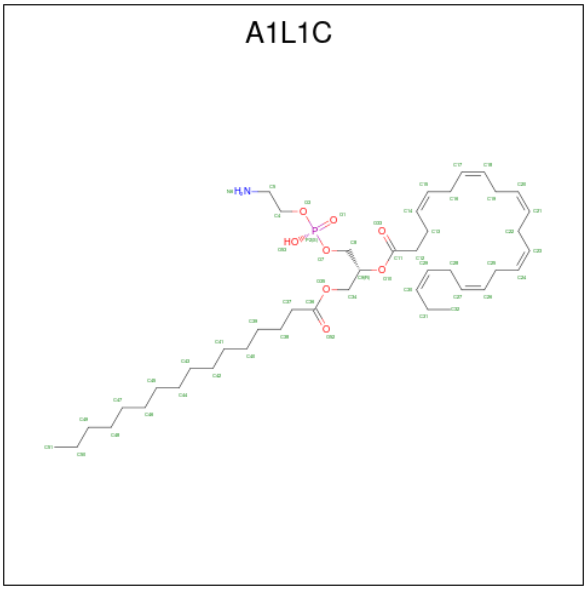
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 49	C 39	N 1	O 8	P 1	0
3	A	1	Total 49	C 39	N 1	O 8	P 1	0
3	A	1	Total 49	C 39	N 1	O 8	P 1	0
3	B	1	Total 49	C 39	N 1	O 8	P 1	0
3	B	1	Total 49	C 39	N 1	O 8	P 1	0
3	B	1	Total 49	C 39	N 1	O 8	P 1	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



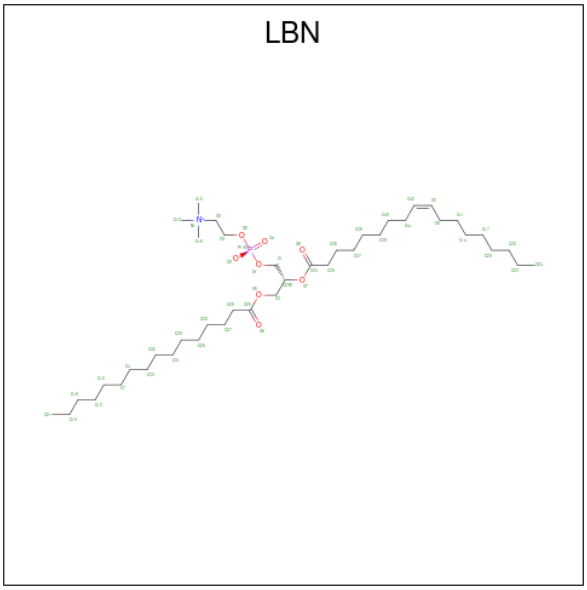
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	

- Molecule 5 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] (4 {Z},7 {Z},10 {Z},13 {Z},16 {Z},19 {Z})-docosa-4,7,10,13,16,19-hexaenoate (three-letter code: A1L1C) (formula: $C_{43}H_{74}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: $C_{42}H_{82}NO_8P$).



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Na	0
			1	1	
7	B	1	Total	Na	0
			1	1	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	O	0
			1	1	

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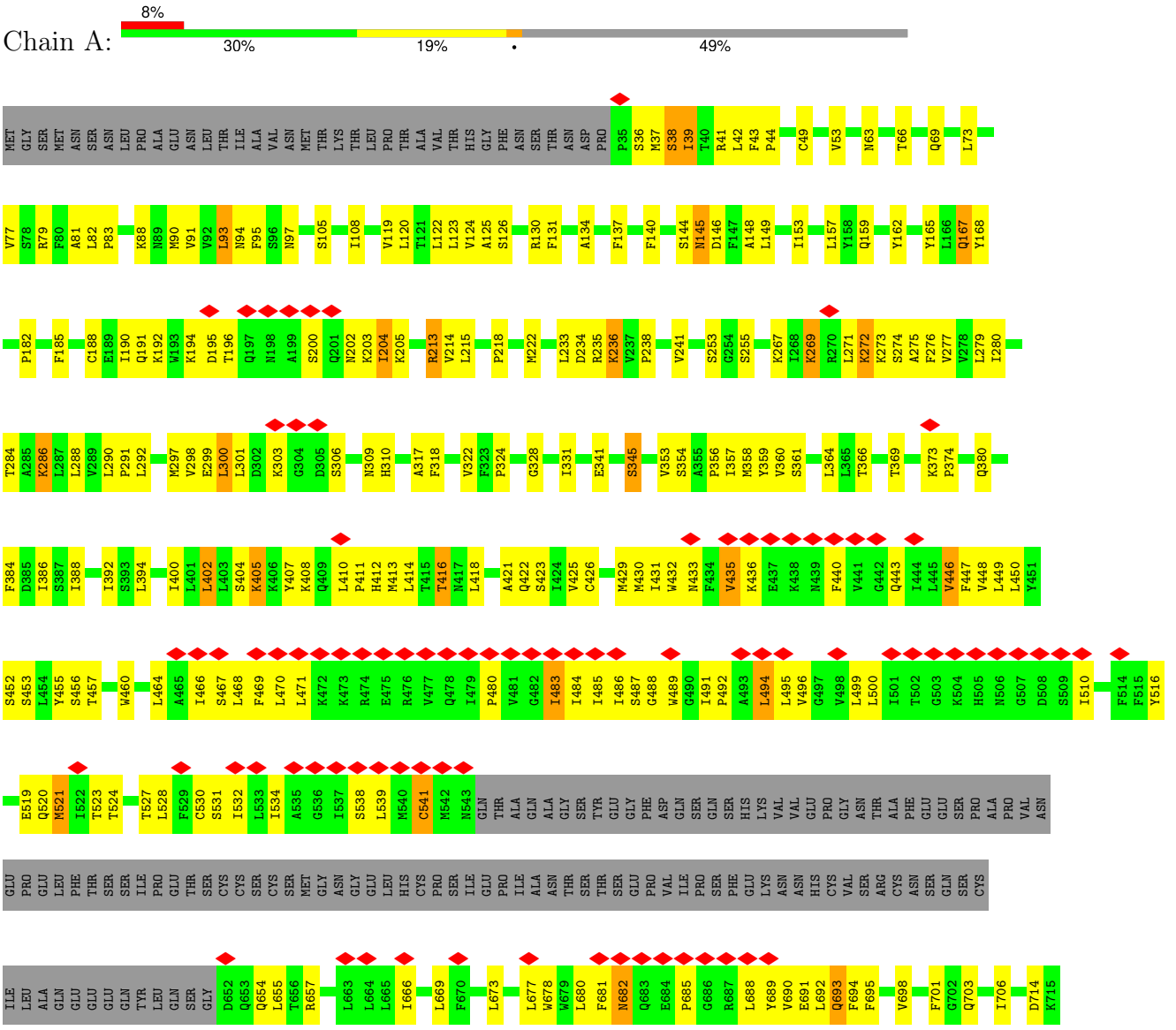
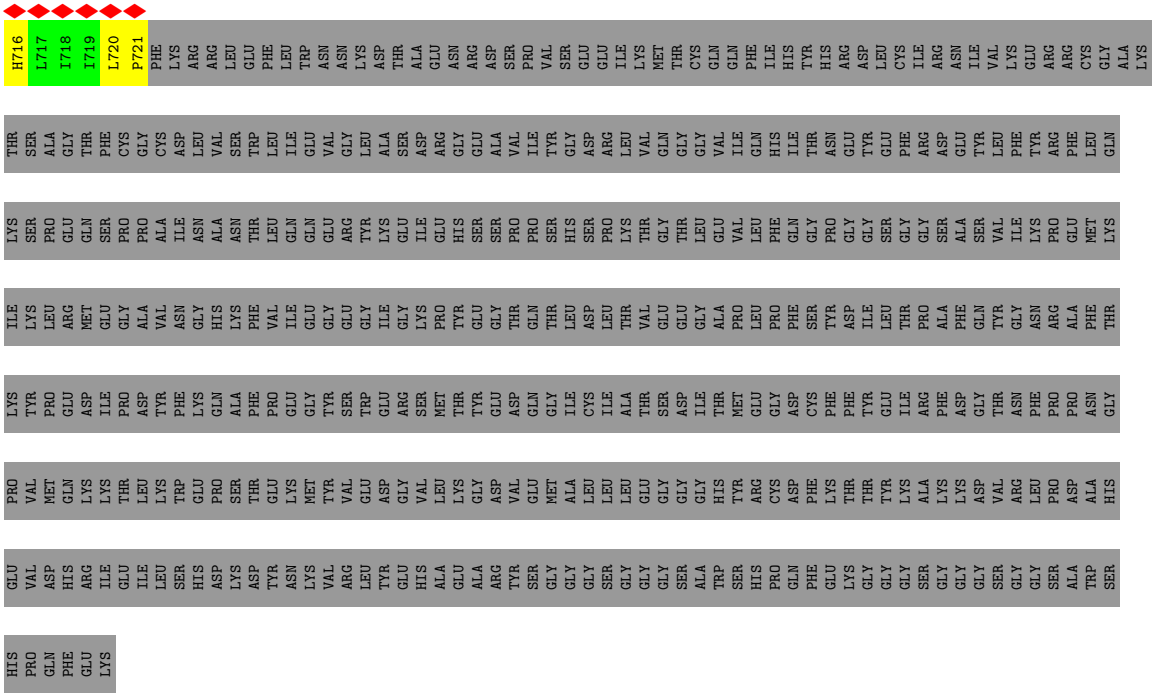
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
8	B	1	1	1	0

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.

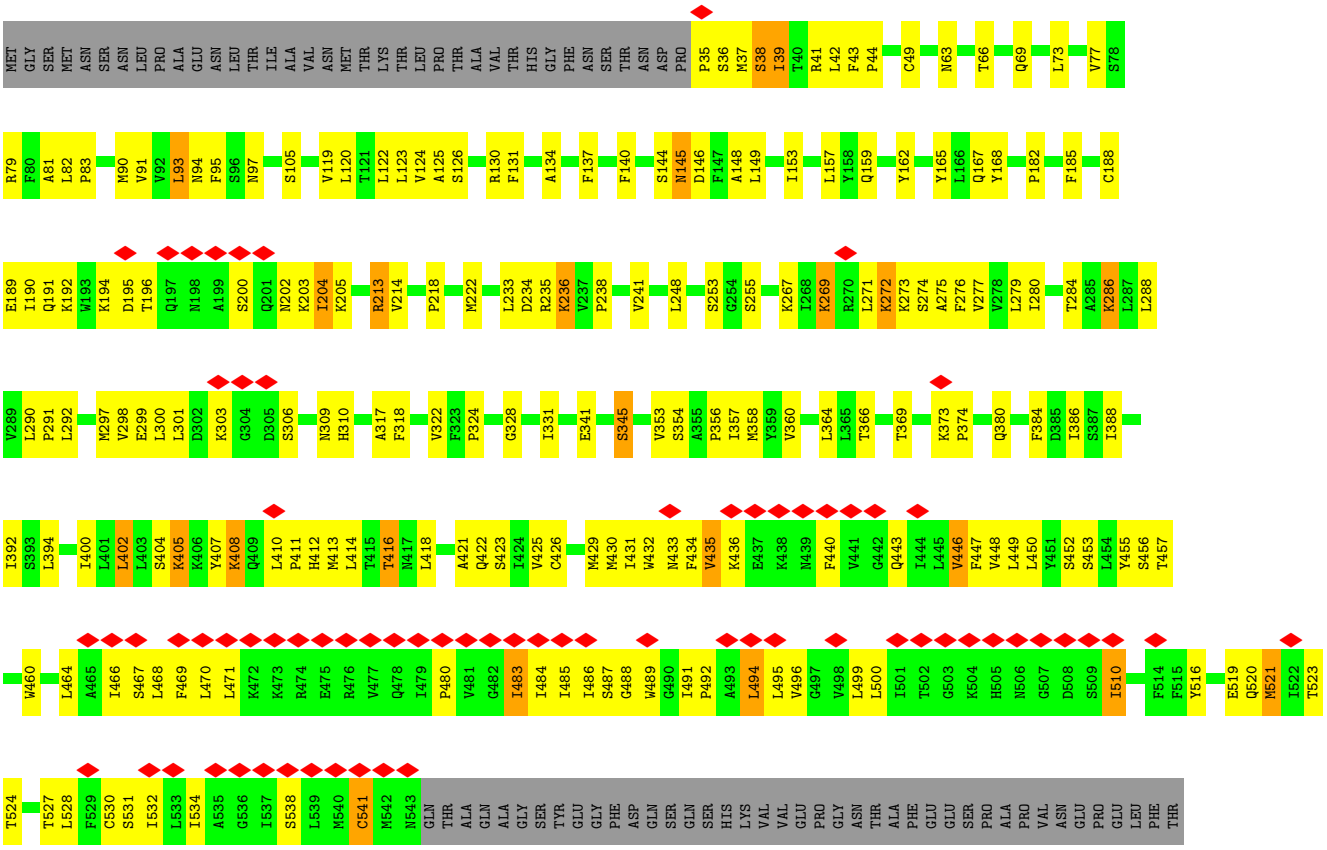
• Molecule 1: Lysosomal cholesterol signaling protein,Fluorescent Protein

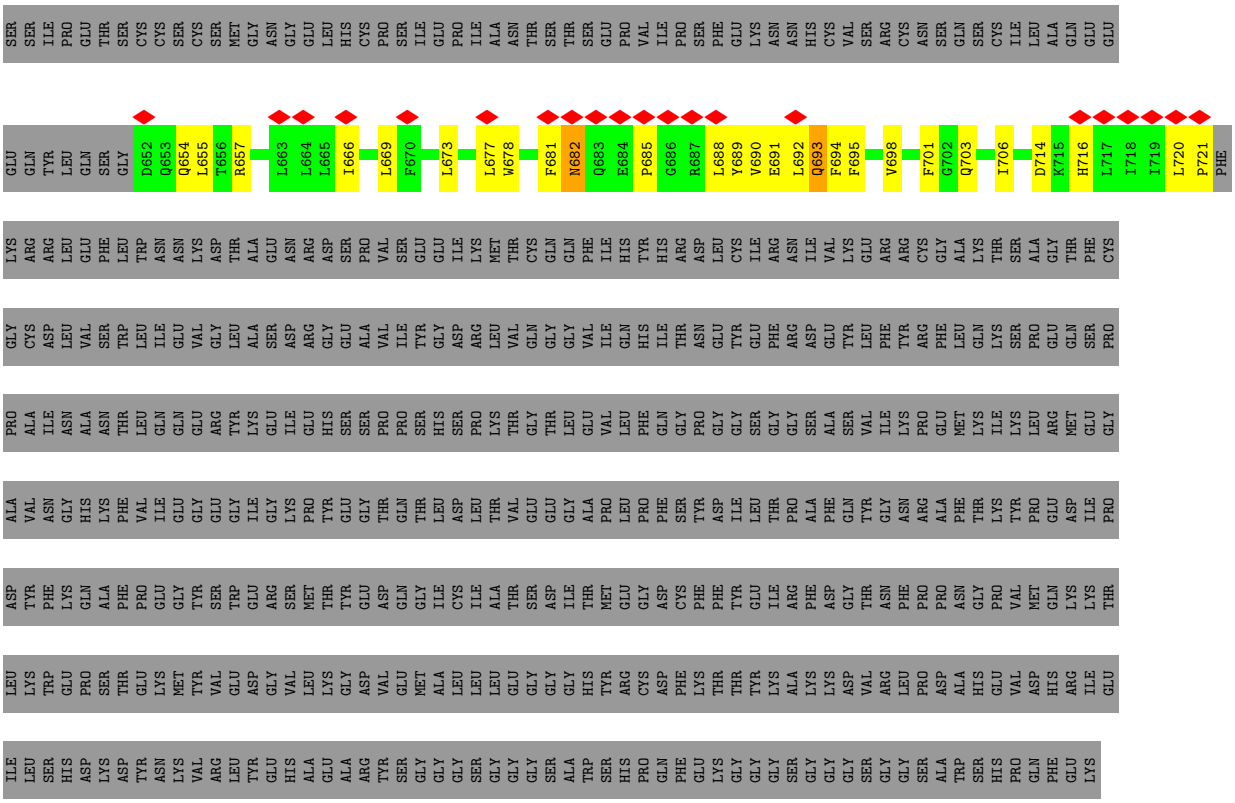




• Molecule 1: Lysosomal cholesterol signaling protein,Fluorescent Protein

Chain B:




SER SER ILE PRO GLU THR SER CYS CYS SER CYS SER MET GLY ASN GLY GLU LEU HIS CYS PRO SER ILE GLU PRO ILE ALA ASN THR SER THR SER GLU PRO VAL ILE PRO SER PHE GLU LYS ASN ASN HIS CYS VAL SER ARG CYS ASN SER GLN SER CYS ILE LEU ALA GLN GLU GLU
GLU GLN TYR LEU GLN SER GLY D652 Q653 Q654 L655 T656 R657 L663 L664 L665 I666 L669 F670 L673 L677 W678 F681 N682 Q683 E684 P685 G686 R687 L688 Y689 V690 E691 L692 Q693 F694 F695 V698 F701 G702 Q703 I706 D714 K715 H716 L717 I718 I719 L720 P721 PHE
LYS ARG ARG LEU GLU PHE LEU TRP ASN ASN LYS ASP THR ALA GLU ASN ARG ASP SER PRO VAL SER GLU GLU ILE LYS MET THR CYS GLN GLN PHE ILE HIS TYR HIS ARG ASP LEU CYS ILE ARG ASN ILE VAL LYS GLU ARG ARG CYS GLY ALA LYS THR SER ALA GLY THR PHE CYS
GLY CYS ASP LEU VAL SER TRP LEU ILE GLU VAL GLY LEU ALA SER ASP ARG GLY GLU ALA VAL ILE TYR GLY ASP ARG LEU VAL GLN GLY GLY VAL ILE GLN HIS ILE THR ASN GLU TYR GLU PHE ARG ASP GLU TYR LEU PHE TYR ARG PHE LEU GLN LYS SER PRO GLU GLN SER PRO
PRO ALA ILE ASN ALA ASN THR LEU GLN GLN GLU GLU ARG TYR LYS GLU ILE GLU HIS SER SER PRO PRO SER HIS SER PRO LYS THR GLY THR LEU GLU VAL LEU PHE GLN GLY PRO GLY GLY SER GLY GLY SER ALA SER VAL ILE LYS PRO GLU MET LYS ILE LYS LEU ARG MET GLU GLY
ALA VAL ASN GLY HIS LYS PHE VAL ILE GLU GLY GLU GLY ILE GLY LYS PRO TYR GLU GLY THR GLN THR LEU ASP LEU THR VAL GLU GLU GLY ALA PRO LEU PRO PHE SER TYR ASP ILE LEU THR PRO ALA PHE GLN TYR GLY ASN ARG ALA PHE THR LYS TYR PRO GLU ASP ILE PRO
ASP TYR PHE LYS GLN ALA PHE PRO GLU GLY TYR SER TRP GLU ARG SER MET THR TYR GLU ASP GLN GLY ILE CYS ILE ALA THR SER ASP ILE THR MET GLU GLY ASP CYS PHE PHE PHE TYR GLU ILE ARG PHE ASP GLY THR ASN PHE PRO PRO ASN GLY PRO VAL MET GLN LYS LYS THR
LEU LYS TRP GLU PRO SER THR GLU LYS MET TYR VAL GLU ASP GLY VAL LEU LYS GLY ASP VAL GLU MET ALA LEU LEU LEU GLU GLY GLY GLY HIS TYR ARG CYS ASP PHE LYS THR THR TYR LYS ALA LYS LYS ASP VAL ARG LEU PRO ASP ALA HIS GLU VAL ASP HIS ARG ILE GLU
ILE LEU SER HIS ASP LYS ASP TYR ASN LYS VAL ARG LEU TYR GLU HIS ALA GLU ALA ARG TYR SER GLY GLY GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	355557	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.076	Depositor
Minimum map value	-2.436	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.592	Depositor
Map size (Å)	335.52, 335.52, 335.52	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, NA, LBN, NAG, A1L1C, 6OU

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	0.75	0/4517	0.59	0/6159
1	B	0.75	0/4517	0.59	0/6159
All	All	0.75	0/9034	0.59	0/12318

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4409	0	4477	210	0
1	B	4409	0	4477	204	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	147	0	0	0	0
3	B	147	0	0	0	0
4	A	28	0	45	20	0
4	B	28	0	45	17	0
5	A	53	0	0	6	0
5	B	53	0	0	5	0
6	A	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	52	0	0	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
All	All	9410	0	9070	435	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 24.

All (435) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:LEU:HD13	1:B:655:LEU:HD11	1.24	1.18
1:A:471:LEU:HD13	1:A:655:LEU:HD11	1.24	1.12
1:B:471:LEU:HD13	1:B:655:LEU:CD1	1.80	1.11
1:A:471:LEU:HD13	1:A:655:LEU:CD1	1.80	1.11
4:A:1205:CLR:H12	5:A:1206:A1L1C:C40	1.88	1.02
4:B:1206:CLR:H12	5:B:1207:A1L1C:C40	1.88	1.02
1:B:202:ASN:HB3	1:B:205:LYS:HB3	1.46	0.98
1:A:202:ASN:HB3	1:A:205:LYS:HB3	1.46	0.97
1:A:471:LEU:CD1	1:A:655:LEU:CD2	2.48	0.92
1:B:471:LEU:CD1	1:B:655:LEU:CD2	2.48	0.92
1:A:471:LEU:CD1	1:A:655:LEU:CD1	2.48	0.91
1:B:471:LEU:CD1	1:B:655:LEU:CD1	2.48	0.91
1:B:471:LEU:CD1	1:B:655:LEU:HD11	2.06	0.85
1:A:471:LEU:HD13	1:A:655:LEU:CD2	2.07	0.84
1:B:297:MET:HE3	1:B:300:LEU:HD22	1.60	0.84
1:A:471:LEU:CD1	1:A:655:LEU:HD11	2.06	0.83
1:B:471:LEU:HD13	1:B:655:LEU:CD2	2.07	0.82
1:B:491:ILE:HA	1:B:494:LEU:HD23	1.62	0.81
1:A:471:LEU:CD1	1:A:655:LEU:HD21	2.10	0.81
1:B:471:LEU:CD1	1:B:655:LEU:HD21	2.10	0.81
1:A:131:PHE:HB2	1:A:191:GLN:HB2	1.63	0.79
1:A:491:ILE:HA	1:A:494:LEU:HD23	1.62	0.79
1:B:238:PRO:HB2	1:B:241:VAL:HG22	1.63	0.79
1:A:238:PRO:HB2	1:A:241:VAL:HG22	1.63	0.78
4:A:1205:CLR:C1	5:A:1206:A1L1C:C40	2.61	0.78
1:B:131:PHE:HB2	1:B:191:GLN:HB2	1.63	0.78
1:A:685:PRO:HG2	1:A:689:TYR:CG	2.19	0.78
1:A:471:LEU:HD13	1:A:655:LEU:HD21	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1206:CLR:C1	5:B:1207:A1L1C:C40	2.61	0.77
1:B:105:SER:HB3	1:B:301:LEU:HD11	1.67	0.77
1:B:685:PRO:HG2	1:B:689:TYR:CG	2.19	0.76
1:A:105:SER:HB3	1:A:301:LEU:HD11	1.67	0.76
1:A:297:MET:HE3	1:A:300:LEU:HD22	1.68	0.76
1:B:471:LEU:HD13	1:B:655:LEU:HD21	1.65	0.75
1:B:530:CYS:SG	1:B:531:SER:N	2.60	0.74
1:A:530:CYS:SG	1:A:531:SER:N	2.60	0.73
1:A:519:GLU:O	1:A:523:THR:HG23	1.90	0.72
1:B:519:GLU:O	1:B:523:THR:HG23	1.90	0.71
1:B:485:ILE:HG23	1:B:486:ILE:HD12	1.73	0.71
1:B:41:ARG:HH22	1:B:159:GLN:HG2	1.55	0.71
1:A:485:ILE:HG23	1:A:486:ILE:HD12	1.73	0.70
1:A:41:ARG:HH22	1:A:159:GLN:HG2	1.55	0.70
1:A:471:LEU:CD1	1:A:655:LEU:HD22	2.22	0.70
1:A:360:VAL:HG13	1:A:694:PHE:HE2	1.58	0.69
1:B:471:LEU:CD1	1:B:655:LEU:HD22	2.22	0.69
1:B:360:VAL:HG13	1:B:694:PHE:HE2	1.58	0.68
1:A:354:SER:O	1:A:358:MET:HG3	1.93	0.68
1:B:487:SER:HA	1:B:491:ILE:HG13	1.76	0.68
1:A:149:LEU:HD13	1:A:324:PRO:HG2	1.76	0.68
1:A:234:ASP:HB3	1:A:236:LYS:HE3	1.77	0.67
1:B:435:VAL:HG11	1:B:446:VAL:HG11	1.74	0.67
1:A:435:VAL:HG11	1:A:446:VAL:HG11	1.74	0.67
1:B:288:LEU:HD13	4:B:1206:CLR:H273	1.75	0.67
1:A:487:SER:HA	1:A:491:ILE:HG13	1.76	0.67
1:B:354:SER:O	1:B:358:MET:HG3	1.93	0.67
1:A:288:LEU:HD13	4:A:1205:CLR:H273	1.75	0.67
1:B:149:LEU:HD13	1:B:324:PRO:HG2	1.76	0.67
1:B:234:ASP:HB3	1:B:236:LYS:HE3	1.77	0.67
1:A:94:ASN:HA	1:A:235:ARG:HD2	1.78	0.66
1:A:82:LEU:HB3	1:A:83:PRO:HD3	1.78	0.65
1:B:94:ASN:HA	1:B:235:ARG:HD2	1.78	0.65
4:A:1205:CLR:C2	5:A:1206:A1L1C:C40	2.74	0.65
4:B:1206:CLR:C2	5:B:1207:A1L1C:C40	2.74	0.65
1:A:443:GLN:HA	1:A:446:VAL:CG1	2.27	0.64
1:B:443:GLN:HA	1:B:446:VAL:CG1	2.27	0.64
1:B:471:LEU:CD1	1:B:655:LEU:HD13	2.26	0.64
1:A:455:TYR:HH	1:A:524:THR:HG1	1.45	0.64
1:B:82:LEU:HB3	1:B:83:PRO:HD3	1.78	0.64
1:A:471:LEU:HD12	1:A:655:LEU:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:LEU:HD12	1:B:655:LEU:HD13	1.80	0.64
1:B:447:PHE:HE1	1:B:520:GLN:HE22	1.46	0.63
1:A:447:PHE:HE1	1:A:520:GLN:HE22	1.46	0.63
1:A:471:LEU:CD1	1:A:655:LEU:HD13	2.26	0.63
1:B:471:LEU:HD11	1:B:655:LEU:CD2	2.28	0.63
1:B:460:TRP:HH2	1:B:484:ILE:HA	1.64	0.62
1:A:460:TRP:HH2	1:A:484:ILE:HA	1.64	0.61
1:A:471:LEU:HD11	1:A:655:LEU:CD2	2.28	0.61
1:A:703:GLN:HA	1:A:706:ILE:HD12	1.83	0.61
1:B:471:LEU:HD11	1:B:655:LEU:HD21	1.84	0.60
1:B:233:LEU:HD13	1:B:238:PRO:HD3	1.82	0.60
1:B:703:GLN:HA	1:B:706:ILE:HD12	1.83	0.60
1:A:233:LEU:HD13	1:A:238:PRO:HD3	1.82	0.60
1:B:404:SER:HB3	1:B:716:HIS:HB3	1.83	0.60
1:A:489:TRP:C	1:A:492:PRO:HD2	2.22	0.60
1:A:471:LEU:HD13	1:A:655:LEU:CG	2.31	0.59
1:B:677:LEU:HB3	1:B:681:PHE:CZ	2.37	0.59
1:A:273:LYS:O	1:A:277:VAL:HG23	2.03	0.59
1:A:290:LEU:HB3	1:A:291:PRO:HD3	1.84	0.59
1:A:677:LEU:HB3	1:A:681:PHE:CZ	2.37	0.59
1:B:122:LEU:HD23	1:B:130:ARG:HD2	1.84	0.59
1:A:318:PHE:O	1:A:322:VAL:HG23	2.03	0.59
1:A:404:SER:HB3	1:A:716:HIS:HB3	1.83	0.59
1:B:273:LYS:O	1:B:277:VAL:HG23	2.03	0.59
1:B:466:ILE:HD11	1:B:534:ILE:HG23	1.84	0.59
1:B:489:TRP:C	1:B:492:PRO:HD2	2.22	0.59
1:B:455:TYR:HH	1:B:524:THR:HG1	1.46	0.59
1:A:466:ILE:HD11	1:A:534:ILE:HG23	1.84	0.59
1:B:410:LEU:HD13	1:B:413:MET:HB3	1.84	0.58
1:A:469:PHE:CE1	1:A:541:CYS:HB3	2.38	0.58
1:B:318:PHE:O	1:B:322:VAL:HG23	2.03	0.58
1:B:491:ILE:HB	1:B:492:PRO:HD3	1.85	0.58
1:A:516:TYR:HB2	1:A:520:GLN:HB2	1.85	0.58
1:A:410:LEU:HD13	1:A:413:MET:HB3	1.84	0.58
1:A:491:ILE:HB	1:A:492:PRO:HD3	1.85	0.58
1:B:516:TYR:HB2	1:B:520:GLN:HB2	1.85	0.58
1:A:122:LEU:HD23	1:A:130:ARG:HD2	1.84	0.58
1:A:39:ILE:HG12	1:A:366:THR:HG21	1.86	0.57
1:B:453:SER:O	1:B:457:THR:HG23	2.04	0.57
1:B:492:PRO:HA	1:B:495:LEU:HD12	1.86	0.57
1:B:469:PHE:CE1	1:B:541:CYS:HB3	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LEU:HB3	1:B:291:PRO:HD3	1.84	0.57
1:B:469:PHE:CD1	1:B:541:CYS:HB3	2.39	0.57
1:A:471:LEU:HD11	1:A:655:LEU:HD21	1.84	0.57
1:B:471:LEU:HD13	1:B:655:LEU:CG	2.31	0.57
1:A:357:ILE:HD13	4:A:1205:CLR:H25	1.86	0.57
1:A:453:SER:O	1:A:457:THR:HG23	2.04	0.57
1:A:469:PHE:CD1	1:A:541:CYS:HB3	2.39	0.57
1:B:39:ILE:HG12	1:B:366:THR:HG21	1.86	0.57
1:B:467:SER:O	1:B:471:LEU:HG	2.05	0.57
1:A:91:VAL:O	1:A:235:ARG:HA	2.05	0.57
1:A:492:PRO:HA	1:A:495:LEU:HD12	1.86	0.57
1:B:91:VAL:O	1:B:235:ARG:HA	2.05	0.57
1:B:666:ILE:HA	1:B:669:LEU:HD12	1.87	0.56
1:A:37:MET:HG2	1:A:157:LEU:HD22	1.88	0.56
1:B:357:ILE:HD13	4:B:1206:CLR:H25	1.86	0.56
1:B:440:PHE:HA	1:B:443:GLN:HE21	1.69	0.56
1:A:467:SER:O	1:A:471:LEU:HG	2.05	0.56
1:A:38:SER:HB2	1:A:41:ARG:HG3	1.87	0.56
1:A:306:SER:HB3	1:A:309:ASN:HB2	1.88	0.56
1:B:38:SER:HB2	1:B:41:ARG:HG3	1.88	0.56
1:B:678:TRP:HD1	1:B:689:TYR:CD1	2.24	0.56
1:B:306:SER:HB3	1:B:309:ASN:HB2	1.88	0.56
1:A:440:PHE:HA	1:A:443:GLN:HE21	1.69	0.56
1:A:491:ILE:O	1:A:495:LEU:HG	2.06	0.56
1:A:666:ILE:HA	1:A:669:LEU:HD12	1.87	0.56
1:B:37:MET:HG2	1:B:157:LEU:HD22	1.88	0.55
1:A:678:TRP:HD1	1:A:689:TYR:CD1	2.24	0.55
1:B:284:THR:HG22	4:B:1206:CLR:H221	1.89	0.55
1:B:491:ILE:O	1:B:495:LEU:HG	2.06	0.55
1:B:353:VAL:HG21	4:B:1206:CLR:H122	1.89	0.55
1:A:353:VAL:HG21	4:A:1205:CLR:H122	1.89	0.54
1:B:433:ASN:HA	1:B:436:LYS:HD3	1.89	0.54
1:A:284:THR:HG22	4:A:1205:CLR:H221	1.89	0.54
1:A:394:LEU:HD13	1:A:423:SER:HA	1.90	0.54
1:A:185:PHE:CD2	1:A:213:ARG:HG2	2.43	0.54
1:B:410:LEU:HD12	1:B:411:PRO:HA	1.89	0.53
1:A:410:LEU:HD12	1:A:411:PRO:HA	1.89	0.53
1:B:466:ILE:O	1:B:470:LEU:HG	2.09	0.53
1:A:433:ASN:HA	1:A:436:LYS:HD3	1.89	0.53
1:B:324:PRO:HG3	1:B:354:SER:OG	2.09	0.53
1:A:204:ILE:HD12	1:A:205:LYS:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ILE:HD12	1:B:205:LYS:H	1.73	0.53
1:A:324:PRO:HG3	1:A:354:SER:OG	2.09	0.53
1:A:466:ILE:O	1:A:470:LEU:HG	2.09	0.53
1:A:90:MET:HE3	1:A:95:PHE:HZ	1.74	0.53
1:B:185:PHE:CD2	1:B:213:ARG:HG2	2.43	0.53
1:B:678:TRP:HD1	1:B:689:TYR:HD1	1.56	0.53
1:A:460:TRP:CZ2	1:A:488:GLY:HA3	2.44	0.53
1:A:443:GLN:HA	1:A:446:VAL:HG12	1.90	0.52
1:A:678:TRP:HD1	1:A:689:TYR:HD1	1.56	0.52
1:B:394:LEU:HD13	1:B:423:SER:HA	1.89	0.52
1:B:443:GLN:HA	1:B:446:VAL:HG12	1.90	0.52
1:B:43:PHE:N	1:B:44:PRO:HD2	2.25	0.52
1:A:720:LEU:N	1:A:721:PRO:HD2	2.24	0.52
1:B:412:HIS:NE2	1:B:654:GLN:NE2	2.58	0.51
1:B:460:TRP:CZ2	1:B:488:GLY:HA3	2.44	0.51
1:A:43:PHE:N	1:A:44:PRO:HD2	2.25	0.51
1:A:284:THR:CG2	4:A:1205:CLR:H221	2.41	0.51
1:A:528:LEU:HD13	1:A:673:LEU:CA	2.41	0.51
1:B:90:MET:HE3	1:B:95:PHE:HZ	1.74	0.51
1:B:412:HIS:HD1	1:B:412:HIS:H	1.58	0.51
1:B:528:LEU:HD13	1:B:673:LEU:CA	2.41	0.51
1:B:720:LEU:N	1:B:721:PRO:HD2	2.24	0.51
1:B:185:PHE:CE2	1:B:213:ARG:HG2	2.45	0.51
1:B:413:MET:O	1:B:416:THR:HG22	2.10	0.51
1:A:185:PHE:CE2	1:A:213:ARG:HG2	2.45	0.51
1:A:412:HIS:NE2	1:A:654:GLN:NE2	2.58	0.51
1:A:413:MET:O	1:A:416:THR:HG22	2.10	0.51
1:A:218:PRO:O	1:A:222:MET:HB2	2.11	0.50
1:B:218:PRO:O	1:B:222:MET:HB2	2.11	0.50
1:B:284:THR:CG2	4:B:1206:CLR:H221	2.41	0.50
1:B:405:LYS:HA	1:B:407:TYR:CE1	2.47	0.50
1:B:272:LYS:HG2	1:B:275:ALA:H	1.76	0.50
1:A:432:TRP:HA	1:A:435:VAL:HG12	1.94	0.50
1:B:144:SER:OG	1:B:146:ASP:OD1	2.26	0.50
1:B:446:VAL:HA	1:B:449:LEU:HD21	1.94	0.50
1:A:36:SER:HB2	1:A:162:TYR:HE1	1.77	0.50
1:A:272:LYS:HG2	1:A:275:ALA:H	1.76	0.50
1:B:714:ASP:HB2	1:B:716:HIS:HE1	1.76	0.50
1:A:412:HIS:HD1	1:A:412:HIS:H	1.58	0.50
1:A:435:VAL:HG11	1:A:446:VAL:CG1	2.42	0.50
1:A:446:VAL:HA	1:A:449:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ILE:HD12	1:A:486:ILE:H	1.77	0.50
1:B:386:ILE:HD13	1:B:698:VAL:HA	1.94	0.50
1:B:486:ILE:HD12	1:B:486:ILE:H	1.77	0.50
1:A:714:ASP:HB2	1:A:716:HIS:HE1	1.76	0.49
1:A:280:ILE:HA	4:A:1205:CLR:H152	1.93	0.49
1:A:94:ASN:HD22	1:A:97:ASN:CG	2.16	0.49
1:B:405:LYS:HZ3	1:B:407:TYR:HE1	1.60	0.49
1:A:144:SER:OG	1:A:146:ASP:OD1	2.26	0.49
1:A:357:ILE:O	1:A:361:SER:OG	2.22	0.49
1:A:405:LYS:HZ3	1:A:407:TYR:HE1	1.60	0.49
1:A:688:LEU:HD12	1:A:691:GLU:OE1	2.13	0.49
1:B:280:ILE:HA	4:B:1206:CLR:H152	1.93	0.49
1:A:405:LYS:HA	1:A:407:TYR:CE1	2.47	0.49
1:B:341:GLU:H	1:B:341:GLU:CD	2.16	0.49
1:B:380:GLN:HG3	1:B:436:LYS:HE2	1.95	0.49
1:B:496:VAL:O	1:B:499:LEU:HG	2.13	0.49
1:B:404:SER:O	1:B:405:LYS:HB2	2.13	0.49
1:A:364:LEU:HD11	1:A:695:PHE:CE2	2.48	0.49
1:A:496:VAL:O	1:A:499:LEU:HG	2.13	0.49
1:A:39:ILE:O	1:A:42:LEU:HB3	2.13	0.48
1:A:380:GLN:HG3	1:A:436:LYS:HE2	1.95	0.48
1:B:688:LEU:HD12	1:B:691:GLU:OE1	2.13	0.48
1:B:66:THR:OG1	1:B:69:GLN:HG3	2.13	0.48
1:A:122:LEU:O	1:A:130:ARG:HD3	2.14	0.48
1:B:432:TRP:HA	1:B:435:VAL:HG12	1.94	0.48
1:A:272:LYS:HE2	1:A:272:LYS:H	1.78	0.48
1:A:386:ILE:HD13	1:A:698:VAL:HA	1.94	0.48
1:B:36:SER:HB2	1:B:162:TYR:HE1	1.77	0.48
1:B:272:LYS:H	1:B:272:LYS:HE2	1.78	0.48
1:A:341:GLU:CD	1:A:341:GLU:H	2.16	0.48
1:A:500:LEU:HD13	1:A:516:TYR:OH	2.13	0.48
1:A:404:SER:O	1:A:405:LYS:HB2	2.13	0.48
1:A:685:PRO:HG2	1:A:689:TYR:CD1	2.49	0.48
1:B:122:LEU:O	1:B:130:ARG:HD3	2.14	0.48
1:A:144:SER:HB3	1:A:286:LYS:HE3	1.95	0.48
1:B:685:PRO:HG2	1:B:689:TYR:CD1	2.49	0.48
1:A:452:SER:O	1:A:456:SER:OG	2.21	0.47
1:B:39:ILE:O	1:B:42:LEU:HB3	2.13	0.47
1:B:284:THR:HG22	4:B:1206:CLR:C22	2.45	0.47
1:B:94:ASN:HD22	1:B:97:ASN:CG	2.16	0.47
1:B:466:ILE:HD13	1:B:538:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1205:CLR:H193	4:A:1205:CLR:H111	1.65	0.47
1:B:500:LEU:HD13	1:B:516:TYR:OH	2.13	0.47
4:B:1206:CLR:H22	5:B:1207:A1L1C:C38	2.44	0.47
1:A:66:THR:OG1	1:A:69:GLN:HG3	2.14	0.47
4:B:1206:CLR:H121	4:B:1206:CLR:H212	1.97	0.47
1:A:284:THR:HG22	4:A:1205:CLR:C22	2.44	0.47
1:B:364:LEU:HD11	1:B:695:PHE:CE2	2.48	0.47
1:A:446:VAL:O	1:A:450:LEU:HB2	2.15	0.47
1:B:373:LYS:HB3	1:B:374:PRO:HD3	1.97	0.47
1:B:446:VAL:HA	1:B:449:LEU:CD2	2.45	0.47
1:A:373:LYS:HB3	1:A:374:PRO:HD3	1.97	0.47
1:A:466:ILE:HD13	1:A:538:SER:OG	2.14	0.47
1:B:446:VAL:O	1:B:450:LEU:HB2	2.15	0.47
4:A:1205:CLR:H22	5:A:1206:A1L1C:C38	2.44	0.47
1:A:402:LEU:HA	1:A:407:TYR:CD1	2.50	0.47
1:B:288:LEU:C	1:B:291:PRO:HD2	2.36	0.47
1:B:460:TRP:HZ2	1:B:484:ILE:O	1.98	0.46
1:A:446:VAL:HA	1:A:449:LEU:CD2	2.45	0.46
1:A:447:PHE:HE2	1:A:500:LEU:HD21	1.80	0.46
1:B:144:SER:HB3	1:B:286:LYS:HE3	1.96	0.46
1:B:491:ILE:O	1:B:494:LEU:HG	2.15	0.46
1:A:689:TYR:O	1:A:692:LEU:N	2.49	0.46
4:A:1205:CLR:H121	4:A:1205:CLR:H212	1.97	0.46
1:A:384:PHE:CE2	1:A:388:ILE:HD11	2.50	0.46
1:B:447:PHE:HE2	1:B:500:LEU:HD21	1.80	0.46
1:B:523:THR:O	1:B:527:THR:OG1	2.29	0.46
1:A:131:PHE:CB	1:A:191:GLN:HB2	2.42	0.46
1:A:491:ILE:O	1:A:494:LEU:HG	2.15	0.46
1:B:122:LEU:HG	1:B:134:ALA:HB2	1.98	0.46
1:B:682:ASN:OD1	1:B:685:PRO:HB3	2.16	0.46
4:B:1206:CLR:H22	5:B:1207:A1L1C:C40	2.45	0.46
1:A:528:LEU:HD13	1:A:673:LEU:HA	1.98	0.46
1:B:384:PHE:CE2	1:B:388:ILE:HD11	2.50	0.46
1:B:689:TYR:O	1:B:692:LEU:N	2.49	0.46
1:B:429:MET:HE2	1:B:701:PHE:CZ	2.50	0.46
1:B:528:LEU:HD13	1:B:673:LEU:HA	1.98	0.46
1:A:36:SER:HB2	1:A:162:TYR:CE1	2.51	0.46
1:A:73:LEU:HD11	1:A:255:SER:HB3	1.98	0.46
1:A:404:SER:CB	1:A:716:HIS:HB3	2.46	0.46
1:B:272:LYS:HE2	1:B:272:LYS:HB3	1.57	0.46
1:A:122:LEU:HG	1:A:134:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:C	1:A:291:PRO:HD2	2.36	0.45
1:B:36:SER:HB2	1:B:162:TYR:CE1	2.51	0.45
1:B:402:LEU:HA	1:B:407:TYR:CD1	2.50	0.45
1:B:435:VAL:HG11	1:B:446:VAL:CG1	2.42	0.45
1:A:280:ILE:HA	4:A:1205:CLR:C15	2.46	0.45
1:A:467:SER:HA	1:A:470:LEU:HD12	1.98	0.45
1:B:404:SER:CB	1:B:716:HIS:HB3	2.46	0.45
1:A:429:MET:HE2	1:A:701:PHE:CZ	2.51	0.45
1:A:433:ASN:HA	1:A:436:LYS:CD	2.46	0.45
1:B:125:ALA:O	1:B:130:ARG:HG3	2.17	0.45
1:B:421:ALA:O	1:B:425:VAL:HG23	2.17	0.45
1:A:88:LYS:HE3	1:A:88:LYS:HB3	1.77	0.45
1:A:241:VAL:HG12	6:A:1207:LBN:C10	2.47	0.45
1:A:341:GLU:O	1:A:345:SER:OG	2.25	0.45
1:A:422:GLN:NE2	1:A:703:GLN:HB3	2.32	0.45
1:A:460:TRP:HZ2	1:A:484:ILE:O	1.98	0.45
1:A:682:ASN:OD1	1:A:685:PRO:HB3	2.16	0.45
1:B:341:GLU:O	1:B:345:SER:OG	2.25	0.45
1:B:422:GLN:NE2	1:B:703:GLN:HB3	2.32	0.45
4:B:1206:CLR:H221	4:B:1206:CLR:H162	1.68	0.45
1:B:455:TYR:OH	1:B:524:THR:OG1	2.26	0.45
1:B:433:ASN:HA	1:B:436:LYS:CD	2.46	0.45
1:A:125:ALA:O	1:A:130:ARG:HG3	2.17	0.45
1:A:298:VAL:HG21	1:A:317:ALA:HB2	1.98	0.45
1:A:471:LEU:HD11	1:A:655:LEU:HD22	1.97	0.45
1:B:188:CYS:O	1:B:192:LYS:HG3	2.17	0.45
1:B:279:LEU:HD23	1:B:279:LEU:HA	1.67	0.44
1:B:280:ILE:HA	4:B:1206:CLR:C15	2.46	0.44
1:B:298:VAL:HG21	1:B:317:ALA:HB2	1.98	0.44
4:B:1206:CLR:H213	4:B:1206:CLR:H231	1.56	0.44
1:B:467:SER:HA	1:B:470:LEU:HD12	1.98	0.44
1:B:532:ILE:HD11	1:B:669:LEU:O	2.17	0.44
1:A:105:SER:CB	1:A:301:LEU:HD21	2.48	0.44
1:A:149:LEU:O	1:A:153:ILE:HD12	2.18	0.44
1:A:364:LEU:HD11	1:A:695:PHE:CZ	2.52	0.44
1:A:690:VAL:HA	1:A:693:GLN:HB3	2.00	0.44
1:B:452:SER:O	1:B:456:SER:OG	2.21	0.44
1:A:299:GLU:HA	1:A:310:HIS:NE2	2.33	0.44
4:A:1205:CLR:H221	4:A:1205:CLR:H162	1.68	0.44
4:A:1205:CLR:H213	4:A:1205:CLR:H231	1.56	0.44
1:B:105:SER:CB	1:B:301:LEU:HD21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:LEU:HD11	1:B:695:PHE:CZ	2.52	0.44
1:A:188:CYS:O	1:A:192:LYS:HG3	2.17	0.44
1:B:690:VAL:HA	1:B:693:GLN:HB3	2.00	0.44
4:A:1205:CLR:H22	5:A:1206:A1L1C:C40	2.45	0.44
1:A:414:LEU:HD22	1:A:460:TRP:HZ3	1.83	0.44
1:A:421:ALA:O	1:A:425:VAL:HG23	2.17	0.44
1:A:532:ILE:HD11	1:A:669:LEU:O	2.17	0.44
1:B:192:LYS:O	1:B:196:THR:HG23	2.18	0.44
1:A:105:SER:HB2	1:A:297:MET:HB3	2.00	0.44
1:A:464:LEU:O	1:A:468:LEU:HG	2.18	0.43
1:B:149:LEU:O	1:B:153:ILE:HD12	2.18	0.43
1:B:694:PHE:O	1:B:698:VAL:HG13	2.18	0.43
4:B:1206:CLR:H182	4:B:1206:CLR:H8	1.72	0.43
1:A:77:VAL:HA	1:A:81:ALA:HB3	2.00	0.43
1:A:192:LYS:O	1:A:196:THR:HG23	2.18	0.43
1:B:73:LEU:HD11	1:B:255:SER:HB3	1.98	0.43
1:B:299:GLU:HA	1:B:310:HIS:NE2	2.33	0.43
1:B:485:ILE:HD12	1:B:489:TRP:HB3	2.00	0.43
1:A:407:TYR:O	1:A:413:MET:HA	2.18	0.43
1:B:714:ASP:HB2	1:B:716:HIS:CE1	2.54	0.43
1:B:137:PHE:O	1:B:140:PHE:HB3	2.18	0.43
1:B:408:LYS:HE2	1:B:408:LYS:HB3	1.33	0.43
1:B:414:LEU:HD22	1:B:460:TRP:HZ3	1.83	0.43
1:B:464:LEU:O	1:B:468:LEU:HG	2.18	0.43
1:A:468:LEU:HA	1:A:471:LEU:HD12	2.01	0.43
1:A:539:LEU:HD23	1:A:539:LEU:HA	1.82	0.43
1:A:714:ASP:HB2	1:A:716:HIS:CE1	2.54	0.43
1:B:131:PHE:CB	1:B:191:GLN:HB2	2.42	0.43
1:B:145:ASN:HD21	1:B:148:ALA:HB3	1.84	0.43
1:B:446:VAL:O	1:B:449:LEU:HG	2.18	0.43
1:B:510:ILE:H	1:B:510:ILE:HG12	1.59	0.43
1:B:94:ASN:O	1:B:95:PHE:HB2	2.19	0.43
1:B:353:VAL:O	1:B:356:PRO:HD2	2.19	0.43
1:A:93:LEU:HD22	1:A:95:PHE:CD1	2.53	0.43
1:A:94:ASN:O	1:A:95:PHE:HB2	2.19	0.43
1:A:137:PHE:O	1:A:140:PHE:HB3	2.18	0.43
1:B:93:LEU:HD22	1:B:95:PHE:CD1	2.53	0.43
1:A:388:ILE:O	1:A:392:ILE:HG13	2.19	0.43
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.67	0.43
1:B:190:ILE:O	1:B:194:LYS:HG2	2.19	0.43
1:B:407:TYR:O	1:B:413:MET:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:VAL:O	1:A:449:LEU:HG	2.18	0.43
1:B:49:CYS:HB3	1:B:149:LEU:HD23	2.01	0.43
1:B:241:VAL:HG12	6:B:1201:LBN:C10	2.49	0.43
1:B:410:LEU:CD1	1:B:413:MET:HB3	2.49	0.43
1:B:480:PRO:O	1:B:483:ILE:HG12	2.19	0.43
1:A:483:ILE:HA	1:A:487:SER:OG	2.19	0.42
1:A:528:LEU:HD13	1:A:673:LEU:N	2.34	0.42
4:A:1205:CLR:H183	4:A:1205:CLR:H20	1.76	0.42
1:A:145:ASN:HD21	1:A:148:ALA:HB3	1.84	0.42
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.81	0.42
1:A:384:PHE:HB2	1:A:433:ASN:HD22	1.84	0.42
1:A:410:LEU:CD1	1:A:413:MET:HB3	2.49	0.42
1:A:485:ILE:HD12	1:A:489:TRP:HB3	2.00	0.42
1:B:410:LEU:HD13	1:B:410:LEU:HA	1.86	0.42
1:B:468:LEU:HA	1:B:471:LEU:HD12	2.01	0.42
1:B:483:ILE:HA	1:B:487:SER:OG	2.19	0.42
1:A:272:LYS:HE2	1:A:272:LYS:HB3	1.57	0.42
1:B:105:SER:HB2	1:B:297:MET:HB3	2.00	0.42
1:A:480:PRO:O	1:A:483:ILE:HG12	2.19	0.42
1:B:388:ILE:O	1:B:392:ILE:HG13	2.18	0.42
1:A:39:ILE:H	1:A:39:ILE:HG13	1.48	0.42
1:A:49:CYS:HB3	1:A:149:LEU:HD23	2.01	0.42
1:A:353:VAL:O	1:A:356:PRO:HD2	2.19	0.42
1:A:694:PHE:O	1:A:698:VAL:HG13	2.18	0.42
1:B:384:PHE:HB2	1:B:433:ASN:HD22	1.84	0.42
1:B:528:LEU:HD13	1:B:673:LEU:N	2.34	0.42
1:A:190:ILE:O	1:A:194:LYS:HG2	2.19	0.42
1:B:77:VAL:HA	1:B:81:ALA:HB3	2.00	0.42
1:B:120:LEU:O	1:B:124:VAL:HG22	2.20	0.42
1:B:119:VAL:O	1:B:123:LEU:HG	2.20	0.42
1:A:426:CYS:O	1:A:430:MET:HE2	2.20	0.41
1:B:422:GLN:HE21	1:B:703:GLN:HB3	1.85	0.41
1:B:486:ILE:HD12	1:B:486:ILE:N	2.35	0.41
4:A:1205:CLR:H12	5:A:1206:A1L1C:C41	2.48	0.41
1:A:414:LEU:HD22	1:A:460:TRP:CZ3	2.55	0.41
1:A:202:ASN:HB3	1:A:205:LYS:CB	2.33	0.41
1:A:328:GLY:HA2	1:A:331:ILE:HD12	2.03	0.41
1:A:486:ILE:HD12	1:A:486:ILE:N	2.35	0.41
1:B:414:LEU:HD22	1:B:460:TRP:CZ3	2.55	0.41
1:B:678:TRP:NE1	1:B:685:PRO:HB2	2.36	0.41
1:A:119:VAL:O	1:A:123:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLN:HE21	1:A:167:GLN:HB3	1.55	0.41
1:A:267:LYS:O	1:A:269:LYS:HD2	2.21	0.41
1:A:276:PHE:CZ	1:A:280:ILE:HD11	2.56	0.41
1:A:695:PHE:O	1:A:698:VAL:HG22	2.21	0.41
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.90	0.41
1:B:328:GLY:HA2	1:B:331:ILE:HD12	2.03	0.41
1:A:422:GLN:HE21	1:A:703:GLN:HB3	1.85	0.41
1:B:165:TYR:HA	1:B:168:TYR:CD2	2.56	0.41
1:B:434:PHE:CD1	1:B:434:PHE:N	2.88	0.41
1:A:42:LEU:HD21	1:A:359:TYR:HA	2.03	0.41
1:A:120:LEU:O	1:A:124:VAL:HG22	2.20	0.41
1:B:426:CYS:O	1:B:430:MET:HE2	2.20	0.41
1:A:190:ILE:O	1:A:194:LYS:HE2	2.21	0.41
1:A:182:PRO:HG3	1:A:214:VAL:HG21	2.03	0.41
1:A:373:LYS:HB3	1:A:374:PRO:CD	2.51	0.41
1:B:189:GLU:HA	1:B:192:LYS:HD3	2.03	0.41
1:B:190:ILE:O	1:B:194:LYS:HE2	2.21	0.41
1:B:202:ASN:HB3	1:B:205:LYS:CB	2.33	0.41
1:B:292:LEU:HD23	1:B:318:PHE:HE2	1.85	0.41
1:B:521:MET:HE3	1:B:521:MET:HB2	1.70	0.41
1:A:108:ILE:HG21	1:A:297:MET:HE1	2.03	0.41
1:A:204:ILE:H	1:A:204:ILE:HG13	1.49	0.41
1:A:292:LEU:HD23	1:A:318:PHE:HE2	1.85	0.41
1:B:182:PRO:HG3	1:B:214:VAL:HG21	2.03	0.41
1:A:165:TYR:HA	1:A:168:TYR:CD2	2.56	0.40
1:A:402:LEU:HA	1:A:402:LEU:HD12	1.86	0.40
1:A:460:TRP:CH2	1:A:484:ILE:HA	2.52	0.40
1:A:678:TRP:NE1	1:A:685:PRO:HB2	2.36	0.40
1:A:521:MET:HB3	1:A:680:LEU:HD21	2.04	0.40
1:A:523:THR:O	1:A:527:THR:OG1	2.29	0.40
1:B:276:PHE:CZ	1:B:280:ILE:HD11	2.56	0.40
1:B:695:PHE:O	1:B:698:VAL:HG22	2.21	0.40
1:A:49:CYS:O	1:A:53:VAL:HG23	2.22	0.40
1:B:267:LYS:O	1:B:269:LYS:HD2	2.21	0.40
1:B:35:PRO:HB2	1:B:36:SER:H	1.66	0.40
1:A:384:PHE:O	1:A:388:ILE:HG13	2.22	0.40
4:A:1205:CLR:H211	4:A:1205:CLR:H263	2.03	0.40
1:B:373:LYS:HB3	1:B:374:PRO:CD	2.51	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	575/1144 (50%)	561 (98%)	14 (2%)	0	100	100
1	B	575/1144 (50%)	561 (98%)	14 (2%)	0	100	100
All	All	1150/2288 (50%)	1122 (98%)	28 (2%)	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	467/986 (47%)	425 (91%)	42 (9%)	8	5
1	B	467/986 (47%)	426 (91%)	41 (9%)	8	5
All	All	934/1972 (47%)	851 (91%)	83 (9%)	10	5

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	39	ILE
1	A	63	ASN
1	A	79	ARG
1	A	93	LEU
1	A	126	SER
1	A	145	ASN
1	A	167	GLN

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Mol	Chain	Res	Type
1	A	195	ASP
1	A	200	SER
1	A	203	LYS
1	A	204	ILE
1	A	213	ARG
1	A	236	LYS
1	A	253	SER
1	A	269	LYS
1	A	271	LEU
1	A	272	LYS
1	A	274	SER
1	A	286	LYS
1	A	300	LEU
1	A	303	LYS
1	A	345	SER
1	A	369	THR
1	A	400	ILE
1	A	402	LEU
1	A	405	LYS
1	A	408	LYS
1	A	416	THR
1	A	418	LEU
1	A	431	ILE
1	A	435	VAL
1	A	446	VAL
1	A	448	VAL
1	A	483	ILE
1	A	494	LEU
1	A	510	ILE
1	A	521	MET
1	A	541	CYS
1	A	657	ARG
1	A	682	ASN
1	A	693	GLN
1	B	38	SER
1	B	39	ILE
1	B	63	ASN
1	B	79	ARG
1	B	93	LEU
1	B	126	SER
1	B	145	ASN
1	B	167	GLN

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Mol	Chain	Res	Type
1	B	195	ASP
1	B	200	SER
1	B	203	LYS
1	B	204	ILE
1	B	213	ARG
1	B	236	LYS
1	B	253	SER
1	B	269	LYS
1	B	271	LEU
1	B	272	LYS
1	B	274	SER
1	B	286	LYS
1	B	303	LYS
1	B	345	SER
1	B	369	THR
1	B	400	ILE
1	B	402	LEU
1	B	405	LYS
1	B	408	LYS
1	B	416	THR
1	B	418	LEU
1	B	431	ILE
1	B	435	VAL
1	B	446	VAL
1	B	448	VAL
1	B	483	ILE
1	B	494	LEU
1	B	510	ILE
1	B	521	MET
1	B	541	CYS
1	B	657	ARG
1	B	682	ASN
1	B	693	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	145	ASN
1	A	167	GLN
1	A	202	ASN
1	A	337	ASN

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Mol	Chain	Res	Type
1	A	443	GLN
1	A	654	GLN
1	A	683	GLN
1	A	703	GLN
1	B	94	ASN
1	B	145	ASN
1	B	167	GLN
1	B	202	ASN
1	B	337	ASN
1	B	443	GLN
1	B	654	GLN
1	B	683	GLN
1	B	703	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	A1L1C	B	1207	-	52,52,52	0.33	0	55,57,57	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	6OU	A	1203	-	48,48,48	0.94	2 (4%)	51,53,53	1.12	3 (5%)
3	6OU	B	1204	-	48,48,48	0.94	2 (4%)	51,53,53	1.12	3 (5%)
6	LBN	B	1201	-	51,51,51	1.06	5 (9%)	57,59,59	0.95	3 (5%)
6	LBN	A	1207	-	51,51,51	1.06	6 (11%)	57,59,59	0.95	3 (5%)
4	CLR	A	1205	-	31,31,31	3.91	16 (51%)	48,48,48	2.06	16 (33%)
2	NAG	A	1201	1	14,14,15	0.39	0	17,19,21	0.41	0
3	6OU	B	1205	-	48,48,48	0.91	4 (8%)	51,53,53	0.99	4 (7%)
4	CLR	B	1206	-	31,31,31	3.90	16 (51%)	48,48,48	2.06	15 (31%)
3	6OU	A	1202	-	48,48,48	0.93	2 (4%)	51,53,53	1.09	4 (7%)
5	A1L1C	A	1206	-	52,52,52	0.33	0	55,57,57	0.43	0
3	6OU	B	1203	-	48,48,48	0.93	2 (4%)	51,53,53	1.09	4 (7%)
3	6OU	A	1204	-	48,48,48	0.91	4 (8%)	51,53,53	0.99	4 (7%)
2	NAG	B	1202	1	14,14,15	0.39	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1L1C	B	1207	-	-	22/56/56/56	-
3	6OU	A	1203	-	-	30/52/52/52	-
3	6OU	B	1204	-	-	30/52/52/52	-
6	LBN	B	1201	-	-	27/55/55/55	-
6	LBN	A	1207	-	-	27/55/55/55	-
4	CLR	A	1205	-	-	9/10/68/68	0/4/4/4
2	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
3	6OU	B	1205	-	-	31/52/52/52	-
4	CLR	B	1206	-	-	9/10/68/68	0/4/4/4
3	6OU	A	1202	-	-	25/52/52/52	-
5	A1L1C	A	1206	-	-	23/56/56/56	-
3	6OU	B	1203	-	-	25/52/52/52	-
3	6OU	A	1204	-	-	31/52/52/52	-
2	NAG	B	1202	1	-	2/6/23/26	0/1/1/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1205	CLR	C11-C9	9.05	1.68	1.53
4	B	1206	CLR	C11-C9	9.01	1.68	1.53
4	A	1205	CLR	C12-C13	-8.57	1.39	1.54
4	B	1206	CLR	C12-C13	-8.57	1.39	1.54
4	A	1205	CLR	C10-C9	-7.62	1.43	1.56
4	B	1206	CLR	C10-C9	-7.59	1.44	1.56
4	B	1206	CLR	C8-C14	-6.62	1.41	1.53
4	A	1205	CLR	C8-C14	-6.60	1.41	1.53
4	B	1206	CLR	C12-C11	6.55	1.66	1.53
4	A	1205	CLR	C12-C11	6.54	1.66	1.53
4	A	1205	CLR	C6-C5	-5.95	1.20	1.33
4	B	1206	CLR	C6-C5	-5.93	1.20	1.33
4	B	1206	CLR	C16-C15	5.17	1.68	1.54
4	A	1205	CLR	C16-C15	5.15	1.68	1.54
4	A	1205	CLR	C20-C17	-4.51	1.46	1.54
4	B	1206	CLR	C20-C17	-4.50	1.46	1.54
4	A	1205	CLR	C13-C14	-4.19	1.47	1.55
4	B	1206	CLR	C13-C14	-4.18	1.47	1.55
4	B	1206	CLR	C2-C3	3.86	1.60	1.51
4	A	1205	CLR	C2-C3	3.85	1.60	1.51
4	B	1206	CLR	C8-C9	3.57	1.60	1.53
4	A	1205	CLR	C8-C9	3.55	1.60	1.53
3	A	1202	6OU	O30-C20	-3.41	1.38	1.46
3	B	1203	6OU	O30-C20	-3.41	1.38	1.46
3	B	1204	6OU	O18-C19	-3.37	1.37	1.45
3	A	1203	6OU	O18-C19	-3.33	1.37	1.45
3	B	1204	6OU	O30-C20	-3.04	1.39	1.46
3	A	1203	6OU	O30-C20	-3.03	1.39	1.46
4	B	1206	CLR	O1-C3	-2.96	1.34	1.43
4	A	1205	CLR	O1-C3	-2.93	1.34	1.43
4	B	1206	CLR	C10-C5	-2.93	1.47	1.52
4	A	1205	CLR	C10-C5	-2.90	1.47	1.52
6	B	1201	LBN	O7-C2	-2.90	1.39	1.46
6	A	1207	LBN	O7-C2	-2.89	1.39	1.46
6	B	1201	LBN	O7-C34	2.80	1.42	1.34
3	A	1204	6OU	O30-C20	-2.80	1.40	1.46
3	B	1205	6OU	O30-C20	-2.79	1.40	1.46
6	A	1207	LBN	O7-C34	2.77	1.42	1.34
3	B	1203	6OU	O18-C19	-2.76	1.39	1.45
3	A	1202	6OU	O18-C19	-2.73	1.39	1.45
3	B	1205	6OU	O18-C16	2.42	1.40	1.33
3	A	1204	6OU	O18-C16	2.41	1.40	1.33
6	A	1207	LBN	O5-C25	2.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1201	LBN	O5-C25	2.36	1.40	1.33
4	B	1206	CLR	C15-C14	2.35	1.59	1.54
4	B	1206	CLR	C7-C6	-2.34	1.45	1.50
4	A	1205	CLR	C15-C14	2.34	1.59	1.54
4	A	1205	CLR	C1-C2	2.32	1.58	1.53
4	A	1205	CLR	C7-C6	-2.31	1.45	1.50
4	B	1206	CLR	C1-C2	2.30	1.58	1.53
3	B	1205	6OU	O18-C19	-2.21	1.40	1.45
3	A	1204	6OU	O18-C19	-2.20	1.40	1.45
6	A	1207	LBN	C6-N1	-2.19	1.44	1.51
6	B	1201	LBN	C6-N1	-2.18	1.44	1.51
3	A	1204	6OU	O30-C31	2.09	1.40	1.34
3	B	1205	6OU	O30-C31	2.08	1.40	1.34
6	B	1201	LBN	C18-N1	-2.03	1.44	1.50
6	A	1207	LBN	C18-N1	-2.02	1.44	1.50
6	A	1207	LBN	O5-C3	-2.01	1.40	1.45

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1206	CLR	C15-C14-C8	-5.34	110.59	119.10
4	A	1205	CLR	C15-C14-C8	-5.33	110.60	119.10
4	A	1205	CLR	C13-C17-C20	-5.27	111.36	119.50
4	B	1206	CLR	C13-C17-C20	-5.25	111.39	119.50
4	A	1205	CLR	C11-C9-C8	-4.21	105.90	111.78
4	B	1206	CLR	C10-C9-C8	-4.21	106.57	112.71
4	B	1206	CLR	C11-C9-C8	-4.19	105.93	111.78
4	A	1205	CLR	C10-C9-C8	-4.19	106.59	112.71
3	B	1205	6OU	O30-C31-C33	4.14	120.43	111.48
3	A	1204	6OU	O30-C31-C33	4.13	120.42	111.48
3	B	1203	6OU	O30-C31-C33	4.11	120.36	111.48
3	A	1202	6OU	O30-C31-C33	4.09	120.33	111.48
3	A	1203	6OU	O30-C31-C33	3.71	119.51	111.48
3	B	1204	6OU	O30-C31-C33	3.71	119.51	111.48
4	A	1205	CLR	C11-C9-C10	-3.27	109.05	113.08
4	B	1206	CLR	C11-C9-C10	-3.27	109.05	113.08
4	A	1205	CLR	C12-C13-C14	3.22	112.06	107.25
4	B	1206	CLR	C12-C13-C14	3.21	112.05	107.25
3	A	1202	6OU	O18-C16-C15	3.19	121.56	111.83
3	B	1203	6OU	O18-C16-C15	3.19	121.55	111.83
6	B	1201	LBN	C3-C2-C1	-3.03	104.71	111.78
6	A	1207	LBN	C3-C2-C1	-3.02	104.75	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1206	CLR	C13-C14-C8	-3.00	110.15	114.41
4	A	1205	CLR	C17-C13-C14	3.00	103.54	100.10
4	B	1206	CLR	C17-C13-C14	3.00	103.54	100.10
6	A	1207	LBN	O7-C34-C35	2.99	117.96	111.48
4	A	1205	CLR	C13-C14-C8	-2.99	110.17	114.41
6	B	1201	LBN	O7-C34-C35	2.96	117.88	111.48
4	B	1206	CLR	C12-C11-C9	-2.75	108.46	113.14
4	A	1205	CLR	C12-C11-C9	-2.73	108.49	113.14
4	B	1206	CLR	C16-C17-C20	-2.70	108.10	112.18
4	A	1205	CLR	C16-C17-C20	-2.69	108.10	112.18
6	B	1201	LBN	O5-C25-C26	2.61	119.80	111.83
6	A	1207	LBN	O5-C25-C26	2.61	119.79	111.83
3	A	1202	6OU	C20-O30-C31	-2.60	111.56	117.80
3	B	1203	6OU	C20-O30-C31	-2.60	111.58	117.80
3	A	1203	6OU	C21-C20-C19	-2.48	106.01	111.78
3	B	1204	6OU	C21-C20-C19	-2.47	106.03	111.78
3	B	1205	6OU	O18-C16-C15	2.33	118.94	111.83
3	A	1204	6OU	O18-C16-C15	2.33	118.94	111.83
3	B	1203	6OU	O30-C31-O32	-2.30	118.33	123.70
3	A	1202	6OU	O30-C31-O32	-2.30	118.34	123.70
4	B	1206	CLR	C19-C10-C5	2.29	111.88	108.38
4	A	1205	CLR	C19-C10-C5	2.28	111.86	108.38
4	B	1206	CLR	C12-C13-C17	-2.25	113.29	116.60
4	A	1205	CLR	C12-C13-C17	-2.24	113.31	116.60
4	A	1205	CLR	C21-C20-C22	-2.20	106.94	110.34
4	B	1206	CLR	C19-C10-C9	-2.18	109.21	111.66
4	B	1206	CLR	C21-C20-C22	-2.18	106.96	110.34
4	A	1205	CLR	C19-C10-C9	-2.16	109.24	111.66
3	B	1205	6OU	C20-O30-C31	-2.15	112.66	117.80
3	A	1204	6OU	C20-O30-C31	-2.14	112.67	117.80
3	A	1203	6OU	C19-O18-C16	-2.09	109.47	117.12
3	B	1204	6OU	C19-O18-C16	-2.09	109.47	117.12
3	A	1204	6OU	O30-C31-O32	-2.08	118.83	123.70
3	B	1205	6OU	O30-C31-O32	-2.08	118.85	123.70
4	B	1206	CLR	C23-C24-C25	-2.03	106.88	115.94
4	A	1205	CLR	C23-C24-C25	-2.03	106.88	115.94
4	A	1205	CLR	C8-C7-C6	-2.01	109.98	112.76

There are no chirality outliers.

All (293) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	6OU	C27-O26-P23-O24
3	A	1202	6OU	C27-O26-P23-O25
3	A	1202	6OU	C33-C31-O30-C20
3	A	1203	6OU	C27-O26-P23-O22
3	A	1203	6OU	C27-O26-P23-O24
3	A	1203	6OU	C27-O26-P23-O25
3	A	1203	6OU	O26-C27-C28-N29
3	A	1204	6OU	O18-C19-C20-O30
3	A	1204	6OU	O26-C27-C28-N29
3	B	1203	6OU	C27-O26-P23-O24
3	B	1203	6OU	C27-O26-P23-O25
3	B	1203	6OU	C33-C31-O30-C20
3	B	1204	6OU	C27-O26-P23-O22
3	B	1204	6OU	C27-O26-P23-O24
3	B	1204	6OU	C27-O26-P23-O25
3	B	1204	6OU	O26-C27-C28-N29
3	B	1205	6OU	O18-C19-C20-O30
3	B	1205	6OU	O26-C27-C28-N29
5	A	1206	A1L1C	C4-O3-P2-O1
5	A	1206	A1L1C	C4-O3-P2-O7
5	A	1206	A1L1C	C8-O7-P2-O3
5	B	1207	A1L1C	C4-O3-P2-O1
5	B	1207	A1L1C	C4-O3-P2-O7
5	B	1207	A1L1C	C8-O7-P2-O3
6	A	1207	LBN	C9-O2-P1-O1
6	A	1207	LBN	C9-O2-P1-O3
6	A	1207	LBN	C9-O2-P1-O4
6	B	1201	LBN	C9-O2-P1-O1
6	B	1201	LBN	C9-O2-P1-O3
6	B	1201	LBN	C9-O2-P1-O4
3	A	1202	6OU	O32-C31-O30-C20
3	B	1203	6OU	O32-C31-O30-C20
3	A	1203	6OU	C33-C31-O30-C20
3	A	1204	6OU	C33-C31-O30-C20
3	B	1204	6OU	C33-C31-O30-C20
3	B	1205	6OU	C33-C31-O30-C20
6	A	1207	LBN	C13-C10-C7-C4
6	B	1201	LBN	C13-C10-C7-C4
3	A	1202	6OU	C10-C11-C12-C13
3	A	1202	6OU	C33-C34-C35-C36
3	B	1203	6OU	C10-C11-C12-C13
3	B	1203	6OU	C33-C34-C35-C36
5	A	1206	A1L1C	C46-C47-C48-C49

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Mol	Chain	Res	Type	Atoms
5	B	1207	A1L1C	C46-C47-C48-C49
3	A	1204	6OU	C03-C04-C05-C06
3	B	1205	6OU	C03-C04-C05-C06
3	A	1203	6OU	C44-C45-C46-C47
3	B	1204	6OU	C44-C45-C46-C47
3	A	1202	6OU	C35-C36-C37-C38
3	B	1203	6OU	C35-C36-C37-C38
4	A	1205	CLR	C13-C17-C20-C21
4	B	1206	CLR	C13-C17-C20-C21
3	A	1204	6OU	O32-C31-O30-C20
3	B	1205	6OU	O32-C31-O30-C20
3	A	1204	6OU	C15-C16-O18-C19
3	B	1205	6OU	C15-C16-O18-C19
3	A	1203	6OU	O32-C31-O30-C20
3	B	1204	6OU	O32-C31-O30-C20
3	A	1203	6OU	C13-C14-C15-C16
3	B	1204	6OU	C13-C14-C15-C16
3	A	1202	6OU	C44-C45-C46-C47
3	A	1203	6OU	C34-C35-C36-C37
3	B	1203	6OU	C44-C45-C46-C47
3	B	1204	6OU	C34-C35-C36-C37
6	A	1207	LBN	C35-C34-O7-C2
6	B	1201	LBN	C35-C34-O7-C2
6	A	1207	LBN	O8-C34-O7-C2
6	B	1201	LBN	O8-C34-O7-C2
6	A	1207	LBN	C9-C6-N1-C12
6	B	1201	LBN	C9-C6-N1-C12
3	A	1204	6OU	O17-C16-O18-C19
3	B	1205	6OU	O17-C16-O18-C19
6	B	1201	LBN	C36-C37-C38-C39
6	A	1207	LBN	C36-C37-C38-C39
2	A	1201	NAG	C4-C5-C6-O6
2	B	1202	NAG	C4-C5-C6-O6
4	A	1205	CLR	C17-C20-C22-C23
4	B	1206	CLR	C17-C20-C22-C23
5	A	1206	A1L1C	C44-C45-C46-C47
5	B	1207	A1L1C	C44-C45-C46-C47
3	A	1204	6OU	C07-C08-C09-C10
3	B	1205	6OU	C07-C08-C09-C10
3	A	1203	6OU	C42-C43-C44-C45
3	B	1204	6OU	C42-C43-C44-C45
4	A	1205	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
4	B	1206	CLR	C22-C23-C24-C25
3	A	1204	6OU	C45-C46-C47-C48
3	B	1205	6OU	C45-C46-C47-C48
5	A	1206	A1L1C	C39-C40-C41-C42
5	B	1207	A1L1C	C39-C40-C41-C42
3	A	1202	6OU	C04-C05-C06-C07
3	B	1203	6OU	C04-C05-C06-C07
3	A	1204	6OU	C13-C14-C15-C16
3	B	1205	6OU	C13-C14-C15-C16
3	A	1204	6OU	C08-C09-C10-C11
3	B	1205	6OU	C08-C09-C10-C11
5	A	1206	A1L1C	C41-C42-C43-C44
5	B	1207	A1L1C	C41-C42-C43-C44
3	A	1202	6OU	C46-C47-C48-C49
3	A	1204	6OU	C46-C47-C48-C49
3	B	1205	6OU	C46-C47-C48-C49
3	B	1203	6OU	C46-C47-C48-C49
3	A	1204	6OU	C04-C05-C06-C07
3	B	1205	6OU	C04-C05-C06-C07
3	A	1202	6OU	C03-C04-C05-C06
3	B	1203	6OU	C03-C04-C05-C06
3	A	1203	6OU	C12-C13-C14-C15
3	B	1204	6OU	C12-C13-C14-C15
3	A	1204	6OU	C12-C13-C14-C15
3	B	1205	6OU	C12-C13-C14-C15
6	A	1207	LBN	C9-C6-N1-C15
6	A	1207	LBN	C9-C6-N1-C18
6	B	1201	LBN	C9-C6-N1-C15
6	B	1201	LBN	C9-C6-N1-C18
4	A	1205	CLR	C13-C17-C20-C22
4	B	1206	CLR	C13-C17-C20-C22
3	B	1205	6OU	C33-C34-C35-C36
3	A	1204	6OU	C33-C34-C35-C36
6	A	1207	LBN	C37-C38-C39-C40
6	B	1201	LBN	C37-C38-C39-C40
3	A	1203	6OU	C20-C21-O22-P23
3	B	1204	6OU	C20-C21-O22-P23
3	A	1202	6OU	C07-C08-C09-C10
3	B	1203	6OU	C07-C08-C09-C10
3	A	1202	6OU	C08-C09-C10-C11
3	B	1203	6OU	C08-C09-C10-C11
3	A	1203	6OU	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
3	B	1204	6OU	C01-C02-C03-C04
6	A	1207	LBN	C11-C14-C17-C20
6	B	1201	LBN	C11-C14-C17-C20
5	A	1206	A1L1C	O7-C8-C9-C34
5	B	1207	A1L1C	O7-C8-C9-C34
3	A	1203	6OU	C08-C09-C10-C11
3	B	1204	6OU	C08-C09-C10-C11
3	B	1204	6OU	C15-C16-O18-C19
3	A	1203	6OU	O18-C19-C20-C21
3	A	1204	6OU	O18-C19-C20-C21
3	B	1204	6OU	O18-C19-C20-C21
3	B	1205	6OU	O18-C19-C20-C21
3	A	1203	6OU	C15-C16-O18-C19
6	A	1207	LBN	C26-C27-C28-C29
6	B	1201	LBN	C26-C27-C28-C29
6	B	1201	LBN	C32-C33-C4-C7
4	A	1205	CLR	C16-C17-C20-C21
4	B	1206	CLR	C16-C17-C20-C21
6	A	1207	LBN	C32-C33-C4-C7
3	A	1204	6OU	C37-C38-C39-C40
3	B	1204	6OU	C37-C38-C39-C40
3	B	1205	6OU	C37-C38-C39-C40
5	A	1206	A1L1C	C43-C44-C45-C46
5	B	1207	A1L1C	C43-C44-C45-C46
3	A	1202	6OU	C05-C06-C07-C08
3	B	1203	6OU	C05-C06-C07-C08
3	A	1204	6OU	C36-C37-C38-C39
3	B	1205	6OU	C36-C37-C38-C39
3	A	1203	6OU	C37-C38-C39-C40
5	A	1206	A1L1C	C37-C38-C39-C40
5	B	1207	A1L1C	C37-C38-C39-C40
3	A	1203	6OU	C02-C03-C04-C05
3	B	1204	6OU	C02-C03-C04-C05
3	A	1203	6OU	C45-C46-C47-C48
3	B	1204	6OU	C45-C46-C47-C48
3	A	1204	6OU	C20-C21-O22-P23
3	B	1205	6OU	C20-C21-O22-P23
4	A	1205	CLR	C21-C20-C22-C23
4	B	1206	CLR	C21-C20-C22-C23
2	A	1201	NAG	O5-C5-C6-O6
2	B	1202	NAG	O5-C5-C6-O6
6	A	1207	LBN	C13-C16-C19-C21

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Mol	Chain	Res	Type	Atoms
6	B	1201	LBN	C13-C16-C19-C21
3	A	1204	6OU	C05-C06-C07-C08
3	B	1205	6OU	C05-C06-C07-C08
3	A	1203	6OU	O17-C16-O18-C19
3	B	1204	6OU	O17-C16-O18-C19
3	B	1205	6OU	C43-C44-C45-C46
3	A	1204	6OU	C43-C44-C45-C46
3	A	1203	6OU	C10-C11-C12-C13
3	B	1204	6OU	C10-C11-C12-C13
5	A	1206	A1L1C	C24-C25-C26-C27
5	A	1206	A1L1C	C27-C28-C29-C30
5	B	1207	A1L1C	C24-C25-C26-C27
5	B	1207	A1L1C	C27-C28-C29-C30
3	A	1203	6OU	C11-C12-C13-C14
3	B	1204	6OU	C11-C12-C13-C14
3	A	1204	6OU	C01-C02-C03-C04
3	B	1205	6OU	C01-C02-C03-C04
3	A	1203	6OU	C05-C06-C07-C08
3	B	1204	6OU	C05-C06-C07-C08
3	A	1204	6OU	C14-C15-C16-O18
3	B	1205	6OU	C14-C15-C16-O18
4	A	1205	CLR	C20-C22-C23-C24
4	B	1206	CLR	C20-C22-C23-C24
3	A	1202	6OU	O30-C20-C21-O22
3	A	1203	6OU	O30-C20-C21-O22
3	B	1203	6OU	O30-C20-C21-O22
3	B	1204	6OU	O30-C20-C21-O22
6	A	1207	LBN	C6-C9-O2-P1
6	B	1201	LBN	C6-C9-O2-P1
3	A	1203	6OU	O18-C19-C20-O30
3	B	1204	6OU	O18-C19-C20-O30
3	A	1202	6OU	C12-C13-C14-C15
6	A	1207	LBN	N1-C6-C9-O2
6	B	1201	LBN	N1-C6-C9-O2
3	B	1203	6OU	C12-C13-C14-C15
3	B	1204	6OU	C46-C47-C48-C49
3	A	1203	6OU	C46-C47-C48-C49
3	A	1202	6OU	C19-C20-C21-O22
3	B	1203	6OU	C19-C20-C21-O22
5	A	1206	A1L1C	O7-C8-C9-O10
5	B	1207	A1L1C	O7-C8-C9-O10
6	B	1201	LBN	C31-C32-C33-C4

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Mol	Chain	Res	Type	Atoms
3	A	1202	6OU	C06-C07-C08-C09
6	A	1207	LBN	C31-C32-C33-C4
3	B	1203	6OU	C06-C07-C08-C09
3	A	1202	6OU	C27-O26-P23-O22
3	A	1202	6OU	O26-C27-C28-N29
3	B	1203	6OU	C27-O26-P23-O22
3	B	1203	6OU	O26-C27-C28-N29
5	A	1206	A1L1C	C4-O3-P2-O53
5	A	1206	A1L1C	C8-O7-P2-O1
5	B	1207	A1L1C	C4-O3-P2-O53
5	B	1207	A1L1C	C8-O7-P2-O1
3	A	1204	6OU	C44-C45-C46-C47
3	B	1205	6OU	C44-C45-C46-C47
3	A	1204	6OU	C11-C12-C13-C14
3	B	1205	6OU	C11-C12-C13-C14
3	A	1203	6OU	C19-C20-C21-O22
3	B	1204	6OU	C19-C20-C21-O22
6	A	1207	LBN	C25-C26-C27-C28
6	B	1201	LBN	C25-C26-C27-C28
5	B	1207	A1L1C	C40-C41-C42-C43
5	A	1206	A1L1C	C40-C41-C42-C43
3	A	1202	6OU	C40-C41-C42-C43
3	B	1203	6OU	C40-C41-C42-C43
6	B	1201	LBN	C14-C17-C20-C22
3	A	1204	6OU	C10-C11-C12-C13
3	B	1205	6OU	C10-C11-C12-C13
6	A	1207	LBN	C14-C17-C20-C22
3	A	1203	6OU	C09-C10-C11-C12
3	B	1204	6OU	C09-C10-C11-C12
6	A	1207	LBN	C26-C25-O5-C3
6	B	1201	LBN	C26-C25-O5-C3
6	A	1207	LBN	O6-C25-O5-C3
6	B	1201	LBN	O6-C25-O5-C3
3	A	1204	6OU	C38-C39-C40-C41
3	B	1205	6OU	C38-C39-C40-C41
4	A	1205	CLR	C16-C17-C20-C22
4	B	1206	CLR	C16-C17-C20-C22
6	A	1207	LBN	C1-C2-C3-O5
6	B	1201	LBN	C1-C2-C3-O5
5	A	1206	A1L1C	C36-C37-C38-C39
5	B	1207	A1L1C	C36-C37-C38-C39
3	A	1204	6OU	O30-C20-C21-O22

Continued on next page...

Continued from previous page...

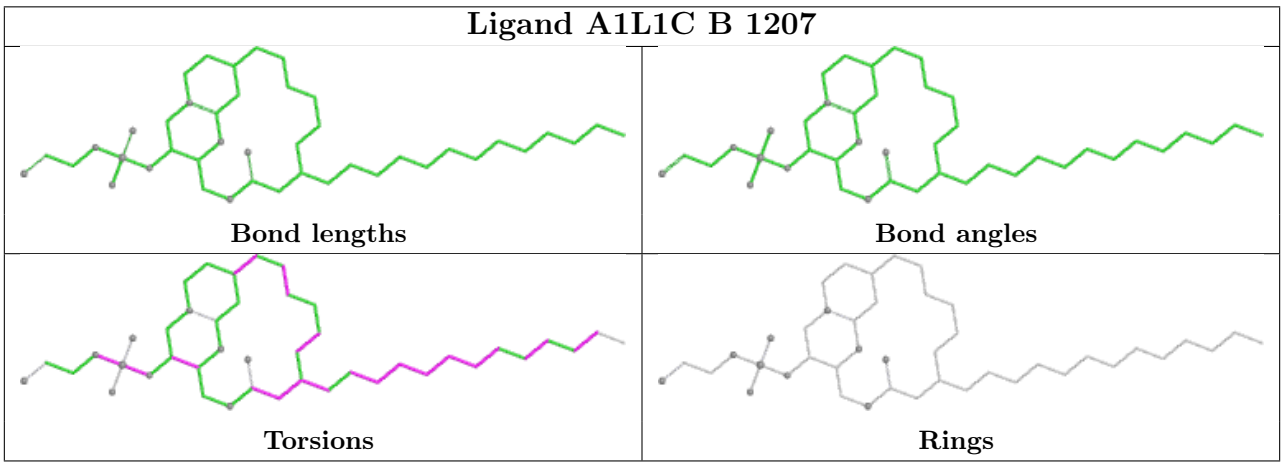
Mol	Chain	Res	Type	Atoms
3	B	1205	6OU	O30-C20-C21-O22
6	A	1207	LBN	C39-C40-C41-C42
6	B	1201	LBN	C39-C40-C41-C42
5	A	1206	A1L1C	C26-C27-C28-C29
4	A	1205	CLR	C23-C24-C25-C27
4	B	1206	CLR	C23-C24-C25-C27
3	A	1204	6OU	C19-C20-C21-O22
3	B	1205	6OU	C19-C20-C21-O22
3	A	1202	6OU	C38-C39-C40-C41
3	B	1203	6OU	C38-C39-C40-C41
5	B	1207	A1L1C	C42-C43-C44-C45
5	A	1206	A1L1C	C42-C43-C44-C45
6	A	1207	LBN	C42-C5-C8-C11
6	B	1201	LBN	C42-C5-C8-C11
3	B	1203	6OU	C11-C12-C13-C14
3	A	1202	6OU	C11-C12-C13-C14
6	A	1207	LBN	C33-C4-C7-C10
6	B	1201	LBN	C33-C4-C7-C10
3	A	1204	6OU	C02-C03-C04-C05
3	B	1205	6OU	C02-C03-C04-C05
3	A	1204	6OU	C14-C15-C16-O17
3	B	1205	6OU	C14-C15-C16-O17
3	A	1203	6OU	C14-C15-C16-O18
3	B	1204	6OU	C14-C15-C16-O18
3	A	1202	6OU	O30-C31-C33-C34
3	B	1203	6OU	O30-C31-C33-C34
5	B	1207	A1L1C	C48-C49-C50-C51
5	A	1206	A1L1C	C48-C49-C50-C51
5	A	1206	A1L1C	O35-C36-C37-C38
5	B	1207	A1L1C	O35-C36-C37-C38
5	A	1206	A1L1C	C29-C30-C31-C32
5	B	1207	A1L1C	C29-C30-C31-C32
5	A	1206	A1L1C	O52-C36-C37-C38
5	B	1207	A1L1C	O52-C36-C37-C38
3	A	1202	6OU	O32-C31-C33-C34
3	B	1203	6OU	O32-C31-C33-C34
3	A	1203	6OU	C03-C04-C05-C06
3	B	1204	6OU	C03-C04-C05-C06
6	A	1207	LBN	O7-C34-C35-C36
6	B	1201	LBN	O7-C34-C35-C36

There are no ring outliers.

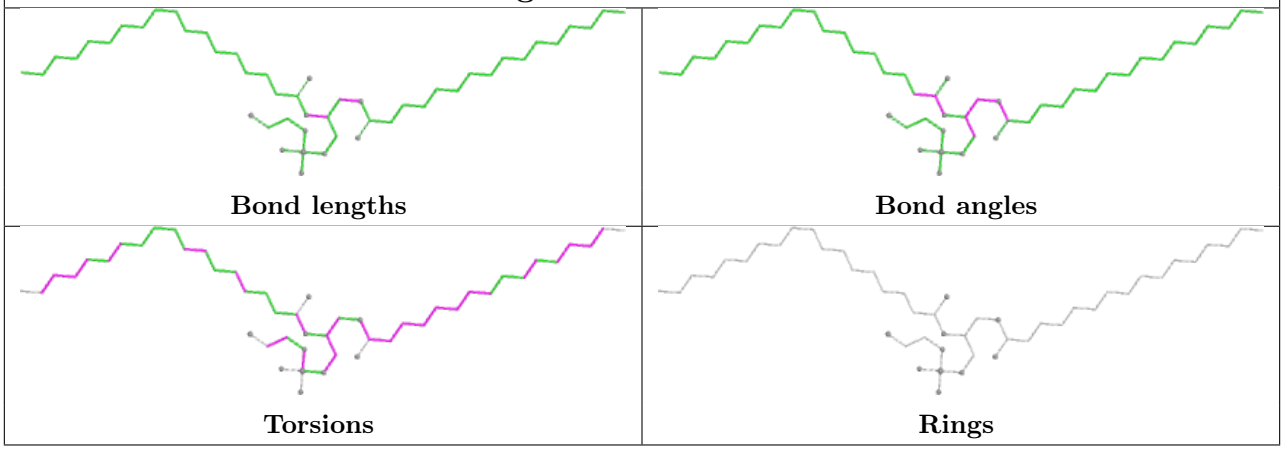
6 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1207	A1L1C	5	0
6	B	1201	LBN	1	0
6	A	1207	LBN	1	0
4	A	1205	CLR	20	0
4	B	1206	CLR	17	0
5	A	1206	A1L1C	6	0

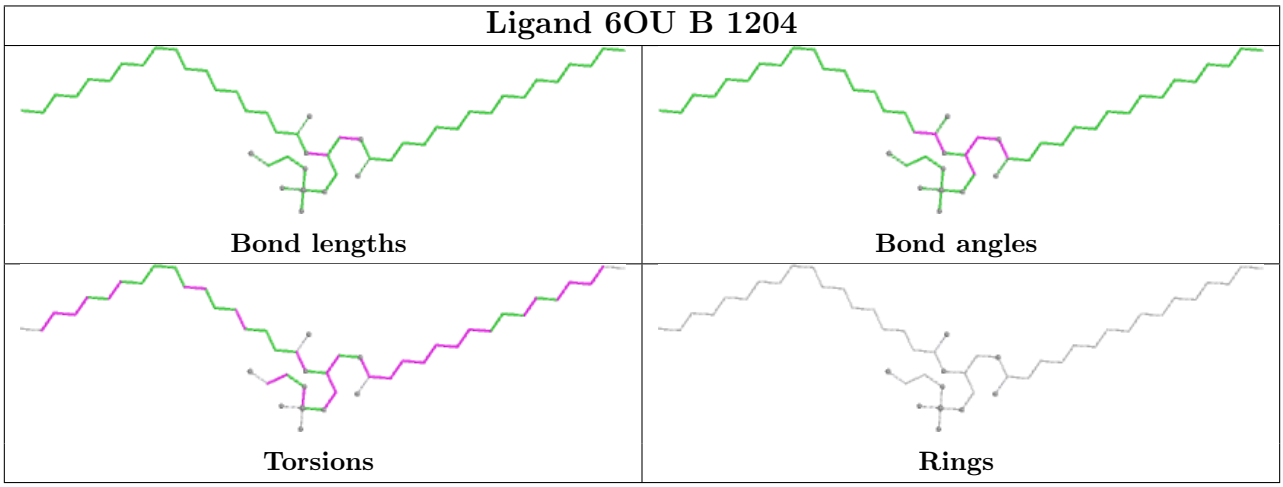
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



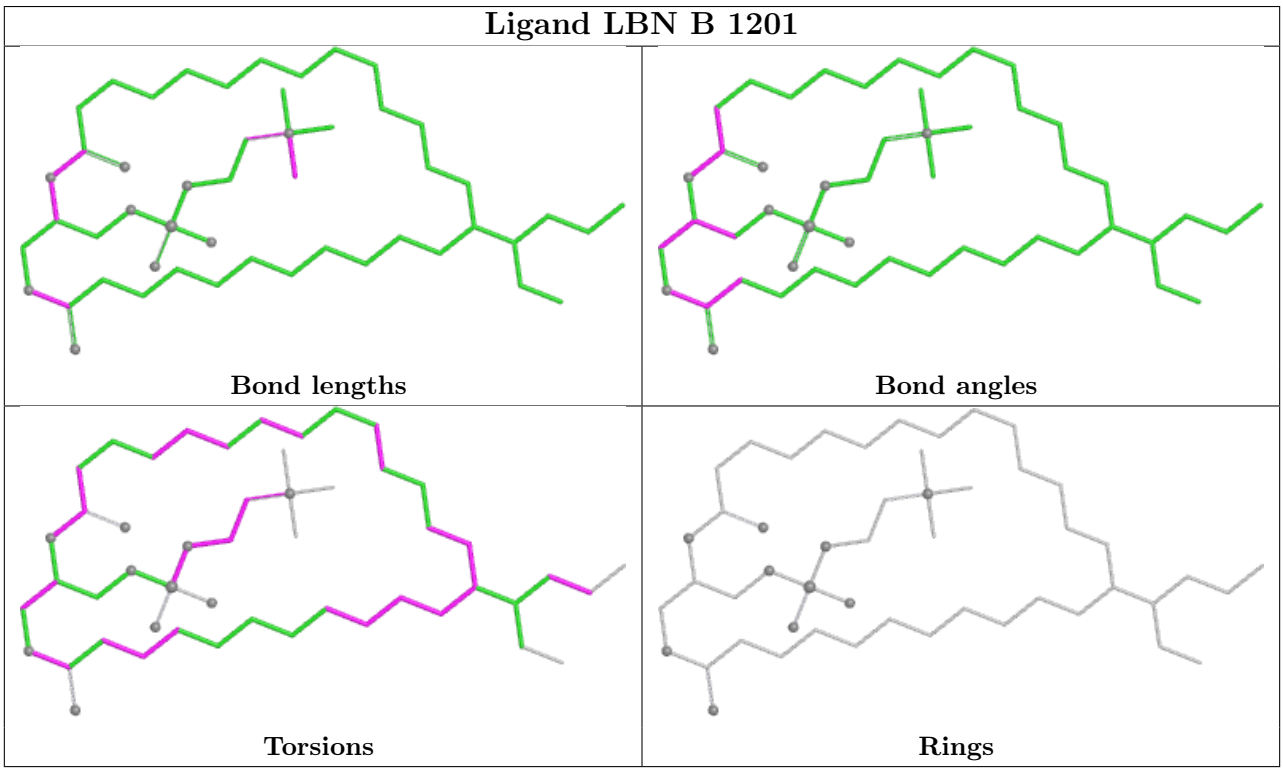
Ligand 6OU A 1203



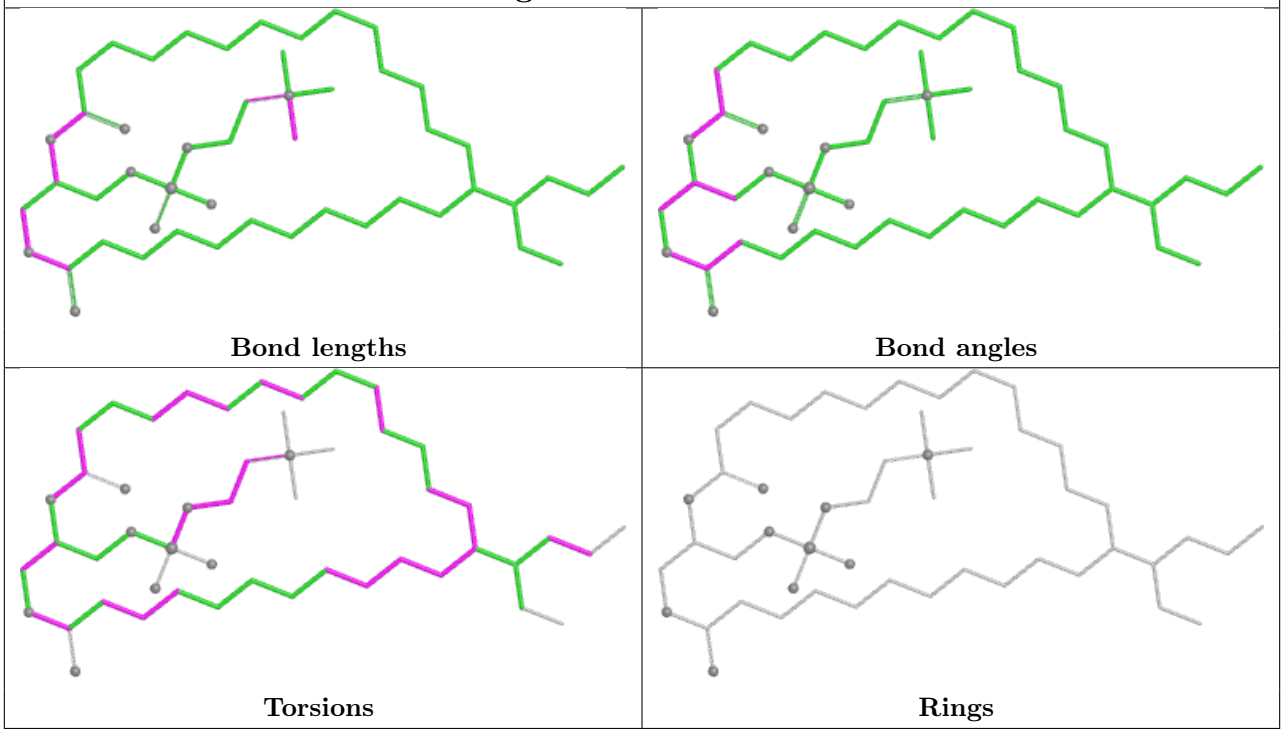
Ligand 6OU B 1204



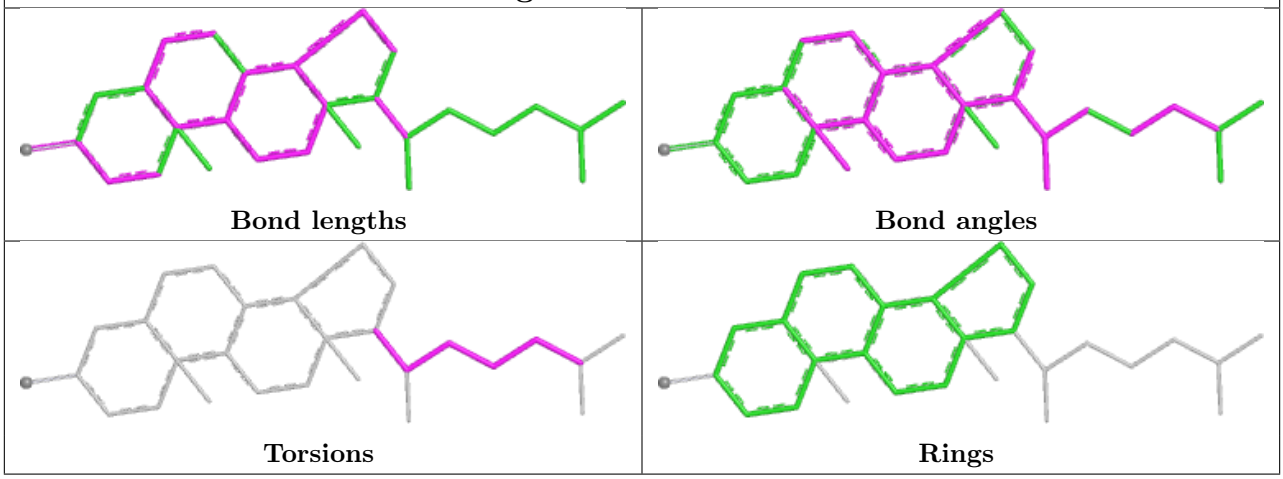
Ligand LBN B 1201



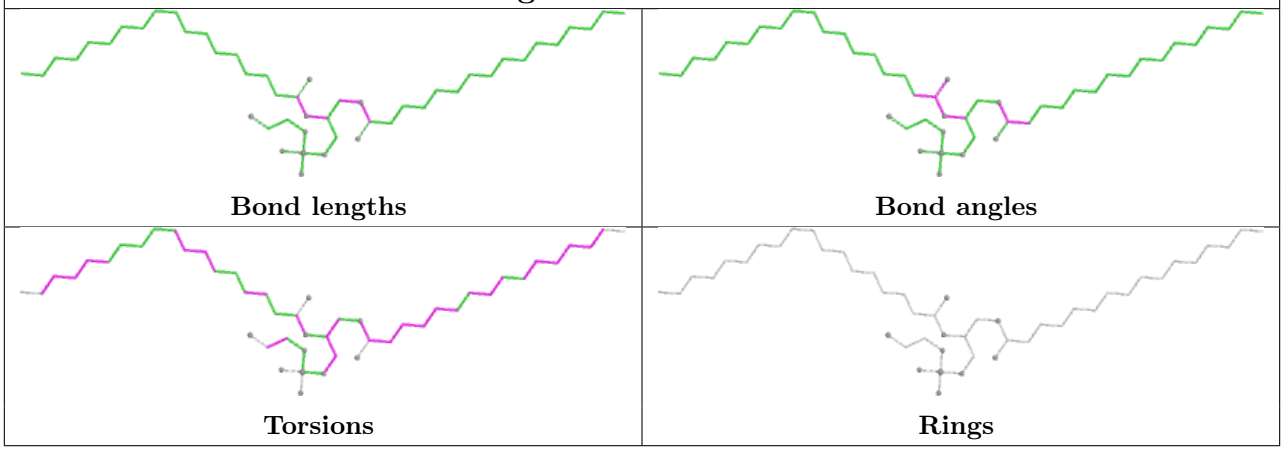
Ligand LBN A 1207



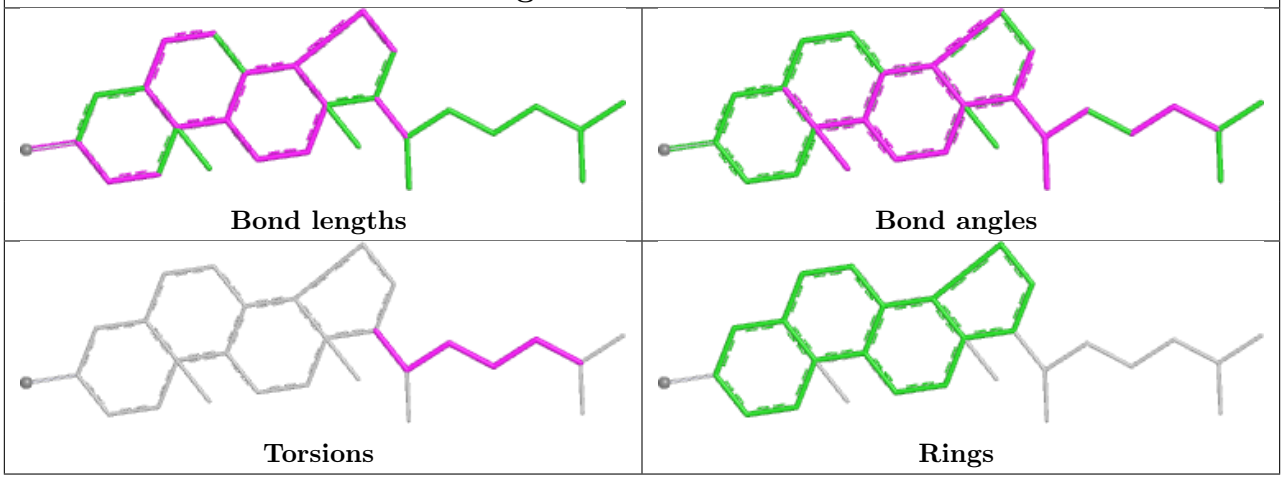
Ligand CLR A 1205



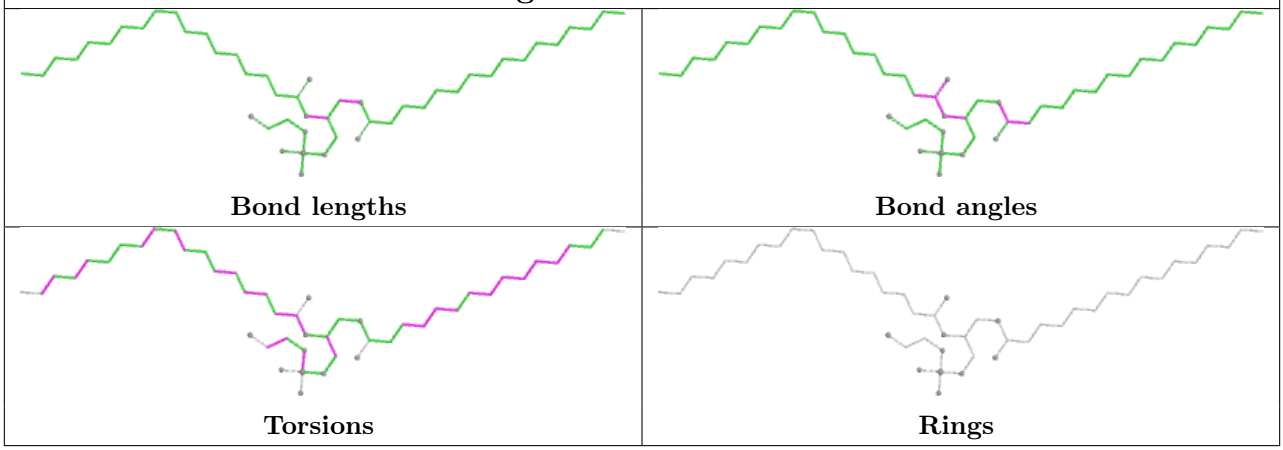
Ligand 6OU B 1205



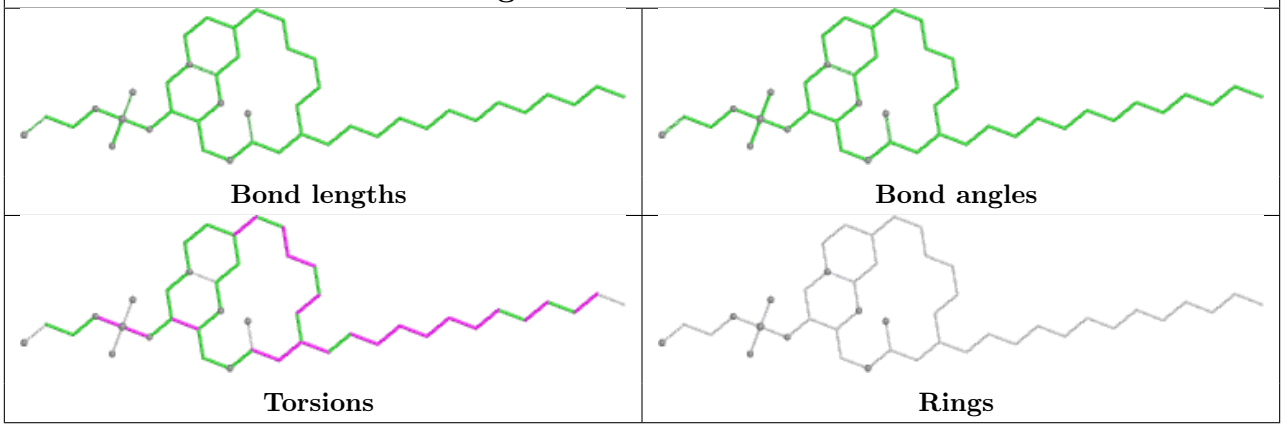
Ligand CLR B 1206

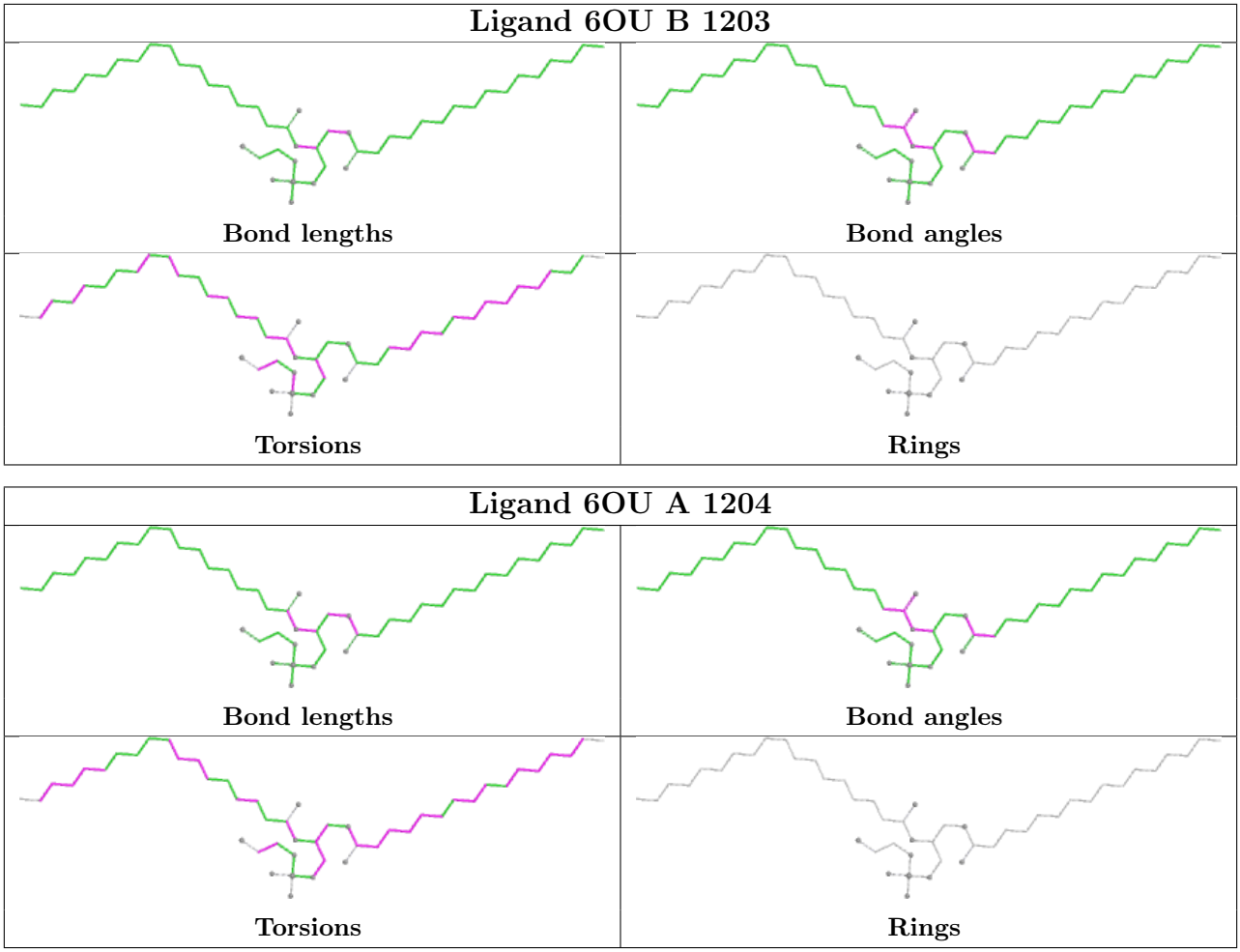


Ligand 6OU A 1202



Ligand A1L1C A 1206





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.

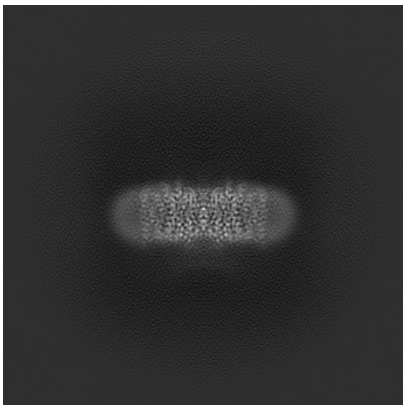
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39851. These allow visual inspection of the internal detail of the map and identification of artifacts.

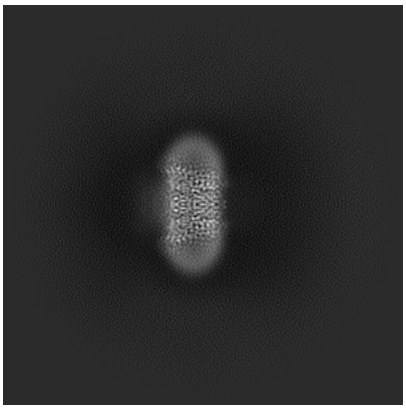
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

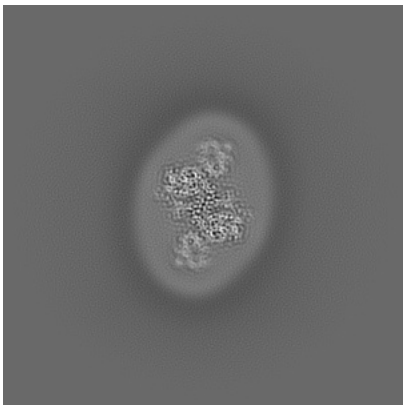
6.1.1 Primary map



X

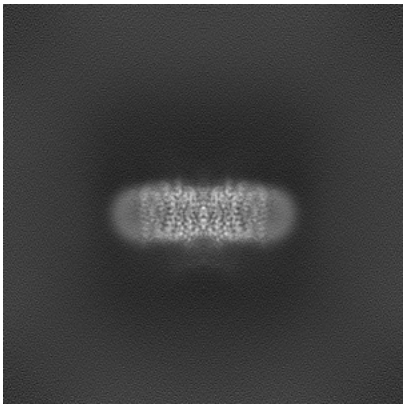


Y

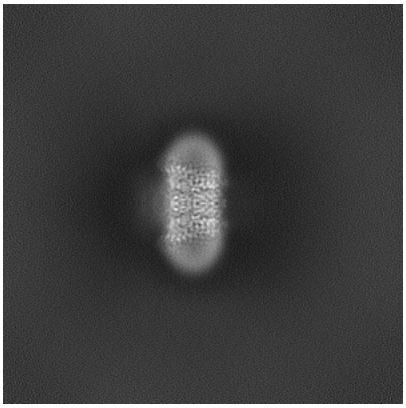


Z

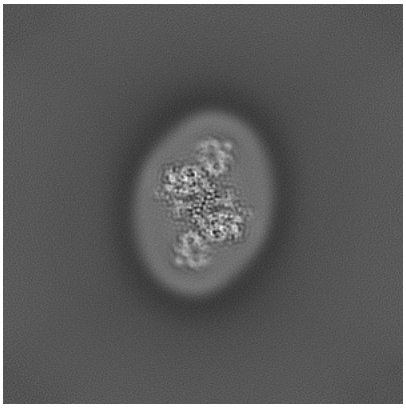
6.1.2 Raw map



X



Y

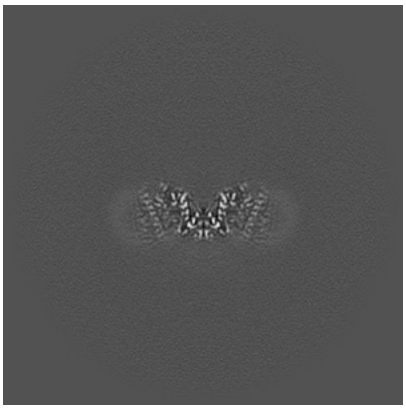


Z

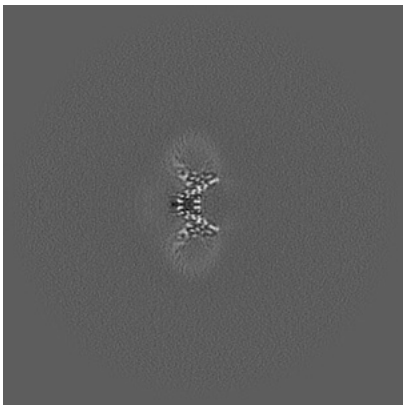
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

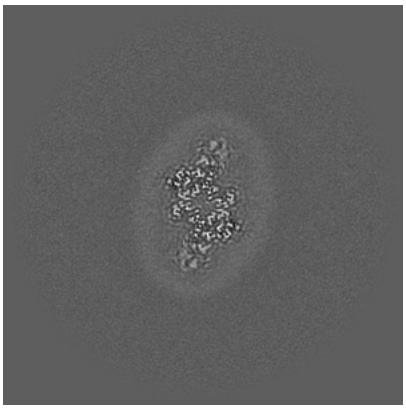
6.2.1 Primary map



X Index: 180

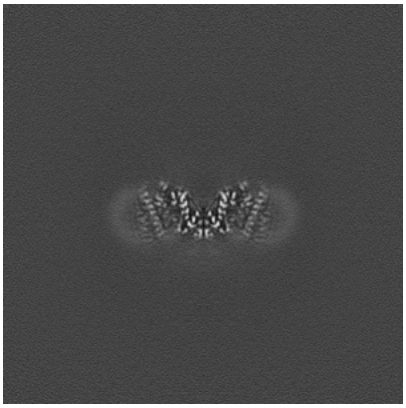


Y Index: 180

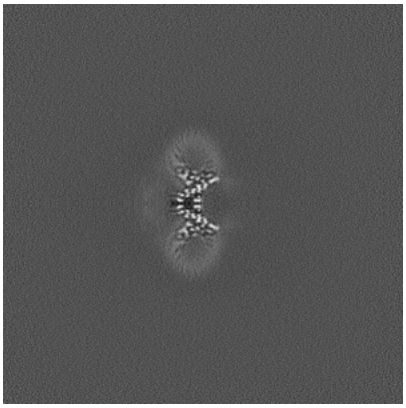


Z Index: 180

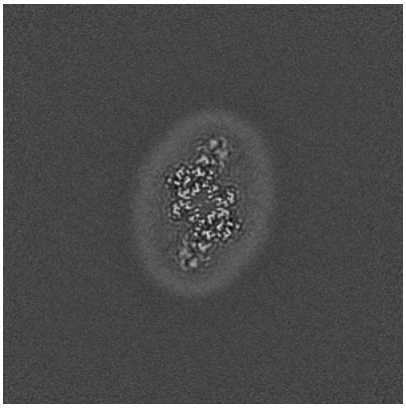
6.2.2 Raw map



X Index: 180



Y Index: 180

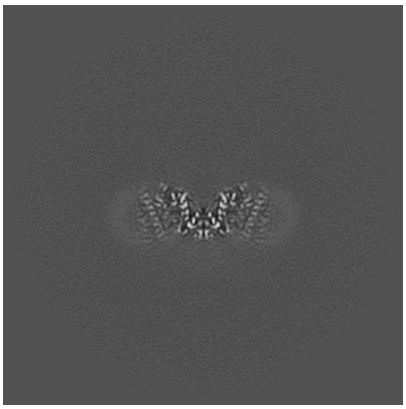


Z Index: 180

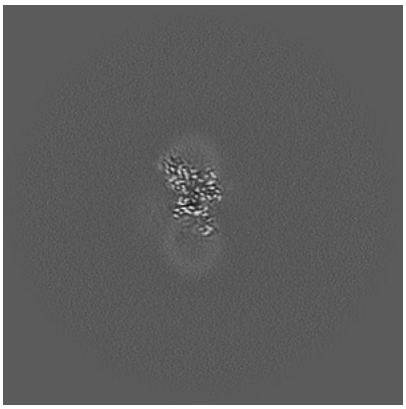
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

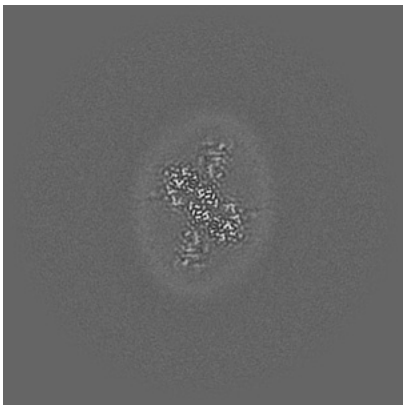
6.3.1 Primary map



X Index: 180

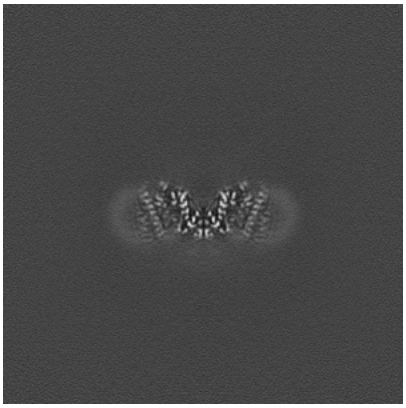


Y Index: 168

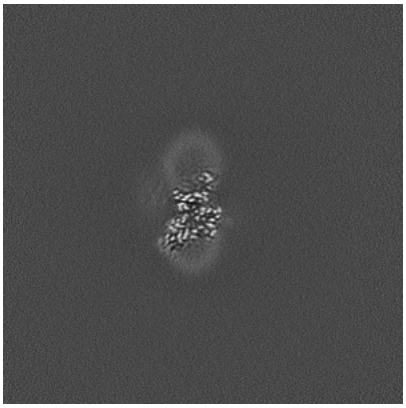


Z Index: 164

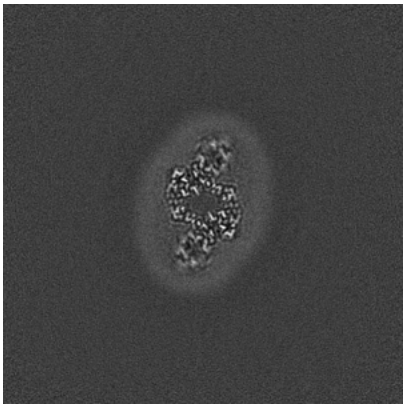
6.3.2 Raw map



X Index: 180



Y Index: 192

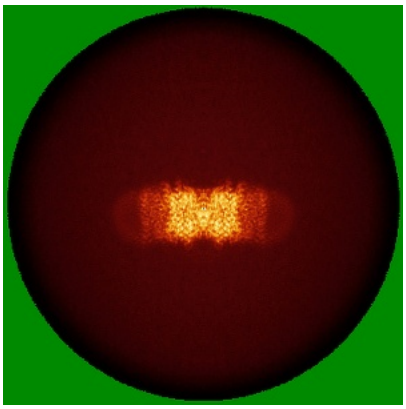


Z Index: 184

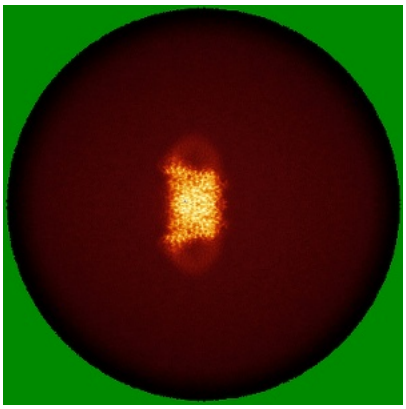
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

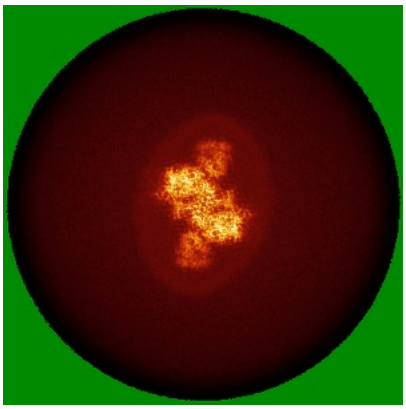
6.4.1 Primary map



X

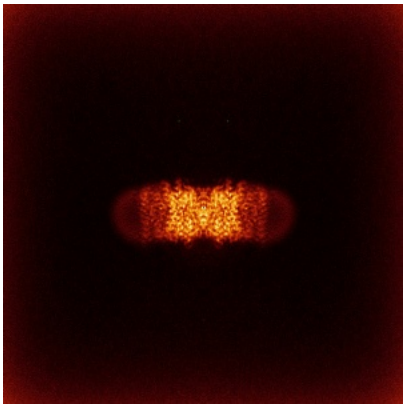


Y

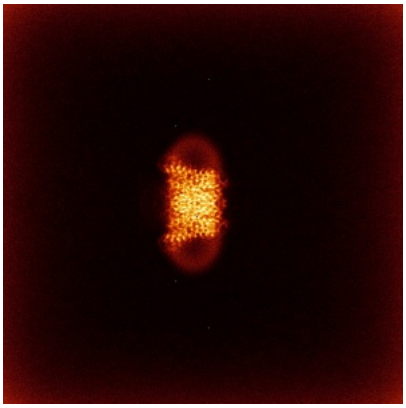


Z

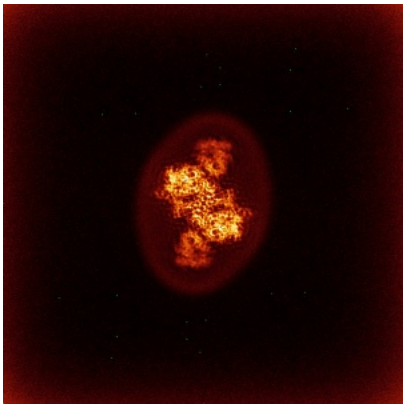
6.4.2 Raw map



X



Y

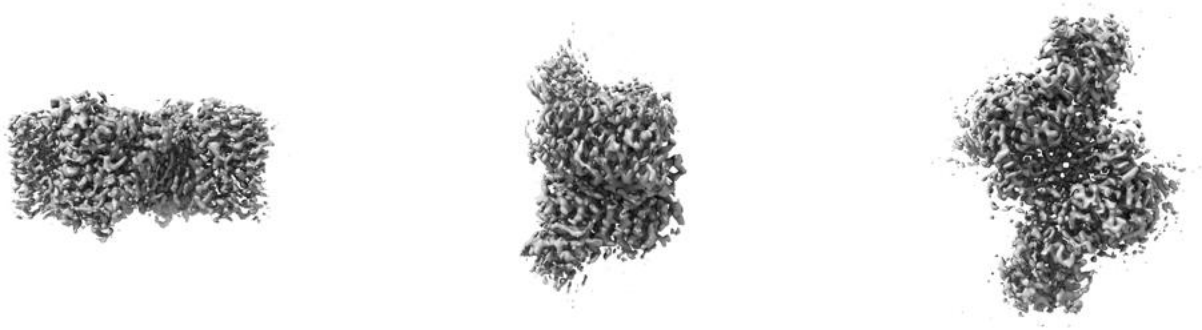


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.592. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

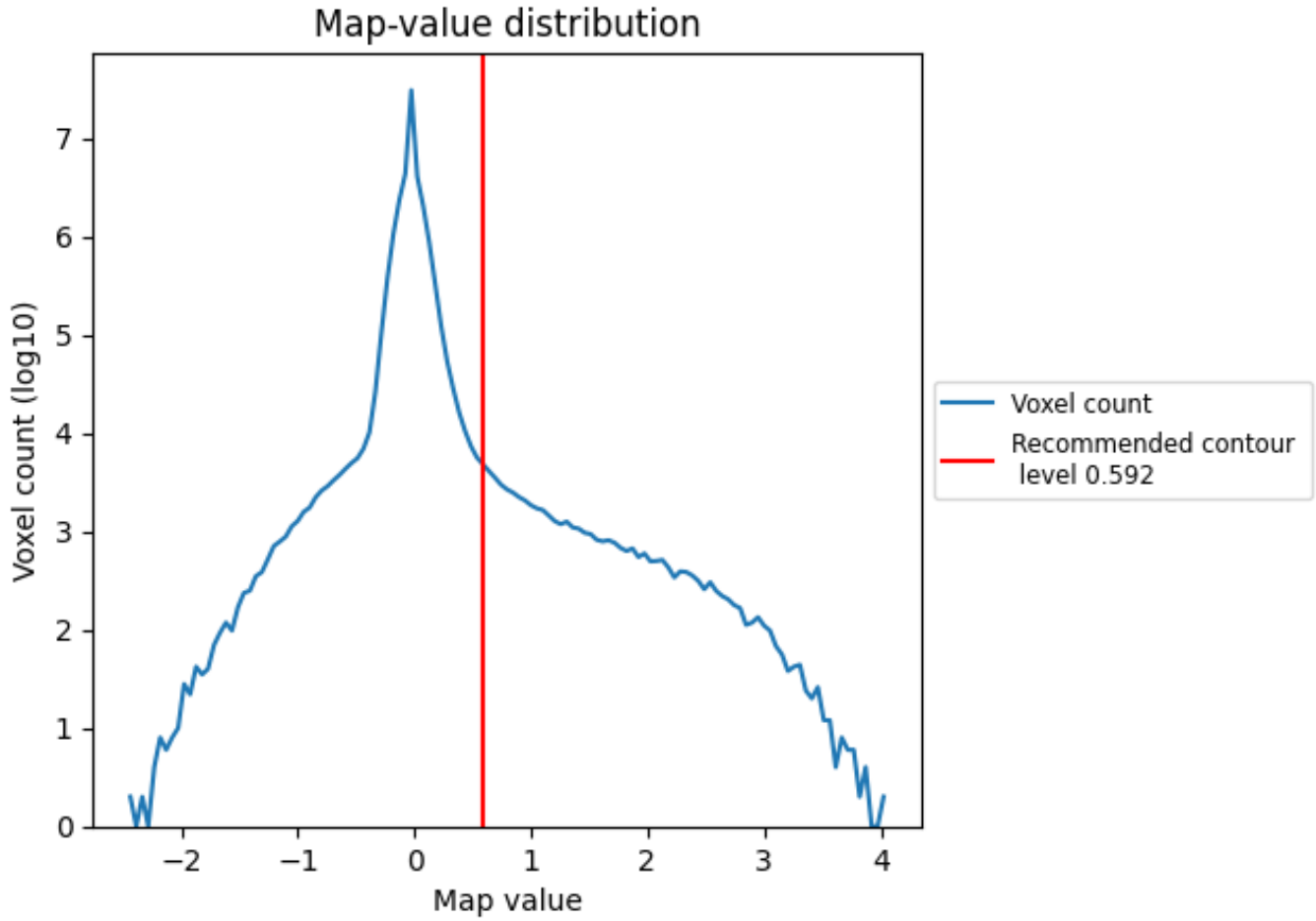
6.6 Mask visualisation (i)

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

7 Map analysis

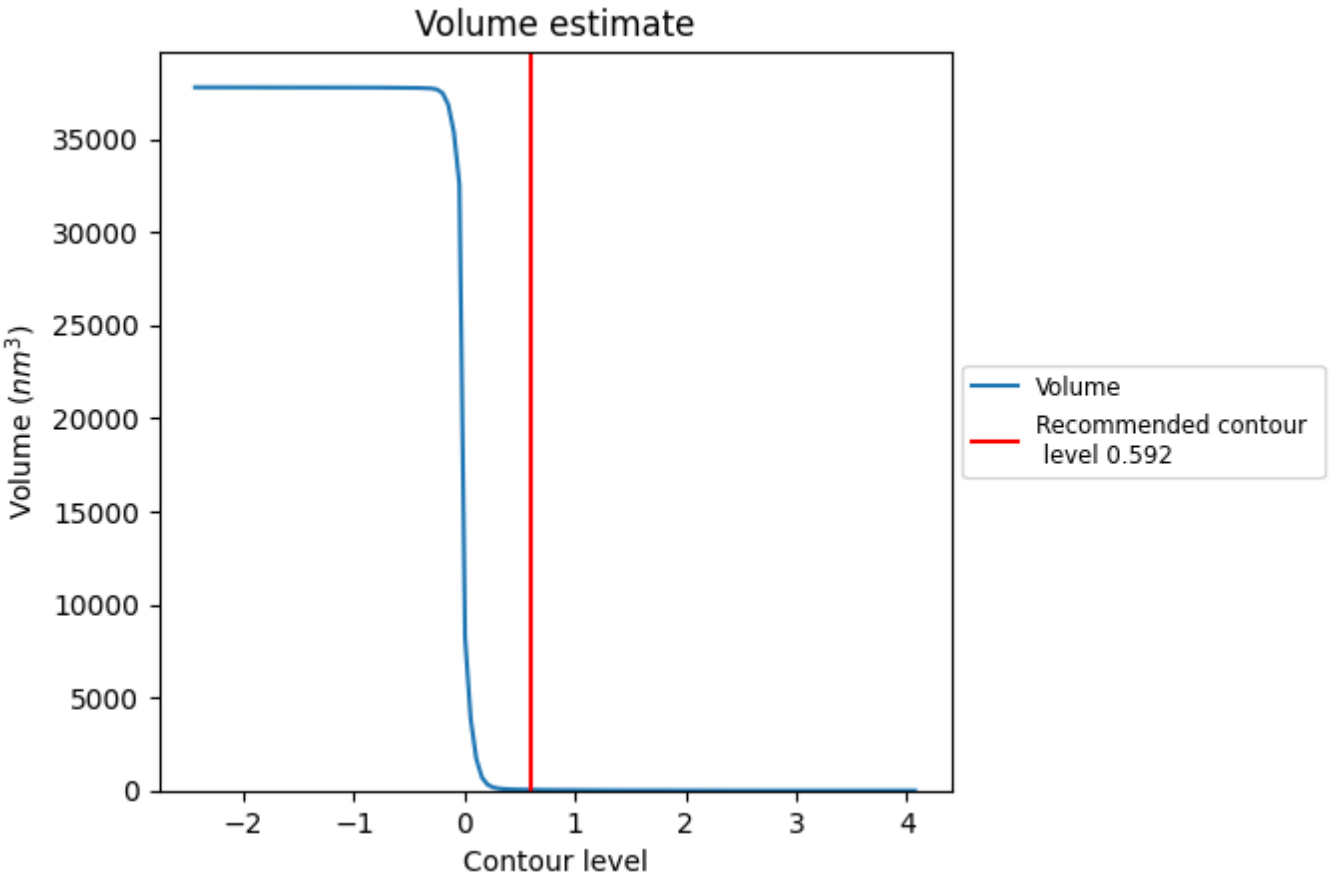
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

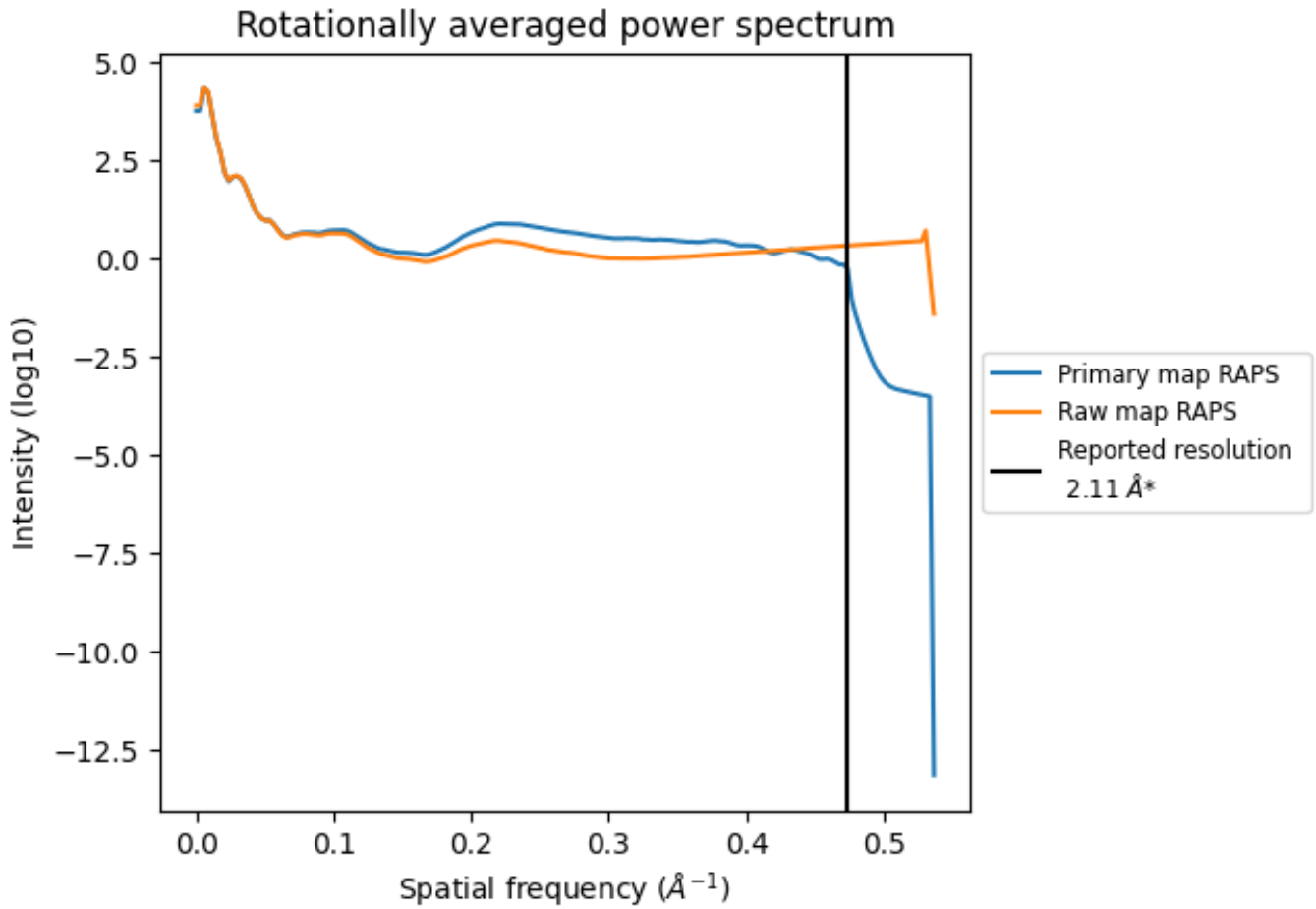
7.2 Volume estimate (i)



The volume at the recommended contour level is 42 nm^3; this corresponds to an approximate mass of 38 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)

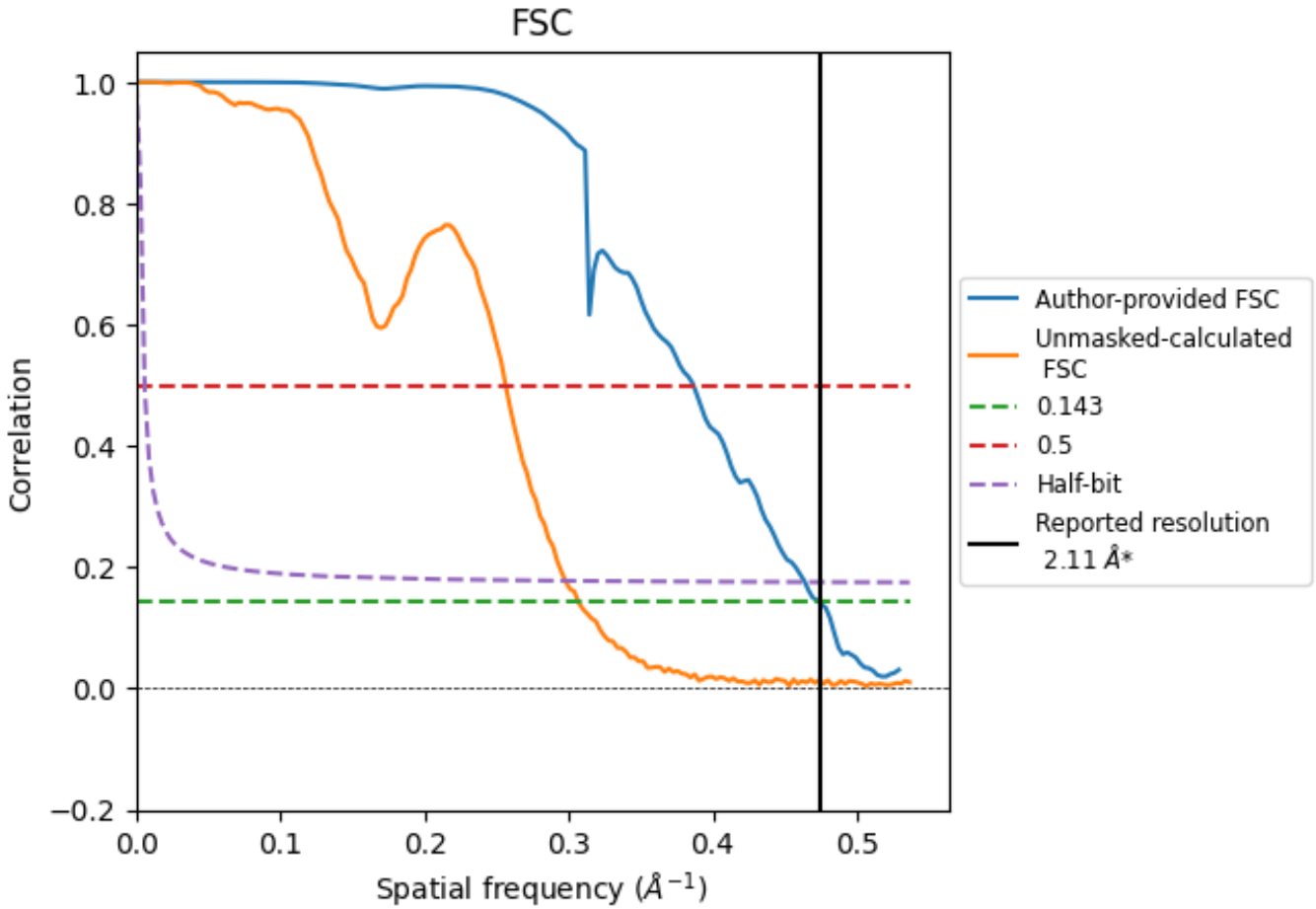


*Reported resolution corresponds to spatial frequency of 0.474 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.474 Å^{-1}

8.2 Resolution estimates (i)

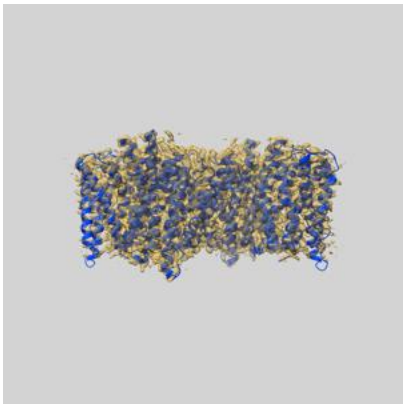
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.11	-	-
Author-provided FSC curve	2.11	2.59	2.16
Unmasked-calculated*	3.26	3.90	3.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.11 by more than 10 %

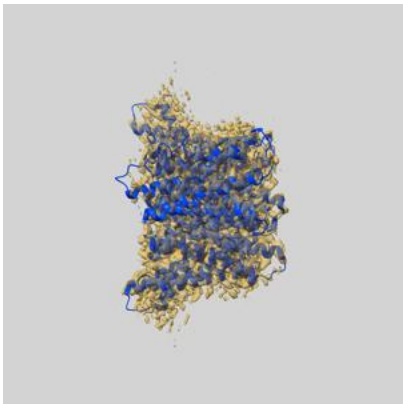
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39851 and PDB model 8Z8Z. Per-residue inclusion information can be found in section 3 on page 8.

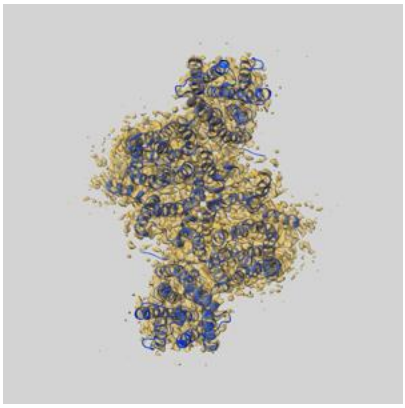
9.1 Map-model overlay



X



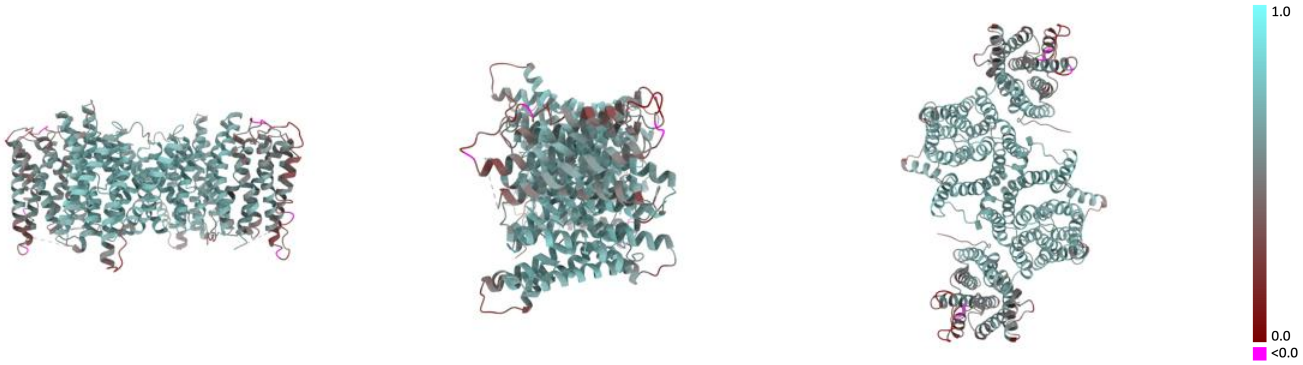
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.592 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.

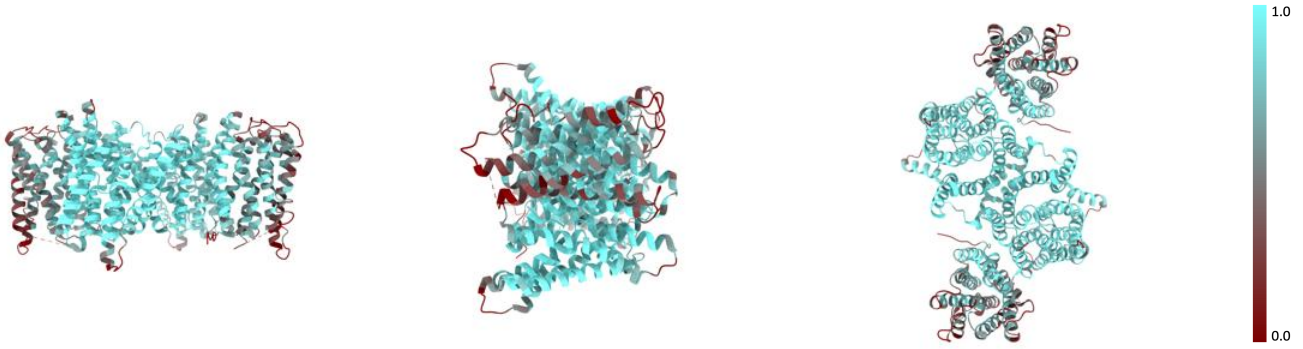
9.2 Q-score mapped to coordinate model (i)



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.

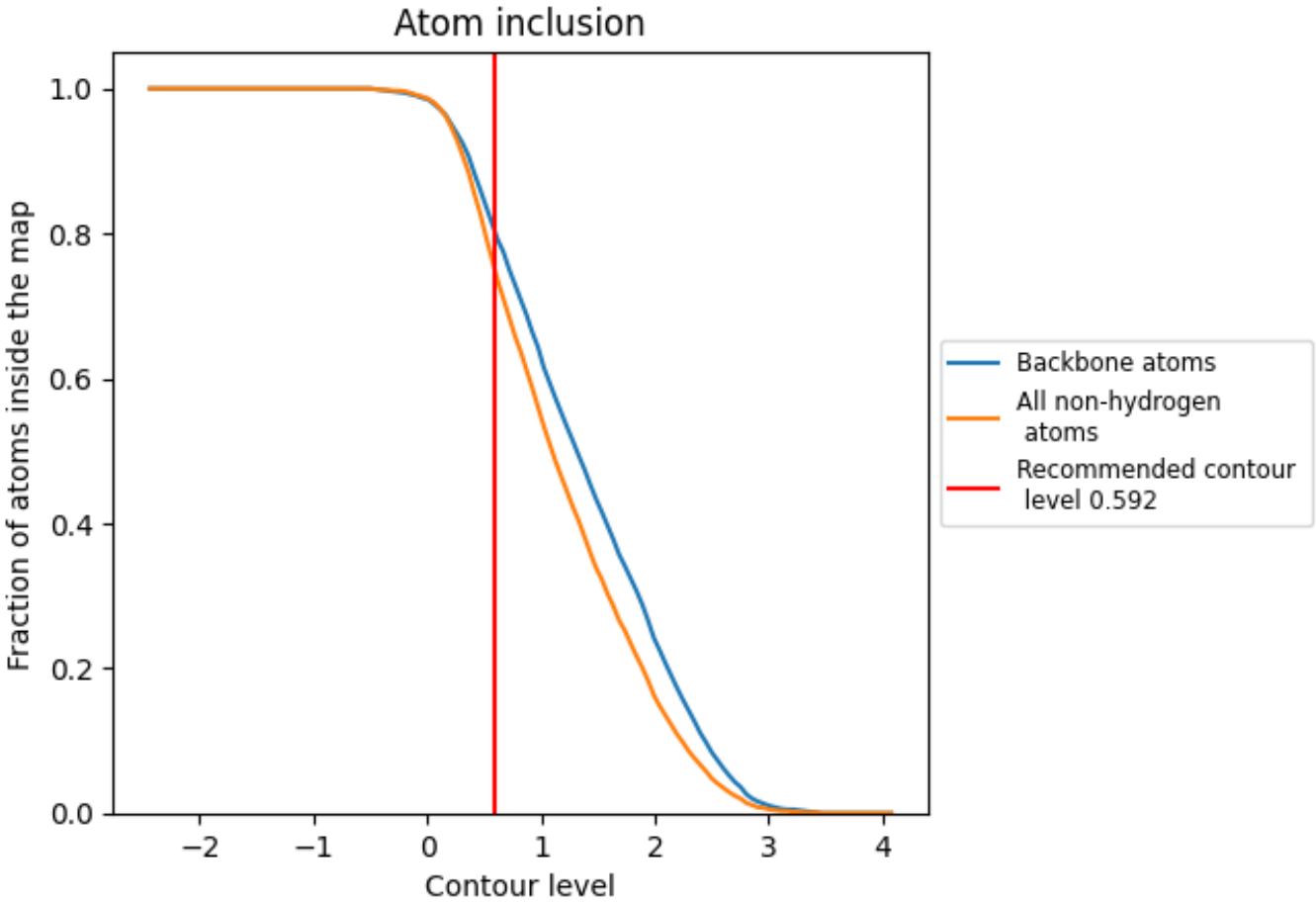
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.592).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.592) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.5890
A	0.7510	0.5890
B	0.7510	0.5880