Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 02:09 AM EDT

PDB ID	:	2FCP
Title	:	FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) FROM E.COLI
Authors	:	Hofmann, E.; Ferguson, A.D.; Diederichs, K.; Welte, W.
Deposited on	:	1998-10-15
Resolution	:	2.50 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:

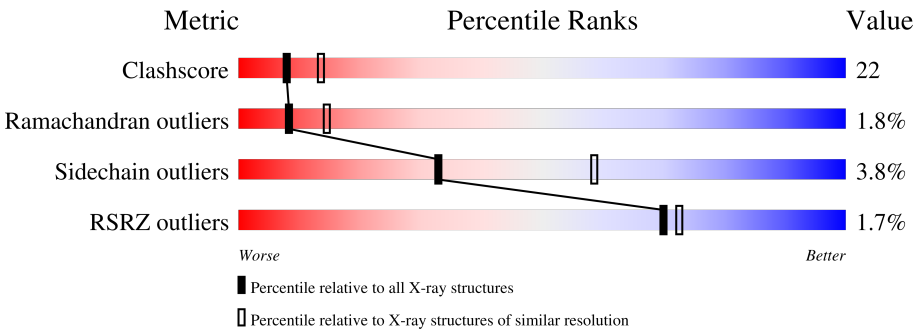
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	723	2%, 62%, 32%, • •
2	B	9	11%, 44%, 44%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	B	6	-	-	X	-
2	GLA	B	8	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LIL	A	804	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5833 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.

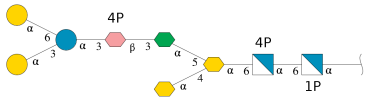
- Molecule 1 is a protein called PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	705	5512	3469	942	1087	14	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP P06971
A	407	HIS	-	insertion	UNP P06971
A	408	HIS	-	insertion	UNP P06971
A	409	HIS	-	insertion	UNP P06971
A	410	HIS	-	insertion	UNP P06971
A	411	HIS	-	insertion	UNP P06971
A	412	HIS	-	insertion	UNP P06971
A	413	GLY	-	insertion	UNP P06971
A	414	SER	-	insertion	UNP P06971

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-4-O-phosphono-D-glycero-beta-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.

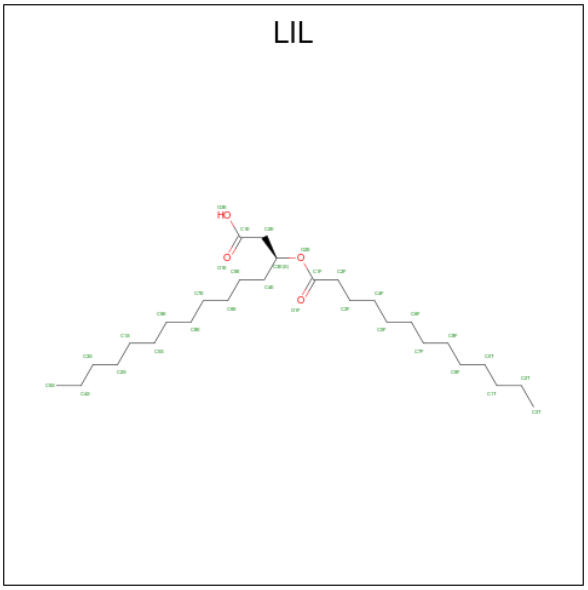


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	9	124	60	2	59	3	0	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

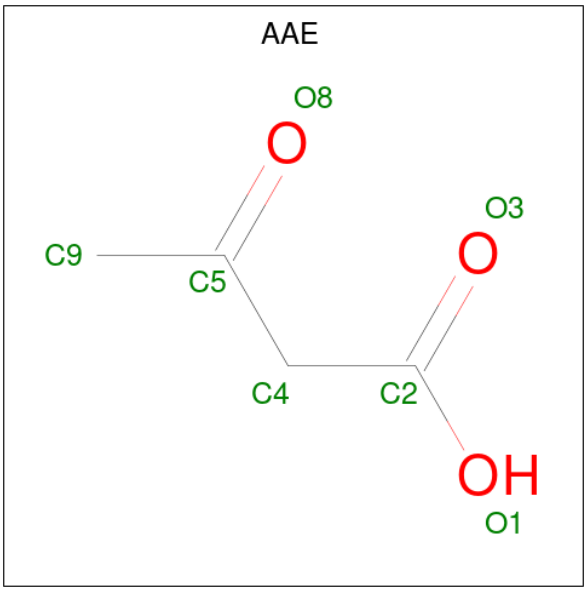
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
3	A	2	2	2	0	0

- Molecule 4 is 2-TRIDECANOYLOXY-PENTADECANOIC ACID (three-letter code: LIL) (formula: $C_{28}H_{54}O_4$).



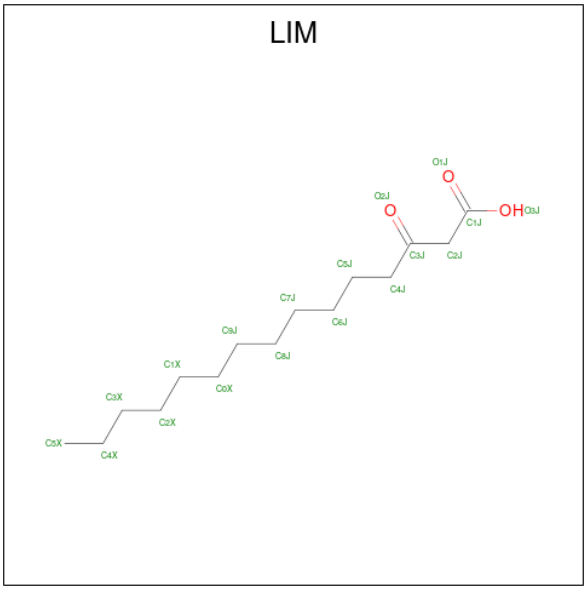
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	31	28	3	0	0
			Total	C	O		
4	A	1	31	28	3	0	0

- Molecule 5 is ACETOACETIC ACID (three-letter code: AAE) (formula: $C_4H_6O_3$).



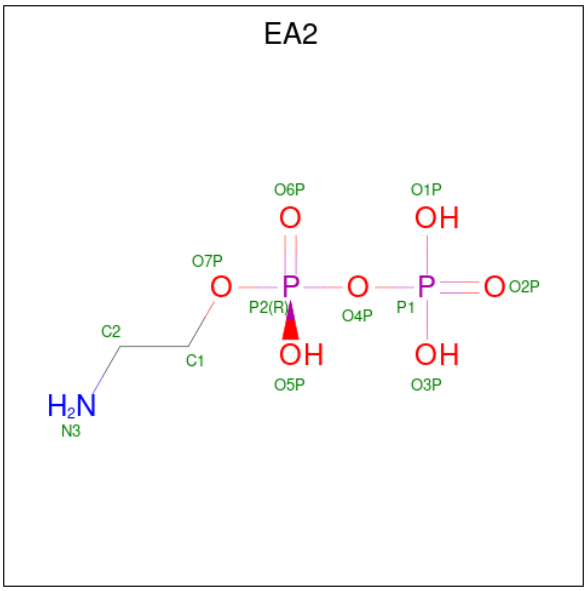
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	4	2	0	0

- Molecule 6 is 3-OXO-PENTADECANOIC ACID (three-letter code: LIM) (formula: $C_{15}H_{28}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	17	15	2	0	0

- Molecule 7 is AMINOETHANOLPYROPHOSPHATE (three-letter code: EA2) (formula: $C_2H_9NO_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	11	2	1	6	2	0	0

- Molecule 8 is water.

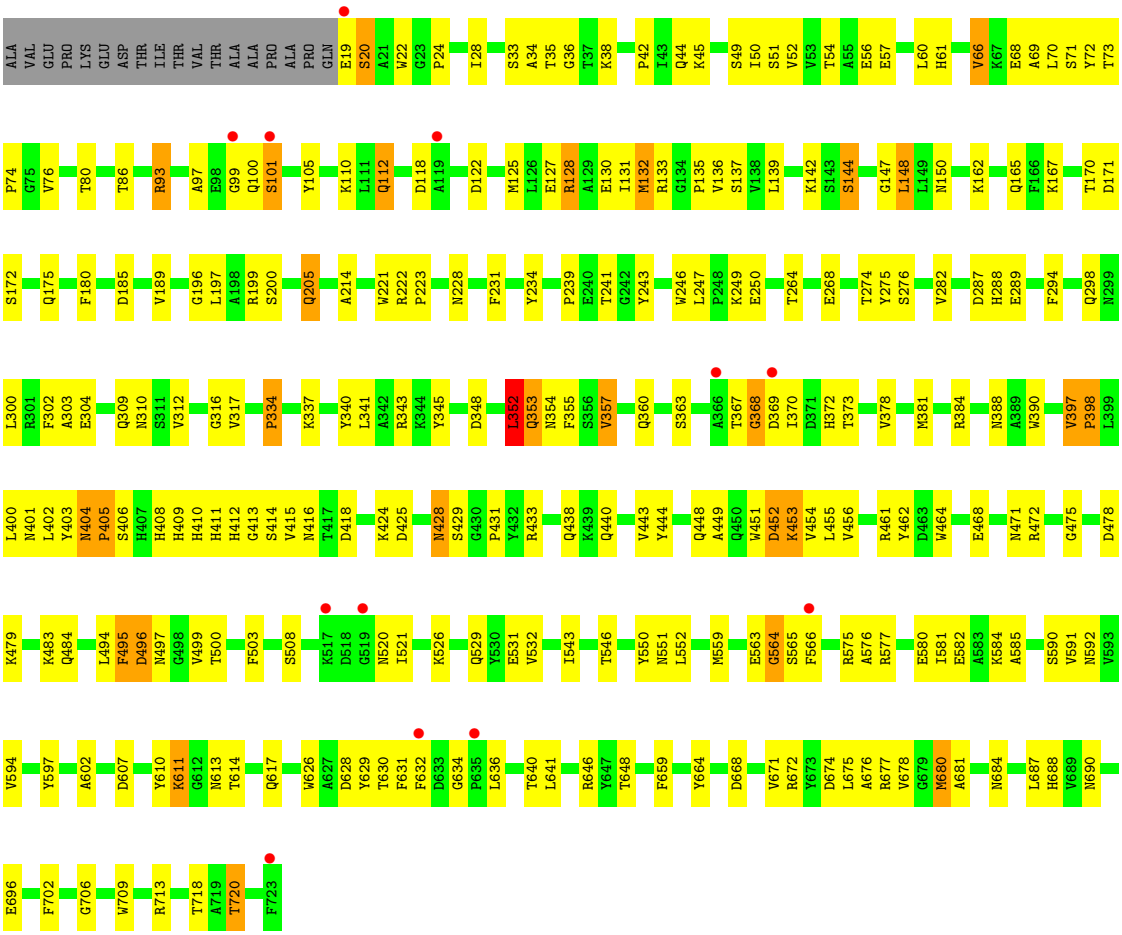
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	99	99	99	0	0

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: PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR)

Chain A: 2% 62% 32%



• Molecule 2: alpha-D-galactopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-4-O-phosphono-D-glycero-beta-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain B: 11% 44% 44%

GP11
GP42
KDO3
GMH4
GPH5
GLC6
GLA7
GLA8
KDO9

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	171.55Å 171.55Å 87.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 43.12 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.50) 98.8 (43.12-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.283 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5833	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: LIM, GPH, EA2, GP4, LIL, GMH, GLA, GLC, KDO, GP1, NI, AAE

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	0.40	0/5652	0.66	1/7680 (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	A	352	LEU	CA-CB-CG	5.59	128.16	115.30

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	5512	0	5213	221	0
2	B	124	0	70	9	0
3	A	2	0	0	0	0
4	A	62	0	106	14	0
5	A	6	0	5	1	0
6	A	17	0	27	5	0
7	A	11	0	6	1	0
8	A	99	0	0	12	0
All	All	5833	0	5427	240	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 22.

All (240) 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:70:LEU:HD13	1:A:131:ILE:HD11	1.32	1.04
1:A:86:THR:HG23	1:A:241:THR:HG21	1.35	1.04
1:A:132:MET:HG2	1:A:136:VAL:HG11	1.50	0.93
1:A:408:HIS:O	1:A:411:HIS:HB3	1.69	0.92
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.57	0.83
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.46	0.80
2:B:6:GLC:C6	2:B:8:GLA:H5	2.12	0.79
1:A:341:LEU:HB2	1:A:402:LEU:HD11	1.62	0.79
1:A:468:GLU:HG3	1:A:479:LYS:HG2	1.66	0.78
1:A:378:VAL:HG12	1:A:443:VAL:HG12	1.65	0.77
1:A:19:GLU:HG3	1:A:632:PHE:CE2	2.20	0.76
2:B:6:GLC:H62	2:B:8:GLA:H5	1.66	0.75
1:A:125:MET:HG3	1:A:234:TYR:HE1	1.53	0.72
1:A:35:THR:HG22	1:A:150:ASN:HD22	1.57	0.70
1:A:713:ARG:HH11	1:A:713:ARG:HG2	1.56	0.70
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.28	0.68
4:A:804:LIL:H9F1	6:A:806:LIM:H5X2	1.75	0.68
1:A:343:ARG:HH11	1:A:400:LEU:HG	1.58	0.67
1:A:565:SER:O	1:A:566:PHE:HB2	1.92	0.67
1:A:298:GLN:HE22	6:A:806:LIM:H3X1	1.59	0.67
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.30	0.67
1:A:668:ASP:OD1	1:A:690:ASN:HA	1.95	0.66
1:A:35:THR:CG2	1:A:150:ASN:HD22	2.08	0.66
1:A:671:VAL:HG22	1:A:687:LEU:HB3	1.78	0.66
1:A:189:VAL:HG23	1:A:222:ARG:O	1.95	0.65
1:A:352:LEU:HB2	1:A:384:ARG:O	1.95	0.65
1:A:135:PRO:HB3	1:A:508:SER:HB3	1.79	0.64
1:A:353:GLN:HG3	8:A:948:HOH:O	1.98	0.64
1:A:408:HIS:O	1:A:411:HIS:CB	2.45	0.63
2:B:6:GLC:C6	2:B:8:GLA:C5	2.77	0.63
1:A:428:ASN:HD22	1:A:429:SER:N	1.95	0.63
1:A:592:ASN:HB2	1:A:628:ASP:OD1	1.99	0.63
1:A:42:PRO:HB2	1:A:44:GLN:NE2	2.13	0.63
1:A:626:TRP:CH2	1:A:628:ASP:HB3	2.32	0.63
1:A:584:LYS:HG2	1:A:594:VAL:HG13	1.81	0.62
1:A:390:TRP:CE2	1:A:424:LYS:HB3	2.34	0.62
1:A:610:TYR:O	1:A:611:LYS:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ARG:HB3	1:A:677:ARG:NH1	2.15	0.62
1:A:428:ASN:HD22	1:A:428:ASN:C	2.03	0.61
2:B:6:GLC:H61	2:B:8:GLA:H3	1.82	0.61
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.82	0.61
1:A:675:LEU:HB2	1:A:684:ASN:HA	1.82	0.61
1:A:35:THR:HG23	1:A:130:GLU:OE1	2.01	0.60
1:A:412:HIS:CD2	1:A:413:GLY:H	2.20	0.60
1:A:702:PHE:CE2	1:A:706:GLY:HA3	2.37	0.60
1:A:71:SER:HB3	1:A:646:ARG:HD3	1.82	0.60
1:A:343:ARG:O	1:A:397:VAL:HG13	2.02	0.60
1:A:401:ASN:OD1	1:A:403:TYR:HB2	2.02	0.60
1:A:676:ALA:CB	1:A:681:ALA:HA	2.32	0.59
1:A:72:TYR:CE2	1:A:626:TRP:HB2	2.37	0.59
1:A:671:VAL:CG2	1:A:687:LEU:HB3	2.32	0.59
1:A:148:LEU:C	1:A:148:LEU:HD23	2.23	0.59
1:A:444:TYR:HB3	1:A:461:ARG:HB2	1.84	0.59
1:A:42:PRO:HB2	1:A:44:GLN:HE22	1.68	0.59
4:A:803:LIL:H9E2	4:A:804:LIL:H0S1	1.84	0.58
1:A:384:ARG:HD3	8:A:948:HOH:O	2.03	0.58
1:A:294:PHE:HE1	1:A:363:SER:HG	1.52	0.57
1:A:529:GLN:HB2	1:A:552:LEU:HD13	1.85	0.57
1:A:132:MET:HG2	1:A:136:VAL:CG1	2.30	0.57
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.39	0.57
1:A:343:ARG:NH1	1:A:400:LEU:HG	2.20	0.57
1:A:51:SER:OG	1:A:133:ARG:NH2	2.37	0.57
1:A:453:LYS:N	1:A:453:LYS:HE2	2.20	0.57
1:A:300:LEU:C	1:A:300:LEU:HD23	2.25	0.57
1:A:264:THR:HA	1:A:709:TRP:CD1	2.40	0.56
1:A:300:LEU:HD12	1:A:357:VAL:CG1	2.35	0.56
1:A:409:HIS:O	1:A:412:HIS:O	2.23	0.56
1:A:73:THR:HG22	8:A:963:HOH:O	2.05	0.56
1:A:142:LYS:HG2	1:A:440:GLN:OE1	2.05	0.56
1:A:249:LYS:HG2	1:A:250:GLU:OE1	2.06	0.55
1:A:97:ALA:HB3	1:A:101:SER:O	2.06	0.55
1:A:132:MET:CG	1:A:136:VAL:HG11	2.30	0.55
1:A:36:GLY:HA2	1:A:132:MET:SD	2.46	0.55
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.37	0.55
1:A:93:ARG:NH2	1:A:531:GLU:OE1	2.30	0.55
1:A:205:GLN:HG3	1:A:243:TYR:HB2	1.88	0.54
1:A:24:PRO:O	1:A:28:ILE:HG12	2.08	0.54
1:A:397:VAL:HG23	1:A:398:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:SER:O	1:A:629:TYR:HA	2.07	0.54
1:A:676:ALA:HB2	1:A:681:ALA:HA	1.90	0.54
1:A:449:ALA:HB3	1:A:456:VAL:CG1	2.38	0.54
1:A:415:VAL:HG22	1:A:416:ASN:N	2.23	0.54
1:A:543:ILE:HG22	1:A:585:ALA:HB1	1.90	0.54
1:A:676:ALA:HA	1:A:680:MET:O	2.08	0.54
1:A:373:THR:HB	1:A:448:GLN:HB2	1.89	0.53
1:A:54:THR:OG1	1:A:57:GLU:HG3	2.08	0.53
1:A:404:ASN:HB2	8:A:910:HOH:O	2.07	0.53
2:B:6:GLC:H62	2:B:8:GLA:C5	2.35	0.53
2:B:6:GLC:H61	2:B:8:GLA:H5	1.88	0.53
1:A:70:LEU:HD22	1:A:131:ILE:HG13	1.90	0.53
1:A:453:LYS:HE2	1:A:453:LYS:H	1.72	0.53
1:A:591:VAL:HG22	1:A:629:TYR:HD1	1.73	0.53
1:A:105:TYR:CZ	1:A:110:LYS:HB2	2.44	0.53
1:A:302:PHE:CZ	4:A:803:LIL:H2E1	2.44	0.52
5:A:805:AAE:O3	2:B:1:GP1:O4	2.27	0.52
1:A:334:PRO:HA	1:A:337:LYS:HE2	1.91	0.52
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.44	0.52
1:A:713:ARG:HG2	1:A:713:ARG:NH1	2.24	0.52
1:A:381:MET:HE3	8:A:970:HOH:O	2.09	0.52
1:A:93:ARG:HG3	1:A:550:TYR:OH	2.10	0.52
1:A:353:GLN:CG	8:A:948:HOH:O	2.58	0.52
4:A:804:LIL:H7F1	6:A:806:LIM:H0X2	1.92	0.51
1:A:110:LYS:HD3	1:A:112:GLN:HG2	1.92	0.51
1:A:546:THR:HG22	1:A:582:GLU:HB3	1.92	0.51
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.92	0.51
1:A:228:ASN:HB3	1:A:287:ASP:OD1	2.11	0.51
1:A:575:ARG:CZ	1:A:577:ARG:HE	2.23	0.51
7:A:807:EA2:O6P	2:B:4:GMH:H6	2.10	0.51
1:A:406:SER:O	1:A:410:HIS:HD2	1.94	0.51
1:A:93:ARG:HH11	1:A:580:GLU:CD	2.13	0.51
1:A:602:ALA:O	1:A:614:THR:HG22	2.10	0.51
1:A:264:THR:HG21	1:A:696:GLU:HG2	1.92	0.51
1:A:472:ARG:HG2	1:A:472:ARG:HH11	1.76	0.51
1:A:671:VAL:HG23	1:A:671:VAL:O	2.11	0.51
1:A:132:MET:O	1:A:147:GLY:HA2	2.11	0.50
1:A:370:ILE:HG12	1:A:451:TRP:CD1	2.47	0.50
1:A:370:ILE:HG12	1:A:451:TRP:HD1	1.76	0.50
1:A:390:TRP:CZ2	1:A:424:LYS:HB2	2.46	0.50
1:A:449:ALA:HB3	1:A:456:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TRP:HE1	1:A:429:SER:CB	2.23	0.50
1:A:404:ASN:O	1:A:406:SER:N	2.45	0.50
1:A:640:THR:HB	1:A:672:ARG:HB3	1.94	0.50
1:A:73:THR:CG2	8:A:963:HOH:O	2.60	0.49
1:A:19:GLU:O	1:A:20:SER:HB3	2.12	0.49
1:A:367:THR:HG22	1:A:367:THR:O	2.13	0.49
1:A:35:THR:HG22	1:A:150:ASN:ND2	2.28	0.49
1:A:196:GLY:HA2	1:A:214:ALA:O	2.13	0.49
1:A:60:LEU:HD21	1:A:626:TRP:HH2	1.76	0.49
4:A:803:LIL:C9F	4:A:803:LIL:H2S1	2.43	0.49
1:A:626:TRP:NE1	8:A:902:HOH:O	2.34	0.48
1:A:282:VAL:HG21	4:A:803:LIL:C9E	2.44	0.48
1:A:298:GLN:NE2	6:A:806:LIM:H3X1	2.26	0.48
1:A:388:ASN:HD22	1:A:433:ARG:HG2	1.77	0.48
1:A:142:LYS:O	1:A:142:LYS:HG3	2.12	0.48
1:A:68:GLU:OE1	1:A:68:GLU:N	2.36	0.48
1:A:368:GLY:O	1:A:369:ASP:HB2	2.14	0.48
1:A:495:PHE:HB2	1:A:499:VAL:O	2.14	0.48
1:A:170:THR:HG22	1:A:171:ASP:H	1.78	0.47
1:A:38:LYS:HD3	1:A:360:GLN:HE22	1.79	0.47
1:A:559:MET:SD	1:A:607:ASP:HA	2.54	0.47
1:A:231:PHE:CZ	4:A:803:LIL:H4S2	2.48	0.47
1:A:440:GLN:HA	1:A:464:TRP:O	2.13	0.47
1:A:453:LYS:HE2	1:A:453:LYS:CA	2.43	0.47
1:A:19:GLU:HG3	1:A:632:PHE:CZ	2.48	0.47
1:A:462:TYR:OH	1:A:483:LYS:HB3	2.14	0.47
1:A:316:GLY:O	1:A:341:LEU:HD12	2.15	0.47
1:A:345:TYR:CD1	1:A:345:TYR:C	2.88	0.47
1:A:165:GLN:HG3	1:A:720:THR:HB	1.97	0.47
1:A:390:TRP:CZ3	1:A:431:PRO:HG3	2.50	0.47
1:A:590:SER:HB2	1:A:630:THR:O	2.15	0.47
1:A:641:LEU:CD2	1:A:671:VAL:HG12	2.45	0.47
1:A:93:ARG:HG3	1:A:550:TYR:CZ	2.49	0.47
1:A:142:LYS:NZ	1:A:438:GLN:OE1	2.48	0.46
1:A:246:TRP:O	1:A:247:LEU:HD23	2.15	0.46
1:A:45:LYS:HB3	1:A:455:LEU:CD2	2.45	0.46
1:A:50:ILE:HB	1:A:132:MET:CE	2.44	0.46
1:A:304:GLU:HA	1:A:352:LEU:O	2.16	0.46
4:A:803:LIL:H2S1	4:A:803:LIL:H9F2	1.98	0.46
1:A:412:HIS:CG	1:A:413:GLY:N	2.84	0.46
1:A:648:THR:HB	1:A:664:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD21	1:A:626:TRP:CH2	2.50	0.46
1:A:137:SER:HB2	1:A:508:SER:HA	1.96	0.46
1:A:413:GLY:O	1:A:414:SER:HB2	2.15	0.46
1:A:520:ASN:ND2	8:A:911:HOH:O	2.49	0.46
1:A:93:ARG:NH1	1:A:580:GLU:OE1	2.48	0.46
1:A:303:ALA:O	1:A:353:GLN:HA	2.16	0.46
4:A:803:LIL:H8E1	4:A:804:LIL:H8E1	1.97	0.45
1:A:425:ASP:HB3	1:A:428:ASN:ND2	2.32	0.45
1:A:22:TRP:CD1	1:A:60:LEU:HD22	2.52	0.45
1:A:282:VAL:HG21	4:A:803:LIL:H9E1	1.99	0.45
1:A:563:GLU:O	1:A:564:GLY:C	2.56	0.45
1:A:61:HIS:HD2	8:A:997:HOH:O	2.00	0.45
1:A:170:THR:HG22	1:A:171:ASP:N	2.31	0.45
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.37	0.45
1:A:197:LEU:C	1:A:197:LEU:HD12	2.38	0.44
1:A:199:ARG:HD2	8:A:990:HOH:O	2.16	0.44
1:A:288:HIS:HD2	1:A:289:GLU:N	2.15	0.44
1:A:629:TYR:HE2	1:A:631:PHE:CE1	2.35	0.44
1:A:137:SER:CB	1:A:508:SER:HA	2.47	0.44
1:A:99:GLY:O	1:A:100:GLN:HB2	2.17	0.44
1:A:415:VAL:HG22	1:A:416:ASN:H	1.81	0.44
1:A:51:SER:OG	1:A:73:THR:HG23	2.17	0.44
1:A:80:THR:CG2	1:A:617:GLN:NE2	2.80	0.44
1:A:678:VAL:HG12	1:A:678:VAL:O	2.18	0.44
1:A:60:LEU:O	1:A:688:HIS:HE1	2.01	0.43
1:A:171:ASP:O	1:A:172:SER:HB2	2.18	0.43
1:A:575:ARG:HG2	1:A:576:ALA:N	2.33	0.43
1:A:137:SER:OG	1:A:508:SER:HA	2.19	0.43
1:A:50:ILE:HB	1:A:132:MET:HE3	2.01	0.43
1:A:52:VAL:HG22	1:A:130:GLU:HG2	2.00	0.43
1:A:452:ASP:C	1:A:454:VAL:H	2.21	0.43
1:A:484:GLN:OE1	1:A:526:LYS:HE2	2.19	0.43
1:A:247:LEU:HD21	1:A:268:GLU:HG3	2.00	0.43
1:A:631:PHE:HB2	1:A:636:LEU:O	2.19	0.43
1:A:690:ASN:O	1:A:713:ARG:HA	2.17	0.43
1:A:49:SER:HB3	1:A:133:ARG:NH1	2.33	0.43
1:A:97:ALA:HA	1:A:144:SER:HB2	2.00	0.43
1:A:309:GLN:HG2	1:A:348:ASP:HB3	2.00	0.43
1:A:355:PHE:CE2	1:A:357:VAL:HG22	2.53	0.43
1:A:456:VAL:HG13	1:A:456:VAL:O	2.18	0.43
1:A:409:HIS:C	1:A:411:HIS:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TRP:CE2	1:A:424:LYS:CB	3.02	0.42
1:A:66:VAL:O	1:A:69:ALA:HB3	2.19	0.42
1:A:249:LYS:HD2	1:A:659:PHE:CD2	2.55	0.42
1:A:402:LEU:C	1:A:405:PRO:HD2	2.39	0.42
1:A:478:ASP:HB3	1:A:521:ILE:HD11	2.01	0.42
1:A:646:ARG:HG3	1:A:646:ARG:HH11	1.84	0.42
1:A:167:LYS:CG	1:A:718:THR:HG23	2.50	0.42
1:A:503:PHE:HB2	1:A:532:VAL:HG12	2.02	0.42
1:A:73:THR:HG23	1:A:74:PRO:HD2	2.01	0.42
1:A:239:PRO:O	1:A:276:SER:HB3	2.20	0.42
1:A:451:TRP:O	1:A:452:ASP:O	2.38	0.42
1:A:677:ARG:CB	1:A:677:ARG:HH11	2.32	0.42
1:A:529:GLN:HA	1:A:551:ASN:O	2.20	0.42
4:A:804:LIL:H9F1	6:A:806:LIM:C5X	2.48	0.42
1:A:317:VAL:HA	1:A:340:TYR:O	2.20	0.42
1:A:390:TRP:CH2	1:A:431:PRO:HG3	2.55	0.42
1:A:495:PHE:HB3	1:A:496:ASP:H	1.49	0.41
1:A:74:PRO:HB2	1:A:580:GLU:HB3	2.02	0.41
1:A:127:GLU:O	1:A:128:ARG:HB3	2.20	0.41
1:A:453:LYS:HE2	1:A:453:LYS:HA	2.02	0.41
4:A:803:LIL:C8E	4:A:804:LIL:H0S1	2.50	0.41
1:A:494:LEU:HA	1:A:500:THR:HG23	2.02	0.41
1:A:122:ASP:O	1:A:125:MET:HG2	2.21	0.41
1:A:471:ASN:O	1:A:475:GLY:N	2.54	0.41
1:A:495:PHE:HD2	1:A:497:ASN:OD1	2.04	0.41
1:A:199:ARG:HG2	1:A:200:SER:N	2.36	0.41
1:A:312:VAL:HG11	1:A:343:ARG:HH21	1.86	0.41
1:A:563:GLU:O	1:A:564:GLY:O	2.38	0.41
1:A:33:SER:OG	1:A:34:ALA:N	2.54	0.40
1:A:56:GLU:CD	1:A:56:GLU:H	2.24	0.40
4:A:803:LIL:H2E2	4:A:804:LIL:H4E2	2.03	0.40
4:A:803:LIL:H3E1	4:A:803:LIL:H2F2	1.85	0.40
1:A:300:LEU:HD12	1:A:357:VAL:HG13	2.02	0.40
1:A:74:PRO:HA	8:A:916:HOH:O	2.21	0.40
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.56	0.40
1:A:611:LYS:C	1:A:613:ASN:H	2.24	0.40
1:A:352:LEU:C	1:A:352:LEU:HD12	2.42	0.40
1:A:581:ILE:HG12	1:A:597:TYR:HB3	2.03	0.40
2:B:3:KDO:H7	2:B:4:GMH:C1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	703/723 (97%)	633 (90%)	57 (8%)	13 (2%)	8 14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	452	ASP
1	A	564	GLY
1	A	634	GLY
1	A	418	ASP
1	A	611	LYS
1	A	680	MET
1	A	495	PHE
1	A	674	ASP
1	A	398	PRO
1	A	334	PRO
1	A	368	GLY
1	A	405	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	585/599 (98%)	563 (96%)	22 (4%)	33 58

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	76	VAL
1	A	93	ARG
1	A	101	SER
1	A	112	GLN
1	A	118	ASP
1	A	128	ARG
1	A	132	MET
1	A	144	SER
1	A	148	LEU
1	A	205	GLN
1	A	275	TYR
1	A	352	LEU
1	A	353	GLN
1	A	354	ASN
1	A	357	VAL
1	A	397	VAL
1	A	404	ASN
1	A	428	ASN
1	A	453	LYS
1	A	496	ASP
1	A	720	THR

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

Mol	Chain	Res	Type
1	A	150	ASN
1	A	165	GLN
1	A	202	ASN
1	A	205	GLN
1	A	288	HIS
1	A	310	ASN
1	A	328	GLN
1	A	353	GLN
1	A	354	ASN
1	A	388	ASN
1	A	410	HIS
1	A	412	HIS
1	A	416	ASN
1	A	428	ASN
1	A	520	ASN
1	A	551	ASN
1	A	688	HIS

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Mol	Chain	Res	Type
1	A	690	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)

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GP1	B	1	5,3,2,6	15,16,16	1.52	2 (13%)	23,24,24	1.02	1 (4%)
2	GP4	B	2	4,2	15,15,16	1.46	1 (6%)	18,22,24	1.03	1 (5%)
2	KDO	B	3	2	15,15,16	0.87	0	19,21,24	0.94	0
2	GMH	B	4	7,2	13,13,14	1.47	3 (23%)	17,18,20	1.27	2 (11%)
2	GPH	B	5	3,2	17,17,18	1.67	2 (11%)	23,25,27	1.15	2 (8%)
2	GLC	B	6	2	11,11,12	0.78	0	15,15,17	1.13	2 (13%)
2	GLA	B	7	2	11,11,12	0.62	0	15,15,17	0.81	1 (6%)
2	GLA	B	8	2	11,11,12	0.50	0	15,15,17	0.77	1 (6%)
2	KDO	B	9	2	15,15,16	0.69	0	19,21,24	0.86	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
2	GP1	B	1	5,3,2,6	-	3/6/27/27	0/1/1/1
2	GP4	B	2	4,2	-	1/7/24/27	0/1/1/1
2	KDO	B	3	2	-	2/10/26/30	0/1/1/1
2	GMH	B	4	7,2	-	0/6/23/26	0/1/1/1
2	GPH	B	5	3,2	-	6/11/28/31	0/1/1/1
2	GLC	B	6	2	-	2/2/19/22	0/1/1/1
2	GLA	B	7	2	-	2/2/19/22	0/1/1/1
2	GLA	B	8	2	-	0/2/19/22	0/1/1/1
2	KDO	B	9	2	-	2/10/26/30	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GPH	P1-O4	-4.87	1.50	1.59
2	B	2	GP4	P4A-O4	-4.79	1.50	1.59
2	B	1	GP1	P4B-O1	-4.33	1.51	1.59
2	B	4	GMH	C2-C3	3.25	1.57	1.52
2	B	1	GP1	C3-C2	2.72	1.57	1.53
2	B	5	GPH	C2-C3	2.62	1.56	1.52
2	B	4	GMH	C1-C2	2.40	1.57	1.52
2	B	4	GMH	O3-C3	2.09	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	GP4	C1-O5-C5	3.06	116.34	112.19
2	B	8	GLA	C1-O5-C5	2.71	115.86	112.19
2	B	1	GP1	C4-C3-C2	-2.68	106.46	111.07
2	B	4	GMH	O3-C3-C2	2.56	114.89	109.99
2	B	6	GLC	C1-O5-C5	2.56	115.66	112.19
2	B	7	GLA	C1-O5-C5	2.53	115.62	112.19
2	B	4	GMH	C3-C4-C5	2.36	115.07	109.68
2	B	5	GPH	C2-C3-C4	2.12	114.67	110.41
2	B	5	GPH	C1-C2-C3	2.08	112.22	109.67
2	B	6	GLC	C1-C2-C3	-2.00	107.21	109.67

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	GP1	C1-O1-P4B-O7B

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Mol	Chain	Res	Type	Atoms
2	B	2	GP4	C4-O4-P4A-O7A
2	B	3	KDO	O6-C6-C7-O7
2	B	5	GPH	C4-C5-C6-C7
2	B	5	GPH	C4-C5-C6-O6
2	B	5	GPH	O5-C5-C6-O6
2	B	9	KDO	C6-C7-C8-O8
2	B	9	KDO	O7-C7-C8-O8
2	B	6	GLC	O5-C5-C6-O6
2	B	1	GP1	C4-C5-C6-O6
2	B	1	GP1	O5-C5-C6-O6
2	B	7	GLA	O5-C5-C6-O6
2	B	6	GLC	C4-C5-C6-O6
2	B	7	GLA	C4-C5-C6-O6
2	B	5	GPH	C3-C4-O4-P1
2	B	3	KDO	O6-C6-C7-C8
2	B	5	GPH	O5-C5-C6-C7
2	B	5	GPH	C5-C4-O4-P1

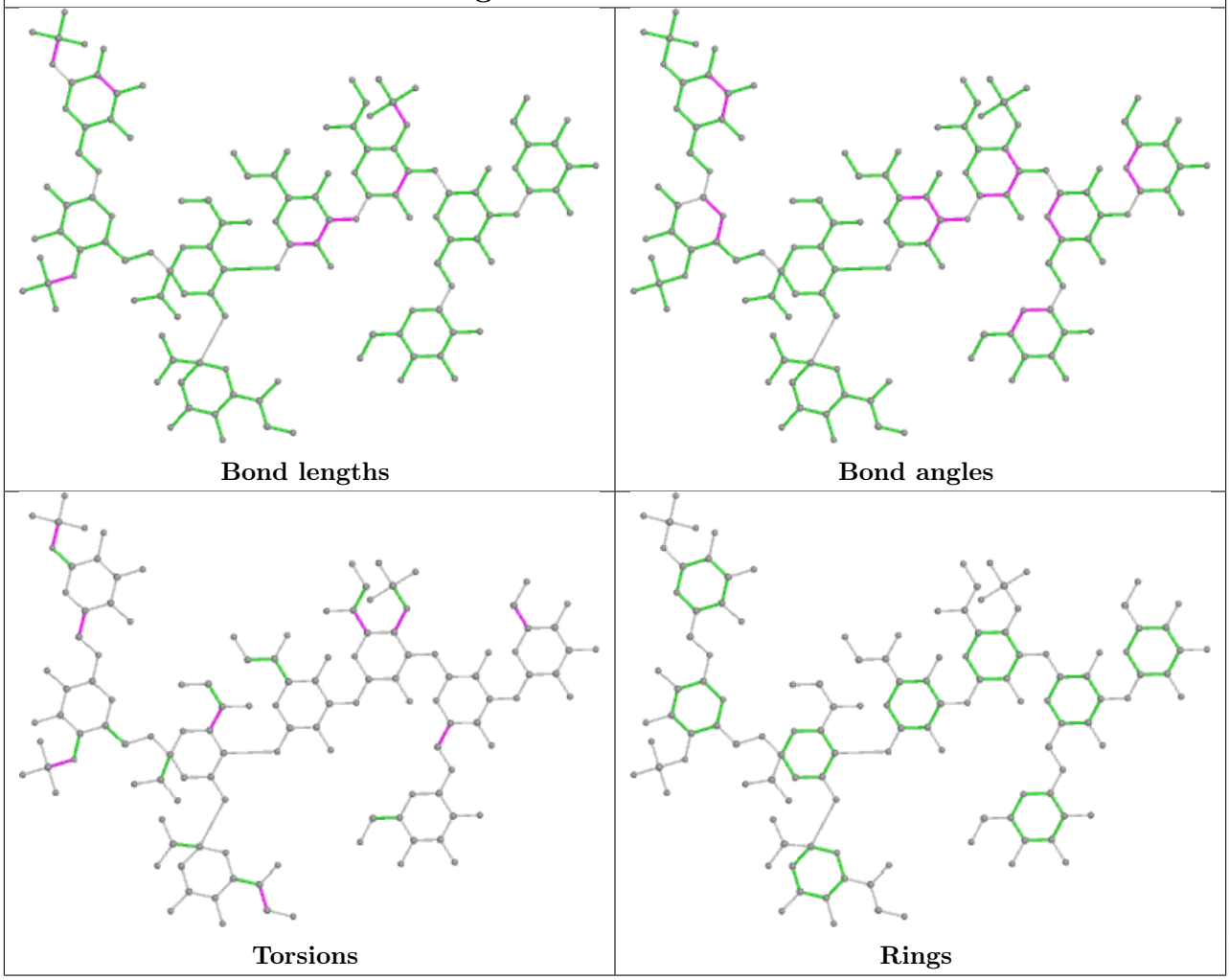
There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	GMH	2	0
2	B	6	GLC	6	0
2	B	3	KDO	1	0
2	B	8	GLA	6	0
2	B	1	GP1	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 oligosaccharide.

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
6	LIM	A	806	2	15,16,17	3.36	1 (6%)	16,16,18	2.30	4 (25%)
5	AAE	A	805	2	4,5,6	3.05	1 (25%)	5,5,7	2.52	2 (40%)
4	LIL	A	804	2	30,30,31	0.71	1 (3%)	30,31,33	1.04	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	LIL	A	803	2	30,30,31	0.77	1 (3%)	30,31,33	1.07	2 (6%)
7	EA2	A	807	2	6,10,11	1.28	1 (16%)	7,13,16	1.04	1 (14%)

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
6	LIM	A	806	2	-	3/14/15/16	-
5	AAE	A	805	2	-	1/2/3/4	-
4	LIL	A	804	2	1/1/2/3	3/31/31/32	-
4	LIL	A	803	2	-	5/31/31/32	-
7	EA2	A	807	2	-	0/8/10/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	806	LIM	O2J-C3J	12.94	1.43	1.21
5	A	805	AAE	O8-C5	5.79	1.44	1.21
4	A	803	LIL	O2E-C1F	3.81	1.45	1.34
4	A	804	LIL	O2E-C1F	3.38	1.43	1.34
7	A	807	EA2	P2-O7P	-2.13	1.50	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	806	LIM	O2J-C3J-C2J	-6.98	109.36	120.83
5	A	805	AAE	O8-C5-C9	-4.38	110.27	121.40
6	A	806	LIM	O2J-C3J-C4J	-4.38	109.86	121.44
4	A	803	LIL	O2E-C1F-O1F	-4.34	113.21	123.70
4	A	804	LIL	O2E-C1F-O1F	-4.08	113.85	123.70
6	A	806	LIM	C2J-C3J-C4J	-2.76	110.02	118.22
5	A	805	AAE	O8-C5-C4	-2.76	111.35	121.16
6	A	806	LIM	O1J-C1J-C2J	-2.32	120.17	126.64
7	A	807	EA2	P2-O7P-C1	-2.09	111.29	121.59
4	A	803	LIL	O1E-C1E-C2E	-2.02	119.55	125.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	804	LIL	C3E

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	LIL	O1F-C1F-O2E-C3E
4	A	803	LIL	C2F-C1F-O2E-C3E
4	A	804	LIL	O2E-C3E-C4E-C5E
4	A	803	LIL	C1F-C2F-C3F-C4F
4	A	804	LIL	C1F-C2F-C3F-C4F
4	A	803	LIL	C1S-C0S-C9E-C8E
6	A	806	LIM	C1X-C2X-C3X-C4X
6	A	806	LIM	O2J-C3J-C4J-C5J
4	A	804	LIL	C2F-C1F-O2E-C3E
4	A	803	LIL	C4F-C5F-C6F-C7F
6	A	806	LIM	C1J-C2J-C3J-O2J
5	A	805	AAE	C2-C4-C5-C9

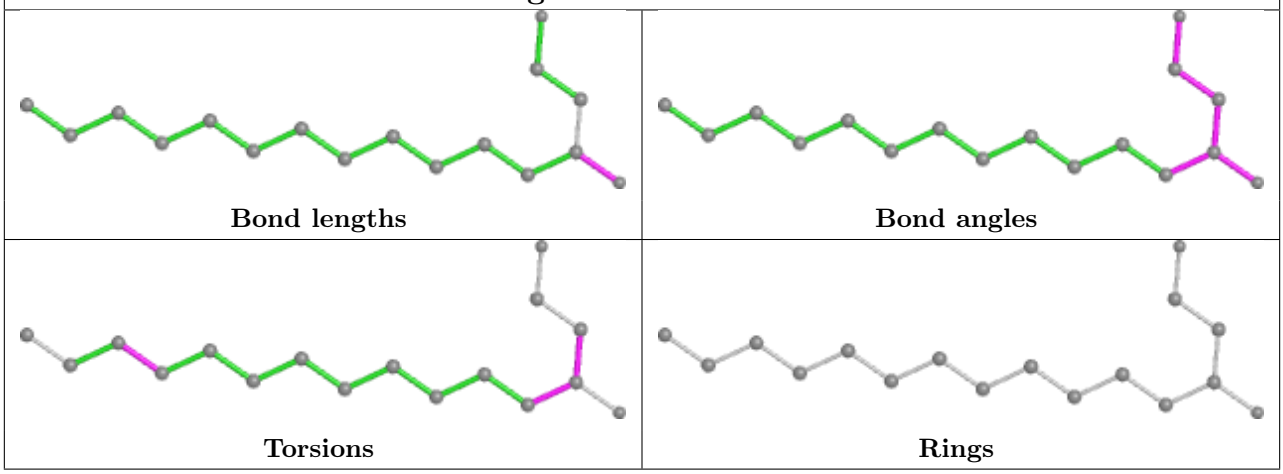
There are no ring outliers.

5 monomers are involved in 18 short contacts:

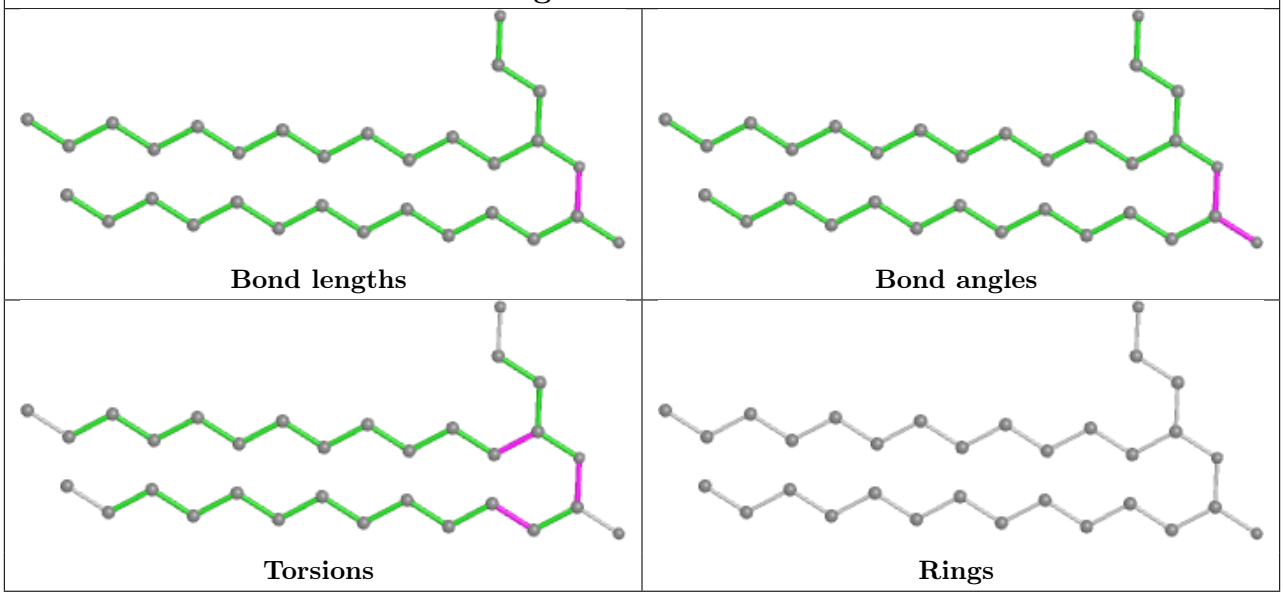
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	806	LIM	5	0
5	A	805	AAE	1	0
4	A	804	LIL	7	0
4	A	803	LIL	11	0
7	A	807	EA2	1	0

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.

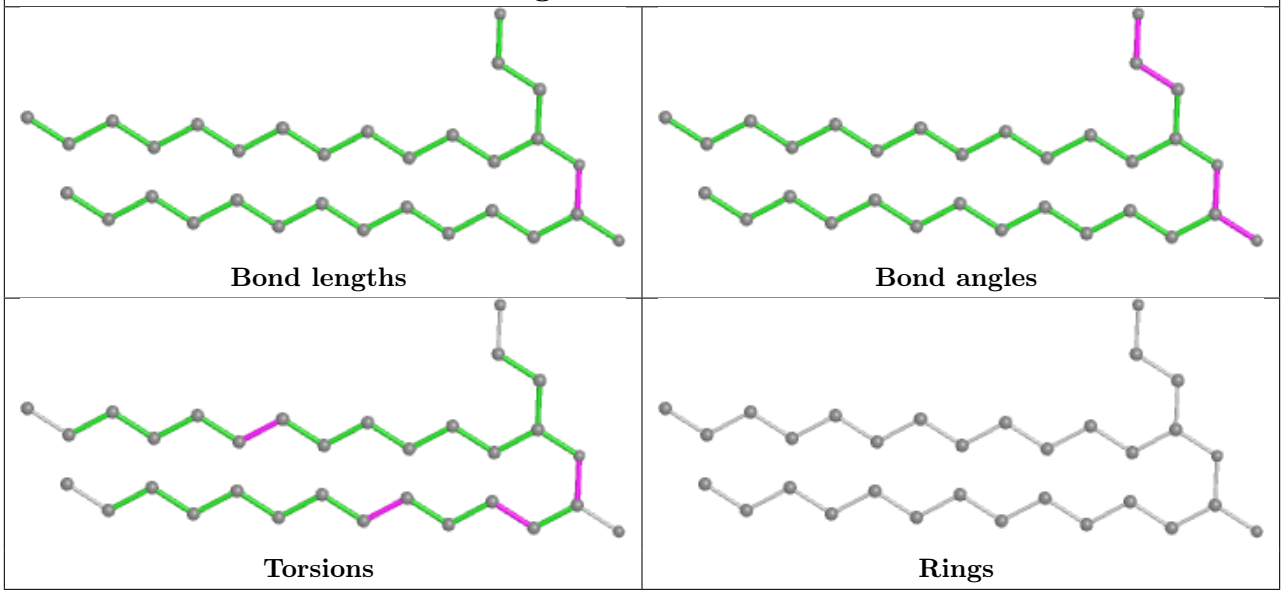
Ligand LIM A 806



Ligand LIL A 804



Ligand LIL A 803



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	705/723 (97%)	-0.12	12 (1%) 70 72	35, 64, 99, 119	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	LYS	4.2
1	A	723	PHE	3.6
1	A	19	GLU	3.6
1	A	635	PRO	3.0
1	A	519	GLY	2.7
1	A	566	PHE	2.6
1	A	632	PHE	2.5
1	A	119	ALA	2.4
1	A	366	ALA	2.3
1	A	99	GLY	2.3
1	A	101	SER	2.0
1	A	369	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)

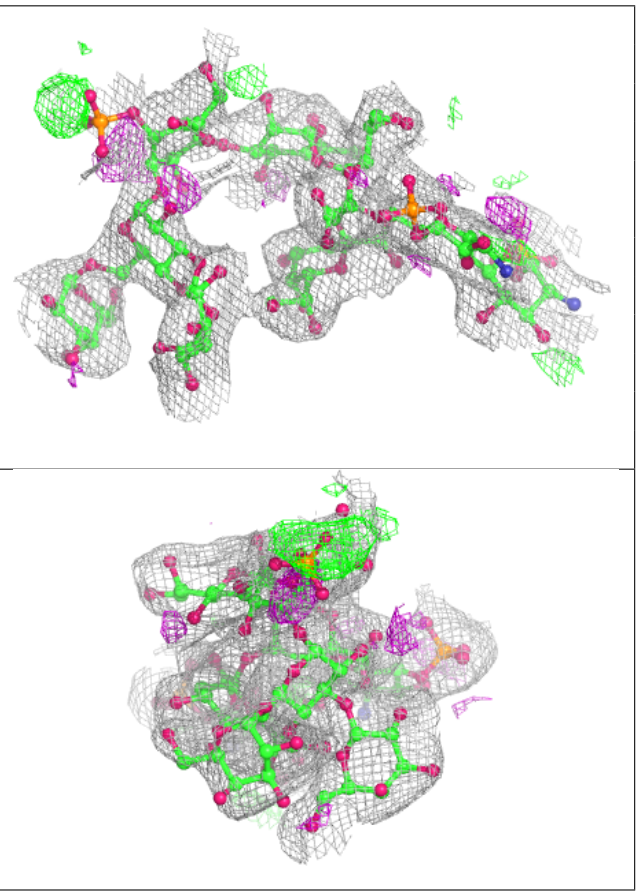
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GPH	B	5	17/18	0.87	0.18	52,84,106,113	0
2	GLA	B	8	11/12	0.88	0.31	101,111,120,120	0
2	GLA	B	7	11/12	0.89	0.31	97,110,116,117	0
2	KDO	B	9	15/16	0.91	0.20	69,78,84,87	0
2	GLC	B	6	11/12	0.92	0.31	80,98,107,114	0
2	GMH	B	4	13/14	0.96	0.12	44,58,75,81	0
2	GP1	B	1	16/16	0.96	0.10	53,65,80,83	0
2	GP4	B	2	15/16	0.96	0.13	35,53,71,81	0
2	KDO	B	3	15/16	0.98	0.11	49,60,76,92	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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



6.4 Ligands (i)

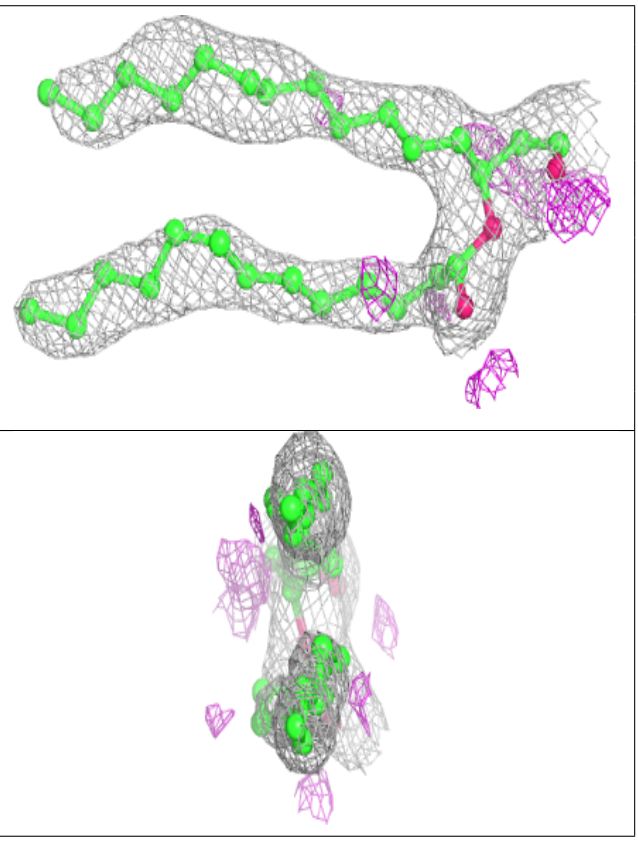
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	AAE	A	805	6/7	0.82	0.25	82,95,101,105	0
3	NI	A	802	1/1	0.84	0.11	120,120,120,120	0
4	LIL	A	803	31/32	0.90	0.27	65,82,92,95	0
3	NI	A	801	1/1	0.90	0.05	100,100,100,100	0
7	EA2	A	807	11/12	0.94	0.15	59,102,120,120	0
6	LIM	A	806	17/18	0.95	0.21	57,69,86,97	0
4	LIL	A	804	31/32	0.95	0.18	46,65,74,84	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.

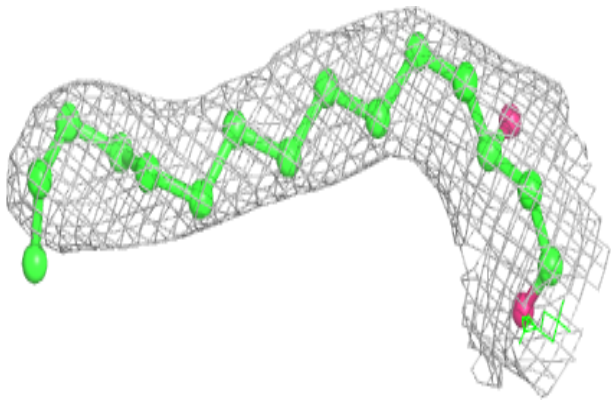
Electron density around LIL A 803:

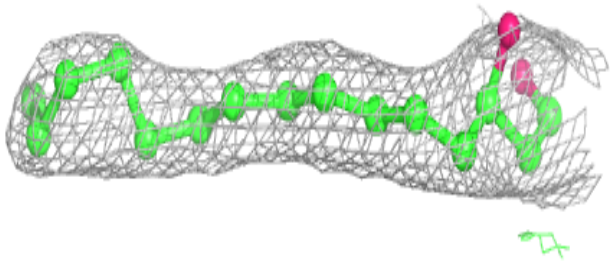
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

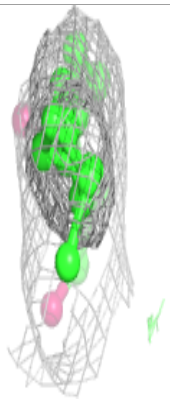


Electron density around LIM A 806:

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

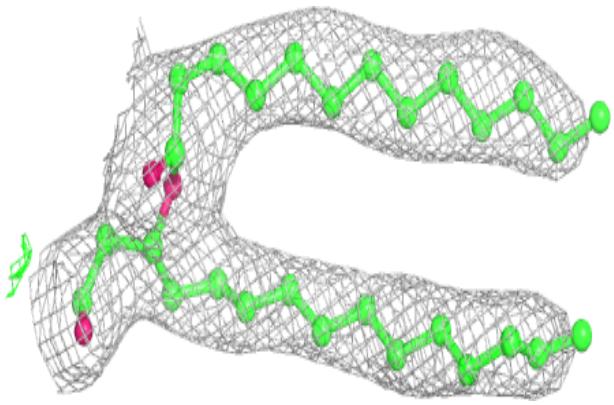


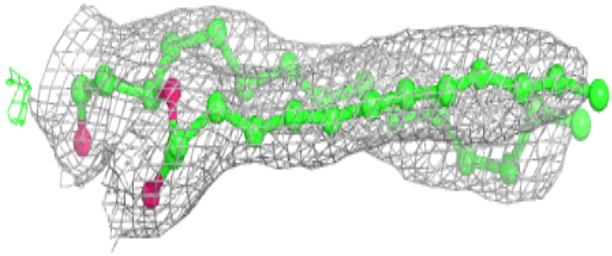


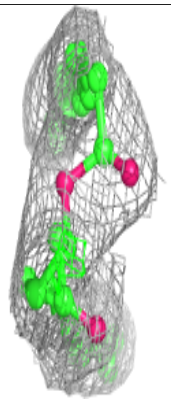


Electron density around LIL A 804:

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







6.5 Other polymers (i)

There are no such residues in this entry.