



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:10 PM UTC

PDB ID : 4R0C / pdb_00004r0c
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

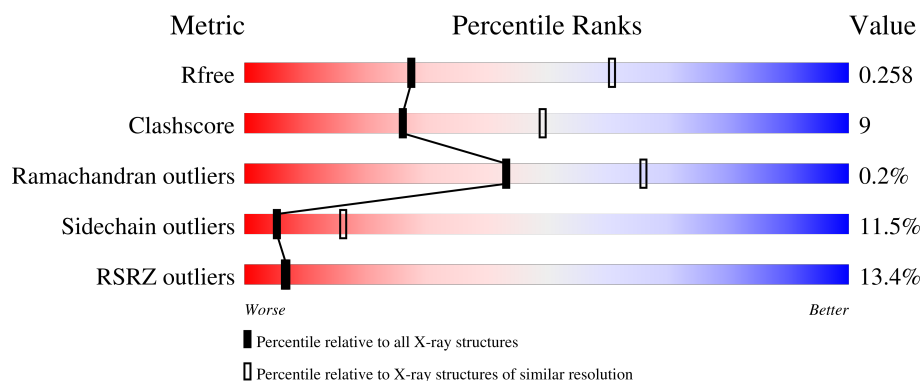
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 $\leq 5\%$. 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	11% 70% 23% • •
1	B	492	20% 65% 26% • 5%
1	C	492	9% 73% 20% • •
1	D	492	11% 73% 21% • •

2 Entry composition

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.

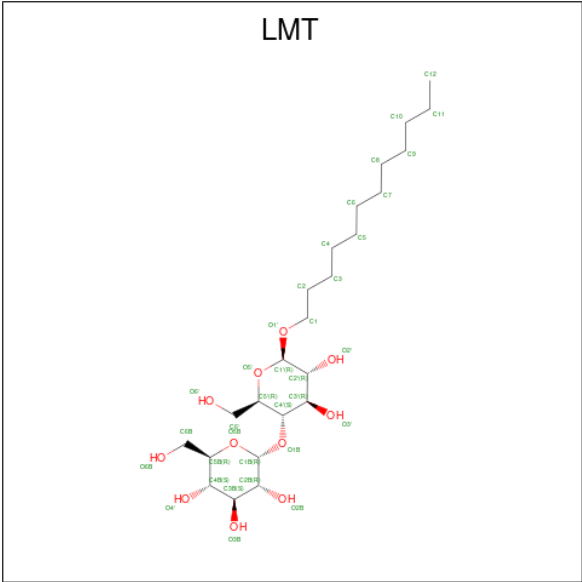
- Molecule 1 is a protein called AbgT putative transporter family.

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

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

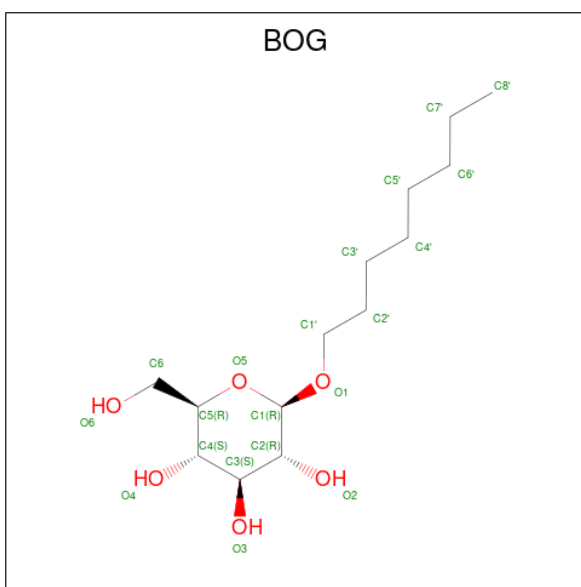
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



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

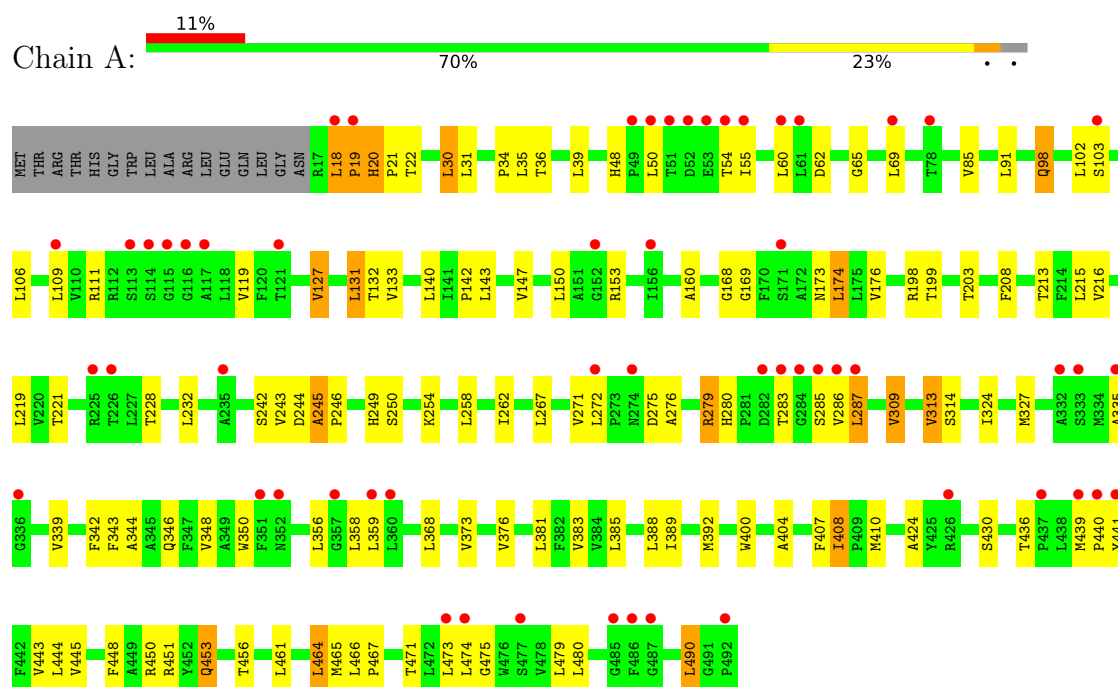
- Molecule 5 is water.

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

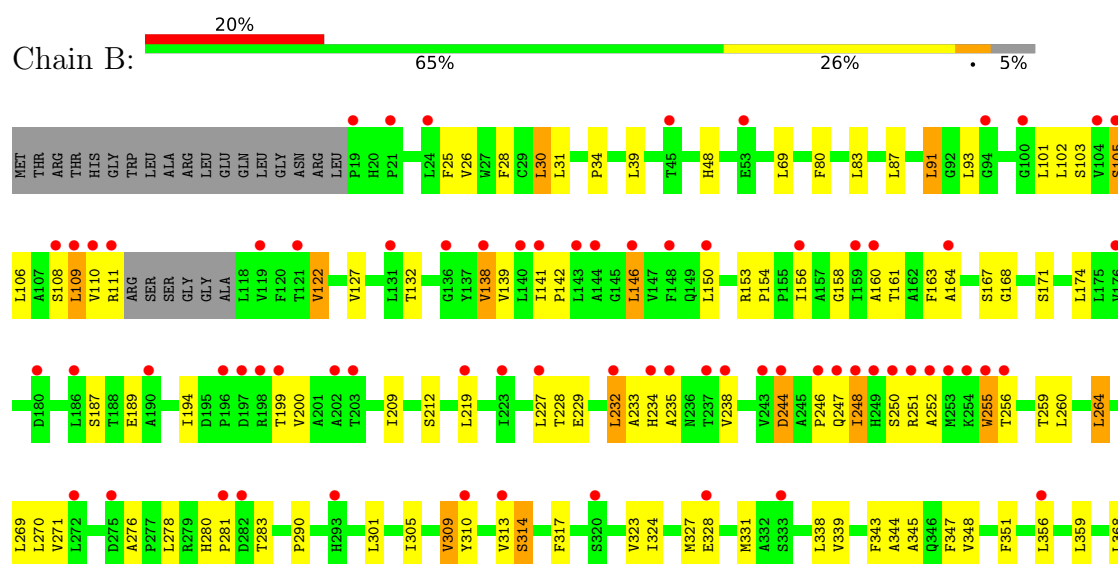
3 Residue-property plots

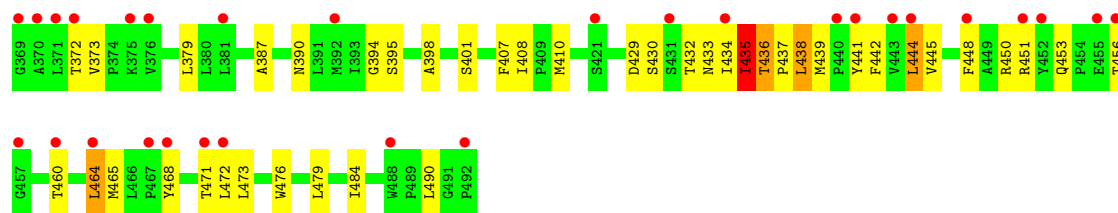
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

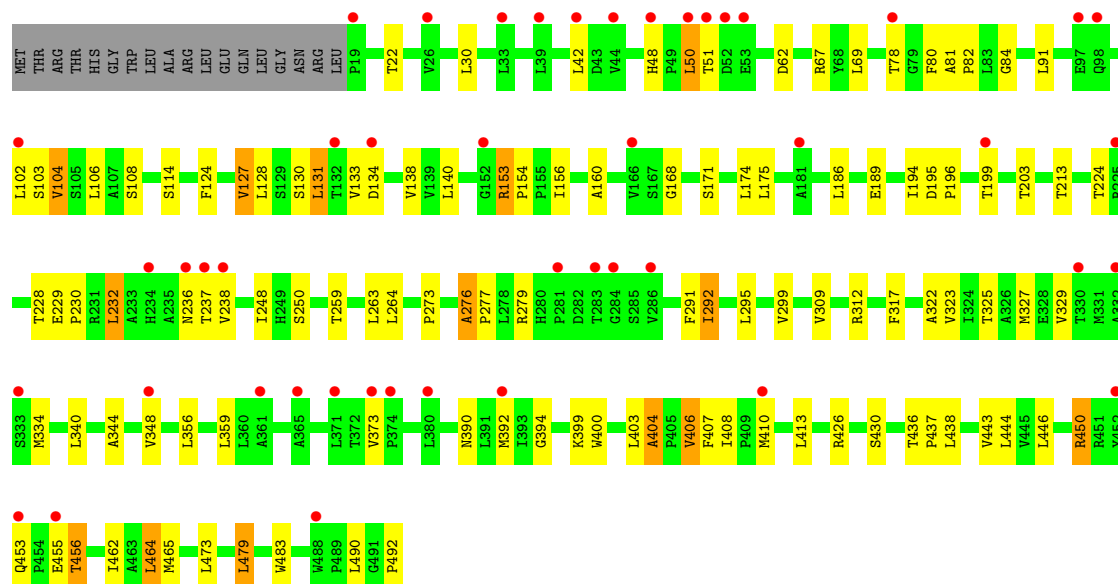
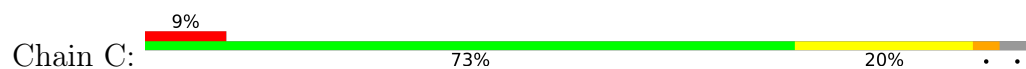


• Molecule 1: AbgT putative transporter family

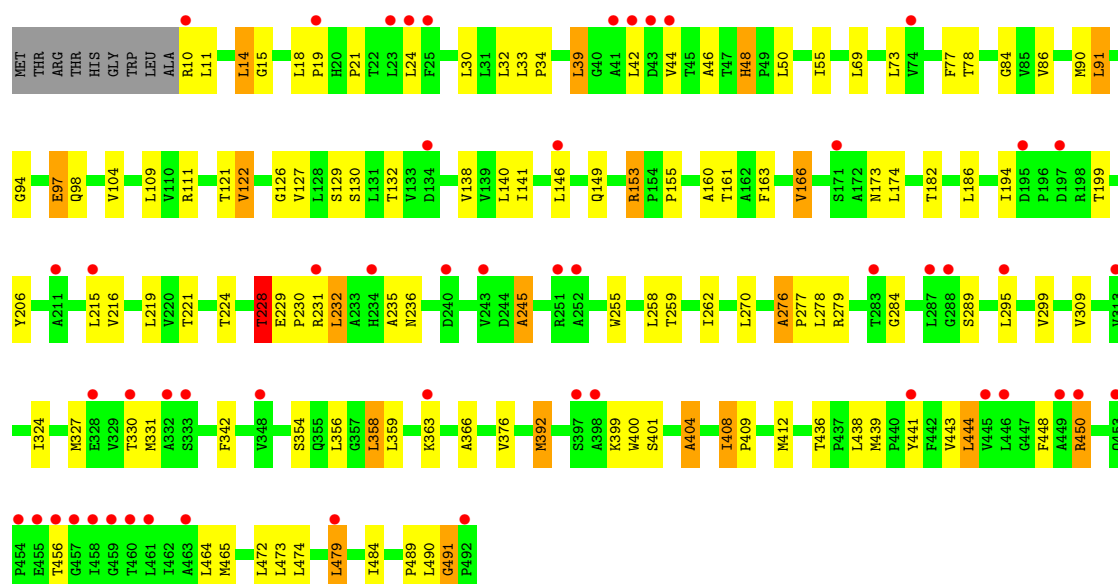
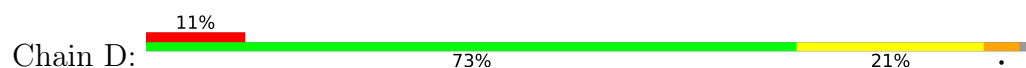




• Molecule 1: AbgT putative transporter family



• Molecule 1: AbgT putative transporter family



4 Data and refinement statistics

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 48.43 – 2.96	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.43-2.96) 95.7 (48.43-2.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.206 , 0.250 0.215 , 0.258	Depositor DCC
R_{free} test set	3769 reflections (4.08%)	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)	0.24 , 19.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, LMT, 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	0.58	0/3594	0.96	6/4933 (0.1%)
1	B	0.60	0/3538	0.99	5/4857 (0.1%)
1	C	0.58	0/3575	0.96	11/4907 (0.2%)
1	D	0.59	0/3651	0.97	13/5009 (0.3%)
All	All	0.59	0/14358	0.97	35/19706 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	THR	CA-C-N	8.06	128.25	119.87
1	A	436	THR	C-N-CA	8.06	128.25	119.87
1	D	48	HIS	CA-C-N	6.69	126.38	119.82
1	D	48	HIS	C-N-CA	6.69	126.38	119.82
1	D	228	THR	N-CA-C	6.59	118.25	111.14
1	B	250	SER	N-CA-C	-6.19	104.53	111.28
1	C	81	ALA	CA-C-N	-5.99	113.51	119.56
1	C	81	ALA	C-N-CA	-5.99	113.51	119.56
1	B	435	ILE	N-CA-C	5.99	118.00	111.77
1	D	404	ALA	CA-C-N	-5.98	113.52	119.56
1	D	404	ALA	C-N-CA	-5.98	113.52	119.56
1	D	491	GLY	N-CA-C	-5.95	100.20	112.34
1	B	138	VAL	N-CA-C	5.79	115.98	110.42
1	D	276	ALA	CA-C-N	5.76	125.62	119.28
1	D	276	ALA	C-N-CA	5.76	125.62	119.28
1	C	195	ASP	CA-C-N	5.75	127.03	119.84
1	C	195	ASP	C-N-CA	5.75	127.03	119.84
1	C	403	LEU	N-CA-C	5.73	117.99	111.11
1	D	436	THR	CA-C-N	5.71	125.33	119.56
1	D	436	THR	C-N-CA	5.71	125.33	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	THR	N-CA-C	5.55	117.02	110.97
1	C	404	ALA	CA-C-N	-5.51	113.99	119.56
1	C	404	ALA	C-N-CA	-5.51	113.99	119.56
1	A	153	ARG	CA-C-N	-5.39	114.83	120.38
1	A	153	ARG	C-N-CA	-5.39	114.83	120.38
1	B	48	HIS	CA-C-N	5.39	125.21	119.28
1	B	48	HIS	C-N-CA	5.39	125.21	119.28
1	C	276	ALA	CA-C-N	5.29	126.45	119.84
1	C	276	ALA	C-N-CA	5.29	126.45	119.84
1	C	134	ASP	N-CA-C	5.25	119.77	112.90
1	C	140	LEU	N-CA-C	5.16	116.59	111.07
1	D	245	ALA	N-CA-C	-5.13	98.47	109.81
1	A	20	HIS	N-CA-C	-5.07	101.57	108.11
1	D	141	ILE	CA-C-N	-5.06	114.45	119.56
1	D	141	ILE	C-N-CA	-5.06	114.45	119.56

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	3510	0	3679	79	0
1	B	3455	0	3621	91	0
1	C	3491	0	3656	51	0
1	D	3567	0	3737	64	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	274	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 (274) 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:160:ALA:HA	1:B:465:MET:HE1	1.51	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:D:163:PHE:HD2	1:D:465:MET:HE3	1.40	0.87
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:D:91:LEU:HD13	1:D:331:MET:HE3	1.64	0.79
1:B:252:ALA:HB2	1:B:313:VAL:HG23	1.66	0.77
1:A:160:ALA:HA	1:A:465:MET:HE1	1.67	0.76
1:D:160:ALA:HA	1:D:465:MET:HE1	1.67	0.75
1:A:244:ASP:C	1:A:245:ALA:O	2.25	0.74
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:C:160:ALA:HA	1:C:465:MET:HE1	1.74	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:464:LEU:HD13	1:A:465:MET:HE2	1.80	0.64
1:A:272:LEU:O	1:A:279:ARG:NH1	2.31	0.64
1:A:48:HIS:CE1	1:A:50:LEU:HB2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:464:LEU:HD13	1:B:465:MET:HE2	1.87	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:D:163:PHE:CD2	1:D:465:MET:HE3	2.32	0.55
1:B:331:MET:HE2	1:B:331:MET:HA	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:PHE:CD2	1:B:323:VAL:HG22	2.42	0.53
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: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: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:A:407:PHE:HD1	1:A:410:MET:HE2	1.79	0.48
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:C:334:MET:HE3	1:C:334:MET:HB3	1.88	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: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:A:327:MET:HE3	1:B:339:VAL:HG11	1.99	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: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:C:464:LEU:HD13	1:C:465:MET:HE2	1.99	0.44
1:B:163:PHE:HD2	1:B:465:MET:HE3	1.82	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:244:ASP:O	1:A:245:ALA:C	2.58	0.44
1:A:324:ILE:HA	1:A:327:MET:HE2	2.00	0.44
1:A:339:VAL:HG11	1:B:327:MET:HE3	2.00	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: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:407:PHE:HD1	1:B:410:MET:HE2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:126:GLY:O	1:D:129:SER:OG	2.35	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:D:186:LEU:HD22	1:D:401:SER:HA	2.01	0.42
1:A:343:PHE:CE2	1:B:327:MET:HE1	2.55	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:368:LEU:CD1	1:B:410:MET:HE3	2.50	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: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:A:467:PRO:O	1:A:471:THR:OG1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	30	53
1	B	464/492 (94%)	440 (95%)	23 (5%)	1 (0%)	43	66
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%)	43	66

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

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%)	325 (88%)	44 (12%)	5	15
1	B	364/382 (95%)	320 (88%)	44 (12%)	5	14
1	C	367/382 (96%)	324 (88%)	43 (12%)	5	16
1	D	375/382 (98%)	337 (90%)	38 (10%)	7	20
All	All	1475/1528 (96%)	1306 (88%)	169 (12%)	5	16

All (169) 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	69	LEU
1	A	85	VAL
1	A	98	GLN
1	A	103	SER
1	A	127	VAL
1	A	131	LEU
1	A	133	VAL
1	A	140	LEU
1	A	150	LEU
1	A	174	LEU
1	A	176	VAL
1	A	198	ARG
1	A	199	THR
1	A	203	THR
1	A	215	LEU
1	A	232	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	368	LEU
1	A	373	VAL
1	A	376	VAL
1	A	381	LEU
1	A	388	LEU
1	A	408	ILE
1	A	443	VAL
1	A	444	LEU
1	A	450	ARG
1	A	453	GLN
1	A	464	LEU
1	A	466	LEU
1	A	473	LEU
1	A	474	LEU
1	A	479	LEU

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Mol	Chain	Res	Type
1	A	490	LEU
1	B	30	LEU
1	B	39	LEU
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	122	VAL
1	B	127	VAL
1	B	146	LEU
1	B	150	LEU
1	B	156	ILE
1	B	171	SER
1	B	174	LEU
1	B	194	ILE
1	B	199	THR
1	B	227	LEU
1	B	232	LEU
1	B	238	VAL
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	271	VAL
1	B	309	VAL
1	B	314	SER
1	B	356	LEU
1	B	359	LEU
1	B	372	THR
1	B	373	VAL
1	B	408	ILE
1	B	435	ILE
1	B	436	THR
1	B	438	LEU
1	B	444	LEU
1	B	451	ARG
1	B	460	THR
1	B	464	LEU

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Mol	Chain	Res	Type
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	69	LEU
1	C	91	LEU
1	C	103	SER
1	C	104	VAL
1	C	108	SER
1	C	114	SER
1	C	127	VAL
1	C	130	SER
1	C	131	LEU
1	C	133	VAL
1	C	138	VAL
1	C	153	ARG
1	C	156	ILE
1	C	174	LEU
1	C	199	THR
1	C	232	LEU
1	C	236	ASN
1	C	237	THR
1	C	238	VAL
1	C	250	SER
1	C	264	LEU
1	C	292	ILE
1	C	309	VAL
1	C	356	LEU
1	C	359	LEU
1	C	373	VAL
1	C	399	LYS
1	C	406	VAL
1	C	408	ILE
1	C	410	MET
1	C	436	THR
1	C	443	VAL
1	C	444	LEU
1	C	450	ARG
1	C	456	THR

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Mol	Chain	Res	Type
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	97	GLU
1	D	104	VAL
1	D	122	VAL
1	D	127	VAL
1	D	138	VAL
1	D	140	LEU
1	D	146	LEU
1	D	153	ARG
1	D	166	VAL
1	D	174	LEU
1	D	199	THR
1	D	206	TYR
1	D	221	THR
1	D	228	THR
1	D	231	ARG
1	D	232	LEU
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	443	VAL
1	D	444	LEU
1	D	450	ARG
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	316	GLN
1	A	355	GLN
1	B	247	GLN
1	B	293	HIS
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 oligosaccharides 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	$\# Z > 2$
3	LMT	A	802	-	23,23,36	1.99	7 (30%)	28,28,47	0.89	1 (3%)
3	LMT	A	804	-	13,13,36	1.12	2 (15%)	12,12,47	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	A	805	-	34,34,36	3.44	13 (38%)	42,42,47	1.09	2 (4%)
4	BOG	D	802	-	20,20,20	0.94	0	25,25,25	0.91	1 (4%)
3	LMT	A	806	-	13,13,36	1.15	2 (15%)	12,12,47	0.64	0
3	LMT	C	803	-	15,15,36	1.06	2 (13%)	14,14,47	0.85	0
3	LMT	C	805	-	14,14,36	1.33	2 (14%)	13,13,47	0.98	1 (7%)
4	BOG	C	804	-	20,20,20	0.92	0	25,25,25	1.62	3 (12%)
4	BOG	A	803	-	11,11,20	0.35	0	10,10,25	0.94	1 (10%)
4	BOG	C	802	-	20,20,20	1.00	0	25,25,25	1.40	2 (8%)

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

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

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	805	LMT	O1B-C1B	-13.84	1.19	1.43
3	A	805	LMT	C4B-C3B	-8.17	1.39	1.53
3	A	802	LMT	O1'-C1'	4.71	1.48	1.40
3	A	805	LMT	O3'-C3'	-4.65	1.31	1.43
3	A	805	LMT	O1'-C1'	4.59	1.47	1.40
3	A	805	LMT	C5B-C4B	-4.58	1.44	1.52
3	A	802	LMT	O3'-C3'	-4.31	1.32	1.43
3	A	805	LMT	O5'-C1'	-3.53	1.32	1.41
3	A	805	LMT	C1B-C2B	-3.49	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	LMT	O5'-C1'	-3.41	1.33	1.41
3	A	802	LMT	O5'-C5'	-3.40	1.36	1.44
3	A	805	LMT	O5'-C5'	-3.39	1.36	1.44
3	C	805	LMT	O1'-C1'	2.75	1.48	1.40
3	A	805	LMT	O2B-C2B	2.65	1.48	1.43
3	A	805	LMT	C2B-C3B	-2.50	1.49	1.53
3	A	806	LMT	C6-C5	2.27	1.63	1.51
3	A	804	LMT	C6-C5	2.26	1.63	1.51
3	A	802	LMT	C1'-C2'	-2.25	1.45	1.52
3	A	802	LMT	C6-C5	2.23	1.62	1.51
3	A	804	LMT	C7-C6	2.21	1.62	1.51
3	A	806	LMT	C7-C6	2.21	1.62	1.51
3	C	803	LMT	C6-C5	2.17	1.62	1.51
3	A	805	LMT	C6-C5	2.17	1.62	1.51
3	A	805	LMT	C1'-C2'	-2.13	1.46	1.52
3	C	805	LMT	C6-C5	2.12	1.62	1.51
3	C	803	LMT	C7-C6	2.04	1.62	1.51
3	A	802	LMT	C7-C6	2.04	1.61	1.51
3	A	805	LMT	C7-C6	2.03	1.61	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	804	BOG	C1'-O1-C1	4.72	121.74	113.68
4	C	802	BOG	C1'-O1-C1	4.23	120.91	113.68
4	C	804	BOG	C4-C3-C2	-3.54	104.61	110.83
3	A	805	LMT	C5B-C4B-C3B	-3.18	108.93	113.97
3	A	802	LMT	C1-O1'-C1'	3.09	118.96	113.68
3	A	805	LMT	C1-O1'-C1'	3.05	118.90	113.68
4	C	804	BOG	C1-O5-C5	2.82	119.23	113.72
4	C	802	BOG	C1-O5-C5	-2.52	108.80	113.72
4	D	802	BOG	C1'-O1-C1	2.29	117.59	113.68
3	C	805	LMT	C1'-O1'-C1	2.26	119.76	112.96
4	A	803	BOG	C1-O1-C1'	2.00	119.07	113.13

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'

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

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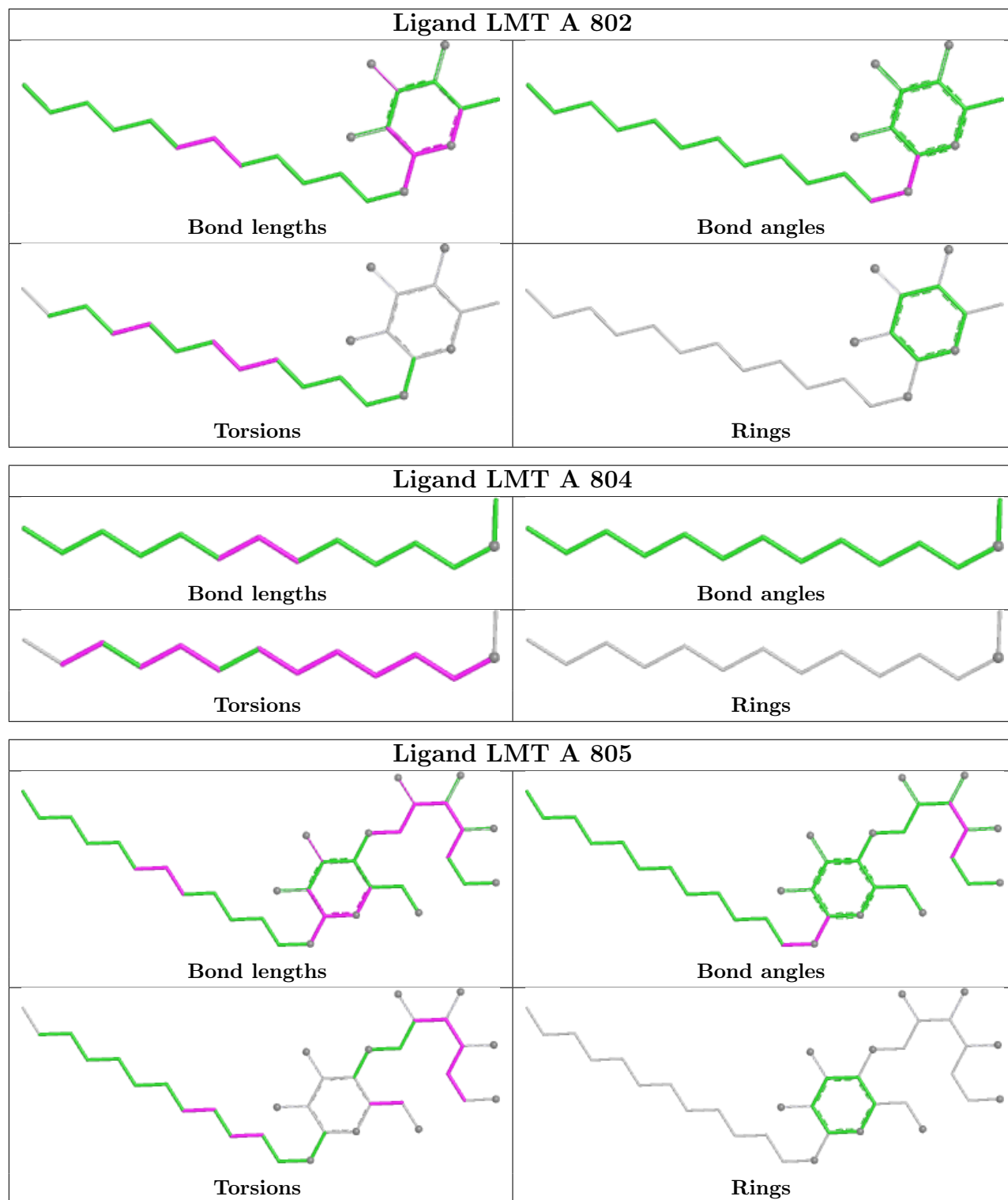
Mol	Chain	Res	Type	Atoms
4	A	803	BOG	C1'-C2'-C3'-C4'
3	A	802	LMT	C7-C8-C9-C10
3	C	803	LMT	C9-C10-C11-C12
3	A	804	LMT	C2-C3-C4-C5
3	A	805	LMT	C3-C4-C5-C6
3	A	806	LMT	C3-C4-C5-C6
4	D	802	BOG	O5-C1-O1-C1'
3	C	803	LMT	C5-C6-C7-C8
3	A	804	LMT	C1-C2-C3-C4
3	A	802	LMT	C3-C4-C5-C6
3	A	804	LMT	C7-C8-C9-C10
4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

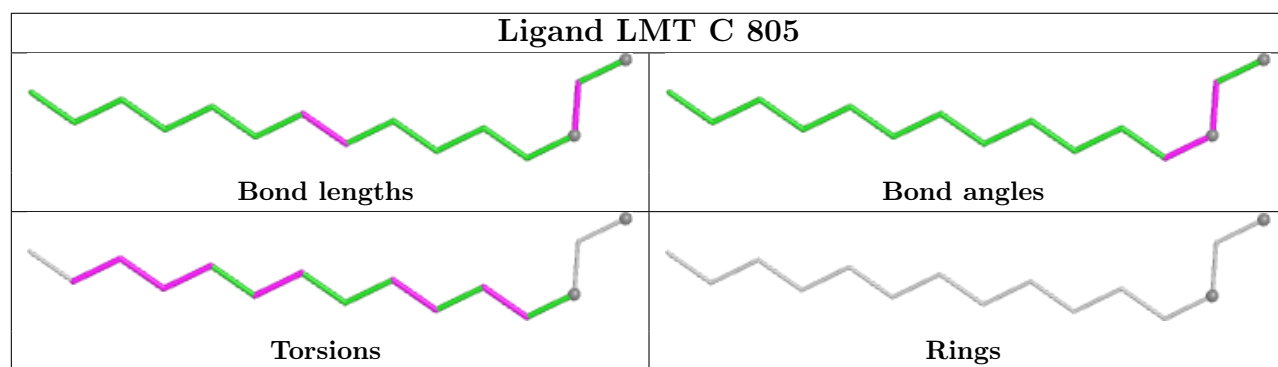
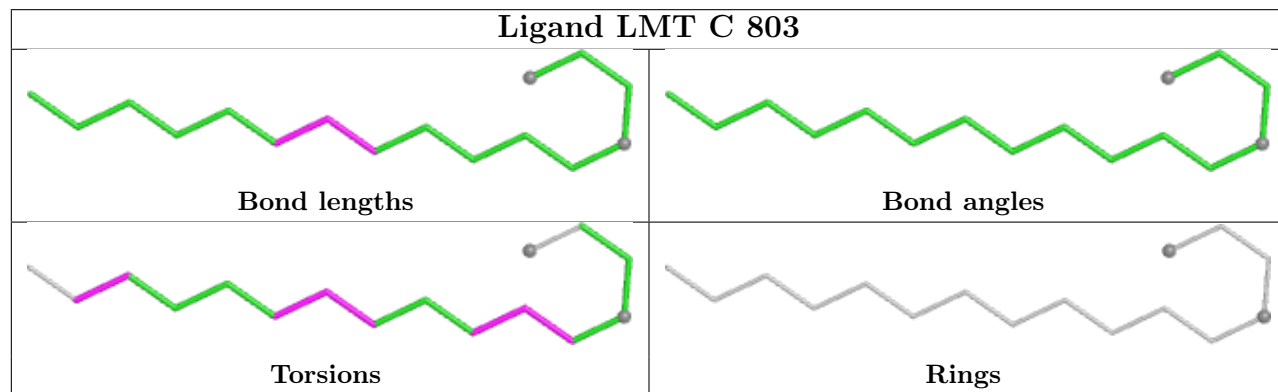
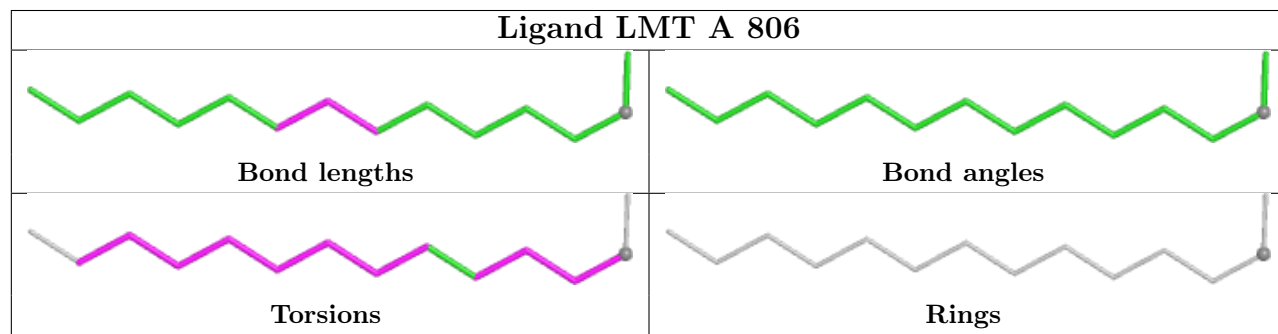
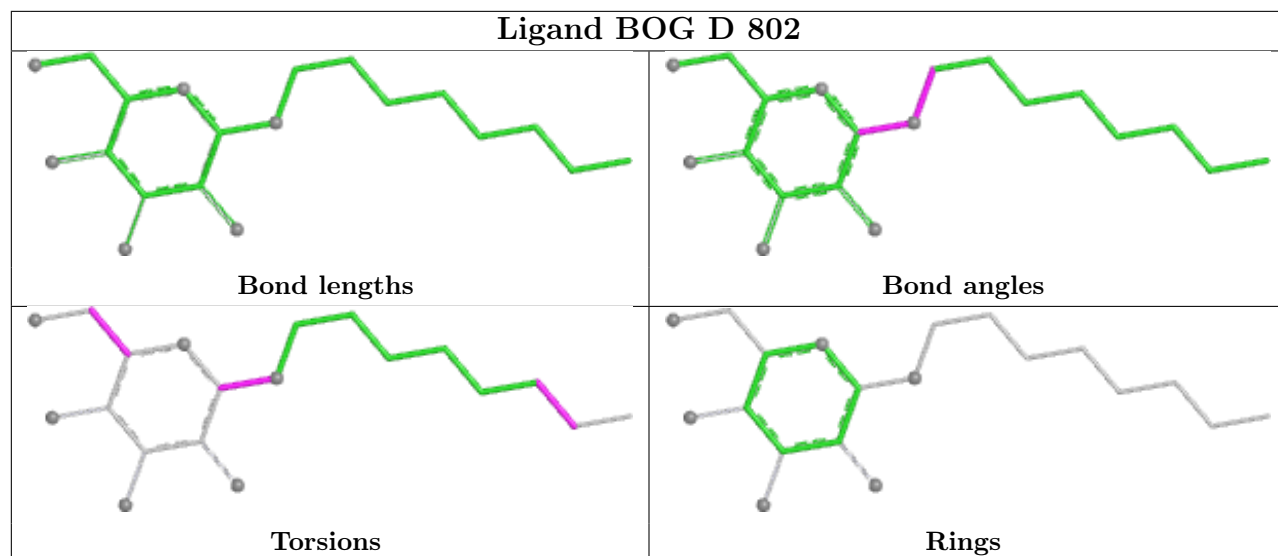
There are no ring outliers.

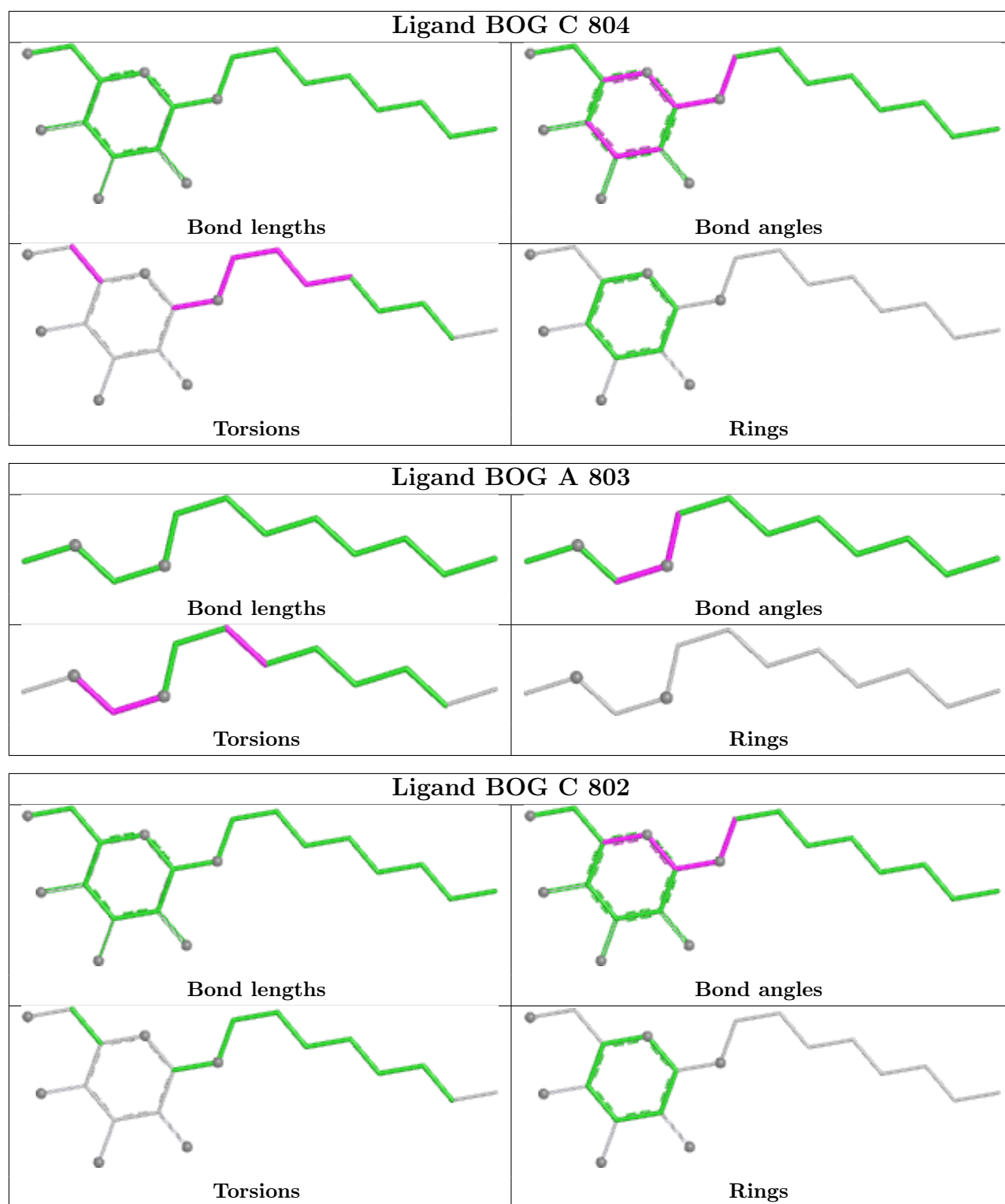
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	LMT	1	0
4	D	802	BOG	1	0
3	C	803	LMT	2	0
4	A	803	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.65	56 (11%) 9 8	48, 72, 109, 126	0
1	B	468/492 (95%)	1.07	100 (21%) 2 2	44, 80, 113, 141	0
1	C	474/492 (96%)	0.54	46 (9%) 13 12	49, 67, 92, 114	0
1	D	483/492 (98%)	0.56	53 (10%) 10 9	50, 67, 104, 139	0
All	All	1901/1968 (96%)	0.70	255 (13%) 7 7	44, 71, 107, 141	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	455	GLU	8.0
1	B	372	THR	7.9
1	B	431	SER	7.7
1	D	454	PRO	7.0
1	B	275	ASP	6.9
1	D	43	ASP	6.9
1	D	453	GLN	6.6
1	B	244	ASP	6.5
1	B	156	ILE	6.4
1	A	117	ALA	6.3
1	D	456	THR	6.2
1	B	108	SER	6.1
1	B	247	GLN	5.9
1	D	459	GLY	5.6
1	B	252	ALA	5.5
1	B	248	ILE	5.3
1	C	333	SER	5.2
1	C	98	GLN	5.2
1	A	285	SER	4.9
1	A	171	SER	4.9
1	C	237	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	333	SER	4.7
1	B	121	THR	4.7
1	B	492	PRO	4.6
1	A	53	GLU	4.6
1	A	333	SER	4.6
1	C	52	ASP	4.5
1	C	134	ASP	4.5
1	C	361	ALA	4.4
1	B	111	ARG	4.4
1	B	197	ASP	4.3
1	A	440	PRO	4.3
1	A	113	SER	4.2
1	C	53	GLU	4.1
1	A	121	THR	4.0
1	A	274	ASN	4.0
1	D	44	VAL	4.0
1	D	460	THR	4.0
1	B	370	ALA	3.9
1	D	463	ALA	3.9
1	D	42	LEU	3.9
1	A	50	LEU	3.9
1	A	116	GLY	3.9
1	A	351	PHE	3.9
1	A	272	LEU	3.8
1	B	110	VAL	3.8
1	B	281	PRO	3.8
1	B	109	LEU	3.8
1	B	371	LEU	3.8
1	A	284	GLY	3.8
1	B	464	LEU	3.8
1	C	42	LEU	3.8
1	B	471	THR	3.8
1	B	223	ILE	3.8
1	B	141	ILE	3.7
1	B	146	LEU	3.7
1	D	450	ARG	3.7
1	C	236	ASN	3.6
1	A	286	VAL	3.6
1	C	44	VAL	3.5
1	B	104	VAL	3.5
1	C	238	VAL	3.5
1	A	226	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	445	VAL	3.5
1	C	453	GLN	3.4
1	A	49	PRO	3.4
1	B	255	TRP	3.4
1	A	335	ALA	3.4
1	B	138	VAL	3.3
1	B	144	ALA	3.3
1	B	227	LEU	3.3
1	C	380	LEU	3.3
1	A	426	ARG	3.3
1	B	254	LYS	3.3
1	B	24	LEU	3.3
1	D	243	VAL	3.2
1	D	330	THR	3.2
1	D	446	LEU	3.2
1	A	283	THR	3.2
1	B	440	PRO	3.2
1	D	457	GLY	3.2
1	A	282	ASP	3.2
1	A	69	LEU	3.2
1	C	373	VAL	3.2
1	A	114	SER	3.1
1	D	348	VAL	3.1
1	B	53	GLU	3.1
1	C	51	THR	3.1
1	C	284	GLY	3.1
1	D	252	ALA	3.0
1	B	443	VAL	3.0
1	D	333	SER	3.0
1	B	455	GLU	3.0
1	B	460	THR	3.0
1	B	243	VAL	3.0
1	C	234	HIS	3.0
1	C	348	VAL	3.0
1	A	109	LEU	3.0
1	B	467	PRO	3.0
1	A	78	THR	3.0
1	C	332	ALA	3.0
1	C	286	VAL	3.0
1	B	293	HIS	3.0
1	B	176	VAL	2.9
1	C	455	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	54	THR	2.9
1	B	143	LEU	2.9
1	A	485	GLY	2.9
1	B	468	TYR	2.9
1	A	51	THR	2.9
1	B	237	THR	2.9
1	A	360	LEU	2.9
1	D	197	ASP	2.9
1	B	421	SER	2.9
1	B	448	PHE	2.9
1	A	357	GLY	2.8
1	B	253	MET	2.8
1	B	434	ILE	2.8
1	C	26	VAL	2.8
1	A	235	ALA	2.8
1	A	492	PRO	2.8
1	B	328	GLU	2.8
1	A	55	ILE	2.8
1	A	441	TYR	2.7
1	A	359	LEU	2.7
1	B	131	LEU	2.7
1	D	441	TYR	2.7
1	C	330	THR	2.7
1	C	152	GLY	2.7
1	A	19	PRO	2.7
1	D	25	PHE	2.7
1	D	332	ALA	2.7
1	B	249	HIS	2.7
1	B	105	SER	2.7
1	B	159	ILE	2.7
1	D	41	ALA	2.7
1	A	439	MET	2.7
1	D	19	PRO	2.7
1	B	180	ASP	2.7
1	A	156	ILE	2.6
1	B	472	LEU	2.7
1	C	410	MET	2.6
1	B	136	GLY	2.6
1	D	288	GLY	2.6
1	B	456	THR	2.6
1	A	18	LEU	2.6
1	B	313	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	458	ILE	2.6
1	B	160	ALA	2.6
1	A	152	GLY	2.6
1	D	134	ASP	2.6
1	B	488	TRP	2.6
1	B	441	TYR	2.6
1	B	140	LEU	2.6
1	D	283	THR	2.6
1	C	97	GLU	2.6
1	B	444	LEU	2.5
1	C	50	LEU	2.5
1	B	232	LEU	2.5
1	B	203	THR	2.5
1	C	78	THR	2.5
1	B	272	LEU	2.5
1	D	23	LEU	2.5
1	B	100	GLY	2.5
1	A	225	ARG	2.5
1	B	21	PRO	2.4
1	B	250	SER	2.4
1	B	198	ARG	2.4
1	C	102	LEU	2.4
1	D	313	VAL	2.4
1	C	199	THR	2.4
1	A	352	ASN	2.4
1	B	119	VAL	2.4
1	A	115	GLY	2.3
1	A	332	ALA	2.3
1	B	45	THR	2.3
1	B	199	THR	2.3
1	B	19	PRO	2.3
1	D	492	PRO	2.3
1	B	376	VAL	2.3
1	D	10	ARG	2.3
1	A	52	ASP	2.3
1	B	235	ALA	2.3
1	C	33	LEU	2.3
1	B	234	HIS	2.3
1	A	487	GLY	2.3
1	D	195	ASP	2.3
1	A	287	LEU	2.3
1	A	474	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	150	LEU	2.3
1	C	371	LEU	2.3
1	C	48	HIS	2.3
1	A	437	PRO	2.3
1	C	19	PRO	2.3
1	D	74	VAL	2.3
1	D	240	ASP	2.3
1	D	287	LEU	2.3
1	D	363	LYS	2.3
1	B	256	THR	2.3
1	C	488	TRP	2.3
1	C	166	VAL	2.3
1	A	486	PHE	2.2
1	C	392	MET	2.2
1	D	24	LEU	2.2
1	D	295	LEU	2.2
1	C	132	THR	2.2
1	B	310	TYR	2.2
1	B	457	GLY	2.2
1	B	202	ALA	2.2
1	C	181	ALA	2.2
1	D	328	GLU	2.2
1	A	61	LEU	2.2
1	C	281	PRO	2.2
1	C	374	PRO	2.2
1	B	94	GLY	2.2
1	B	392	MET	2.2
1	D	397	SER	2.2
1	B	186	LEU	2.2
1	C	39	LEU	2.2
1	B	251	ARG	2.2
1	D	231	ARG	2.2
1	B	196	PRO	2.2
1	B	452	TYR	2.2
1	D	211	ALA	2.2
1	C	283	THR	2.1
1	B	381	LEU	2.1
1	D	215	LEU	2.1
1	A	103	SER	2.1
1	B	164	ALA	2.1
1	B	190	ALA	2.1
1	B	320	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	461	LEU	2.1
1	B	451	ARG	2.1
1	D	234	HIS	2.1
1	A	60	LEU	2.1
1	B	356	LEU	2.1
1	B	369	GLY	2.1
1	C	225	ARG	2.1
1	A	477	SER	2.1
1	D	171	SER	2.1
1	B	238	VAL	2.1
1	A	473	LEU	2.1
1	C	365	ALA	2.1
1	B	246	PRO	2.0
1	D	479	LEU	2.0
1	A	336	GLY	2.0
1	B	375	LYS	2.0
1	C	452	TYR	2.0
1	B	219	LEU	2.0
1	D	146	LEU	2.0
1	D	251	ARG	2.0
1	B	148	PHE	2.0
1	D	398	ALA	2.0
1	D	449	ALA	2.0
1	B	282	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

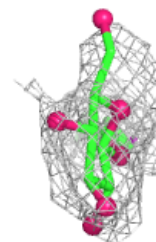
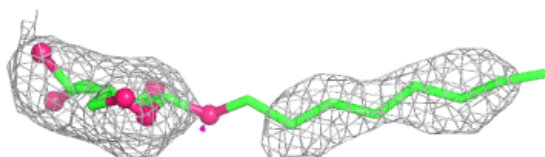
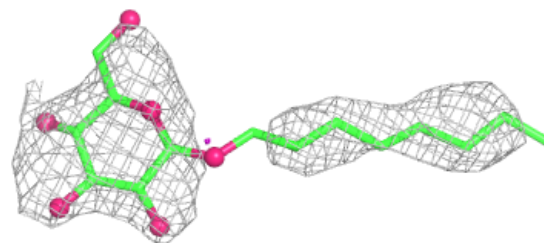
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BOG	C	802	20/20	0.74	0.20	76,100,110,111	0
3	LMT	A	804	14/35	0.76	0.26	70,75,79,90	0
3	LMT	A	805	34/35	0.77	0.17	67,106,122,127	0
4	BOG	D	802	20/20	0.81	0.19	62,70,76,80	0
3	LMT	C	803	16/35	0.85	0.23	59,71,94,96	0
4	BOG	C	804	20/20	0.86	0.16	71,86,101,105	0
3	LMT	A	806	14/35	0.86	0.21	55,67,81,89	0
4	BOG	A	803	12/20	0.87	0.20	66,85,101,102	0
2	NA	B	801	1/1	0.88	0.08	64,64,64,64	0
3	LMT	A	802	23/35	0.88	0.14	60,89,119,120	0
3	LMT	C	805	15/35	0.90	0.18	64,68,96,97	0
2	NA	A	801	1/1	0.96	0.06	61,61,61,61	0
2	NA	C	801	1/1	0.97	0.07	58,58,58,58	0
2	NA	D	801	1/1	0.99	0.02	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.

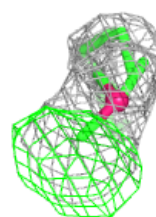
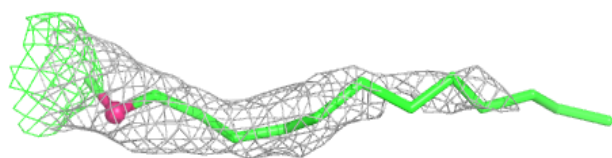
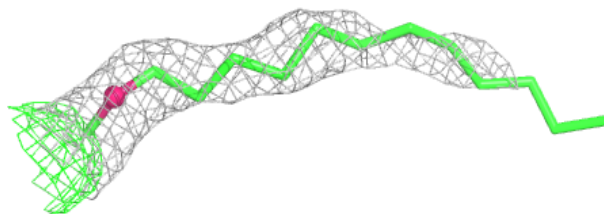
Electron density around BOG C 802:

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

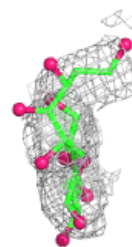
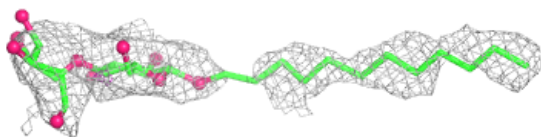
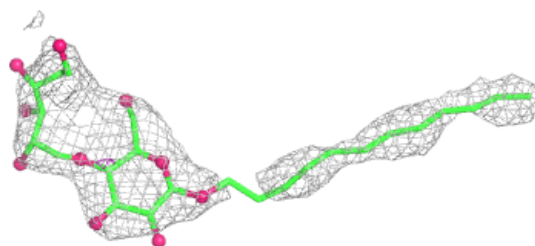


Electron density around LMT A 804:

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

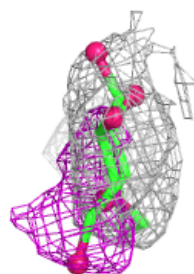
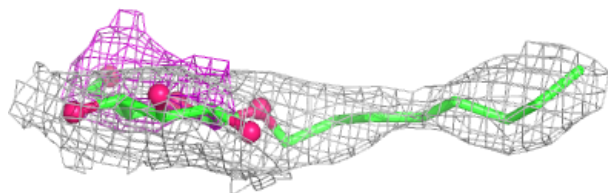
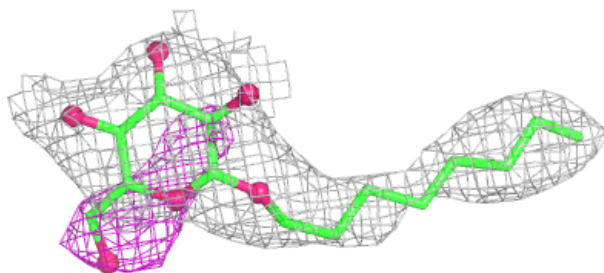
**Electron density around LMT A 805:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

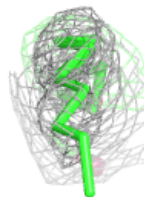
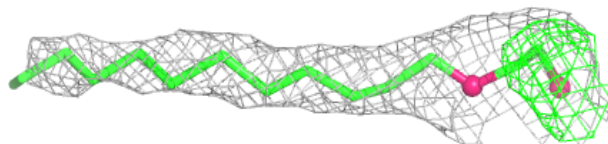
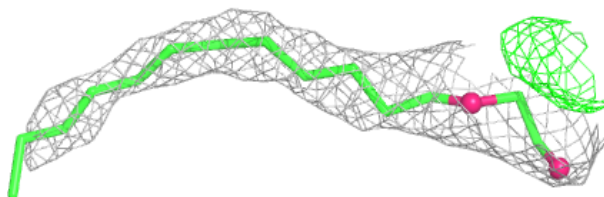


Electron density around BOG D 802:

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

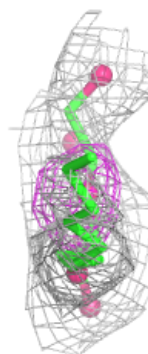
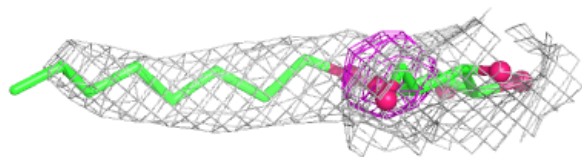
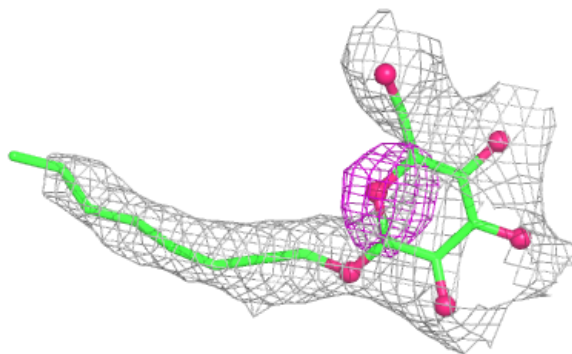
**Electron density around LMT C 803:**

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

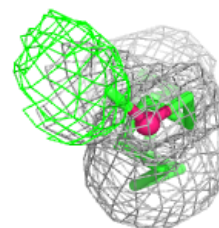
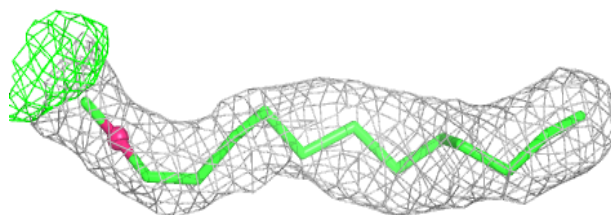
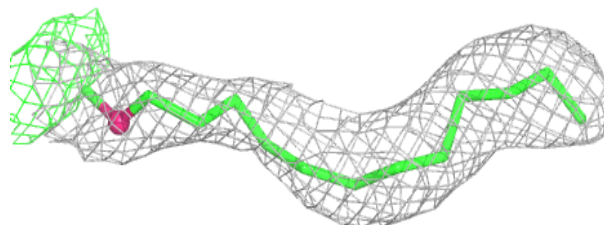


Electron density around BOG C 804:

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

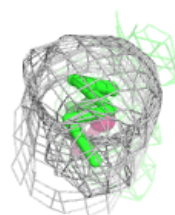
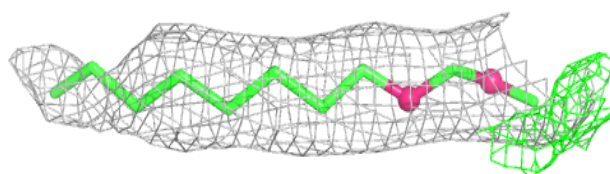
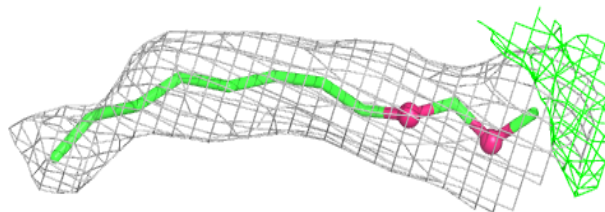
**Electron density around LMT A 806:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

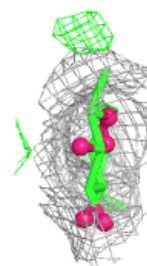
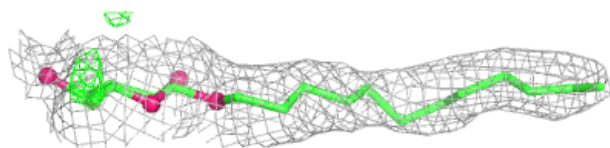
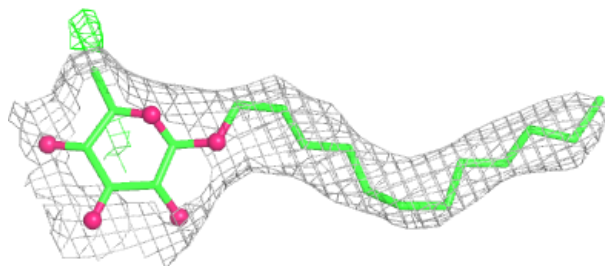


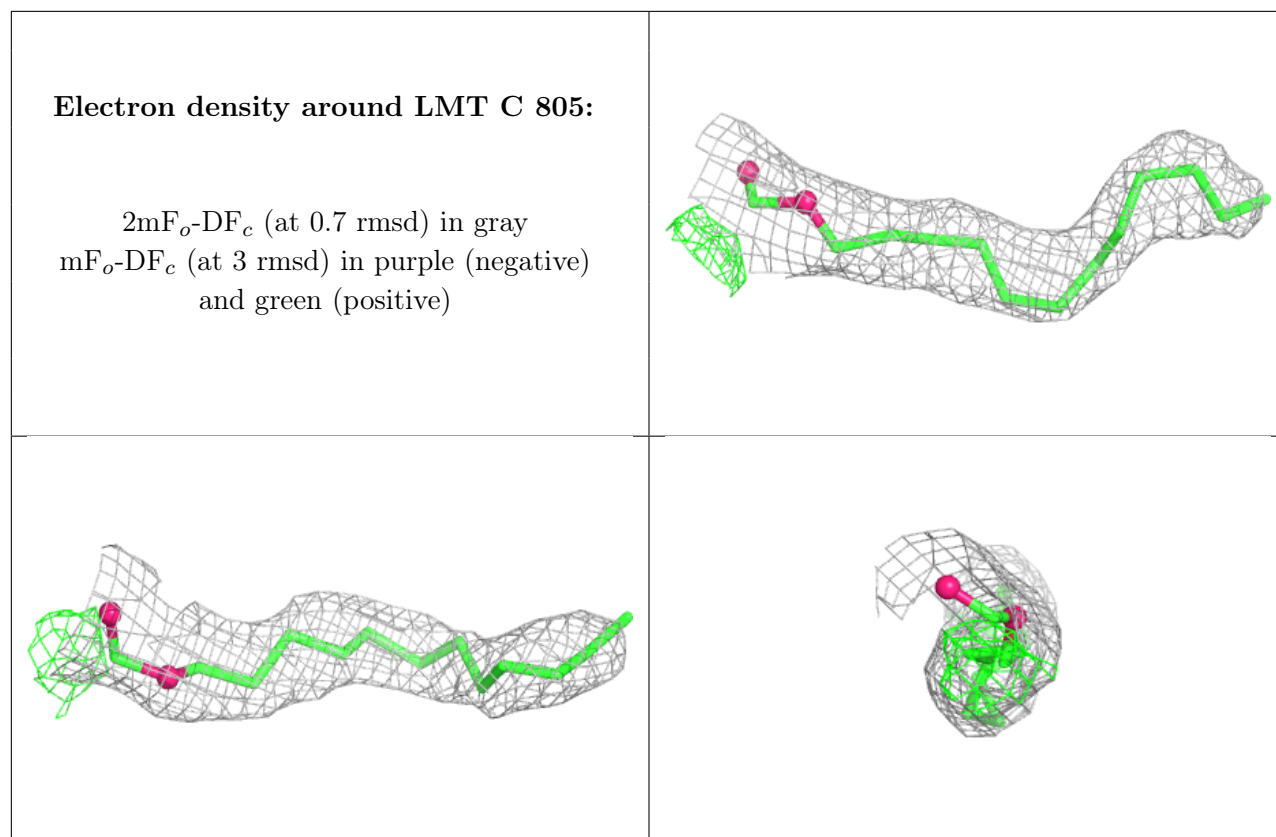
Electron density around BOG A 803:

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

**Electron density around LMT 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.