Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 08:19 PM EST

PDB ID	:	4R0C
Title	:	Crystal structure of the Alcanivorax borkumensis YdaH transporter reveals an unusual topology
Authors	:	Su, C.-C.; Bolla, J.R.; Yu, E.W.
Deposited on	:	2014-07-30
Resolution	:	2.96 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (i)) were used in the production of this report:

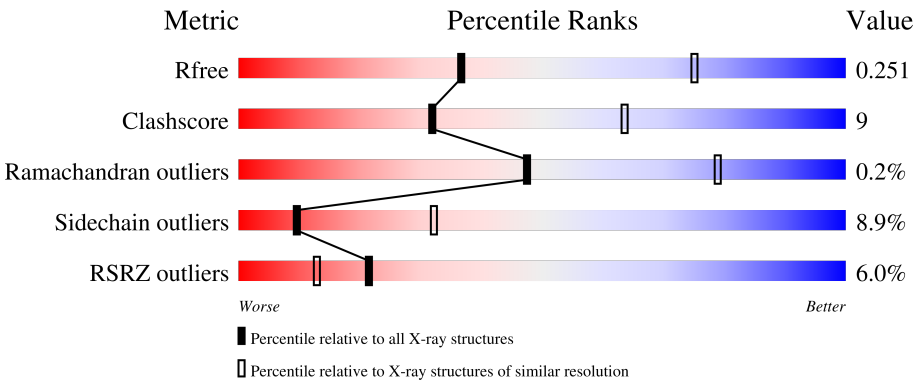
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	492	6% 74% 20% • •
1	B	492	8% 67% 24% • 5%
1	C	492	4% 76% 19% • •
1	D	492	6% 74% 22% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14273 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

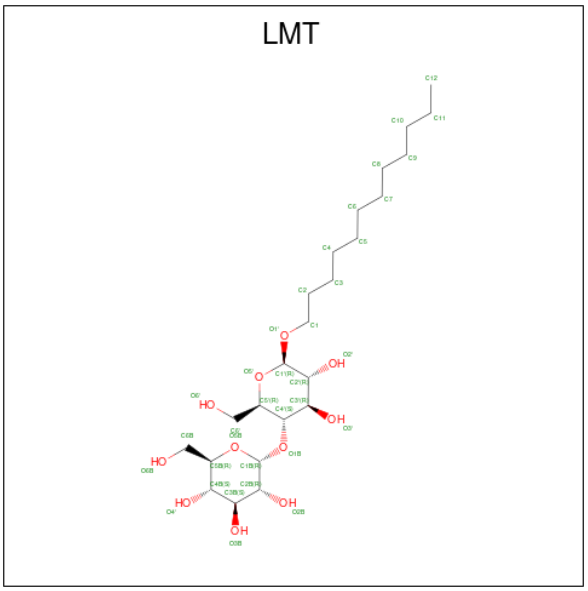
- Molecule 1 is a protein called AbgT putative transporter family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	476	3510	2321	567	609	13	0	0	0
1	B	468	3455	2290	553	599	13	0	0	0
1	C	474	3491	2309	562	607	13	0	0	0
1	D	483	3567	2355	579	620	13	0	0	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

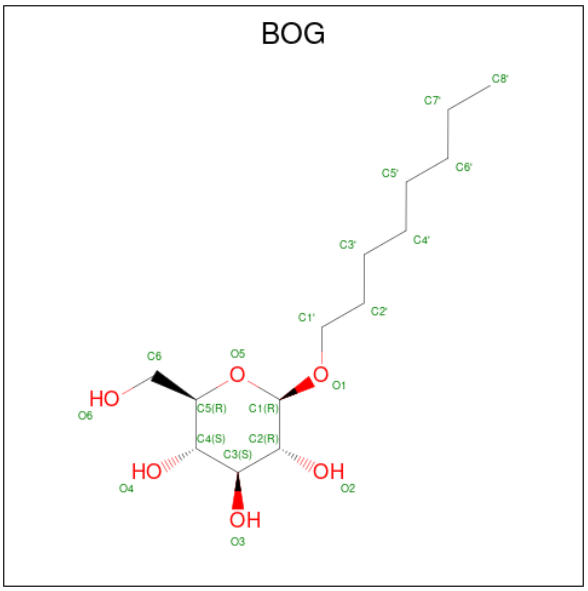
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	23	18	5	0	0
			Total	C	O		
3	A	1	14	13	1	0	0
			Total	C	O		
3	A	1	34	24	10	0	0
			Total	C	O		
3	A	1	14	13	1	0	0
			Total	C	O		
3	C	1	16	14	2	0	0
			Total	C	O		
3	C	1	15	13	2	0	0

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	12	10	2	0	0
			Total	C	O		
4	C	1	20	14	6	0	0
			Total	C	O		
4	C	1	20	14	6	0	0
			Total	C	O		
4	D	1	20	14	6	0	0

- Molecule 5 is water.

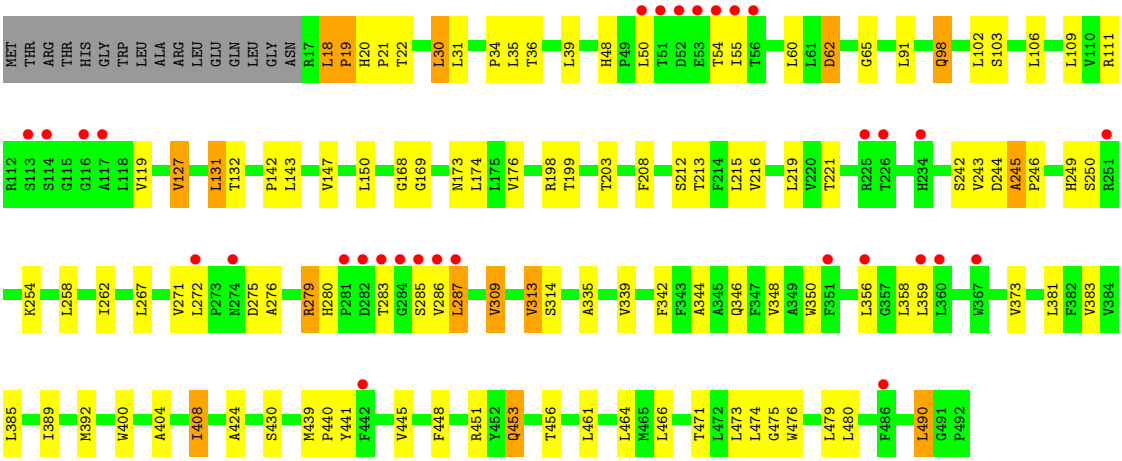
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	12	12	12	0	0
			Total	O		
5	B	15	15	15	0	0
			Total	O		
5	C	15	15	15	0	0
			Total	O		
5	D	16	16	16	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

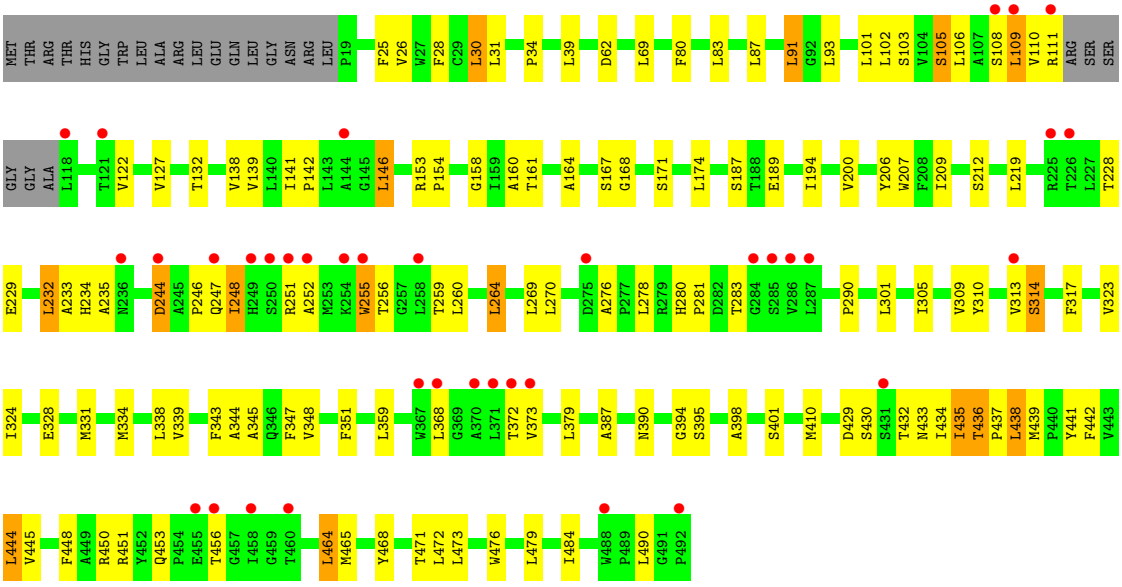
• Molecule 1: AbgT putative transporter family

Chain A:



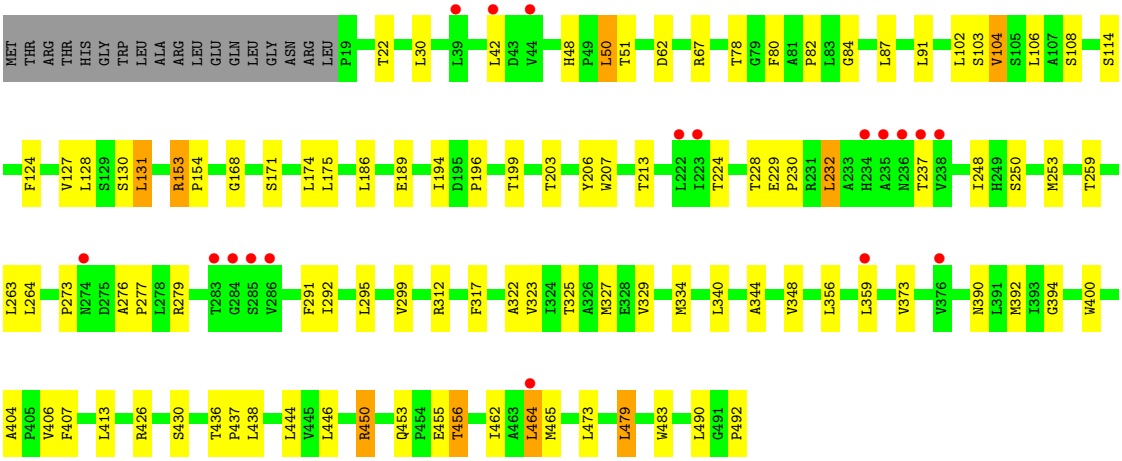
• Molecule 1: AbgT putative transporter family

Chain B:



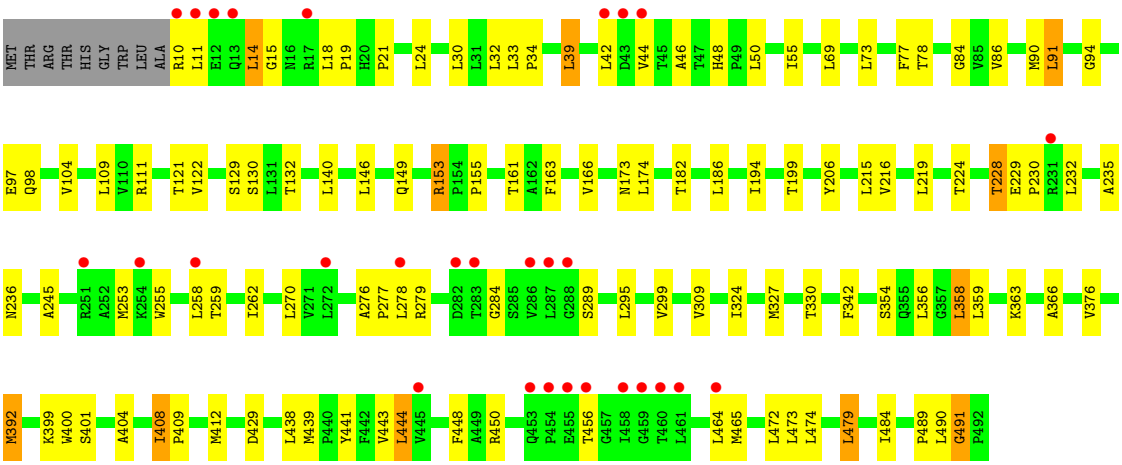
• Molecule 1: AbgT putative transporter family

Chain C:



• Molecule 1: AbgT putative transporter family

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.14Å 200.98Å 101.49Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	48.43 – 2.96 49.18 – 2.96	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.43-2.96) 95.8 (49.18-2.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.206 , 0.250 0.211 , 0.251	Depositor DCC
R_{free} test set	3769 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	76.2	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14273	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: LMT, NA, BOG

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	0.43	0/3594	0.62	0/4933
1	B	0.43	0/3538	0.62	0/4857
1	C	0.42	0/3575	0.62	0/4907
1	D	0.43	0/3651	0.62	1/5009 (0.0%)
All	All	0.43	0/14358	0.62	1/19706 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	491	GLY	N-CA-C	-5.16	100.20	113.10

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	3510	0	3679	71	0
1	B	3455	0	3621	87	0
1	C	3491	0	3656	50	0
1	D	3567	0	3737	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	85	0	124	1	0
3	C	31	0	51	2	0
4	A	12	0	17	1	0
4	C	40	0	56	0	0
4	D	20	0	28	1	0
5	A	12	0	0	1	0
5	B	15	0	0	0	0
5	C	15	0	0	0	0
5	D	16	0	0	0	0
All	All	14273	0	14969	260	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 9.

All (260) 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:A:245:ALA:HB1	1:A:246:PRO:HD3	1.28	1.15
1:A:245:ALA:HB1	1:A:246:PRO:CD	1.82	1.09
1:A:20:HIS:ND1	1:A:21:PRO:HD2	1.69	1.06
1:B:248:ILE:H	1:B:248:ILE:CD1	1.68	1.05
1:A:245:ALA:CB	1:A:246:PRO:CD	2.43	0.96
1:A:20:HIS:CE1	1:A:21:PRO:HD2	2.03	0.93
1:B:248:ILE:HD12	1:B:248:ILE:N	1.83	0.92
1:B:248:ILE:CD1	1:B:248:ILE:N	2.30	0.92
1:A:244:ASP:O	1:A:245:ALA:O	1.86	0.92
1:B:248:ILE:H	1:B:248:ILE:HD13	1.38	0.86
1:A:20:HIS:ND1	1:A:21:PRO:CD	2.42	0.82
1:B:252:ALA:HB2	1:B:313:VAL:HG23	1.66	0.77
1:C:102:LEU:HD22	3:C:803:LMT:H121	1.73	0.69
1:B:102:LEU:HD13	1:B:132:THR:HG22	1.74	0.69
1:A:244:ASP:C	1:A:245:ALA:O	2.25	0.69
1:C:127:VAL:HG21	1:C:213:THR:HG23	1.74	0.69
1:A:174:LEU:HD13	1:A:213:THR:HG21	1.77	0.67
1:B:122:VAL:HG11	1:B:161:THR:HG23	1.77	0.67
1:C:450:ARG:NH1	1:C:456:THR:O	2.26	0.66
1:B:390:ASN:ND2	1:B:429:ASP:O	2.29	0.65
1:B:278:LEU:HD13	1:B:290:PRO:HB2	1.77	0.65
1:A:272:LEU:O	1:A:279:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:HIS:CE1	1:A:50:LEU:HB2	2.34	0.63
1:A:283:THR:HG22	1:A:285:SER:H	1.64	0.62
1:A:245:ALA:CB	1:A:246:PRO:HD2	2.29	0.62
1:B:164:ALA:HA	1:B:434:ILE:HG21	1.81	0.62
1:C:48:HIS:CE1	1:C:50:LEU:HB2	2.35	0.62
1:D:15:GLY:HA3	1:D:438:LEU:HD21	1.81	0.62
1:B:246:PRO:HG2	1:C:196:PRO:HD2	1.82	0.61
1:A:242:SER:HB3	1:A:451:ARG:HH21	1.65	0.60
1:B:108:SER:OG	1:B:247:GLN:NE2	2.35	0.60
1:B:252:ALA:CB	1:B:313:VAL:HG23	2.30	0.60
1:C:437:PRO:HD3	1:C:462:ILE:HD11	1.84	0.59
1:D:111:ARG:NH2	1:D:245:ALA:HB3	2.18	0.59
1:B:437:PRO:HG2	1:B:438:LEU:HD13	1.85	0.58
1:A:246:PRO:CD	1:A:246:PRO:O	2.50	0.58
1:D:18:LEU:HG	1:D:19:PRO:HD2	1.86	0.58
1:C:259:THR:HG22	1:C:263:LEU:HD12	1.85	0.57
1:A:111:ARG:NH2	1:A:245:ALA:HB3	2.19	0.57
3:A:802:LMT:H32	4:A:803:BOG:H1'2	1.87	0.57
1:C:446:LEU:O	1:C:450:ARG:HG2	2.05	0.57
1:D:149:GLN:NE2	1:D:235:ALA:HB1	2.20	0.57
1:B:87:LEU:HD11	1:B:338:LEU:HD21	1.86	0.57
1:A:127:VAL:HG21	1:A:213:THR:HG23	1.87	0.56
1:B:228:THR:O	1:B:232:LEU:HB2	2.05	0.56
1:C:154:PRO:HB2	1:C:232:LEU:HD12	1.86	0.56
1:C:273:PRO:O	1:C:279:ARG:HD2	2.05	0.56
1:C:453:GLN:O	1:C:456:THR:HG22	2.06	0.56
1:B:450:ARG:HG2	1:B:456:THR:HG23	1.87	0.56
1:A:62:ASP:HB3	1:A:65:GLY:H	1.71	0.56
1:D:73:LEU:HD22	4:D:802:BOG:H3'2	1.88	0.55
1:C:124:PHE:CE2	1:C:128:LEU:HD11	2.42	0.55
1:B:146:LEU:HD12	1:C:50:LEU:HD13	1.89	0.55
1:D:48:HIS:CD2	1:D:358:LEU:HD21	2.42	0.54
1:C:168:GLY:O	1:C:430:SER:HB3	2.07	0.54
1:B:138:VAL:HG12	1:B:444:LEU:HD11	1.90	0.54
1:C:312:ARG:HD2	1:C:317:PHE:HB2	1.89	0.54
1:A:280:HIS:HB3	1:A:283:THR:HB	1.90	0.54
1:D:149:GLN:HB2	1:D:155:PRO:HB3	1.89	0.54
1:A:20:HIS:ND1	1:A:22:THR:N	2.52	0.54
1:A:142:PRO:HD3	1:A:448:PHE:CE2	2.43	0.53
1:B:317:PHE:CD2	1:B:323:VAL:HG22	2.42	0.53
1:B:464:LEU:HD13	1:B:465:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:HIS:CE1	1:A:22:THR:H	2.27	0.53
1:B:280:HIS:HB3	1:B:283:THR:HB	1.89	0.53
1:B:441:TYR:O	1:B:445:VAL:HG23	2.08	0.53
1:D:439:MET:SD	1:D:441:TYR:HB2	2.48	0.53
1:A:98:GLN:NE2	5:A:905:HOH:O	2.41	0.53
1:B:234:HIS:HA	1:B:235:ALA:HB3	1.89	0.53
1:C:453:GLN:HB3	1:C:456:THR:HG22	1.91	0.52
1:B:259:THR:HG21	1:B:309:VAL:HG11	1.90	0.52
1:B:472:LEU:O	1:B:476:TRP:HB2	2.10	0.52
1:C:22:THR:HG23	1:C:340:LEU:HA	1.92	0.52
1:B:453:GLN:O	1:B:456:THR:HG22	2.10	0.52
1:C:171:SER:HB3	1:C:426:ARG:HE	1.74	0.52
1:B:344:ALA:O	1:B:348:VAL:HG23	2.10	0.52
1:B:310:TYR:O	1:B:314:SER:HB3	2.10	0.52
1:D:228:THR:HG23	1:D:232:LEU:HD22	1.92	0.52
1:A:242:SER:HB3	1:A:451:ARG:NH2	2.25	0.52
1:B:160:ALA:HA	1:B:465:MET:HE1	1.91	0.52
1:A:245:ALA:HB1	1:A:246:PRO:HD2	1.82	0.51
1:A:168:GLY:HA2	1:A:430:SER:O	2.11	0.51
1:B:444:LEU:HD13	1:B:448:PHE:HE2	1.75	0.51
1:B:153:ARG:HB3	1:B:229:GLU:OE2	2.11	0.50
1:D:55:ILE:HD13	1:D:358:LEU:HG	1.93	0.50
1:B:25:PHE:CZ	1:B:401:SER:HB2	2.46	0.50
1:B:110:VAL:O	1:B:111:ARG:HB2	2.12	0.50
1:A:91:LEU:HD11	1:B:339:VAL:HG22	1.94	0.50
1:D:46:ALA:HB3	1:D:55:ILE:HD12	1.93	0.50
1:B:437:PRO:HA	1:B:442:PHE:CD2	2.47	0.50
1:A:106:LEU:O	1:A:109:LEU:HB2	2.12	0.49
1:A:453:GLN:HB3	1:A:456:THR:HG23	1.93	0.49
1:C:317:PHE:HB3	1:C:322:ALA:HB3	1.94	0.49
1:B:331:MET:HE1	1:B:334:MET:HG3	1.94	0.49
1:D:94:GLY:O	1:D:98:GLN:HB2	2.12	0.49
1:D:279:ARG:NE	1:D:284:GLY:O	2.45	0.49
1:A:246:PRO:HD2	1:A:246:PRO:O	2.13	0.49
1:D:489:PRO:HB2	1:D:491:GLY:O	2.12	0.49
1:A:267:LEU:O	1:A:271:VAL:HG12	2.11	0.49
1:A:385:LEU:O	1:A:389:ILE:HG13	2.13	0.49
1:B:435:ILE:CG1	1:B:435:ILE:O	2.58	0.49
1:C:82:PRO:HG3	1:C:186:LEU:HD23	1.94	0.49
1:D:33:LEU:HB2	1:D:34:PRO:HD3	1.95	0.48
1:D:270:LEU:HB3	1:D:278:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ARG:HD2	1:C:229:GLU:OE2	2.13	0.48
1:A:143:LEU:O	1:A:147:VAL:HG23	2.14	0.48
1:A:30:LEU:O	1:A:34:PRO:HD3	2.14	0.48
1:A:439:MET:HG2	1:A:440:PRO:HD2	1.96	0.48
1:B:83:LEU:HD11	1:B:338:LEU:HD23	1.95	0.48
1:A:20:HIS:CG	1:A:21:PRO:CD	2.96	0.48
1:A:20:HIS:CG	1:A:21:PRO:HD2	2.43	0.48
1:A:102:LEU:HD13	1:A:132:THR:HG22	1.94	0.48
1:C:344:ALA:O	1:C:348:VAL:HG23	2.13	0.48
1:A:287:LEU:HD12	1:A:287:LEU:HA	1.77	0.48
1:C:203:THR:O	1:C:492:PRO:HD2	2.13	0.48
1:D:48:HIS:HE1	1:D:50:LEU:HB2	1.79	0.48
1:D:48:HIS:CE1	1:D:50:LEU:HB2	2.48	0.47
1:C:392:MET:HA	1:C:438:LEU:HD12	1.96	0.47
1:D:32:LEU:HD23	1:D:32:LEU:HA	1.75	0.47
1:A:169:GLY:HA3	1:A:216:VAL:HG11	1.97	0.47
1:B:80:PHE:CD1	1:B:345:ALA:HB2	2.50	0.47
1:C:84:GLY:HA3	1:D:78:THR:HG21	1.97	0.47
1:A:31:LEU:O	1:A:34:PRO:HD2	2.15	0.47
1:C:400:TRP:CE2	1:C:404:ALA:HB2	2.50	0.47
1:D:153:ARG:NH1	1:D:229:GLU:OE2	2.42	0.47
1:D:259:THR:HG21	1:D:309:VAL:HG21	1.97	0.47
1:B:244:ASP:OD1	1:B:244:ASP:N	2.48	0.46
1:C:390:ASN:OD1	1:C:394:GLY:HA2	2.15	0.46
1:A:344:ALA:O	1:A:348:VAL:HG23	2.15	0.46
1:B:209:ILE:HA	1:B:212:SER:HB2	1.96	0.46
1:D:229:GLU:HB3	1:D:230:PRO:HD3	1.97	0.46
1:C:80:PHE:CE2	1:C:189:GLU:HG3	2.50	0.46
1:A:127:VAL:CG2	1:A:213:THR:HG23	2.46	0.46
1:C:406:VAL:HG12	1:C:407:PHE:CD2	2.50	0.46
1:B:465:MET:O	1:B:468:TYR:N	2.48	0.46
1:D:14:LEU:HD21	1:D:392:MET:HB3	1.96	0.46
1:D:258:LEU:O	1:D:262:ILE:HG13	2.16	0.46
1:C:295:LEU:O	1:C:299:VAL:HG23	2.15	0.46
1:A:404:ALA:O	1:A:408:ILE:HB	2.16	0.46
1:B:270:LEU:O	1:B:276:ALA:HB1	2.15	0.46
1:A:20:HIS:ND1	1:A:21:PRO:N	2.64	0.45
1:A:249:HIS:CD2	1:A:314:SER:HA	2.51	0.45
1:D:163:PHE:HD2	1:D:465:MET:CE	2.29	0.45
1:B:103:SER:HB3	1:B:139:VAL:HG11	1.98	0.45
1:B:387:ALA:HB1	1:B:432:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PHE:CE2	1:B:189:GLU:HG3	2.52	0.45
1:B:154:PRO:HG2	1:B:232:LEU:HB3	1.98	0.45
1:B:270:LEU:O	1:B:278:LEU:HB2	2.17	0.45
1:B:167:SER:OG	1:B:433:ASN:HB3	2.17	0.45
1:D:276:ALA:HB3	1:D:279:ARG:HD2	1.98	0.45
1:B:160:ALA:HA	1:B:465:MET:CE	2.47	0.45
1:B:264:LEU:HD12	1:B:264:LEU:HA	1.66	0.45
1:B:168:GLY:HA2	1:B:430:SER:O	2.16	0.45
1:D:354:SER:OG	1:D:356:LEU:HG	2.17	0.45
1:C:224:THR:HA	1:C:228:THR:HB	1.99	0.44
1:A:60:LEU:HD11	1:A:350:TRP:HB3	1.99	0.44
1:A:119:VAL:HG12	1:A:221:THR:HG23	2.00	0.44
1:B:301:LEU:O	1:B:305:ILE:HG13	2.18	0.44
1:C:67:ARG:NH2	1:D:277:PRO:HA	2.32	0.44
1:B:30:LEU:O	1:B:34:PRO:HD2	2.17	0.44
1:B:255:TRP:CE3	1:B:255:TRP:HA	2.53	0.44
1:B:187:SER:HB3	1:B:200:VAL:HG21	2.00	0.44
1:D:10:ARG:CZ	1:D:14:LEU:HB2	2.48	0.44
1:A:208:PHE:HB2	1:A:490:LEU:HD12	1.99	0.43
1:D:129:SER:OG	1:D:166:VAL:HG22	2.17	0.43
1:B:368:LEU:HD11	1:B:410:MET:HE3	2.00	0.43
1:A:35:LEU:HD23	1:A:39:LEU:HD13	1.98	0.43
1:B:439:MET:SD	1:B:441:TYR:HB2	2.58	0.43
1:A:275:ASP:OD1	1:A:275:ASP:N	2.39	0.43
1:A:276:ALA:HB3	1:A:279:ARG:HD2	2.00	0.43
1:B:324:ILE:O	1:B:328:GLU:HG3	2.18	0.43
1:B:390:ASN:OD1	1:B:394:GLY:HA2	2.17	0.43
1:D:91:LEU:HD12	1:D:327:MET:HB3	2.00	0.43
1:D:109:LEU:O	1:D:121:THR:HG21	2.19	0.43
1:B:436:THR:HG23	1:B:439:MET:HB2	2.00	0.43
1:C:104:VAL:HG13	1:C:248:ILE:HG12	2.00	0.43
1:D:216:VAL:HG22	1:D:472:LEU:HD22	2.00	0.43
1:A:309:VAL:O	1:A:313:VAL:HG13	2.19	0.43
1:B:347:PHE:O	1:B:351:PHE:HB2	2.19	0.43
1:D:194:ILE:HG12	1:D:409:PRO:HB3	2.00	0.43
1:A:441:TYR:O	1:A:445:VAL:HG23	2.19	0.43
1:B:28:PHE:HB3	1:B:347:PHE:CD1	2.53	0.43
1:B:101:LEU:O	1:B:105:SER:HB2	2.19	0.43
1:D:444:LEU:HD22	1:D:448:PHE:CZ	2.54	0.43
1:D:484:ILE:HD13	1:D:484:ILE:HA	1.88	0.43
1:A:131:LEU:HD22	1:A:173:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:THR:O	1:B:259:THR:OG1	2.22	0.42
1:D:295:LEU:O	1:D:299:VAL:HG23	2.19	0.42
1:A:55:ILE:HD13	1:A:358:LEU:HG	2.00	0.42
1:B:430:SER:O	1:B:433:ASN:HB2	2.18	0.42
1:B:450:ARG:HD3	1:B:456:THR:O	2.19	0.42
1:B:111:ARG:NH2	1:C:50:LEU:O	2.30	0.42
1:B:154:PRO:HB3	1:B:232:LEU:HD12	2.00	0.42
1:D:90:MET:O	1:D:330:THR:HG21	2.20	0.42
1:D:149:GLN:HE22	1:D:236:ASN:N	2.17	0.42
1:B:246:PRO:CG	1:C:196:PRO:HD2	2.47	0.42
1:B:280:HIS:ND1	1:B:281:PRO:HD2	2.34	0.42
1:C:87:LEU:HD23	1:C:334:MET:HE2	2.01	0.42
1:D:186:LEU:HD22	1:D:401:SER:HA	2.01	0.42
1:C:131:LEU:HD21	1:C:175:LEU:HB2	2.02	0.42
1:C:325:THR:O	1:C:329:VAL:HG23	2.20	0.42
1:D:130:SER:HB2	1:D:173:ASN:HD22	1.85	0.42
1:B:435:ILE:O	1:B:435:ILE:HG13	2.20	0.42
1:A:219:LEU:HD11	1:A:475:GLY:HA3	2.02	0.41
1:A:480:LEU:HD12	1:A:480:LEU:HA	1.86	0.41
1:B:91:LEU:HD12	1:B:91:LEU:HA	1.85	0.41
1:C:455:GLU:OE1	1:C:455:GLU:N	2.40	0.41
1:A:212:SER:HG	1:A:476:TRP:HE1	1.66	0.41
1:B:219:LEU:HD13	1:B:471:THR:HG22	2.01	0.41
1:B:395:SER:HB3	1:B:398:ALA:HB3	2.01	0.41
1:D:39:LEU:HA	1:D:39:LEU:HD12	1.80	0.41
1:D:122:VAL:HG12	1:D:161:THR:HG22	2.01	0.41
1:A:258:LEU:O	1:A:262:ILE:HG13	2.20	0.41
1:A:383:VAL:HG22	1:A:424:ALA:O	2.20	0.41
1:B:168:GLY:O	1:B:430:SER:HB3	2.21	0.41
1:A:18:LEU:HD11	1:A:392:MET:HB3	2.01	0.41
1:A:400:TRP:CE2	1:A:404:ALA:HB2	2.55	0.41
1:B:158:GLY:HA2	1:B:161:THR:HG22	2.01	0.41
1:B:309:VAL:O	1:B:313:VAL:HG22	2.21	0.41
1:C:291:PHE:CD2	1:C:292:ILE:HD12	2.54	0.41
1:A:36:THR:HG21	1:A:60:LEU:HG	2.02	0.41
1:D:21:PRO:O	1:D:24:LEU:HB2	2.20	0.41
1:A:219:LEU:HD13	1:A:471:THR:HG22	2.02	0.41
1:A:279:ARG:HH21	1:A:286:VAL:HG23	1.85	0.41
1:C:78:THR:HG21	1:D:84:GLY:HA3	2.03	0.41
1:C:229:GLU:HB3	1:C:230:PRO:HD3	2.02	0.41
1:D:215:LEU:O	1:D:219:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:LEU:HD13	1:C:465:MET:HE1	2.01	0.41
1:D:408:ILE:O	1:D:412:MET:HG3	2.21	0.41
1:D:450:ARG:NH1	1:D:456:THR:O	2.52	0.41
1:B:141:ILE:N	1:B:142:PRO:HD2	2.36	0.41
1:D:77:PHE:CD1	1:D:342:PHE:HA	2.56	0.41
1:D:276:ALA:O	1:D:279:ARG:HG2	2.21	0.41
1:D:363:LYS:O	1:D:366:ALA:HB3	2.21	0.41
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.86	0.41
1:B:141:ILE:HD13	1:B:445:VAL:HG13	2.02	0.41
1:D:324:ILE:HD13	1:D:327:MET:CE	2.52	0.41
1:A:335:ALA:O	1:A:339:VAL:HG23	2.21	0.40
1:A:461:LEU:HD12	1:A:461:LEU:HA	1.90	0.40
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.85	0.40
1:B:260:LEU:O	1:B:264:LEU:HB2	2.21	0.40
1:C:276:ALA:HA	1:C:277:PRO:HD2	1.82	0.40
1:C:323:VAL:O	1:C:327:MET:HG3	2.20	0.40
1:D:97:GLU:OE1	1:D:132:THR:HB	2.21	0.40
1:A:19:PRO:HB2	1:A:20:HIS:H	1.67	0.40
1:A:279:ARG:NH2	1:A:286:VAL:HG23	2.36	0.40
1:B:26:VAL:HG22	1:B:343:PHE:CE1	2.56	0.40
1:B:379:LEU:CD1	1:B:484:ILE:HG13	2.51	0.40
1:D:86:VAL:HG21	1:D:182:THR:OG1	2.22	0.40
1:D:224:THR:HA	1:D:228:THR:HB	2.02	0.40
1:D:255:TRP:O	1:D:259:THR:HG23	2.21	0.40
1:C:106:LEU:HD21	3:C:803:LMT:H111	2.02	0.40
1:C:295:LEU:HD12	1:C:295:LEU:HA	1.76	0.40
1:D:279:ARG:HA	1:D:289:SER:HB2	2.03	0.40
1:A:342:PHE:O	1:A:346:GLN:HG2	2.21	0.40
1:B:111:ARG:HH12	1:C:51:THR:HA	1.86	0.40
1:D:479:LEU:HD23	1:D:479:LEU:HA	1.98	0.40
1:C:194:ILE:HD12	1:C:413:LEU:HD21	2.04	0.40
1:C:479:LEU:O	1:C:483:TRP:HB2	2.22	0.40
1:D:400:TRP:CE2	1:D:404:ALA:HB2	2.57	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 X-ray entries followed by that with respect to entries of similar resolution.

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	474/492 (96%)	448 (94%)	24 (5%)	2 (0%)	34	69
1	B	464/492 (94%)	440 (95%)	23 (5%)	1 (0%)	47	79
1	C	472/492 (96%)	454 (96%)	18 (4%)	0	100	100
1	D	481/492 (98%)	471 (98%)	10 (2%)	0	100	100
All	All	1891/1968 (96%)	1813 (96%)	75 (4%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ALA
1	A	19	PRO
1	B	233	ALA

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 X-ray entries followed by that with respect to entries of similar resolution.

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	369/382 (97%)	336 (91%)	33 (9%)	9	32
1	B	364/382 (95%)	328 (90%)	36 (10%)	8	27
1	C	367/382 (96%)	335 (91%)	32 (9%)	10	33
1	D	375/382 (98%)	344 (92%)	31 (8%)	11	35
All	All	1475/1528 (96%)	1343 (91%)	132 (9%)	9	32

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	30	LEU
1	A	54	THR
1	A	62	ASP
1	A	98	GLN
1	A	103	SER
1	A	127	VAL
1	A	131	LEU
1	A	150	LEU
1	A	176	VAL
1	A	198	ARG
1	A	199	THR
1	A	203	THR
1	A	215	LEU
1	A	243	VAL
1	A	250	SER
1	A	254	LYS
1	A	279	ARG
1	A	287	LEU
1	A	309	VAL
1	A	313	VAL
1	A	356	LEU
1	A	359	LEU
1	A	373	VAL
1	A	381	LEU
1	A	408	ILE
1	A	453	GLN
1	A	464	LEU
1	A	466	LEU
1	A	473	LEU
1	A	474	LEU
1	A	479	LEU
1	A	490	LEU
1	B	30	LEU
1	B	39	LEU
1	B	62	ASP
1	B	69	LEU
1	B	91	LEU
1	B	93	LEU
1	B	105	SER
1	B	106	LEU
1	B	109	LEU
1	B	127	VAL

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Mol	Chain	Res	Type
1	B	146	LEU
1	B	171	SER
1	B	174	LEU
1	B	194	ILE
1	B	206	TYR
1	B	207	TRP
1	B	232	LEU
1	B	244	ASP
1	B	248	ILE
1	B	251	ARG
1	B	255	TRP
1	B	264	LEU
1	B	269	LEU
1	B	314	SER
1	B	359	LEU
1	B	372	THR
1	B	373	VAL
1	B	435	ILE
1	B	436	THR
1	B	438	LEU
1	B	444	LEU
1	B	451	ARG
1	B	464	LEU
1	B	473	LEU
1	B	479	LEU
1	B	490	LEU
1	C	30	LEU
1	C	42	LEU
1	C	50	LEU
1	C	62	ASP
1	C	91	LEU
1	C	103	SER
1	C	104	VAL
1	C	108	SER
1	C	114	SER
1	C	130	SER
1	C	131	LEU
1	C	153	ARG
1	C	174	LEU
1	C	199	THR
1	C	206	TYR
1	C	207	TRP

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Mol	Chain	Res	Type
1	C	232	LEU
1	C	237	THR
1	C	250	SER
1	C	253	MET
1	C	264	LEU
1	C	356	LEU
1	C	359	LEU
1	C	373	VAL
1	C	436	THR
1	C	444	LEU
1	C	450	ARG
1	C	456	THR
1	C	464	LEU
1	C	473	LEU
1	C	479	LEU
1	C	490	LEU
1	D	11	LEU
1	D	14	LEU
1	D	30	LEU
1	D	39	LEU
1	D	42	LEU
1	D	44	VAL
1	D	69	LEU
1	D	91	LEU
1	D	104	VAL
1	D	140	LEU
1	D	146	LEU
1	D	153	ARG
1	D	174	LEU
1	D	199	THR
1	D	206	TYR
1	D	228	THR
1	D	253	MET
1	D	358	LEU
1	D	359	LEU
1	D	376	VAL
1	D	392	MET
1	D	399	LYS
1	D	408	ILE
1	D	429	ASP
1	D	443	VAL
1	D	444	LEU

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Mol	Chain	Res	Type
1	D	464	LEU
1	D	473	LEU
1	D	474	LEU
1	D	479	LEU
1	D	490	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	247	GLN
1	C	58	HIS
1	C	205	ASN
1	D	149	GLN
1	D	236	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)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	BOG	C	802	-	20,20,20	1.03	1 (5%)	25,25,25	1.39	2 (8%)
3	LMT	A	805	-	34,34,36	3.30	11 (32%)	41,42,47	0.97	1 (2%)
3	LMT	C	805	-	14,14,36	1.26	1 (7%)	12,13,47	1.01	1 (8%)
4	BOG	A	803	-	11,11,20	0.35	0	10,10,25	0.94	0
4	BOG	C	804	-	20,20,20	0.95	2 (10%)	25,25,25	1.63	3 (12%)
3	LMT	A	806	-	13,13,36	1.06	1 (7%)	12,12,47	0.63	0
3	LMT	C	803	-	15,15,36	0.98	0	14,14,47	0.86	0
3	LMT	A	802	-	23,23,36	1.98	6 (26%)	28,28,47	0.89	1 (3%)
4	BOG	D	802	-	20,20,20	0.96	1 (5%)	25,25,25	0.91	1 (4%)
3	LMT	A	804	-	13,13,36	1.02	1 (7%)	12,12,47	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BOG	C	802	-	-	0/11/31/31	0/1/1/1
3	LMT	A	805	-	-	15/31/51/61	0/1/1/2
3	LMT	C	805	-	-	6/11/12/61	-
4	BOG	A	803	-	-	3/9/9/31	-
4	BOG	C	804	-	-	8/11/31/31	0/1/1/1
3	LMT	A	806	-	-	10/11/11/61	-
3	LMT	C	803	-	-	5/13/13/61	-
3	LMT	A	802	-	-	3/13/33/61	0/1/1/2
4	BOG	D	802	-	-	5/11/31/31	0/1/1/1
3	LMT	A	804	-	-	9/11/11/61	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	805	LMT	O1B-C1B	-13.18	1.19	1.43
3	A	805	LMT	C4B-C3B	-7.61	1.39	1.53
3	A	805	LMT	O3'-C3'	-4.90	1.31	1.43
3	A	802	LMT	O1'-C1'	4.60	1.48	1.40
3	A	802	LMT	O3'-C3'	-4.54	1.32	1.43
3	A	805	LMT	O1'-C1'	4.48	1.47	1.40
3	A	805	LMT	C5B-C4B	-4.31	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	805	LMT	O5'-C1'	-3.58	1.32	1.41
3	A	802	LMT	O5'-C1'	-3.46	1.33	1.41
3	A	805	LMT	O5'-C5'	-3.40	1.36	1.44
3	A	802	LMT	O5'-C5'	-3.38	1.36	1.44
3	A	805	LMT	C1B-C2B	-3.35	1.47	1.51
3	C	805	LMT	O1'-C1'	2.69	1.48	1.40
3	A	805	LMT	O2B-C2B	2.62	1.48	1.43
3	A	805	LMT	C2B-C3B	-2.34	1.49	1.53
3	A	802	LMT	C1'-C2'	-2.28	1.45	1.52
3	A	805	LMT	C1'-C2'	-2.16	1.46	1.52
4	C	802	BOG	O2-C2	-2.11	1.38	1.43
4	C	804	BOG	O3-C3	-2.10	1.38	1.43
4	D	802	BOG	O2-C2	-2.07	1.38	1.43
3	A	806	LMT	C6-C5	2.05	1.63	1.51
4	C	804	BOG	O2-C2	-2.04	1.38	1.43
3	A	804	LMT	C6-C5	2.03	1.63	1.51
3	A	802	LMT	C6-C5	2.01	1.62	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	804	BOG	C1'-O1-C1	4.76	121.74	113.84
4	C	802	BOG	C1'-O1-C1	4.26	120.91	113.84
4	C	804	BOG	C4-C3-C2	-3.56	104.61	110.82
3	A	802	LMT	C1-O1'-C1'	3.09	118.96	113.84
3	A	805	LMT	C1-O1'-C1'	3.05	118.90	113.84
4	C	804	BOG	C1-O5-C5	2.82	119.23	113.69
4	C	802	BOG	C1-O5-C5	-2.49	108.80	113.69
4	D	802	BOG	C1'-O1-C1	2.26	117.59	113.84
3	C	805	LMT	C1'-O1'-C1	2.22	119.76	112.84

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	805	LMT	O2B-C2B-C3B-O3B
3	A	805	LMT	C2B-C3B-C4B-C5B
3	A	805	LMT	C2B-C3B-C4B-O4'
3	A	805	LMT	O3B-C3B-C4B-C5B
3	A	805	LMT	O3B-C3B-C4B-O4'
4	C	804	BOG	O5-C1-O1-C1'
3	A	805	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
4	C	804	BOG	C4-C5-C6-O6
4	D	802	BOG	O5-C5-C6-O6
3	A	805	LMT	C1B-C2B-C3B-O3B
3	A	805	LMT	C1B-C2B-C3B-C4B
3	A	805	LMT	C4'-C5'-C6'-O6'
4	A	803	BOG	O1-C1-O5-C5
4	D	802	BOG	C4-C5-C6-O6
4	C	804	BOG	O5-C5-C6-O6
3	A	805	LMT	O2B-C2B-C3B-C4B
3	C	805	LMT	O1'-C1-C2-C3
3	C	803	LMT	O1'-C1-C2-C3
3	A	804	LMT	O1'-C1-C2-C3
3	A	802	LMT	C4-C5-C6-C7
3	A	806	LMT	C11-C10-C9-C8
3	A	804	LMT	C6-C7-C8-C9
3	A	806	LMT	C6-C7-C8-C9
3	A	806	LMT	C7-C8-C9-C10
3	C	805	LMT	C2-C3-C4-C5
3	C	805	LMT	C7-C8-C9-C10
3	A	805	LMT	O4'-C4B-C5B-C6B
3	C	805	LMT	C5-C6-C7-C8
3	C	803	LMT	C1-C2-C3-C4
3	A	804	LMT	C4-C5-C6-C7
4	A	803	BOG	O5-C1-O1-C1'
3	A	804	LMT	C2-C1-O1'-C1'
3	A	806	LMT	C2-C1-O1'-C1'
3	A	805	LMT	C1-C2-C3-C4
3	C	803	LMT	C4-C5-C6-C7
3	A	806	LMT	C1-C2-C3-C4
4	D	802	BOG	C5'-C6'-C7'-C8'
3	A	806	LMT	C9-C10-C11-C12
3	A	805	LMT	C3B-C4B-C5B-C6B
4	C	804	BOG	C2'-C3'-C4'-C5'
4	D	802	BOG	C2-C1-O1-C1'
4	C	804	BOG	O1-C1'-C2'-C3'
3	A	805	LMT	C4B-C5B-C6B-O6B
3	C	805	LMT	C9-C10-C11-C12
3	A	806	LMT	C4-C5-C6-C7
3	A	802	LMT	C7-C8-C9-C10
3	C	803	LMT	C9-C10-C11-C12
4	C	804	BOG	C2'-C1'-O1-C1
3	A	804	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	805	LMT	C3-C4-C5-C6
4	A	803	BOG	C1'-C2'-C3'-C4'
3	A	806	LMT	C3-C4-C5-C6
4	D	802	BOG	O5-C1-O1-C1'
3	C	803	LMT	C5-C6-C7-C8
3	A	804	LMT	C1-C2-C3-C4
3	A	802	LMT	C3-C4-C5-C6
3	A	804	LMT	C7-C8-C9-C10
4	C	804	BOG	C2-C1-O1-C1'
3	A	806	LMT	O1'-C1-C2-C3
3	A	804	LMT	C3-C4-C5-C6
3	C	805	LMT	C11-C10-C9-C8
3	A	806	LMT	C5-C6-C7-C8
4	C	804	BOG	C1'-C2'-C3'-C4'
3	A	804	LMT	C9-C10-C11-C12

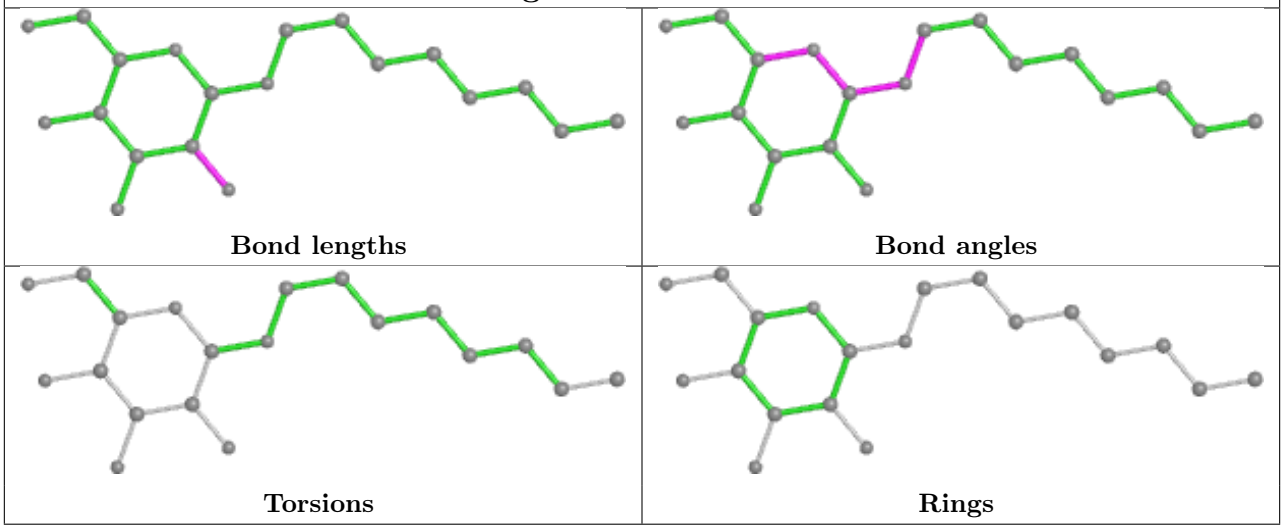
There are no ring outliers.

4 monomers are involved in 4 short contacts:

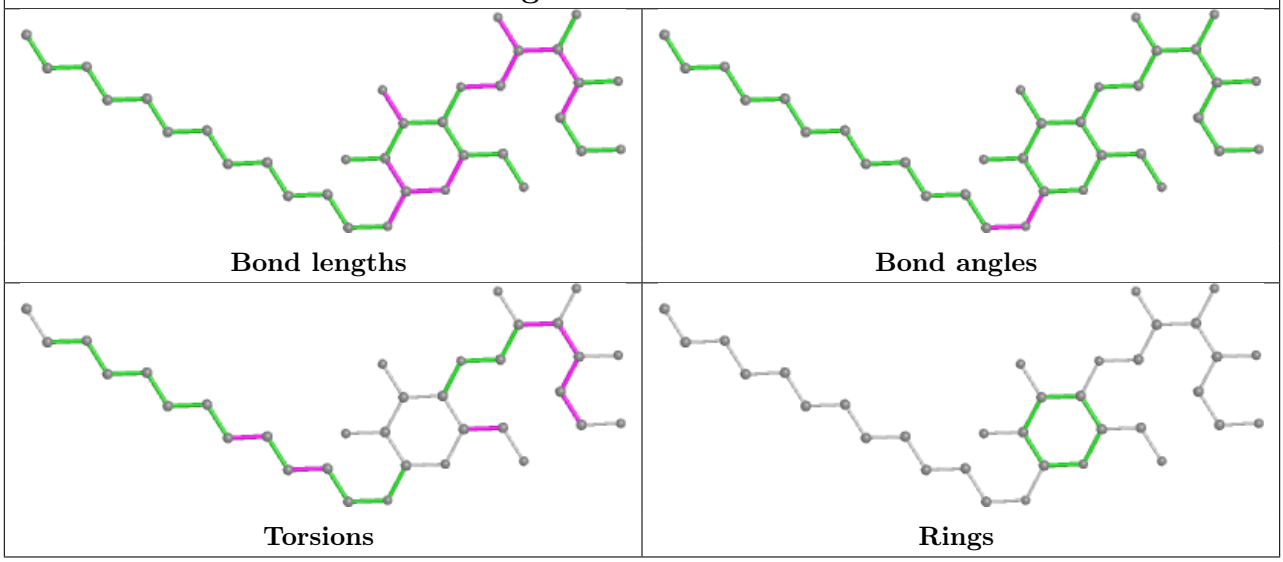
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	BOG	1	0
3	C	803	LMT	2	0
3	A	802	LMT	1	0
4	D	802	BOG	1	0

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

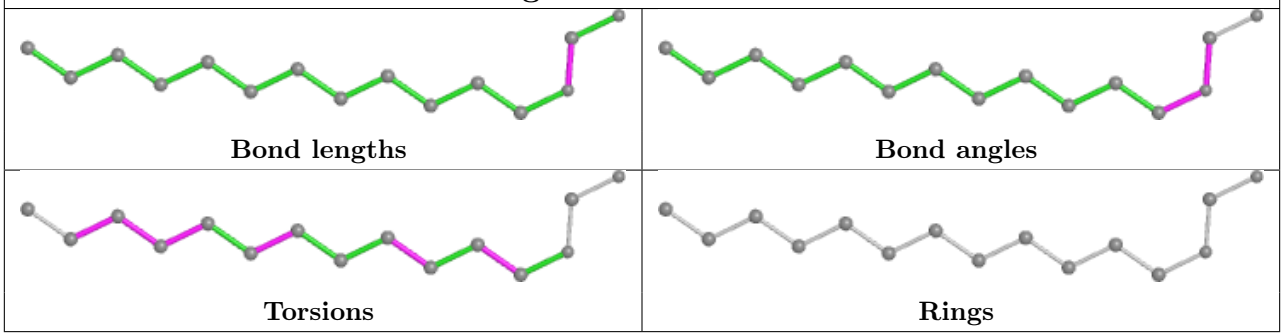
Ligand BOG C 802



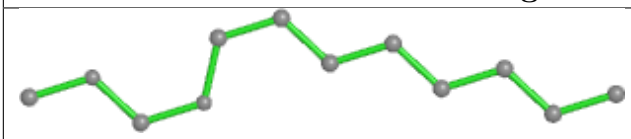
Ligand LMT A 805



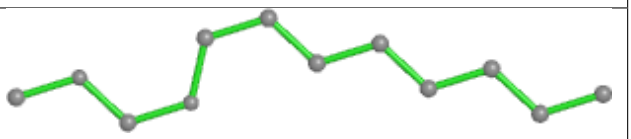
Ligand LMT C 805



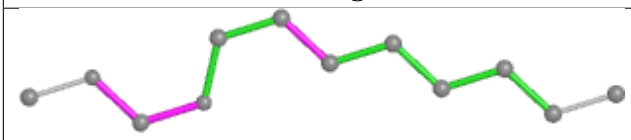
Ligand BOG A 803



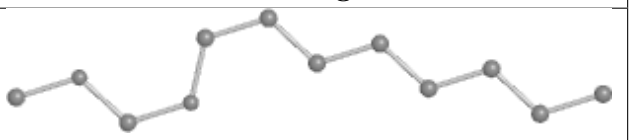
Bond lengths



Bond angles

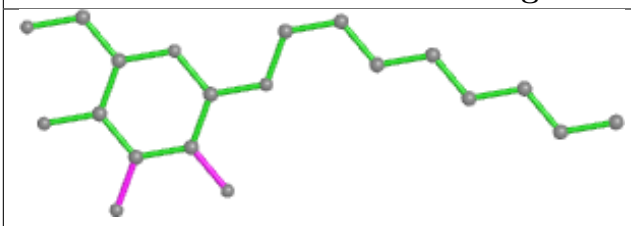


Torsions

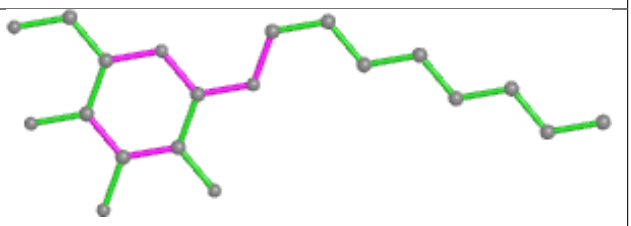


Rings

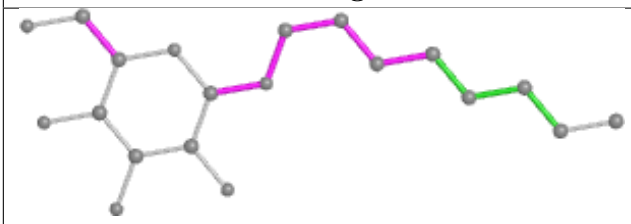
Ligand BOG C 804



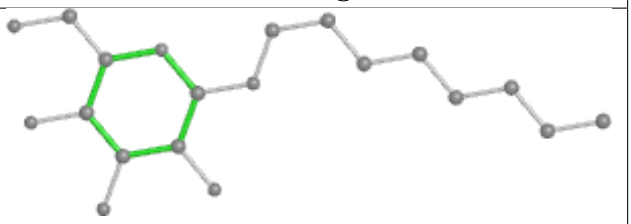
Bond lengths



Bond angles

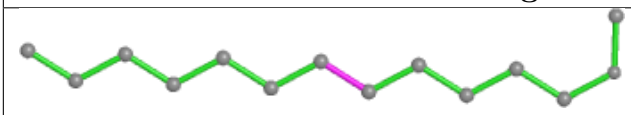


Torsions

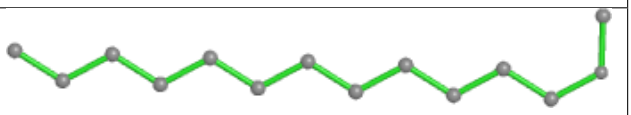


Rings

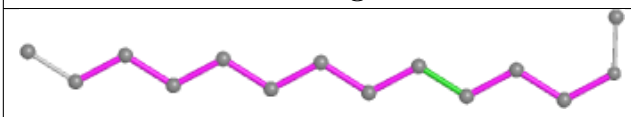
Ligand LMT A 806



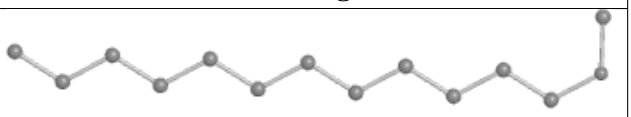
Bond lengths



Bond angles

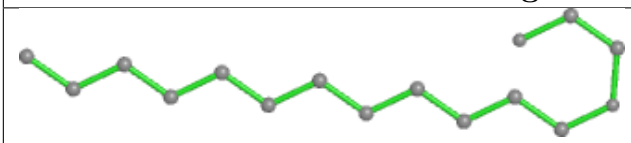


Torsions

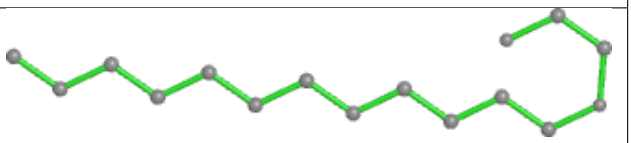


Rings

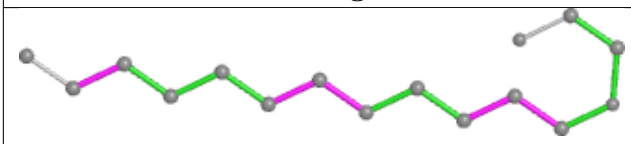
Ligand LMT C 803



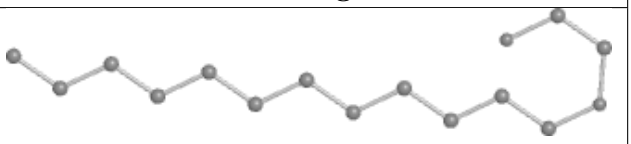
Bond lengths



Bond angles

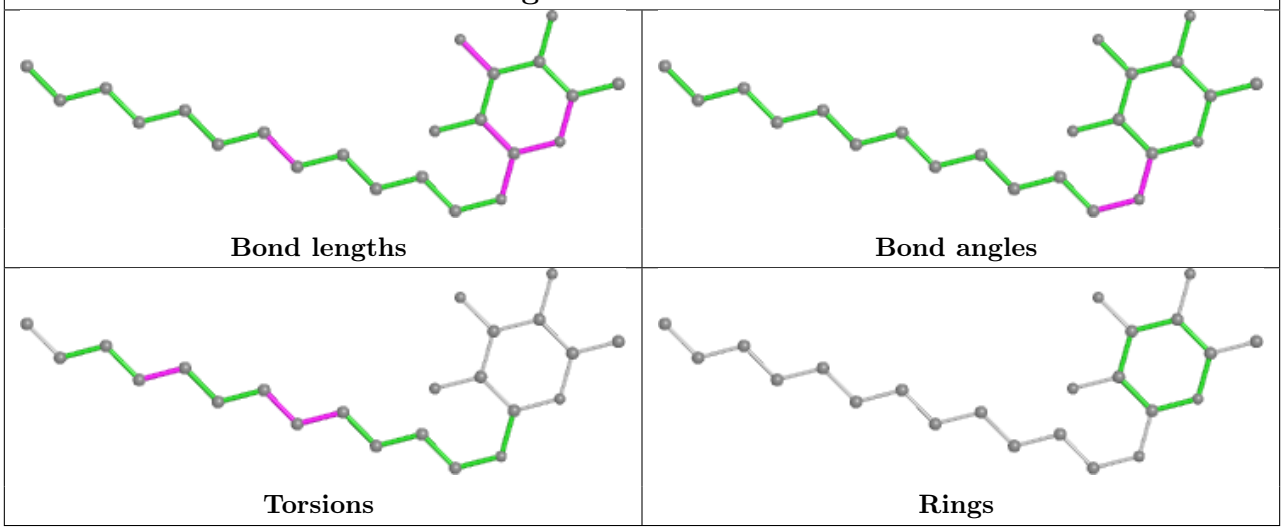


Torsions

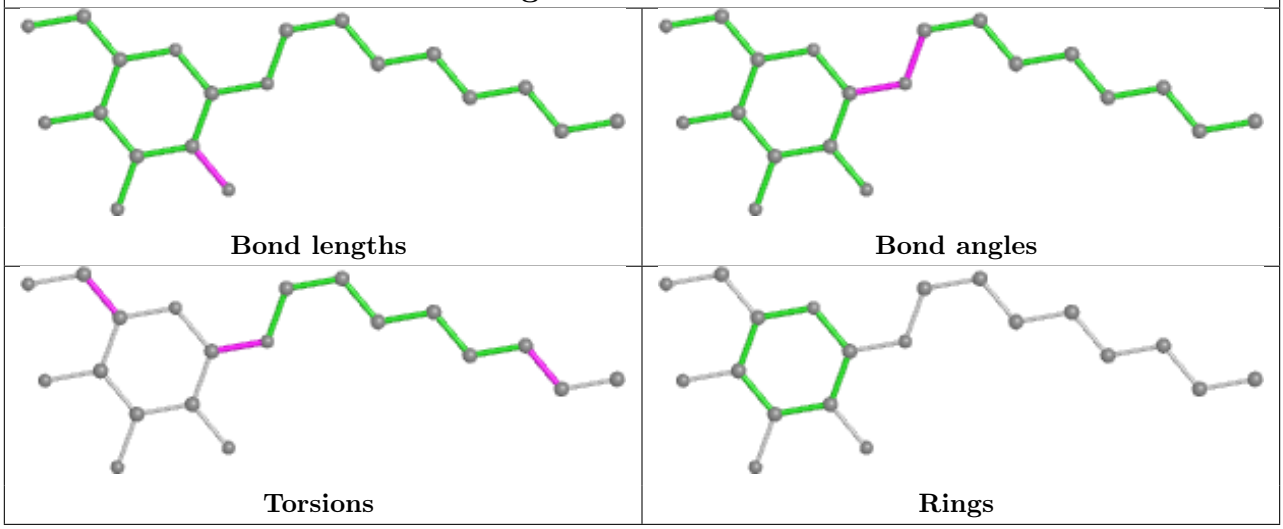


Rings

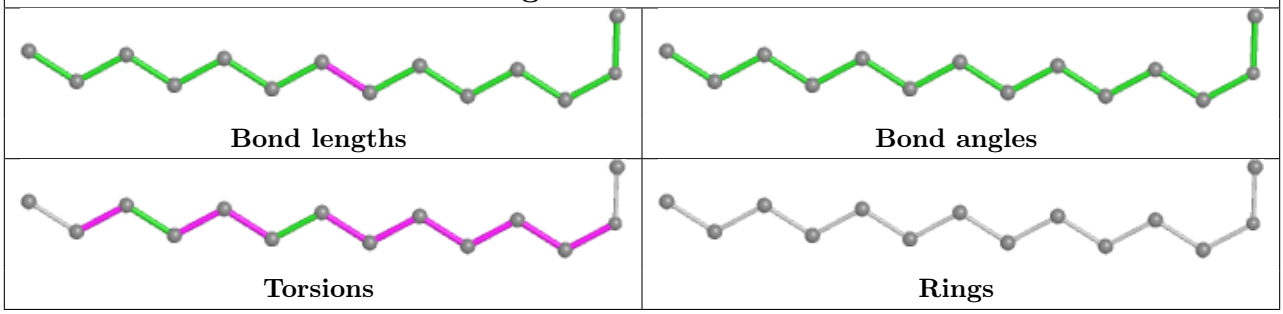
Ligand LMT A 802



Ligand BOG D 802



Ligand LMT A 804



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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	476/492 (96%)	0.11	31 (6%)	18	11	48, 72, 109, 126	0
1	B	468/492 (95%)	0.18	37 (7%)	12	7	44, 80, 113, 141	0
1	C	474/492 (96%)	0.06	18 (3%)	40	26	49, 67, 92, 114	0
1	D	483/492 (98%)	0.13	29 (6%)	21	13	50, 67, 104, 139	0
All	All	1901/1968 (96%)	0.12	115 (6%)	21	13	44, 71, 107, 141	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ALA	5.9
1	B	275	ASP	5.9
1	B	247	GLN	5.3
1	B	372	THR	5.1
1	B	286	VAL	4.8
1	A	51	THR	4.7
1	D	456	THR	4.6
1	D	282	ASP	4.3
1	D	283	THR	4.3
1	B	254	LYS	4.3
1	C	44	VAL	4.2
1	A	282	ASP	4.1
1	D	455	GLU	4.1
1	C	284	GLY	4.0
1	C	234	HIS	4.0
1	B	255	TRP	3.9
1	A	50	LEU	3.8
1	D	286	VAL	3.8
1	A	367	TRP	3.8
1	D	43	ASP	3.7
1	A	53	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	287	LEU	3.7
1	B	371	LEU	3.7
1	B	287	LEU	3.6
1	A	486	PHE	3.6
1	A	116	GLY	3.6
1	B	488	TRP	3.5
1	A	285	SER	3.5
1	C	237	THR	3.5
1	D	460	THR	3.4
1	A	274	ASN	3.4
1	D	458	ILE	3.4
1	D	42	LEU	3.4
1	B	252	ALA	3.4
1	A	287	LEU	3.4
1	C	236	ASN	3.4
1	D	288	GLY	3.4
1	D	44	VAL	3.3
1	C	42	LEU	3.3
1	B	284	GLY	3.3
1	B	250	SER	3.2
1	A	55	ILE	3.2
1	D	453	GLN	3.2
1	B	109	LEU	3.2
1	B	456	THR	3.2
1	D	12	GLU	3.1
1	B	249	HIS	3.1
1	B	121	THR	3.1
1	A	286	VAL	3.0
1	D	459	GLY	3.0
1	B	108	SER	3.0
1	A	114	SER	3.0
1	B	367	TRP	3.0
1	A	54	THR	3.0
1	C	283	THR	3.0
1	C	286	VAL	2.9
1	D	454	PRO	2.9
1	B	285	SER	2.9
1	A	360	LEU	2.9
1	B	251	ARG	2.9
1	B	111	ARG	2.8
1	B	460	THR	2.8
1	A	52	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	236	ASN	2.7
1	B	258	LEU	2.7
1	D	258	LEU	2.6
1	A	113	SER	2.6
1	B	225	ARG	2.6
1	C	285	SER	2.6
1	D	17	ARG	2.6
1	A	283	THR	2.5
1	B	244	ASP	2.5
1	D	254	LYS	2.5
1	A	272	LEU	2.5
1	C	235	ALA	2.5
1	C	223	ILE	2.4
1	A	351	PHE	2.4
1	A	234	HIS	2.4
1	C	274	ASN	2.4
1	D	464	LEU	2.4
1	D	251	ARG	2.4
1	B	373	VAL	2.3
1	C	238	VAL	2.3
1	D	231	ARG	2.3
1	D	278	LEU	2.3
1	B	455	GLU	2.3
1	A	251	ARG	2.3
1	C	39	LEU	2.3
1	C	222	LEU	2.3
1	D	445	VAL	2.3
1	D	13	GLN	2.2
1	D	10	ARG	2.2
1	A	356	LEU	2.2
1	A	56	THR	2.2
1	A	226	THR	2.2
1	B	118	LEU	2.2
1	A	359	LEU	2.2
1	B	492	PRO	2.2
1	B	370	ALA	2.1
1	A	281	PRO	2.1
1	D	11	LEU	2.1
1	B	313	VAL	2.1
1	B	226	THR	2.1
1	D	461	LEU	2.1
1	A	442	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	225	ARG	2.1
1	B	144	ALA	2.1
1	B	368	LEU	2.0
1	D	272	LEU	2.0
1	C	376	VAL	2.0
1	C	359	LEU	2.0
1	B	431	SER	2.0
1	B	458	ILE	2.0
1	C	464	LEU	2.0
1	A	284	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	A	801	1/1	0.79	0.18	61,61,61,61	0
3	LMT	A	804	14/35	0.80	0.73	70,75,79,90	0
3	LMT	A	806	14/35	0.81	0.34	55,67,81,89	0
3	LMT	A	805	34/35	0.83	0.48	67,106,122,127	0
4	BOG	C	804	20/20	0.83	0.52	71,86,101,105	0
4	BOG	C	802	20/20	0.84	0.51	76,100,110,111	0
2	NA	B	801	1/1	0.89	0.11	64,64,64,64	0
4	BOG	D	802	20/20	0.90	0.33	62,70,76,80	0
3	LMT	A	802	23/35	0.91	0.22	60,89,119,120	0
3	LMT	C	805	15/35	0.91	0.29	64,68,96,97	0
4	BOG	A	803	12/20	0.91	0.16	66,85,101,102	0
3	LMT	C	803	16/35	0.92	0.48	59,71,94,96	0
2	NA	C	801	1/1	0.96	0.13	58,58,58,58	0

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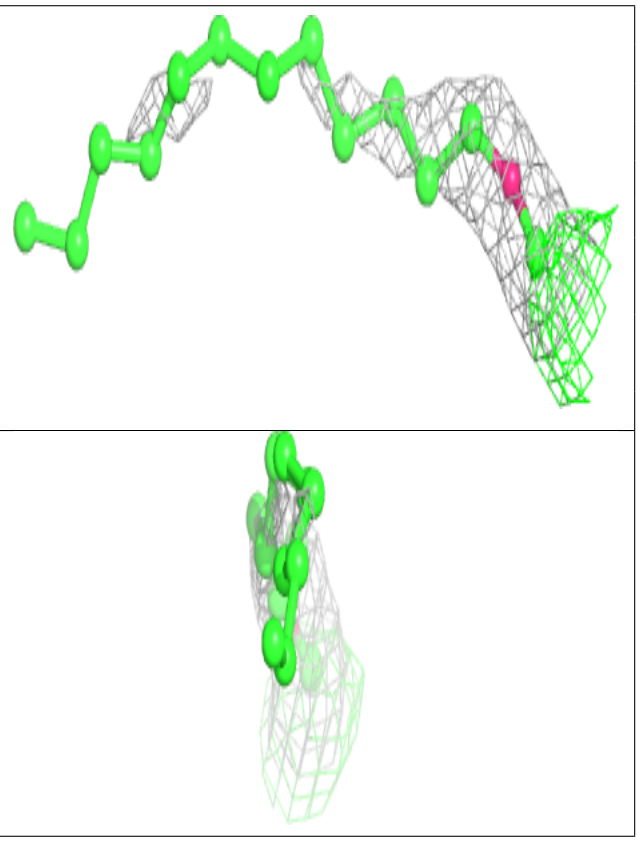
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	D	801	1/1	0.98	0.07	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

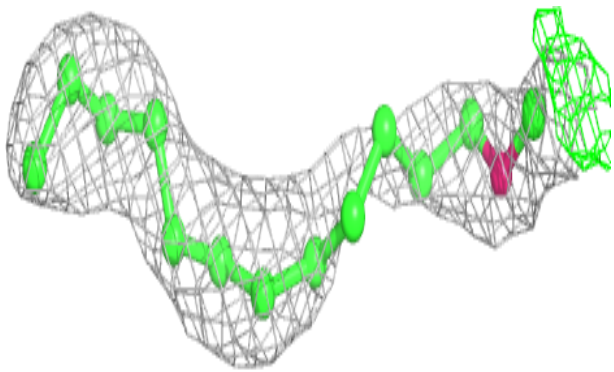
Electron density around LMT A 804:

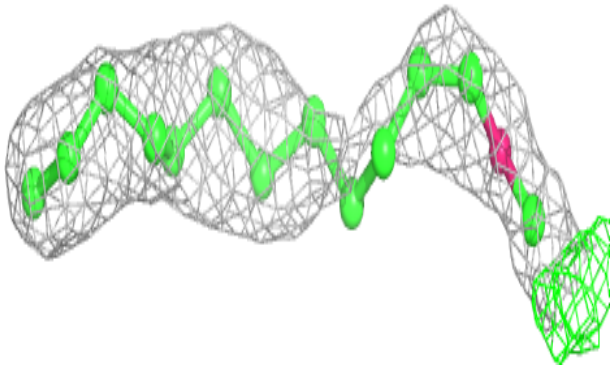
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

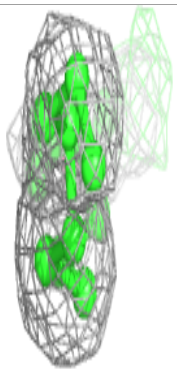


Electron density around LMT A 806:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

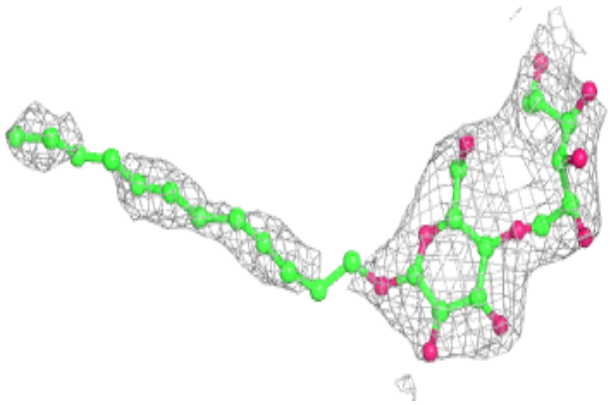


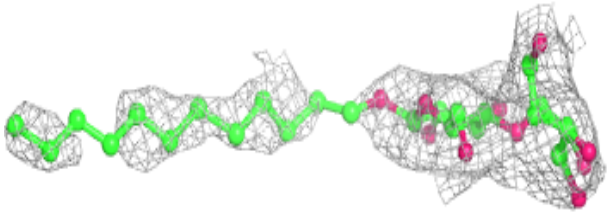


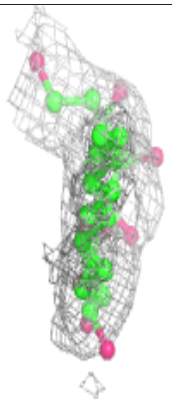


Electron density around LMT A 805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

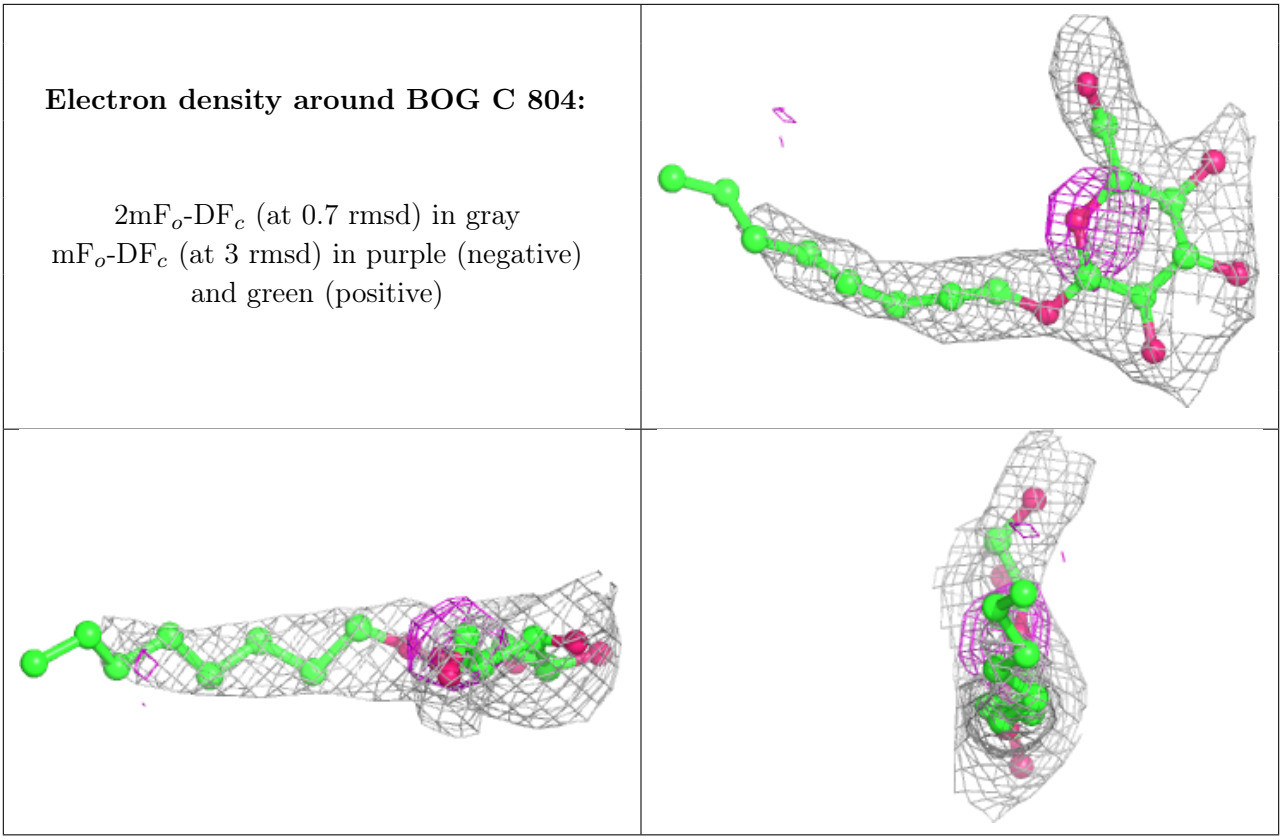






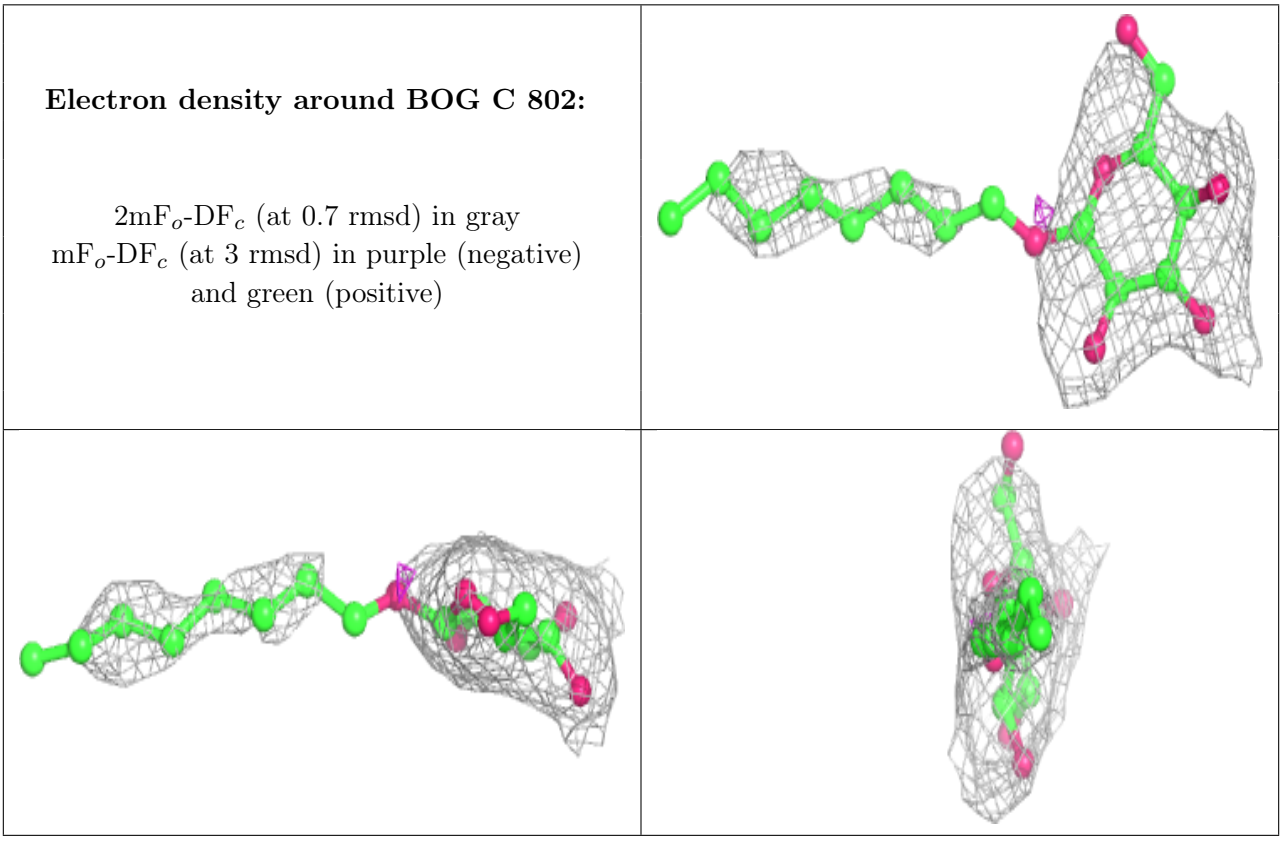
Electron density around BOG C 804:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



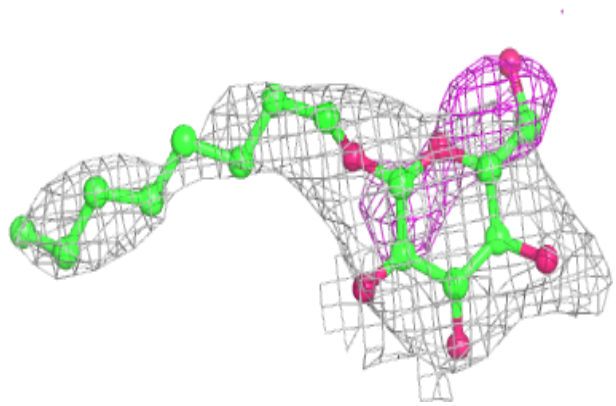
Electron density around BOG C 802:

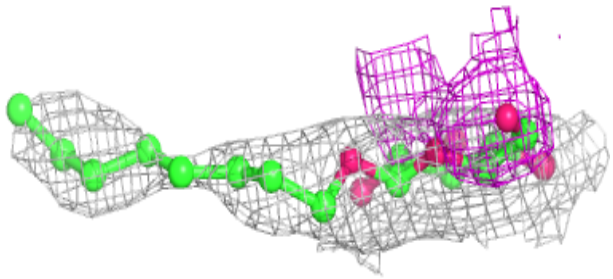
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

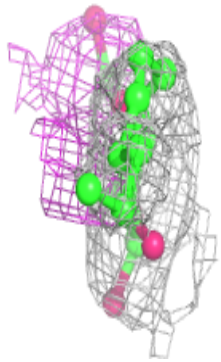


Electron density around BOG D 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

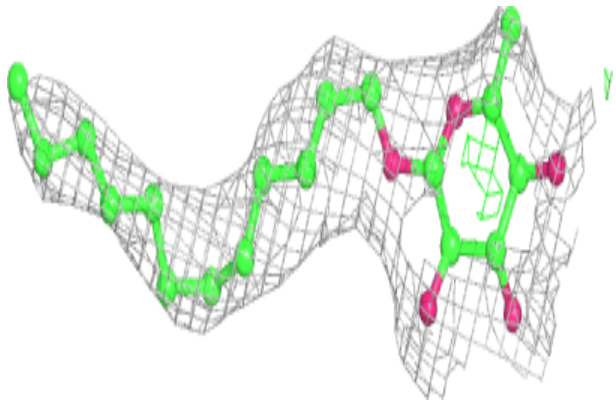


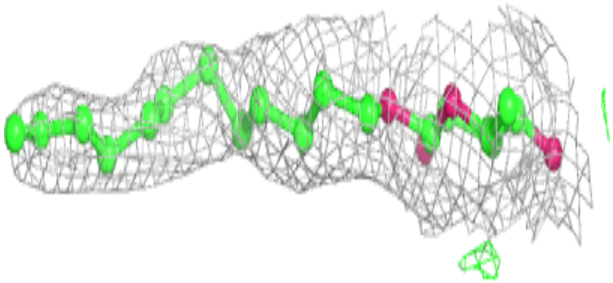


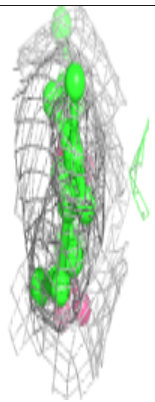


Electron density around LMT A 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

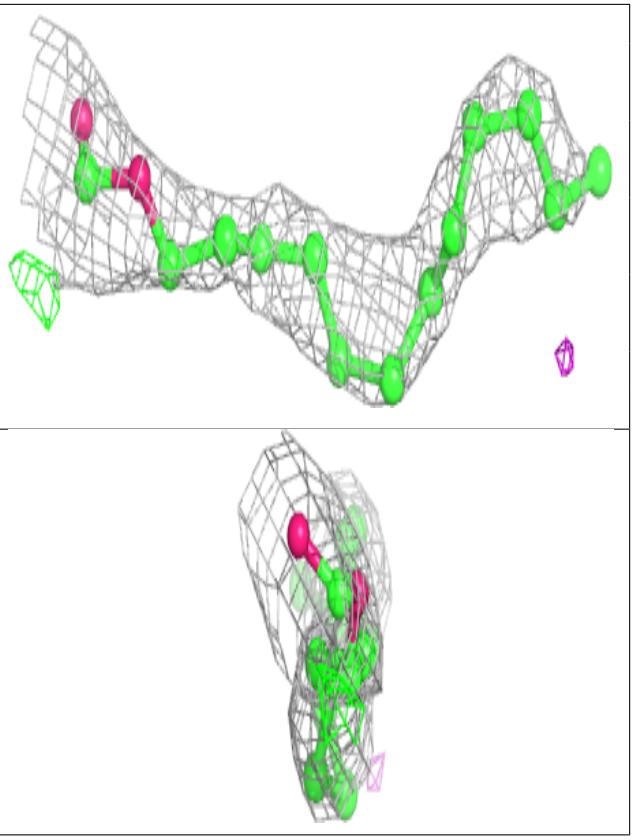






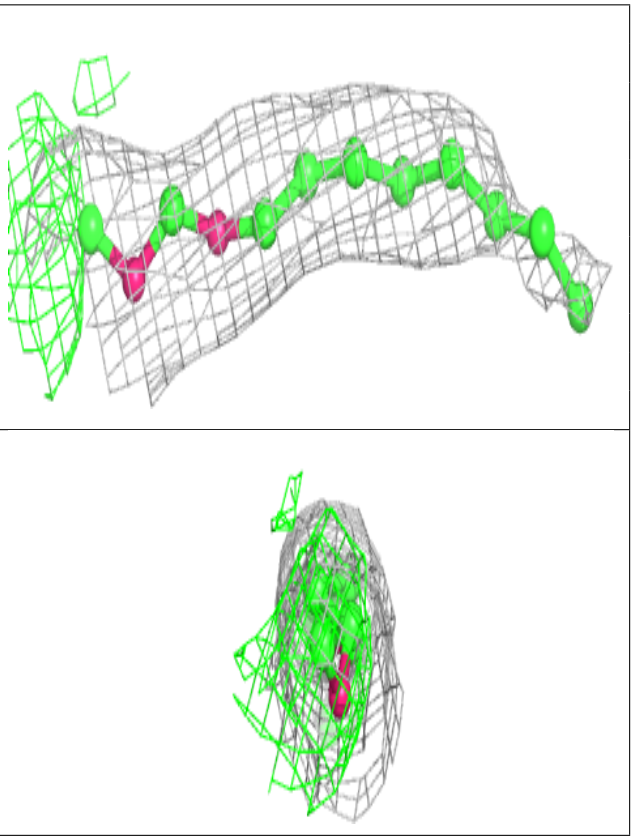
Electron density around LMT C 805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



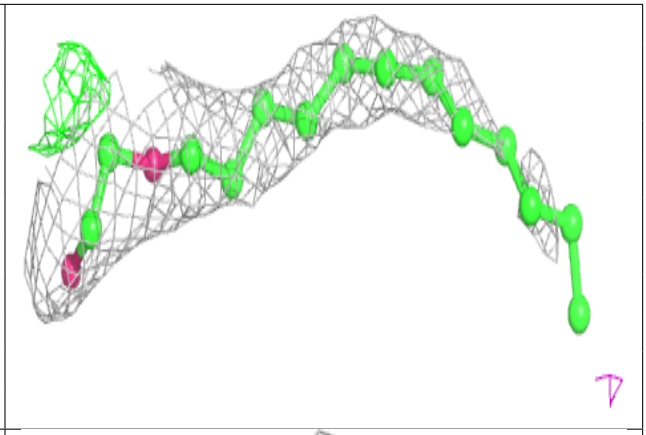
Electron density around BOG A 803:

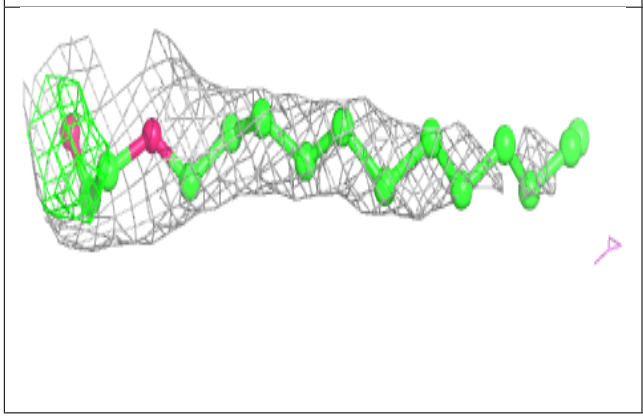
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

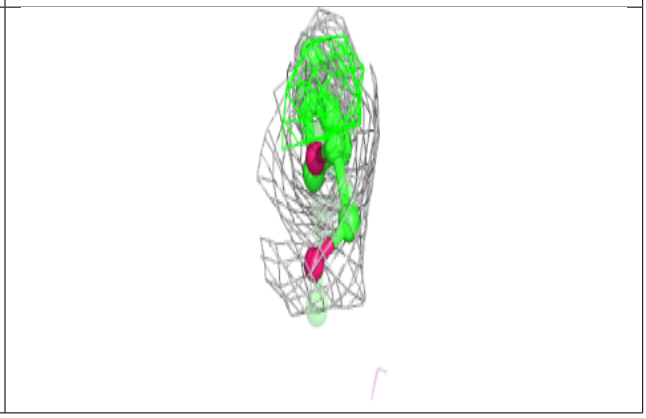


Electron density around LMT C 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.