Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2020 – 07:10 PM BST

PDB ID	:	4IRJ
Title	:	Structure of the mouse CD1d-4ClPhC-alpha-GalCer-iNKT TCR complex
Authors	:	Nemcovic, M.; Zajonc, D.M.
Deposited on	:	2013-01-14
Resolution	:	3.00 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 following versions of software and data (see references (i)) were used in the production of this report:

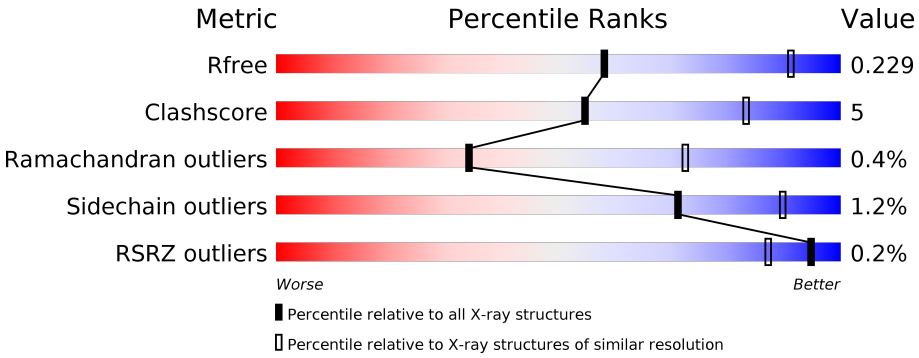
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	285	75% 18% 6%
2	B	99	85% 12% .
3	C	209	86% 11% .
4	D	241	84% 14% ..
5	E	3	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6381 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2103	1345	356	389	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	conflict	UNP P11609
A	280	HIS	-	expression tag	UNP P11609
A	281	HIS	-	expression tag	UNP P11609
A	282	HIS	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	HIS	-	expression tag	UNP P11609

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			748	480	125	137	6			

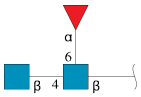
- Molecule 3 is a protein called Valpha14 (mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	202	Total	C	N	O	S	0	0	0
			1518	941	259	310	8			

- Molecule 4 is a protein called Vbeta8.2 (mouse variable domain, human constant domain).

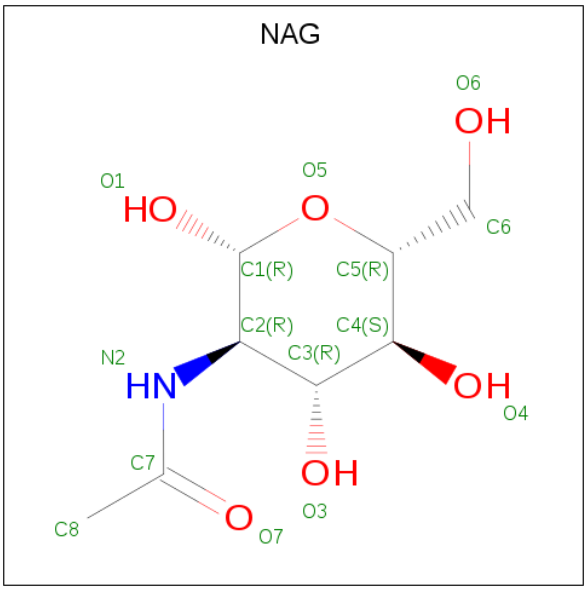
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1863	1170	333	354	6			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



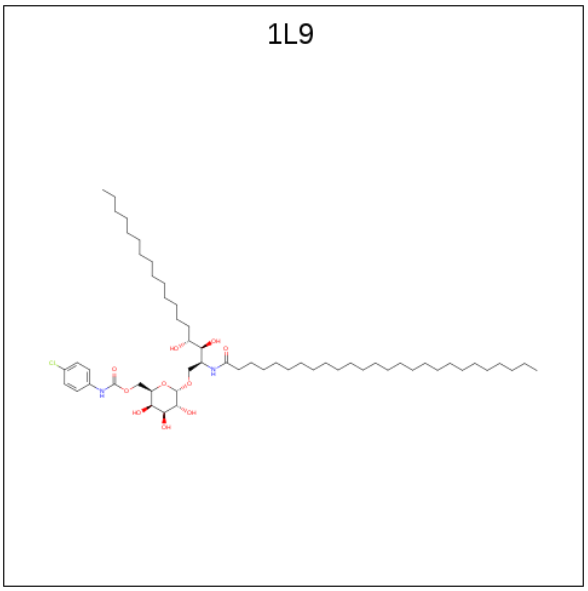
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is N-[(2S,3S,4R)-1-({6-O-[(4-chlorophenyl)carbamoyl]-alpha-D-galactopyranosyl}oxy)-3,4-dihydroxyoctadecan-2-yl]hexacosanamide (three-letter code: 1L9) (formula: $C_{57}H_{103}ClN_2O_{10}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	Cl	N	O	0	0
			70	57	1	2	10		

- Molecule 8 is water.

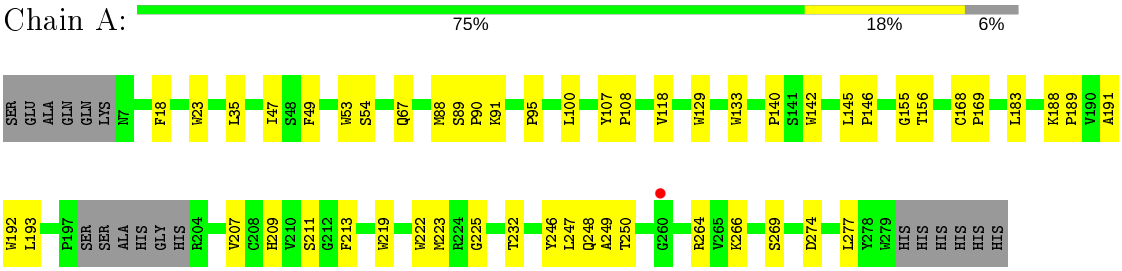
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	O	0	0
			6	6		
8	C	4	Total	O	0	0
			4	4		
8	D	3	Total	O	0	0
			3	3		

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.

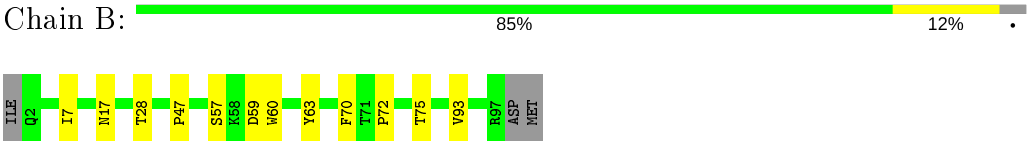
- Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain A:



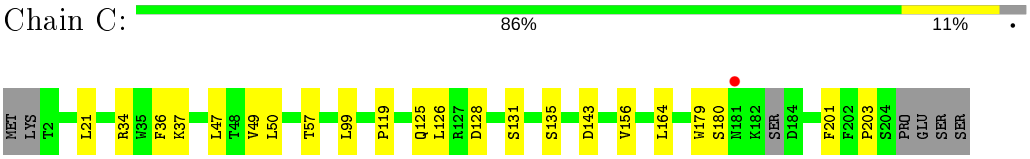
- Molecule 2: Beta-2-microglobulin

Chain B:



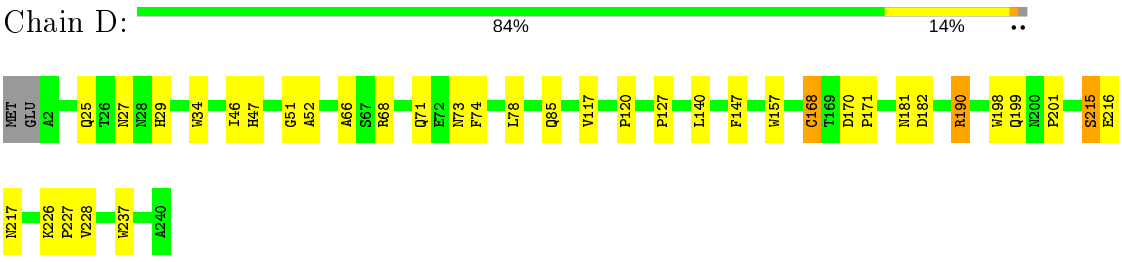
- Molecule 3: Valpha14 (mouse variable domain, human constant domain)

Chain C:



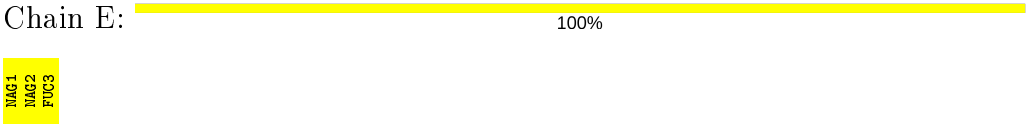
- Molecule 4: Vbeta8.2 (mouse variable domain, human constant domain)

Chain D:



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	79.28Å 191.86Å 151.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.35 – 3.00 38.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.35-3.00) 97.5 (38.35-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	33.70 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.186 , 0.228 0.185 , 0.229	Depositor DCC
R_{free} test set	1185 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6381	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, NAG, 1L9

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	0.67	6/2165 (0.3%)	0.61	0/2952
2	B	0.61	0/774	0.59	0/1062
3	C	0.52	1/1545 (0.1%)	0.59	0/2106
4	D	0.60	4/1914 (0.2%)	0.60	0/2611
All	All	0.61	11/6398 (0.2%)	0.60	0/8731

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	34	TRP	CD2-CE2	5.49	1.48	1.41
1	A	222	TRP	CD2-CE2	5.29	1.47	1.41
3	C	179	TRP	CD2-CE2	5.29	1.47	1.41
1	A	23	TRP	CD2-CE2	5.24	1.47	1.41
4	D	157	TRP	CD2-CE2	5.15	1.47	1.41
4	D	237	TRP	CD2-CE2	5.14	1.47	1.41
1	A	133	TRP	CD2-CE2	5.08	1.47	1.41
4	D	198	TRP	CD2-CE2	5.07	1.47	1.41
1	A	129	TRP	CD2-CE2	5.07	1.47	1.41
1	A	53	TRP	CD2-CE2	5.05	1.47	1.41
1	A	192	TRP	CD2-CE2	5.03	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2103	0	1969	29	0
2	B	748	0	677	4	0
3	C	1518	0	1413	13	0
4	D	1863	0	1764	18	0
5	E	38	0	34	0	0
6	A	28	0	26	0	0
7	A	70	0	103	5	0
8	A	6	0	0	0	0
8	C	4	0	0	0	0
8	D	3	0	0	1	0
All	All	6381	0	5986	64	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 5.

All (64) 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:219:TRP:HB3	1:A:266:LYS:HB2	1.72	0.72
1:A:191:ALA:HA	1:A:209:HIS:O	1.95	0.67
3:C:126:LEU:O	3:C:135:SER:HB2	2.01	0.60
3:C:164:LEU:HB3	4:D:168:CYS:HB3	1.83	0.59
1:A:100:LEU:HD23	7:A:306:1L9:H36	1.86	0.57
4:D:71:GLN:HG3	8:D:302:HOH:O	2.05	0.56
1:A:266:LYS:HG2	1:A:274:ASP:OD1	2.05	0.56
4:D:117:VAL:HG12	4:D:227:PRO:HB2	1.88	0.55
3:C:34:ARG:HD2	3:C:36:PHE:CE2	2.42	0.55
4:D:120:PRO:HB3	4:D:147:PHE:CD1	2.42	0.55
1:A:207:VAL:HG22	1:A:250:THR:HG22	1.89	0.54
3:C:201:PHE:CZ	3:C:203:PRO:HB3	2.43	0.54
1:A:88:MET:CE	1:A:145:LEU:HD23	2.38	0.53
4:D:25:GLN:HE22	4:D:29:HIS:H	1.57	0.53
1:A:88:MET:HE1	1:A:145:LEU:HD23	1.90	0.52
1:A:140:PRO:HB2	1:A:142:TRP:CD1	2.46	0.51
1:A:211:SER:HB2	1:A:246:TYR:CD1	2.47	0.50
4:D:68:ARG:HD2	4:D:73:ASN:O	2.10	0.50
1:A:193:LEU:HG	1:A:277:LEU:HD23	1.93	0.50
2:B:17:ASN:HA	2:B:72:PRO:O	2.12	0.50
4:D:215:SER:C	4:D:217:ASN:H	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HD12	1:A:248:GLN:N	2.27	0.49
1:A:223:MET:HE1	1:A:264:ARG:HD2	1.93	0.49
2:B:7:ILE:HB	2:B:93:VAL:HG21	1.94	0.49
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.93	0.49
3:C:156:VAL:HG22	3:C:180:SER:HB2	1.94	0.49
3:C:128:ASP:HB3	3:C:131:SER:O	2.13	0.48
1:A:247:LEU:HD12	1:A:248:GLN:H	1.79	0.47
1:A:47:ILE:HD12	1:A:67:GLN:HG3	1.98	0.46
4:D:46:ILE:HG22	4:D:47:HIS:CD2	2.50	0.46
4:D:66:ALA:HB1	4:D:74:PHE:CE1	2.51	0.46
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.98	0.45
4:D:120:PRO:HB3	4:D:147:PHE:HB3	1.97	0.45
4:D:181:ASN:O	4:D:182:ASP:HB2	2.17	0.45
3:C:34:ARG:HD2	3:C:36:PHE:CZ	2.52	0.45
4:D:199:GLN:O	4:D:201:PRO:HD3	2.17	0.45
3:C:99:LEU:HA	3:C:99:LEU:HD23	1.75	0.44
1:A:88:MET:O	1:A:91:LYS:HB3	2.17	0.44
4:D:127:PRO:HD3	4:D:140:LEU:HG	1.99	0.44
1:A:89:SER:HB2	1:A:90:PRO:HA	2.00	0.44
3:C:119:PRO:HG3	3:C:143:ASP:HB3	1.98	0.44
3:C:49:VAL:HG13	3:C:49:VAL:O	2.18	0.44
1:A:18:PHE:O	1:A:95:PRO:HA	2.18	0.44
7:A:306:1L9:H97	7:A:306:1L9:H99	1.56	0.44
1:A:118:VAL:HG11	7:A:306:1L9:H73	2.00	0.43
4:D:226:LYS:O	4:D:228:VAL:N	2.51	0.43
2:B:59:ASP:O	2:B:60:TRP:HB2	2.18	0.43
4:D:168:CYS:SG	4:D:190:ARG:HD3	2.59	0.42
4:D:78:LEU:HD23	4:D:85:GLN:OE1	2.19	0.42
3:C:37:LYS:HB2	3:C:47:LEU:HD11	2.00	0.42
1:A:35:LEU:HD12	1:A:183:LEU:HD23	2.00	0.42
1:A:145:LEU:HB3	1:A:146:PRO:HD3	2.01	0.42
1:A:156:THR:HG23	7:A:306:1L9:H50	2.01	0.42
1:A:168:CYS:HB3	1:A:169:PRO:CD	2.50	0.42
1:A:232:THR:HG23	1:A:249:ALA:HB1	2.01	0.42
1:A:211:SER:HB2	1:A:246:TYR:HD1	1.84	0.41
1:A:188:LYS:HA	1:A:269:SER:OG	2.21	0.41
3:C:50:LEU:HD23	3:C:57:THR:HG23	2.02	0.41
4:D:170:ASP:HA	4:D:171:PRO:HD3	1.93	0.41
3:C:125:GLN:C	3:C:126:LEU:HD12	2.41	0.41
1:A:155:GLY:HA3	7:A:306:1L9:O3A	2.20	0.41
1:A:49:PHE:HB3	1:A:54:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:GLY:O	4:D:52:ALA:C	2.59	0.40
2:B:28:THR:HG22	2:B:63:TYR:HB2	2.03	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	263/285 (92%)	254 (97%)	8 (3%)	1 (0%)	34 72
2	B	94/99 (95%)	91 (97%)	2 (2%)	1 (1%)	14 50
3	C	198/209 (95%)	184 (93%)	14 (7%)	0	100 100
4	D	237/241 (98%)	229 (97%)	7 (3%)	1 (0%)	34 72
All	All	792/834 (95%)	758 (96%)	31 (4%)	3 (0%)	34 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	47	PRO
4	D	216	GLU
1	A	225	GLY

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	223/249 (90%)	223 (100%)	0	100	100
2	B	79/93 (85%)	76 (96%)	3 (4%)	33	69
3	C	169/188 (90%)	168 (99%)	1 (1%)	86	95
4	D	200/208 (96%)	196 (98%)	4 (2%)	55	83
All	All	671/738 (91%)	663 (99%)	8 (1%)	71	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	57	SER
2	B	70	PHE
2	B	75	THR
3	C	21	LEU
4	D	27	ASN
4	D	168	CYS
4	D	190	ARG
4	D	215	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
3	C	31	ASN
3	C	53	GLN
4	D	10	ASN
4	D	25	GLN
4	D	116	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)

3 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	$\#\|Z\| > 2$
5	NAG	E	1	1,5	14,14,15	0.57	0	17,19,21	1.24	1 (5%)
5	NAG	E	2	5	14,14,15	0.45	0	17,19,21	1.31	1 (5%)
5	FUC	E	3	5	10,10,11	0.57	0	14,14,16	1.28	2 (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
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	FUC	E	3	5	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C1-O5-C5	3.95	117.55	112.19
5	E	3	FUC	C3-C4-C5	-2.77	105.46	109.77
5	E	3	FUC	C1-C2-C3	2.55	112.80	109.67
5	E	1	NAG	O5-C5-C6	2.22	110.69	107.20

There are no chirality outliers.

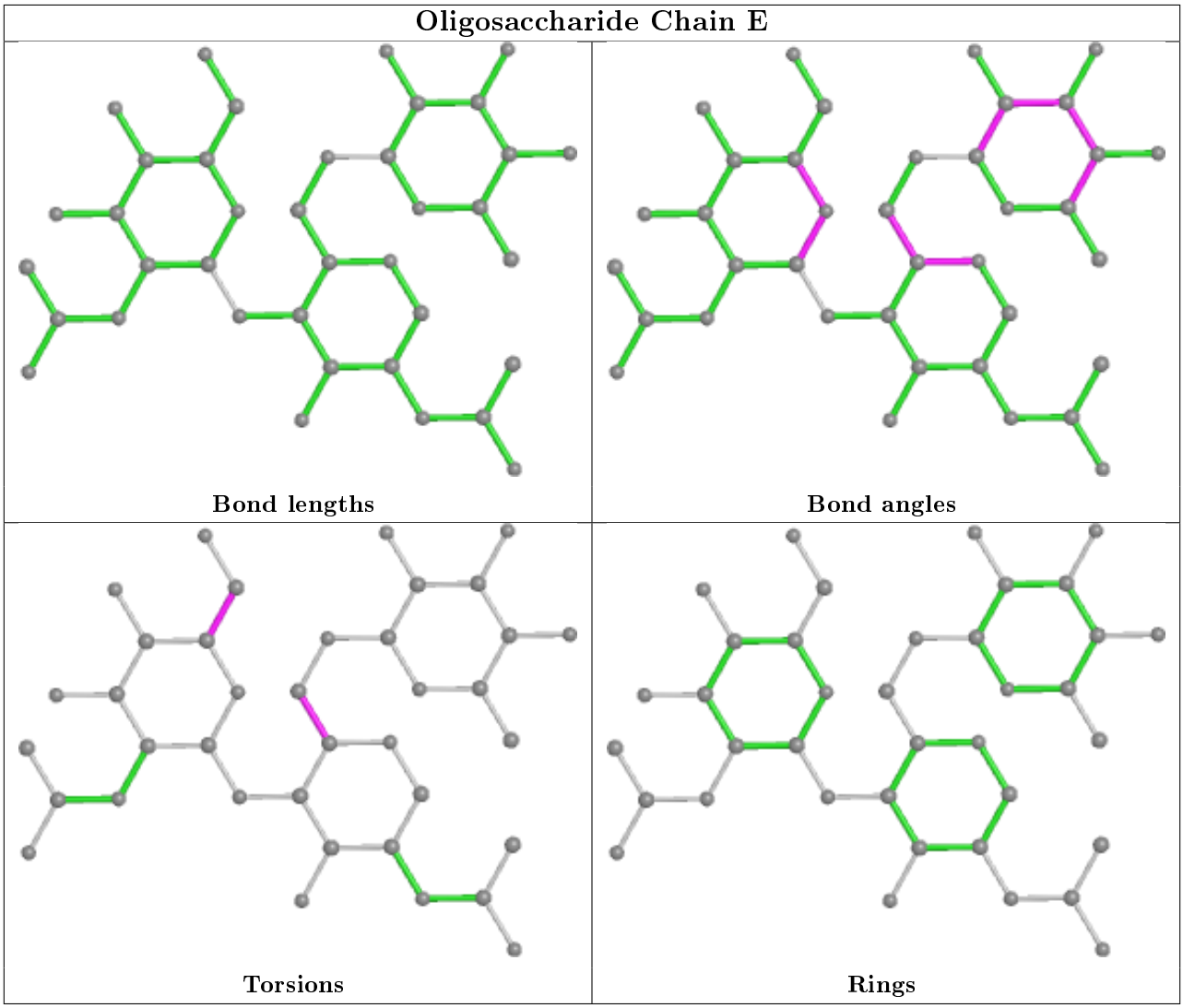
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry (i)

3 ligands 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	$\#\|Z\|>2$
6	NAG	A	302	1	14,14,15	0.50	0	17,19,21	1.24	3 (17%)
6	NAG	A	301	1	14,14,15	0.55	0	17,19,21	1.05	2 (11%)
7	1L9	A	306	-	71,71,71	0.80	2 (2%)	80,84,84	1.36	7 (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
6	NAG	A	302	1	-	0/6/23/26	0/1/1/1
6	NAG	A	301	1	-	2/6/23/26	0/1/1/1
7	1L9	A	306	-	-	28/65/85/85	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	306	1L9	CCU-NCJ	-3.32	1.34	1.41
7	A	306	1L9	O1A-C1A	2.66	1.44	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	306	1L9	OAZ-CCI-NCJ	7.14	120.99	109.32
7	A	306	1L9	CCU-NCJ-CCI	-4.19	119.47	126.36
6	A	301	NAG	C1-O5-C5	2.84	116.03	112.19
7	A	306	1L9	OAZ-CCI-OCK	-2.83	118.83	124.25
7	A	306	1L9	OCK-CCI-NCJ	-2.73	120.18	126.11
7	A	306	1L9	C1-C2-C3	-2.68	107.43	112.71
6	A	301	NAG	O5-C5-C6	2.24	110.71	107.20
7	A	306	1L9	O6A-C5M-C6A	2.23	111.16	106.67
6	A	302	NAG	C1-O5-C5	2.09	115.02	112.19
6	A	302	NAG	C3-C4-C5	-2.07	106.54	110.24
7	A	306	1L9	C6-C5-C4	-2.07	110.78	114.18
6	A	302	NAG	O5-C1-C2	-2.04	108.06	111.29

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	306	1L9	OCK-CCI-OAZ-C6A
7	A	306	1L9	NCJ-CCI-OAZ-C6A
7	A	306	1L9	CCL-CCU-NCJ-CCI
7	A	306	1L9	CCT-CCU-NCJ-CCI
6	A	301	NAG	O5-C5-C6-O6
6	A	301	NAG	C4-C5-C6-O6
7	A	306	1L9	C11-C12-C13-C14
7	A	306	1L9	CAG-CAH-CAI-CAJ
7	A	306	1L9	CAT-CAU-CAV-CAW
7	A	306	1L9	CAH-CAI-CAJ-CAK
7	A	306	1L9	CAQ-CAR-CAS-CAT
7	A	306	1L9	C12-C13-C14-C15
7	A	306	1L9	C9-C10-C11-C12
7	A	306	1L9	CAV-CAW-CAX-CAY
7	A	306	1L9	CAI-CAJ-CAK-CAL
7	A	306	1L9	CAN-CAO-CAP-CAQ
7	A	306	1L9	CAE-CAF-CAG-CAH
7	A	306	1L9	CAJ-CAK-CAL-CAM
7	A	306	1L9	CAP-CAQ-CAR-CAS
7	A	306	1L9	CAW-CAX-CAY-CAZ
7	A	306	1L9	C14-C15-C16-C17
7	A	306	1L9	CAM-CAN-CAO-CAP
7	A	306	1L9	CAO-CAP-CAQ-CAR
7	A	306	1L9	CAK-CAL-CAM-CAN
7	A	306	1L9	O6A-C1A-O1A-C1
7	A	306	1L9	C4A-C5M-C6A-OAZ
7	A	306	1L9	CAU-CAV-CAW-CAX
7	A	306	1L9	C5-C6-C7-C8
7	A	306	1L9	CAF-CAG-CAH-CAI
7	A	306	1L9	C6-C7-C8-C9

There are no ring outliers.

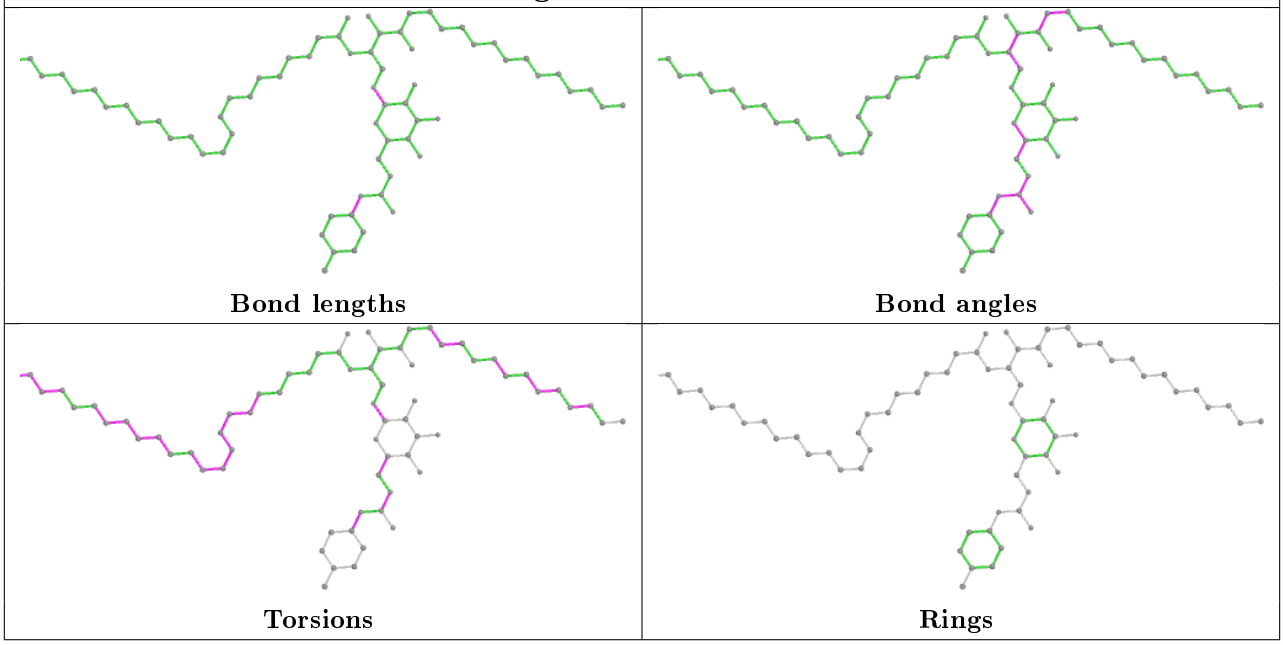
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	306	1L9	5	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 1L9 A 306



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

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, 95^{th} 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	267/285 (93%)	-0.24	1 (0%) 92 79	23, 36, 68, 77	0
2	B	96/99 (96%)	-0.27	0 100 100	30, 41, 55, 66	1 (1%)
3	C	202/209 (96%)	-0.21	1 (0%) 91 75	27, 42, 77, 86	0
4	D	239/241 (99%)	-0.30	0 100 100	27, 39, 58, 85	0
All	All	804/834 (96%)	-0.25	2 (0%) 95 87	23, 39, 70, 86	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	181	ASN	2.2
1	A	260	GLY	2.1

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

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

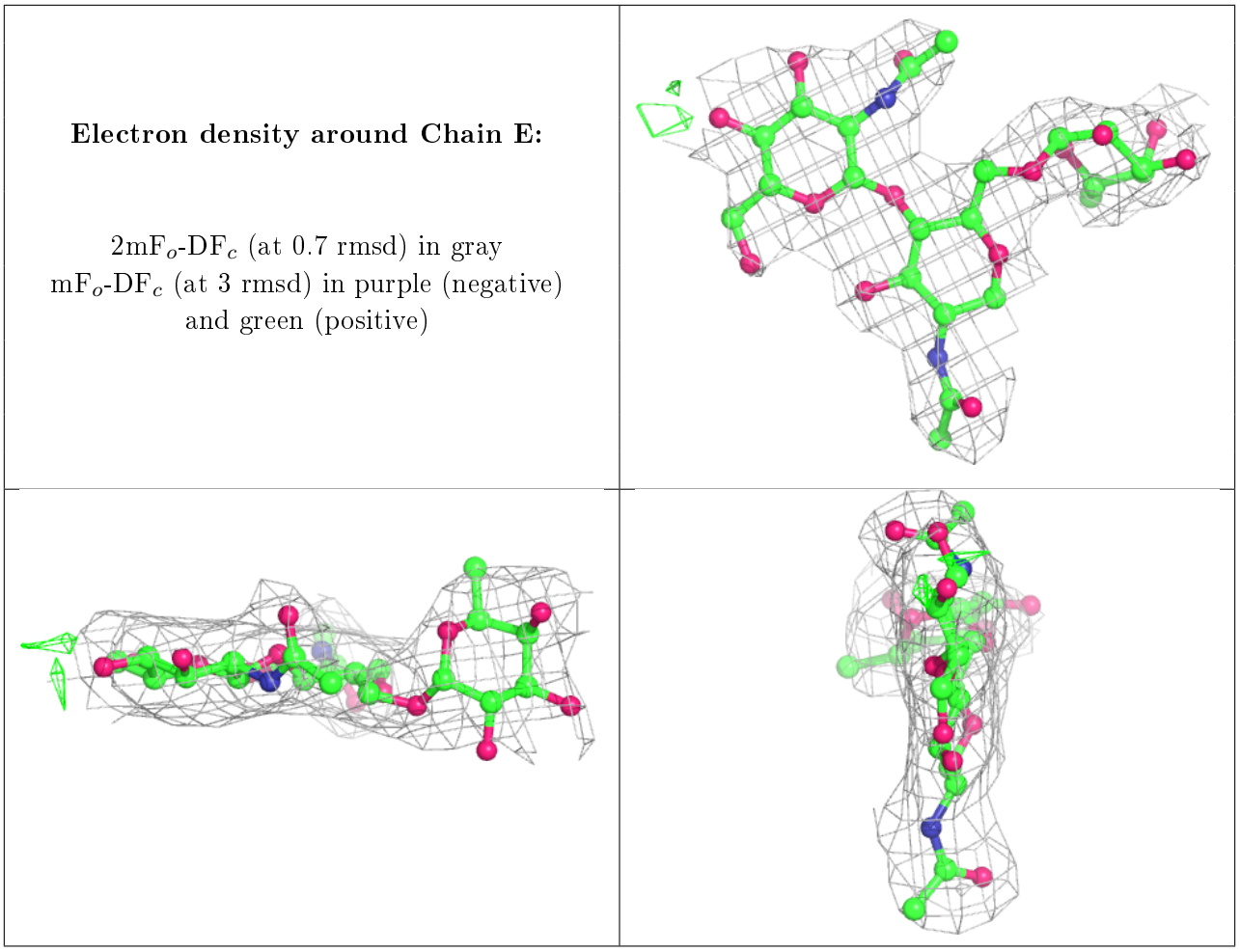
6.3 Carbohydrates

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, 95^{th} 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	NAG	E	2	14/15	0.90	0.30	60,62,66,68	0
5	FUC	E	3	10/11	0.94	0.35	52,55,58,62	0
5	NAG	E	1	14/15	0.96	0.22	43,46,54,55	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands

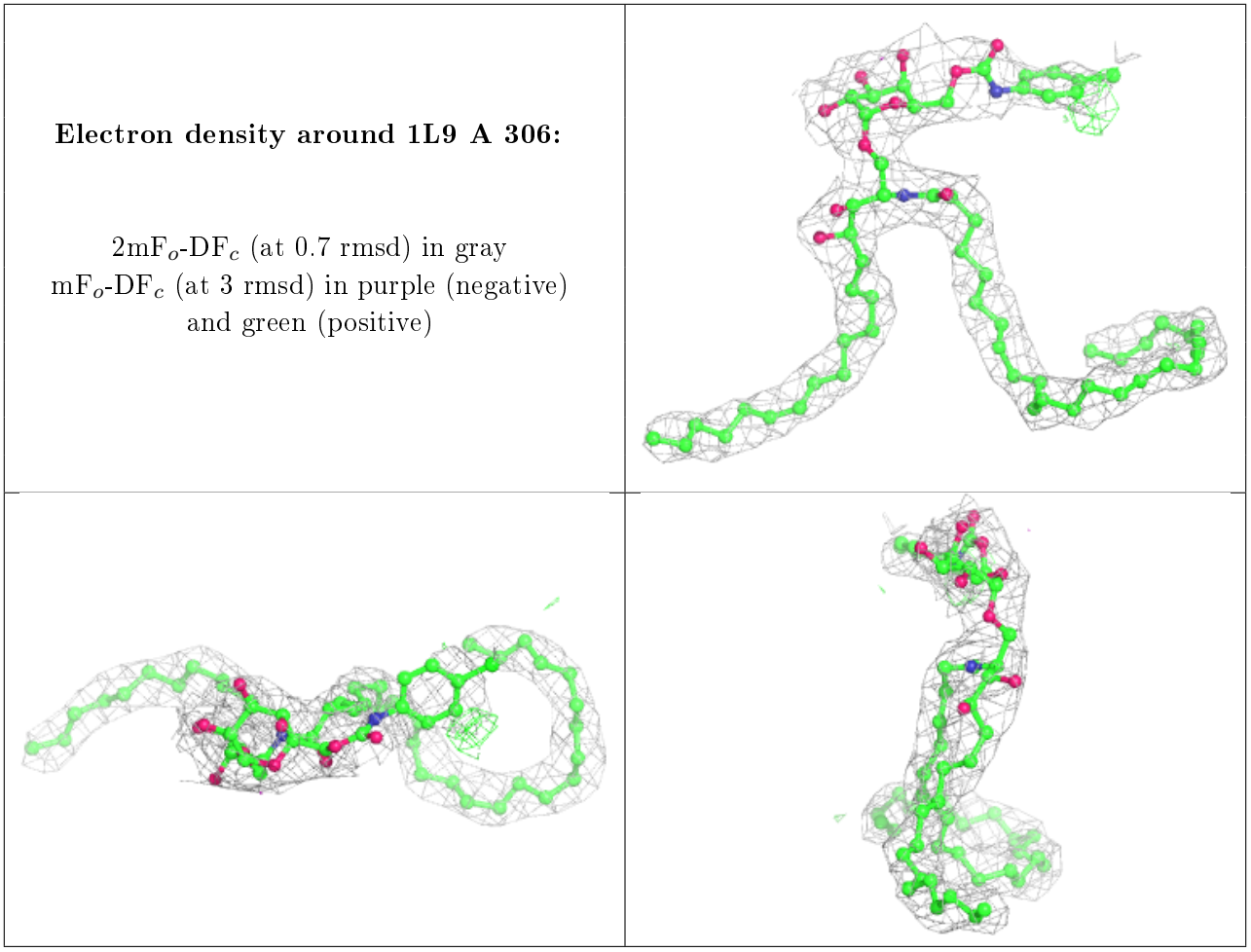
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	NAG	A	301	14/15	0.82	0.31	69,75,80,80	0
6	NAG	A	302	14/15	0.85	0.35	48,51,57,61	0
7	1L9	A	306	70/70	0.93	0.24	36,46,103,117	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 1L9 A 306:

$2mF_o$-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.