wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 10:22 PM EDT

PDB ID	:	1FCP
Title	:	FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) FROM E.COLI IN COMPLEX WITH BOUND FERRICHROME-IRON
Authors	:	Hofmann, E.; Ferguson, A.D.; Diederichs, K.; Welte, W.
Deposited on	:	1998-10-14
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

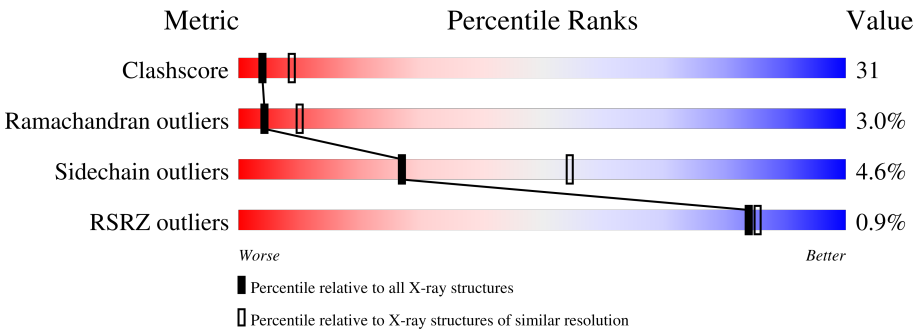
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	705	% 52% 44%
2	B	9	11% 56% 33%

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
4	LIL	A	904	X	-	-	-
5	AAE	A	905	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	FCI	A	750	X	-	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5832 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.

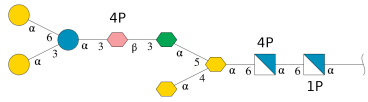
- Molecule 1 is a protein called PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	705	5512	3469	942	1087	4	10	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.

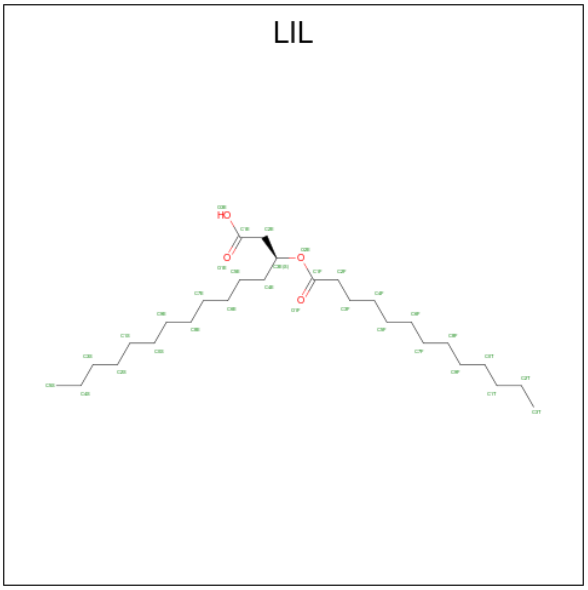


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	9	124	60	2	59	3	0	0	0

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

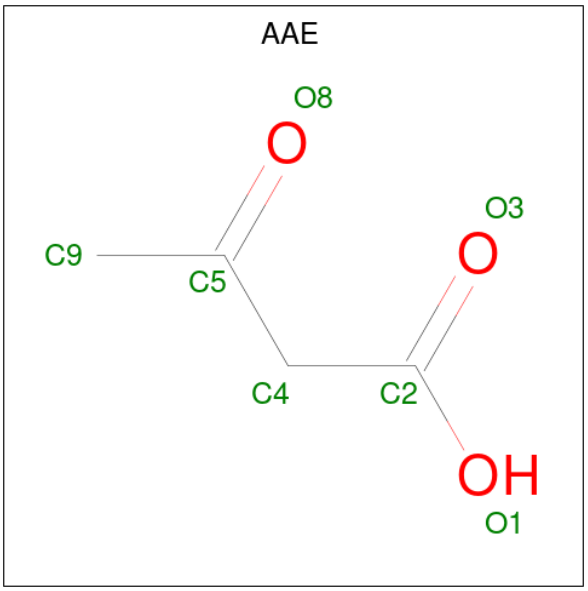
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
3	A	2	2	2	0	0

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



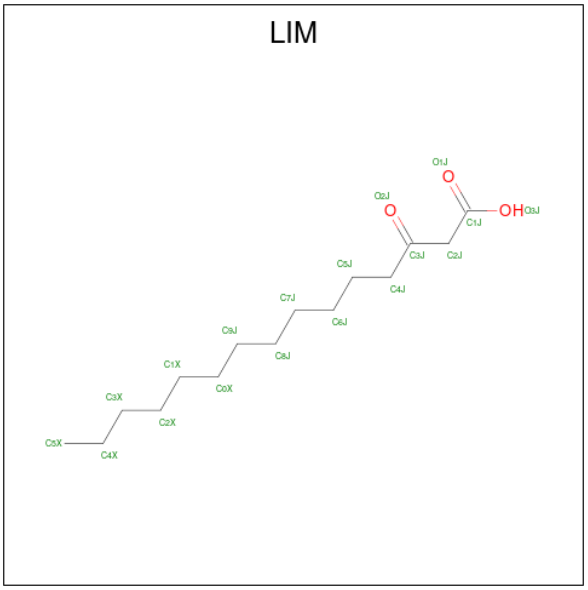
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	31	28	3	0	0
			Total	C	O		
4	A	1	31	28	3	0	0

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



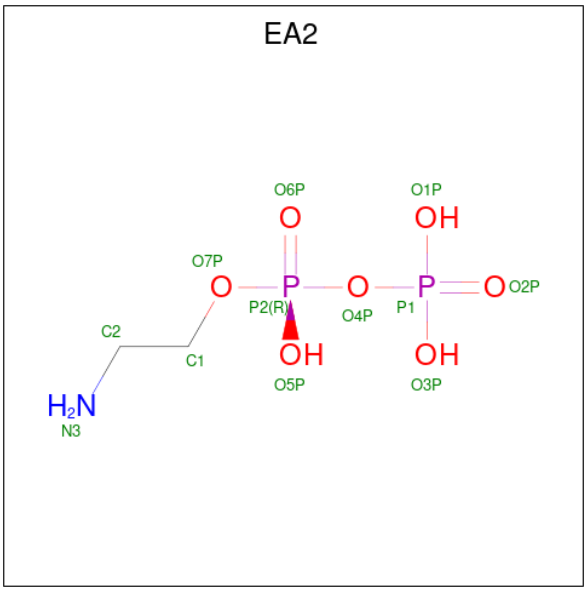
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	4	2	0	0

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



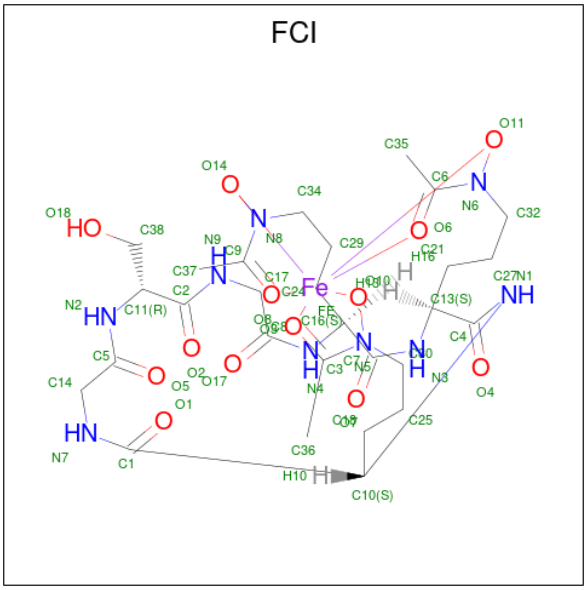
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	17	15	2	0	0

- 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 FERRICROCIN-IRON (three-letter code: FCI) (formula: $C_{28}H_{44}FeN_9O_{13}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
8	A	1	46	24	1	9	12	0	0

- Molecule 9 is water.

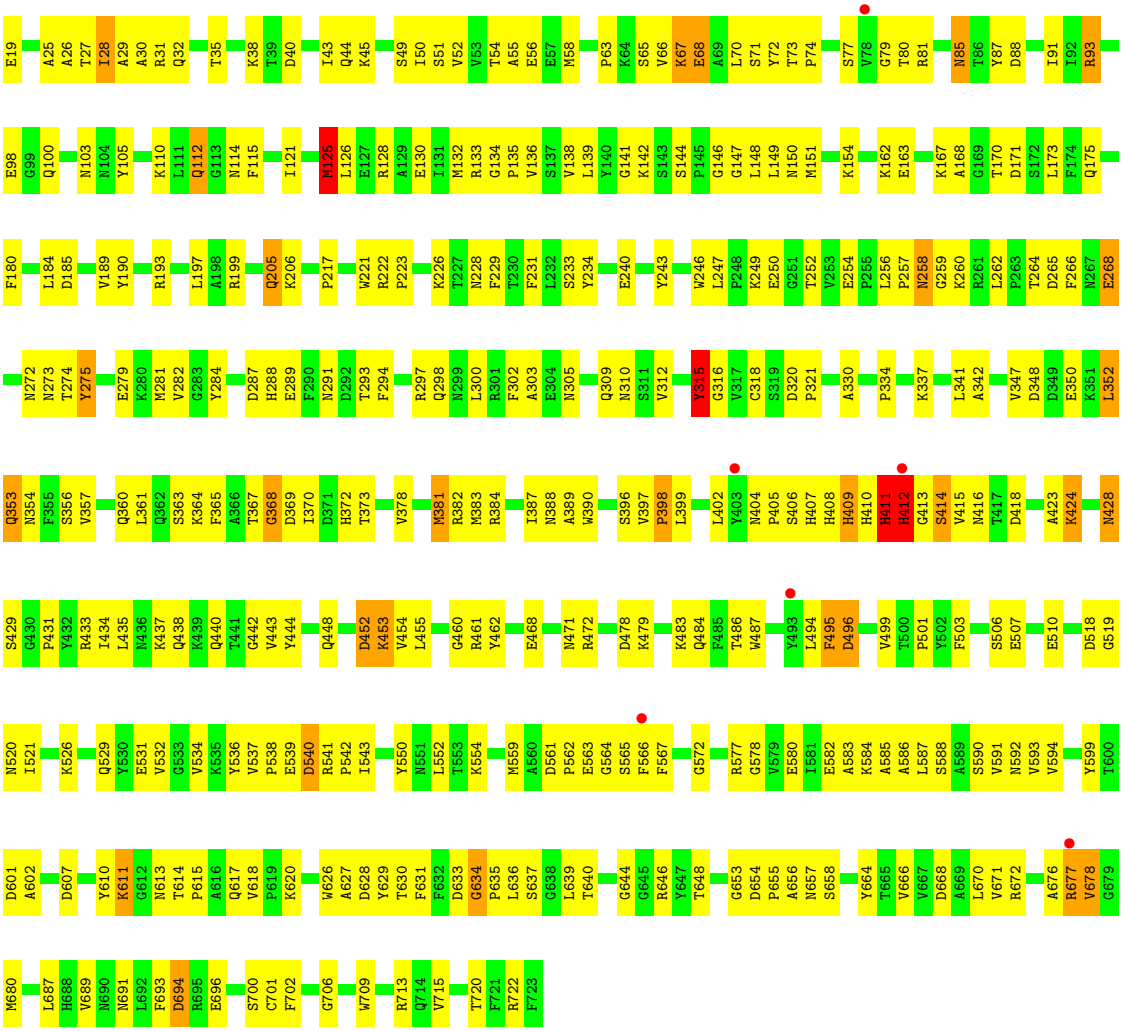
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	52	52	52	0	0

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)

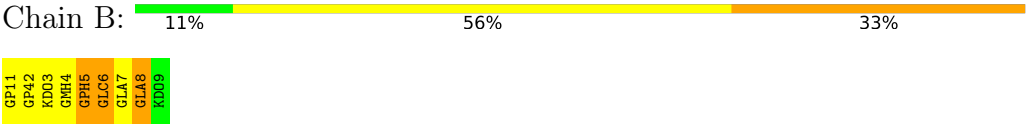
Chain A:



• 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:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	171.40Å 171.40Å 85.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 46.94 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.00-2.70) 97.5 (46.94-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.69Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.232 , 0.281 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	59.8	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5832	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: GMH, EA2, GP4, GPH, LIM, AAE, GLC, GLA, GP1, NI, FCI, LIL, KDO

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	0.45	2/5642 (0.0%)	0.71	8/7650 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	MSE	CG-SE	-5.73	1.75	1.95
1	A	680	MSE	CG-SE	-5.18	1.77	1.95

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	412	HIS	N-CA-C	15.24	152.14	111.00
1	A	412	HIS	CA-C-N	-9.20	97.79	116.20
1	A	409	HIS	N-CA-C	-7.00	92.10	111.00
1	A	411	HIS	N-CA-C	-6.74	92.82	111.00
1	A	412	HIS	CB-CA-C	-6.00	98.41	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	412	HIS	Mainchain

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	329	0
2	B	124	0	70	4	0
3	A	2	0	0	0	0
4	A	62	0	106	16	0
5	A	6	0	5	0	0
6	A	17	0	27	6	0
7	A	11	0	6	0	0
8	A	46	0	31	2	0
9	A	52	0	0	6	0
All	All	5832	0	5458	343	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 31.

The worst 5 of 343 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:410:HIS:HA	1:A:412:HIS:ND1	1.69	1.06
1:A:121:ILE:HB	1:A:151:MSE:HE1	1.40	1.01
1:A:28:ILE:HD12	1:A:28:ILE:H	1.24	1.00
1:A:410:HIS:H	1:A:412:HIS:HB3	1.27	0.97
1:A:410:HIS:CA	1:A:412:HIS:ND1	2.29	0.95

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	703/705 (100%)	624 (89%)	58 (8%)	21 (3%)	4 10

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	PHE
1	A	633	ASP
1	A	634	GLY
1	A	368	GLY
1	A	414	SER

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	585/575 (102%)	558 (95%)	27 (5%)	27 54

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	LEU
1	A	381	MSE
1	A	496	ASP
1	A	354	ASN
1	A	404	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	ASN
1	A	592	ASN
1	A	310	ASN
1	A	328	GLN
1	A	354	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	3,2	15,16,16	1.49	1 (6%)	23,24,24	0.79	0
2	GP4	B	2	2	15,15,16	1.63	2 (13%)	18,22,24	1.11	1 (5%)
2	KDO	B	3	2	15,15,16	0.85	0	19,21,24	1.03	1 (5%)
2	GMH	B	4	2	13,13,14	0.87	0	17,18,20	0.98	1 (5%)
2	GPH	B	5	3,2	17,17,18	1.42	3 (17%)	23,25,27	1.17	3 (13%)
2	GLC	B	6	2	11,11,12	0.71	0	15,15,17	1.23	2 (13%)
2	GLA	B	7	2	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
2	GLA	B	8	2	11,11,12	0.66	0	15,15,17	0.84	1 (6%)
2	KDO	B	9	2	15,15,16	0.69	0	19,21,24	0.98	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	3,2	-	3/6/27/27	0/1/1/1
2	GP4	B	2	2	-	0/7/24/27	0/1/1/1
2	KDO	B	3	2	-	0/10/26/30	0/1/1/1
2	GMH	B	4	2	-	0/6/23/26	0/1/1/1
2	GPH	B	5	3,2	-	0/11/28/31	0/1/1/1
2	GLC	B	6	2	-	0/2/19/22	0/1/1/1
2	GLA	B	7	2	-	2/2/19/22	0/1/1/1
2	GLA	B	8	2	-	1/2/19/22	0/1/1/1
2	KDO	B	9	2	-	2/10/26/30	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GP4	P4A-O4	-4.91	1.50	1.59
2	B	1	GP1	P4B-O1	-4.59	1.50	1.59
2	B	5	GPH	P1-O4	-3.39	1.52	1.59
2	B	2	GP4	C1-C2	2.84	1.55	1.52
2	B	5	GPH	O5-C5	2.59	1.46	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	GP4	C1-O5-C5	3.45	116.87	112.19
2	B	7	GLA	C1-O5-C5	3.43	116.83	112.19
2	B	5	GPH	C6-C5-C4	-2.80	109.27	114.18
2	B	4	GMH	O3-C3-C2	2.79	115.34	109.99
2	B	5	GPH	C1-C2-C3	2.75	113.05	109.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	GP1	C1-O1-P4B-O7B
2	B	1	GP1	C4-C5-C6-O6
2	B	1	GP1	O5-C5-C6-O6
2	B	9	KDO	C6-C7-C8-O8
2	B	9	KDO	O7-C7-C8-O8

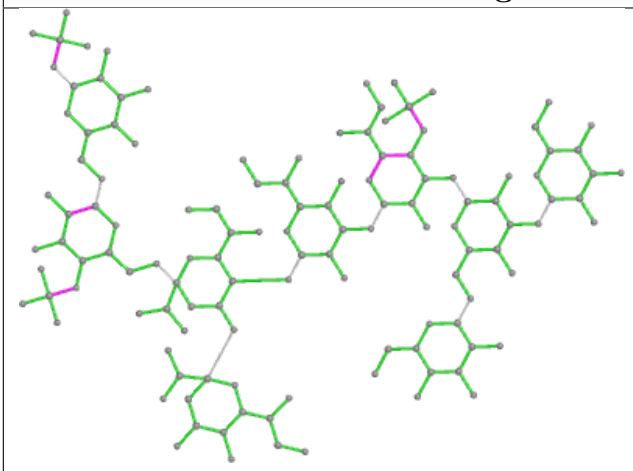
There are no ring outliers.

3 monomers are involved in 4 short contacts:

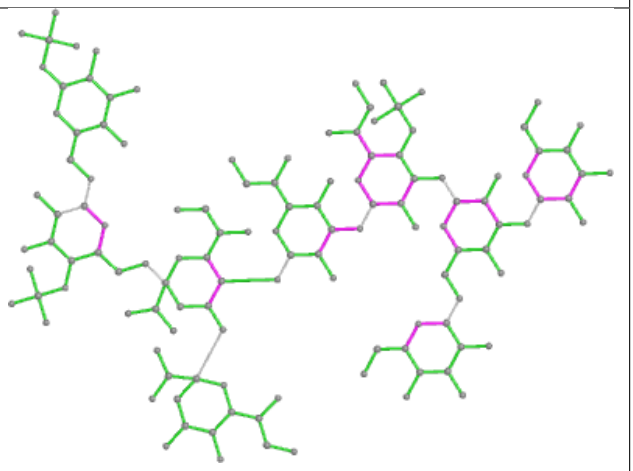
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	GLC	4	0
2	B	5	GPH	1	0
2	B	8	GLA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

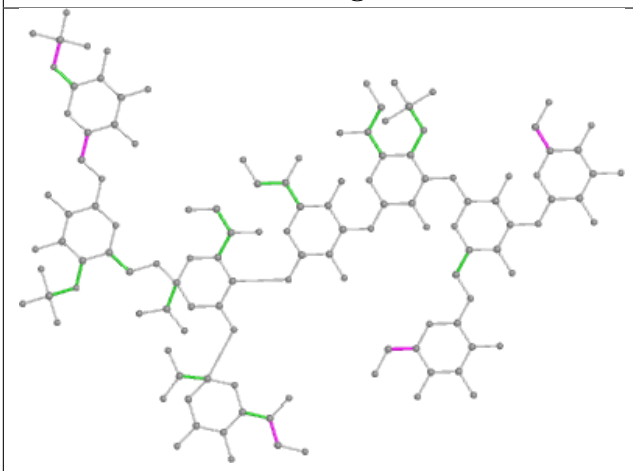
Oligosaccharide Chain B



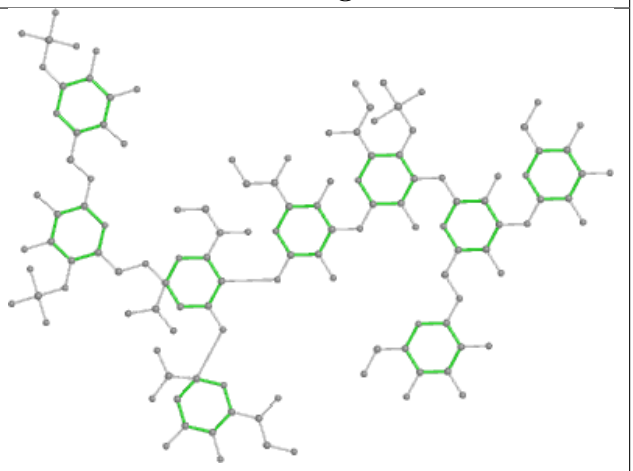
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	LIL	A	904	-	30,30,31	0.71	1 (3%)	30,31,33	1.05	2 (6%)
7	EA2	A	1008	-	6,10,11	1.34	1 (16%)	7,13,16	1.13	1 (14%)
4	LIL	A	903	-	30,30,31	0.79	1 (3%)	30,31,33	1.05	1 (3%)
5	AAE	A	905	-	4,5,6	2.96	1 (25%)	5,5,7	2.89	4 (80%)
6	LIM	A	906	-	15,16,17	3.38	1 (6%)	16,16,18	2.26	4 (25%)
8	FCI	A	750	-	45,51,56	0.42	0	51,78,87	0.63	2 (3%)

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	LIL	A	904	-	1/1/2/3	4/31/31/32	-
7	EA2	A	1008	-	-	1/8/10/11	-
4	LIL	A	903	-	-	5/31/31/32	-
5	AAE	A	905	-	-	2/2/3/4	-
6	LIM	A	906	-	-	3/14/15/16	-
8	FCI	A	750	-	3/3/13/23	6/57/102/116	0/4/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	906	LIM	O2J-C3J	12.96	1.43	1.21
5	A	905	AAE	O8-C5	5.71	1.43	1.21
4	A	903	LIL	O2E-C1F	3.88	1.45	1.34
4	A	904	LIL	O2E-C1F	3.50	1.44	1.34
7	A	1008	EA2	P2-O7P	-2.37	1.49	1.59

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	906	LIM	O2J-C3J-C2J	-6.79	109.68	120.83
5	A	905	AAE	O8-C5-C9	-4.70	109.47	121.40
6	A	906	LIM	O2J-C3J-C4J	-4.35	109.93	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	903	LIL	O2E-C1F-O1F	-4.24	113.46	123.70
4	A	904	LIL	O2E-C1F-O1F	-3.96	114.13	123.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	904	LIL	C3E
8	A	750	FCI	N6
8	A	750	FCI	N8
8	A	750	FCI	N5

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	LIL	O1F-C1F-O2E-C3E
4	A	903	LIL	C2F-C1F-O2E-C3E
8	A	750	FCI	C25-C30-N5-C3
8	A	750	FCI	C24-C16-C7-O7
8	A	750	FCI	C24-C16-C7-N3

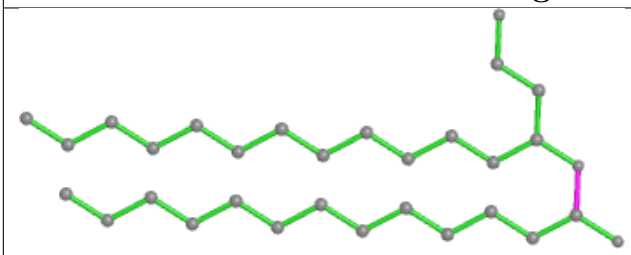
There are no ring outliers.

4 monomers are involved in 20 short contacts:

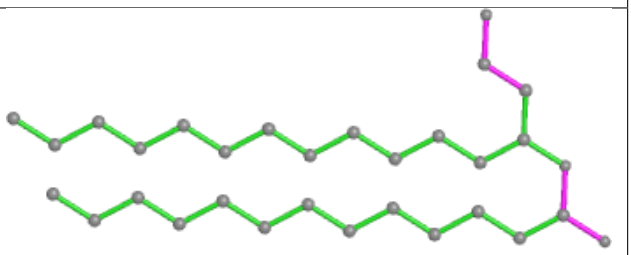
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	904	LIL	8	0
4	A	903	LIL	11	0
6	A	906	LIM	6	0
8	A	750	FCI	2	0

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.

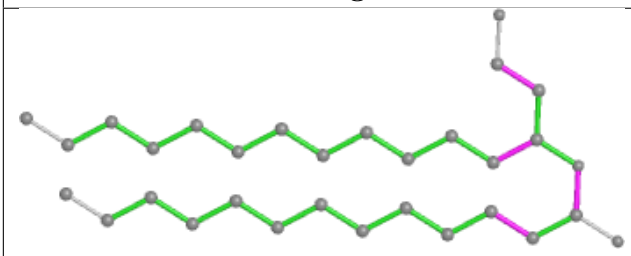
Ligand LIL A 904



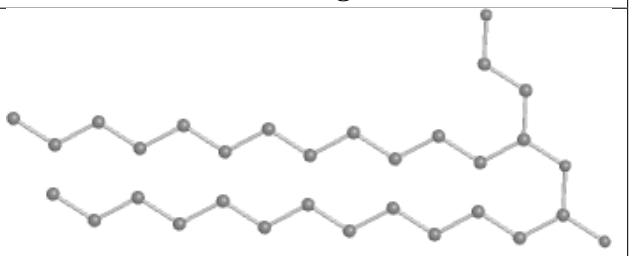
Bond lengths



Bond angles

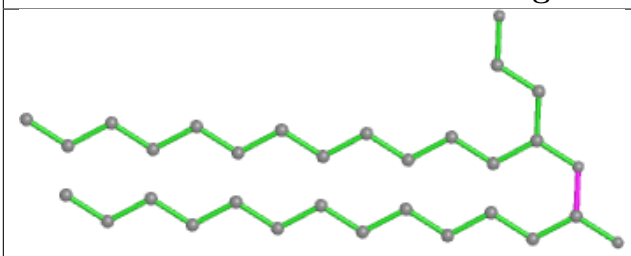


Torsions

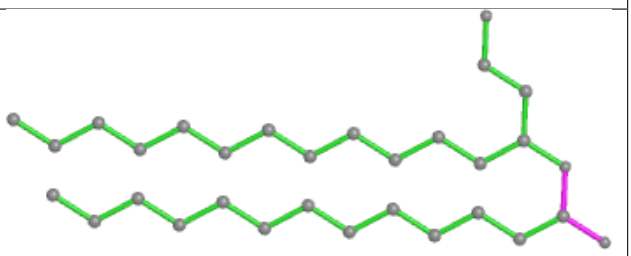


Rings

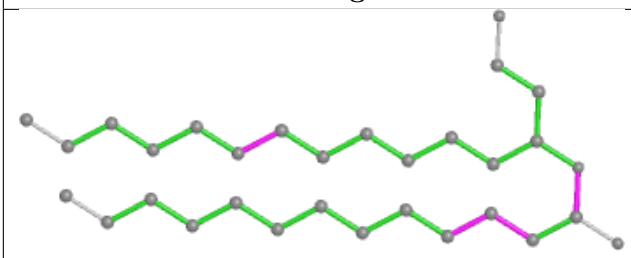
Ligand LIL A 903



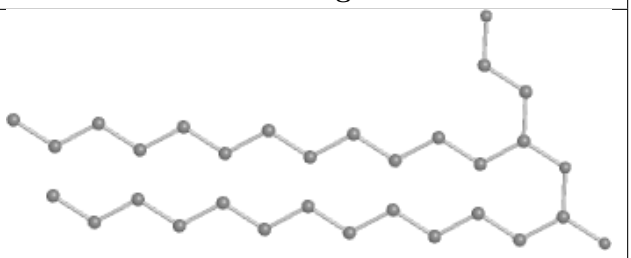
Bond lengths



Bond angles

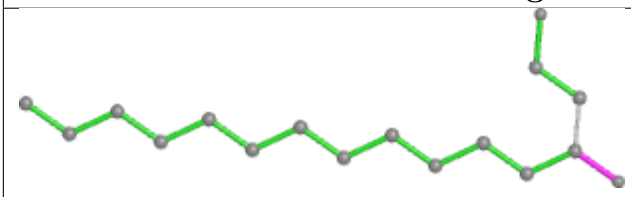


Torsions

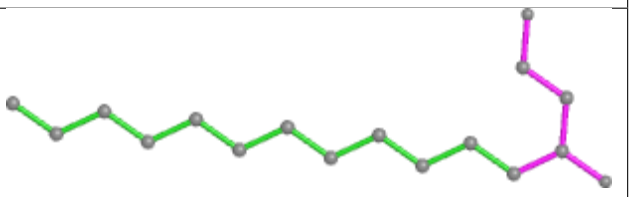


Rings

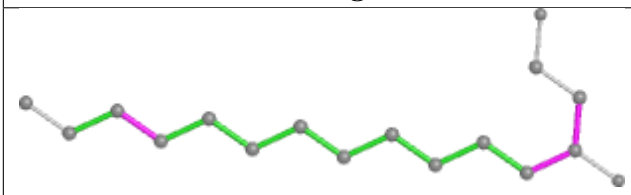
Ligand LIM A 906



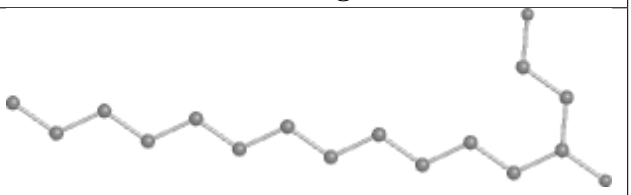
Bond lengths



Bond angles

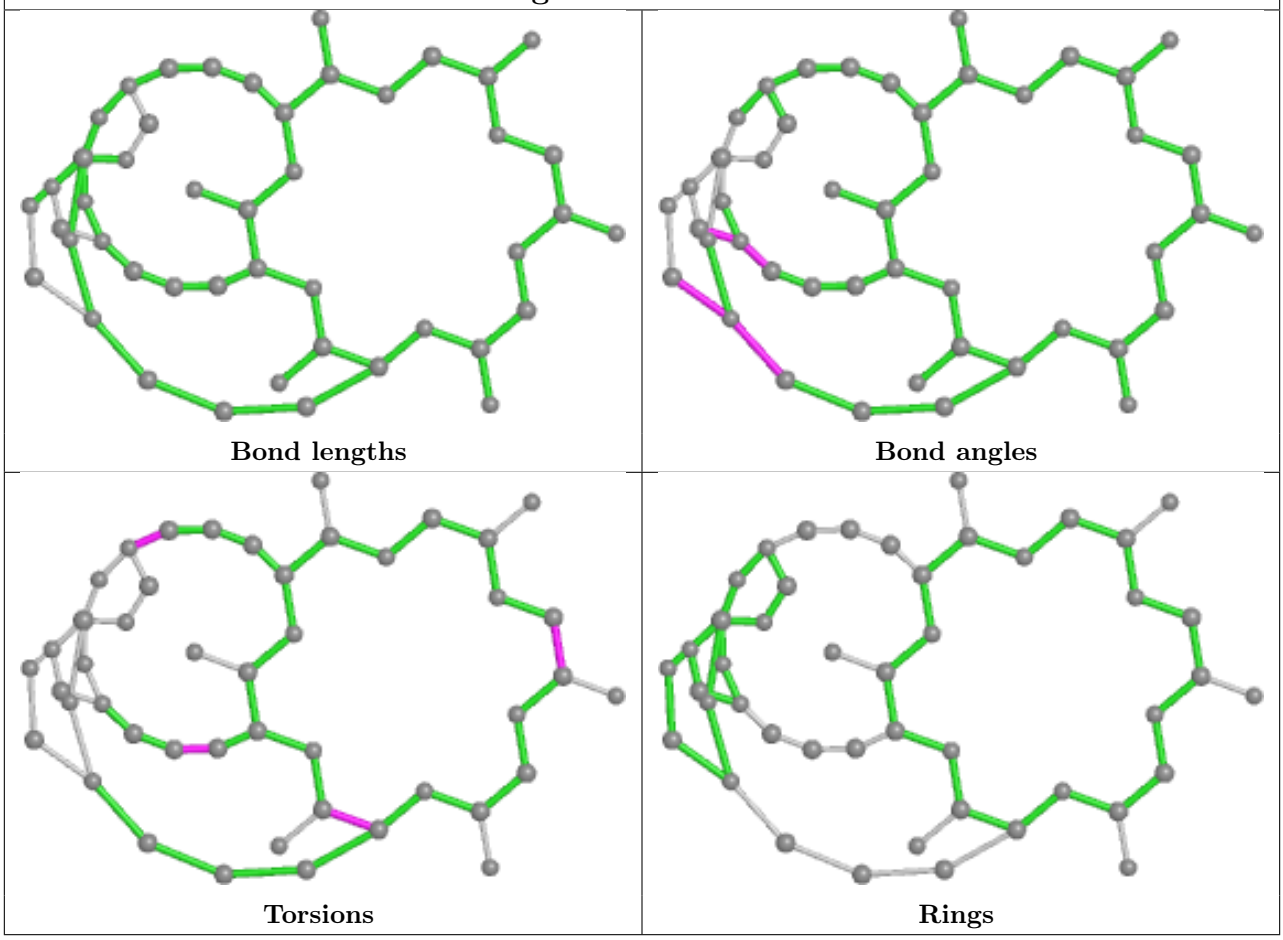


Torsions



Rings

Ligand FCI A 750



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	695/705 (98%)	-0.22	6 (0%) 84 85	31, 62, 94, 113	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	HIS	6.6
1	A	566	PHE	2.9
1	A	493	TYR	2.5
1	A	677	ARG	2.3
1	A	403	TYR	2.3

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	GLA	B	7	11/12	0.82	0.28	74,96,110,120	0
2	GLA	B	8	11/12	0.83	0.21	81,91,107,107	0
2	GPH	B	5	17/18	0.85	0.17	55,82,120,120	0
2	GLC	B	6	11/12	0.90	0.21	74,83,102,110	0
2	KDO	B	9	15/16	0.93	0.13	49,64,80,85	0
2	GMH	B	4	13/14	0.96	0.12	43,59,80,83	0
2	GP1	B	1	16/16	0.97	0.08	50,63,90,103	0

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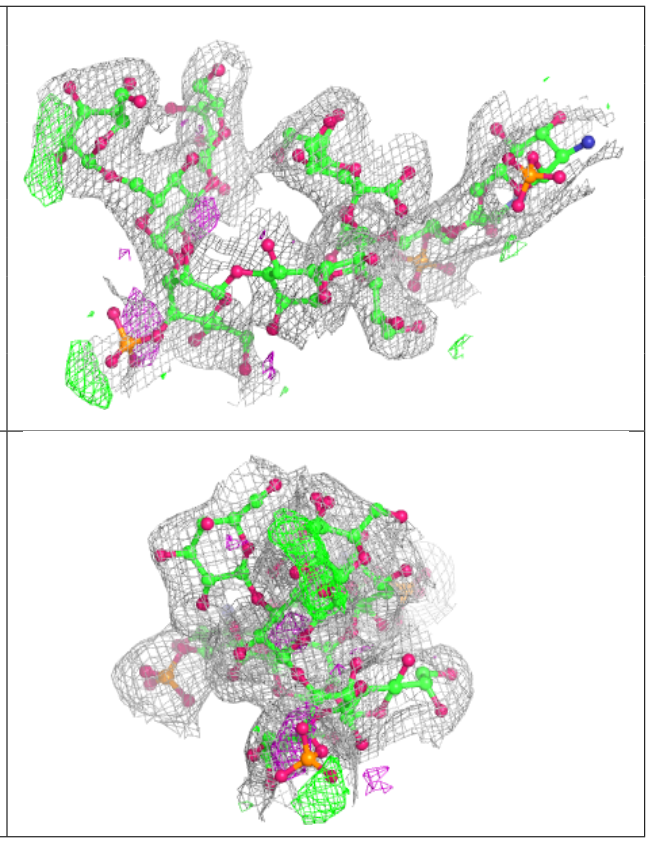
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GP4	B	2	15/16	0.97	0.10	32,46,71,73	0
2	KDO	B	3	15/16	0.97	0.09	45,59,70,92	0

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	905	6/7	0.90	0.20	75,80,86,107	0
4	LIL	A	903	31/32	0.92	0.40	48,78,93,96	0
6	LIM	A	906	17/18	0.93	0.37	54,65,82,97	0
7	EA2	A	1008	11/12	0.93	0.16	52,109,120,120	0
4	LIL	A	904	31/32	0.94	0.30	48,59,76,83	0
3	NI	A	1012	1/1	0.95	0.10	113,113,113,113	0

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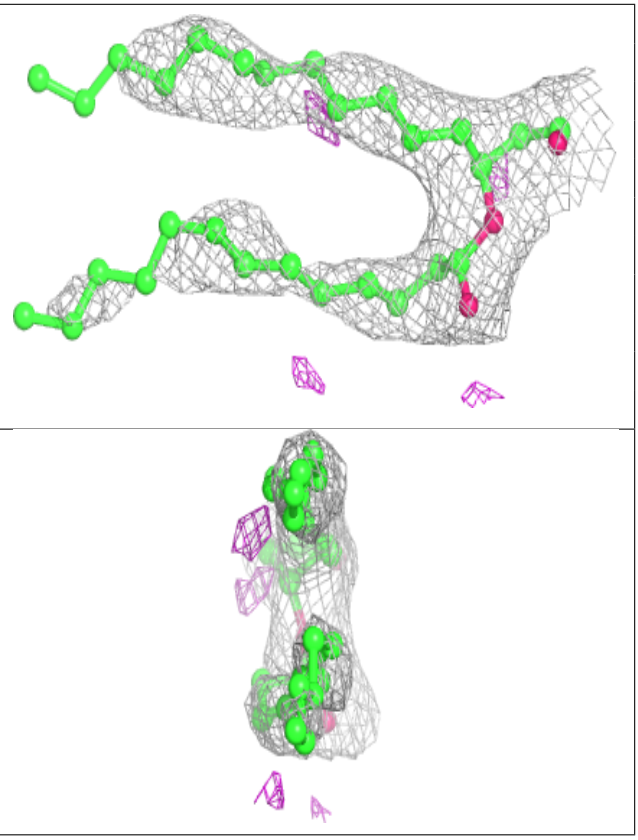
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NI	A	1011	1/1	0.96	0.08	98,98,98,98	0
8	FCI	A	750	46/51	0.98	0.19	21,47,64,69	0

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.

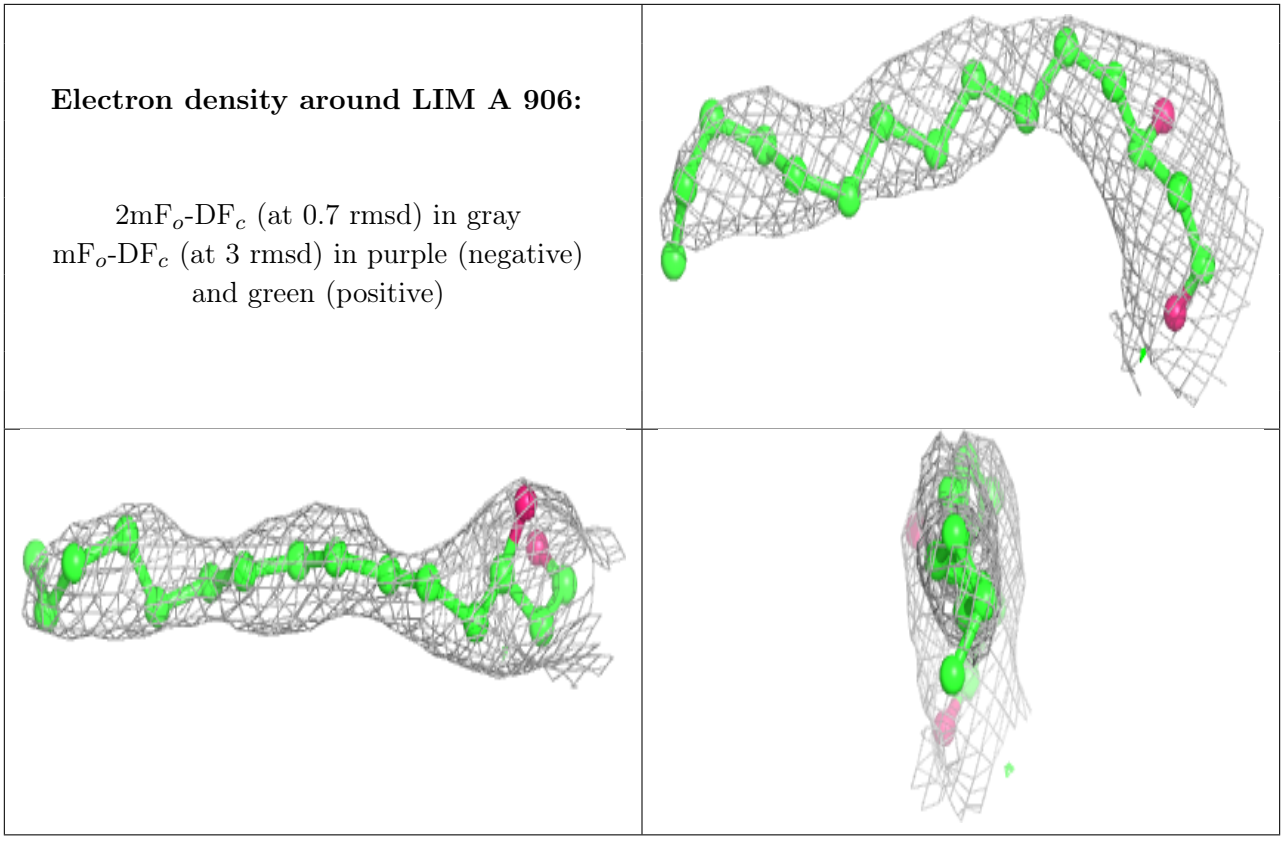
Electron density around LIL A 903:

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



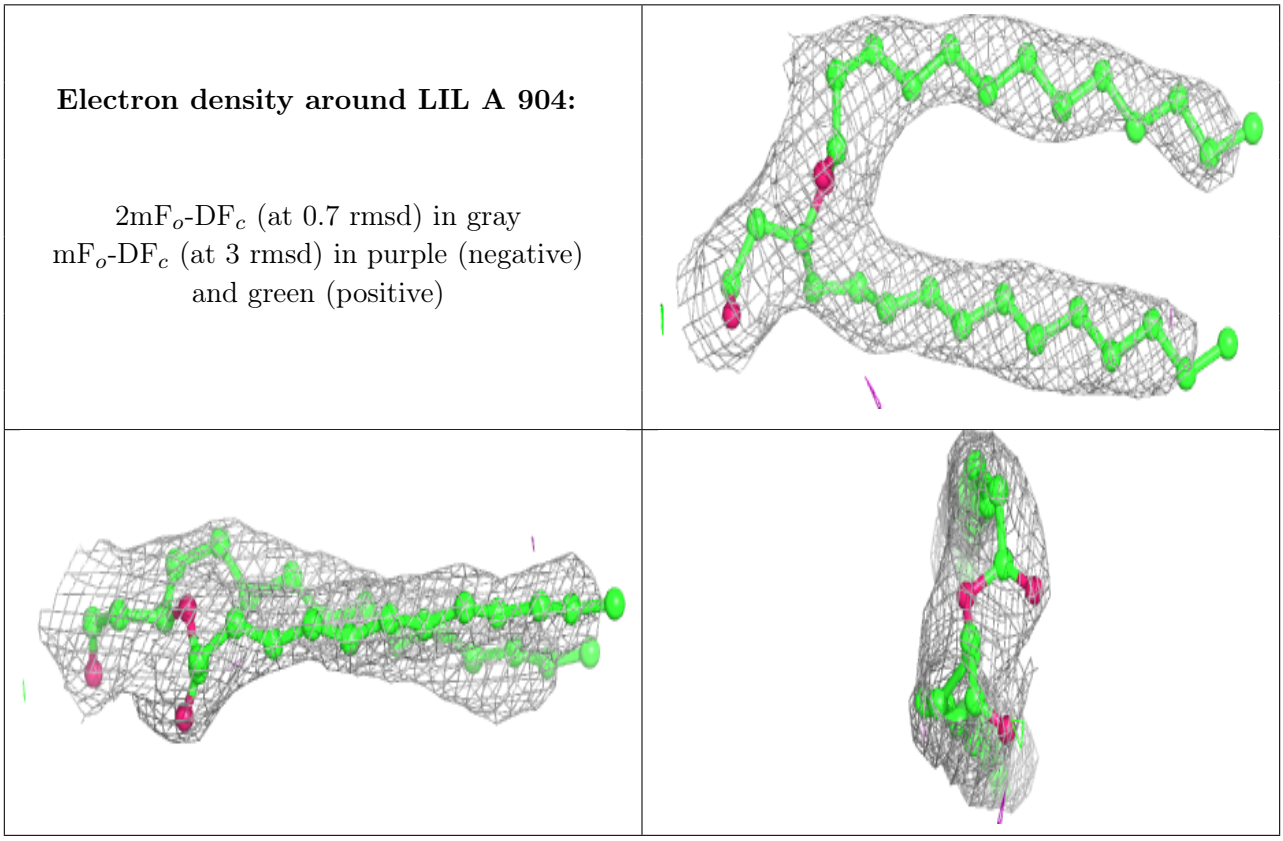
Electron density around LIM A 906:

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



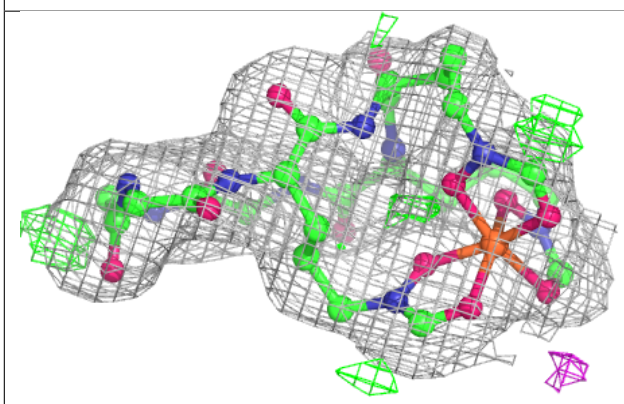
Electron density around LIL A 904:

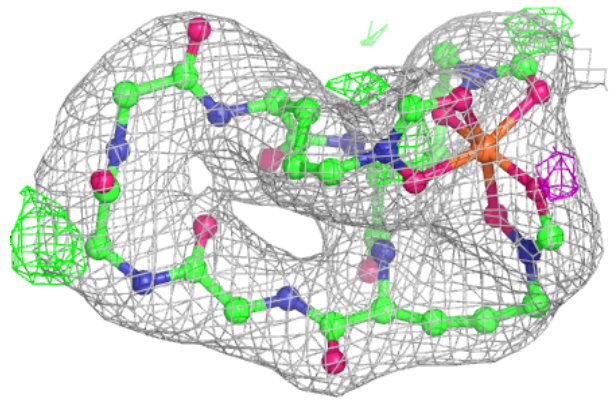
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

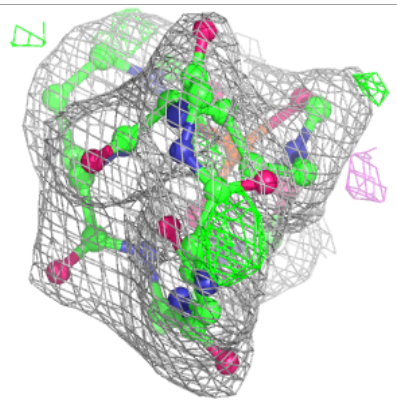


Electron density around FCI A 750:

$2mF_o$-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.