Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 01:07 AM EDT

PDB ID	:	8DV3
Title	:	Crystal structure of human CD1b presenting Phosphatidylinositol C34:1
Authors	:	Farquhar, R.; Rossjohn, J.; Shahine, A.
Deposited on	:	2022-07-28
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

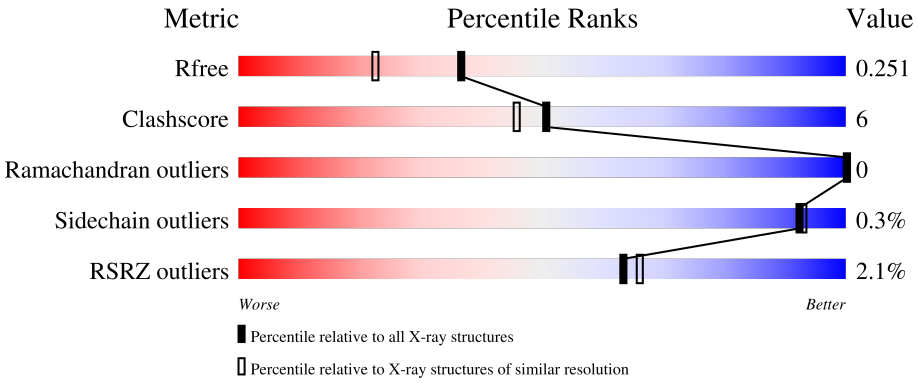
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	300	2% 82% 12% 6%
2	B	101	% 91% 8%
3	C	7	14% 71% 14%
4	D	3	100%

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	FUC	D	3	-	-	-	X
6	CL	A	1213	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 3592 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 T-cell surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	6	0
			2222	1421	378	413	10			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	GLY	-	expression tag	UNP P29016
A	280	SER	-	expression tag	UNP P29016
A	281	GLY	-	expression tag	UNP P29016
A	282	LEU	-	expression tag	UNP P29016
A	283	ASN	-	expression tag	UNP P29016
A	284	ASP	-	expression tag	UNP P29016
A	285	ILE	-	expression tag	UNP P29016
A	286	PHE	-	expression tag	UNP P29016
A	287	GLU	-	expression tag	UNP P29016
A	288	ALA	-	expression tag	UNP P29016
A	289	GLN	-	expression tag	UNP P29016
A	290	LYS	-	expression tag	UNP P29016
A	291	ILE	-	expression tag	UNP P29016
A	292	GLU	-	expression tag	UNP P29016
A	293	TRP	-	expression tag	UNP P29016
A	294	HIS	-	expression tag	UNP P29016
A	295	GLU	-	expression tag	UNP P29016
A	296	HIS	-	expression tag	UNP P29016
A	297	HIS	-	expression tag	UNP P29016
A	298	HIS	-	expression tag	UNP P29016
A	299	HIS	-	expression tag	UNP P29016
A	300	HIS	-	expression tag	UNP P29016
A	301	HIS	-	expression tag	UNP P29016

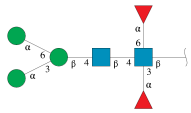
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	2	0
			828	528	142	156	2			

There are 2 discrepancies between the modelled and reference sequences:

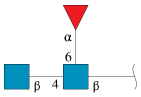
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	PRO	-	expression tag	UNP P61769
B	2	LYS	-	expression tag	UNP P61769

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



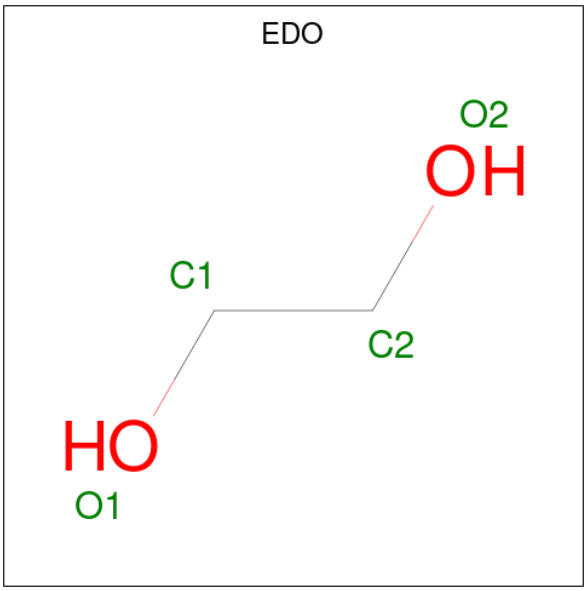
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			81	46	2	33			

- Molecule 4 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
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

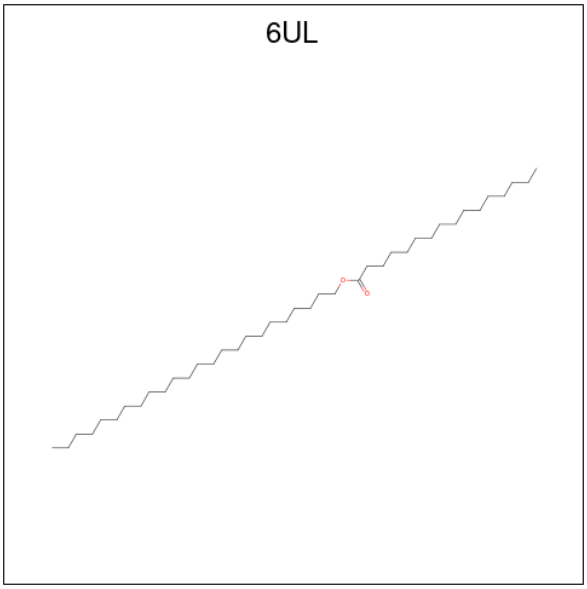
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total Cl 4 4	0	0
6	B	2	Total Cl 2 2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Na 2 2	0	0

- Molecule 8 is TETRACOSYL PALMITATE (three-letter code: 6UL) (formula: $C_{40}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).

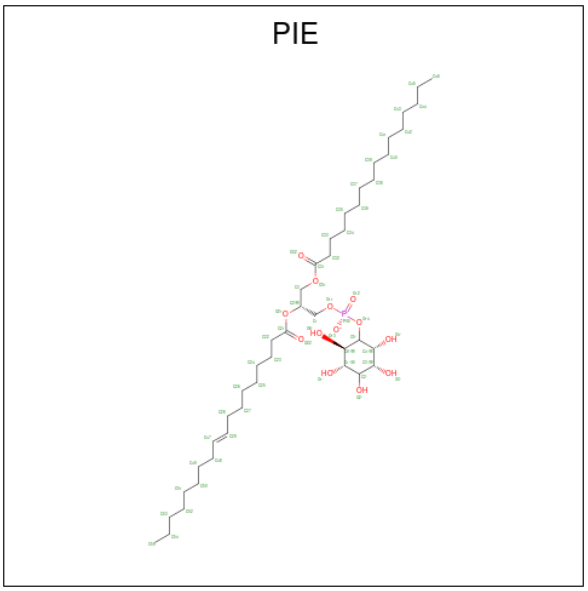


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 32 30 2	0	0

- Molecule 9 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total I 2 2	0	0

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOINOSITOL (three-letter code: PIE) (formula: $C_{43}H_{80}O_{13}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	P	0	0
			57	43	13	1		

- Molecule 11 is water.

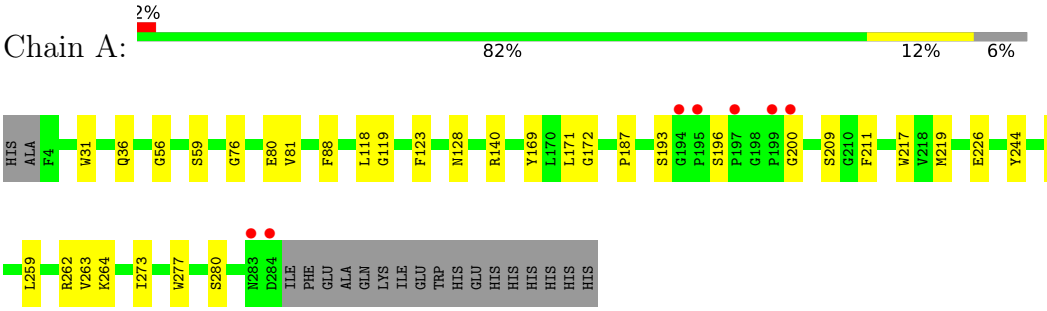
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	216	Total	O	0	0
			216	216		
11	B	84	Total	O	0	0
			84	84		

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.

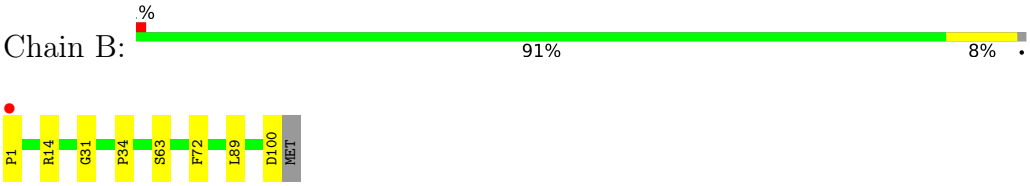
• Molecule 1: T-cell surface glycoprotein CD1b

Chain A:



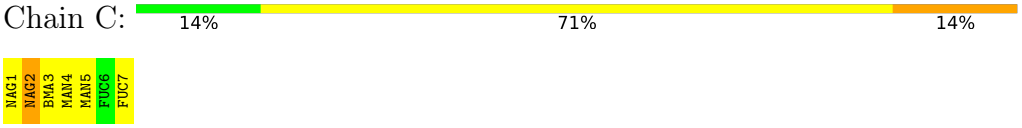
• Molecule 2: Beta-2-microglobulin

Chain B:



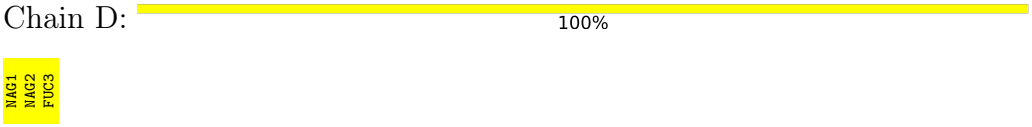
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.82Å 78.63Å 92.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.58 – 1.90 46.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.58-1.90) 99.3 (46.58-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.192 , 0.253 0.191 , 0.251	Depositor DCC
R_{free} test set	996 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3592	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: 6UL, NA, BMA, CL, IOD, FUC, PIE, EDO, MAN, NAG

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	0/2285	0.59	0/3102
2	B	0.38	0/852	0.58	0/1157
All	All	0.40	0/3137	0.59	0/4259

There are no bond length outliers.

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	2222	0	2125	28	0
2	B	828	0	779	8	0
3	C	81	0	70	1	0
4	D	38	0	34	1	0
5	A	24	0	36	4	0
6	A	4	0	0	3	0
6	B	2	0	0	0	0
7	A	2	0	0	0	0
8	A	32	0	57	4	0
9	A	2	0	0	0	0
10	A	57	0	80	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	216	0	0	3	0
11	B	84	0	0	3	0
All	All	3592	0	3181	37	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 6.

All (37) 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)
2:B:89:LEU:O	11:B:301:HOH:O	2.02	0.77
1:A:262[A]:ARG:NH2	11:A:1301:HOH:O	2.21	0.71
2:B:100:ASP:O	11:B:302:HOH:O	2.14	0.64
1:A:123:PHE:CZ	8:A:1205:6UL:HBD2	2.38	0.59
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.86	0.57
1:A:118:LEU:HG	2:B:1:PRO:HB3	1.86	0.56
1:A:128:ASN:ND2	11:A:1309:HOH:O	2.39	0.55
1:A:209:SER:HB2	1:A:244:TYR:HD1	1.73	0.53
1:A:273:ILE:HG12	5:A:1210:EDO:H12	1.91	0.52
1:A:196:SER:OG	1:A:250:ASP:OD1	2.18	0.51
1:A:59:SER:HB2	5:A:1208:EDO:H12	1.92	0.51
1:A:200:GLY:O	1:A:253:ASP:N	2.43	0.50
5:A:1201:EDO:H21	2:B:34:PRO:HG3	1.94	0.50
1:A:171:LEU:HD12	3:C:2:NAG:H82	1.92	0.50
2:B:14:ARG:NH2	11:B:307:HOH:O	2.45	0.50
1:A:81:VAL:HA	8:A:1205:6UL:HAY1	1.94	0.49
1:A:193:SER:HB3	1:A:277:TRP:CH2	2.48	0.49
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.95	0.48
1:A:172:GLY:HA3	6:A:1213:CL:CL	2.51	0.47
8:A:1205:6UL:HAL2	10:A:1212:PIE:H531	1.97	0.47
1:A:119:GLY:HA3	2:B:1:PRO:HA	1.97	0.46
10:A:1212:PIE:O22	10:A:1212:PIE:H31	2.15	0.46
1:A:119:GLY:HA3	2:B:1:PRO:CA	2.45	0.46
1:A:56:GLY:HA3	6:A:1213:CL:CL	2.53	0.45
1:A:76:GLY:O	1:A:80:GLU:HG2	2.18	0.44
1:A:263:VAL:HB	1:A:273:ILE:HB	1.99	0.44
1:A:262[A]:ARG:HE	1:A:262[A]:ARG:HB2	1.52	0.44
1:A:80:GLU:HG3	10:A:1212:PIE:H352	1.99	0.43
1:A:219:MET:HG2	1:A:226:GLU:HB3	2.01	0.43
1:A:280:SER:O	11:A:1302:HOH:O	2.21	0.42
2:B:31:GLY:HA2	2:B:63[A]:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1205:6UL:HAV1	10:A:1212:PIE:H262	2.02	0.42
1:A:251[B]:VAL:HG11	1:A:259:LEU:HD11	2.00	0.42
5:A:1211:EDO:H22	4:D:2:NAG:O4	2.20	0.42
1:A:31:TRP:CZ3	1:A:36:GLN:HB2	2.54	0.42
1:A:169:TYR:O	6:A:1213:CL:CL	2.76	0.41
1:A:88:PHE:HD2	1:A:140:ARG:HG3	1.86	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	285/300 (95%)	281 (99%)	4 (1%)	0	100	100
2	B	100/101 (99%)	97 (97%)	3 (3%)	0	100	100
All	All	385/401 (96%)	378 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	232/247 (94%)	232 (100%)	0	100	100
2	B	92/96 (96%)	91 (99%)	1 (1%)	73	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	324/343 (94%)	323 (100%)	1 (0%)	92 93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	72	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

10 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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.77	1 (7%)	17,19,21	0.83	1 (5%)
3	NAG	C	2	3	14,14,15	0.34	0	17,19,21	0.68	1 (5%)
3	BMA	C	3	3	11,11,12	1.09	1 (9%)	15,15,17	1.11	1 (6%)
3	MAN	C	4	3	11,11,12	0.85	0	15,15,17	1.16	2 (13%)
3	MAN	C	5	3	11,11,12	0.92	0	15,15,17	1.18	1 (6%)
3	FUC	C	6	3	10,10,11	0.75	0	14,14,16	0.90	0
3	FUC	C	7	3	10,10,11	1.77	2 (20%)	14,14,16	1.70	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	1	1,4	14,14,15	0.23	0	17,19,21	0.92	1 (5%)
4	NAG	D	2	4	14,14,15	0.33	0	17,19,21	0.44	0
4	FUC	D	3	4	10,10,11	1.42	3 (30%)	14,14,16	1.11	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
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	FUC	C	6	3	-	-	0/1/1/1
3	FUC	C	7	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	7	FUC	C1-C2	4.07	1.61	1.52
3	C	3	BMA	O5-C1	-2.66	1.39	1.43
4	D	3	FUC	C2-C3	2.49	1.56	1.52
3	C	1	NAG	O5-C1	-2.41	1.39	1.43
3	C	7	FUC	O2-C2	-2.29	1.38	1.43
4	D	3	FUC	O5-C5	2.24	1.48	1.43
4	D	3	FUC	C1-C2	2.05	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	7	FUC	C1-C2-C3	4.61	115.33	109.67
3	C	5	MAN	C1-O5-C5	3.34	116.72	112.19
3	C	4	MAN	C1-O5-C5	3.12	116.42	112.19
3	C	4	MAN	O2-C2-C3	-2.47	105.18	110.14
4	D	1	NAG	C1-O5-C5	2.47	115.54	112.19
3	C	7	FUC	O5-C1-C2	2.35	114.39	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3	BMA	C1-O5-C5	2.28	115.28	112.19
3	C	7	FUC	C3-C4-C5	-2.06	106.57	109.77
3	C	1	NAG	C2-N2-C7	2.01	125.77	122.90
3	C	2	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6

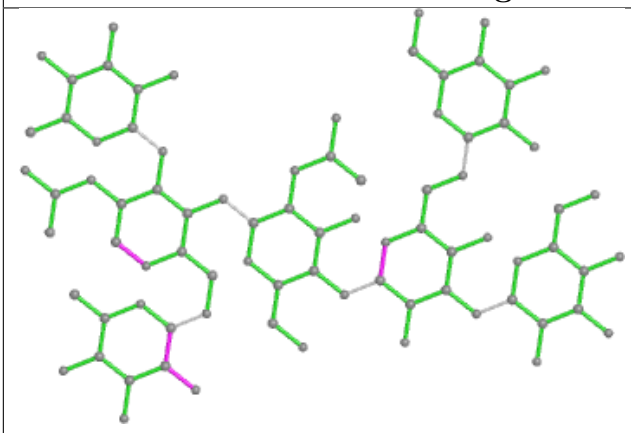
There are no ring outliers.

2 monomers are involved in 2 short contacts:

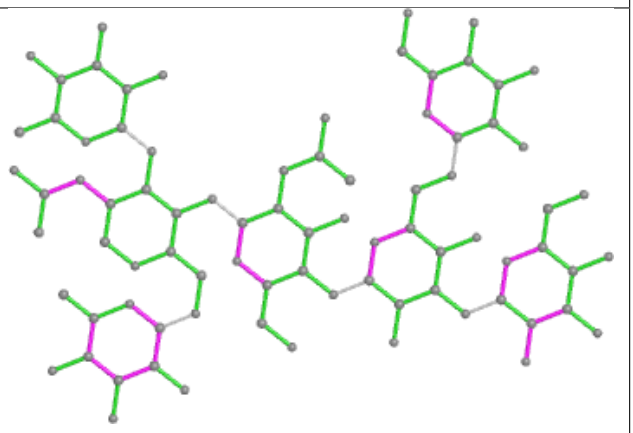
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	1	0
4	D	2	NAG	1	0

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

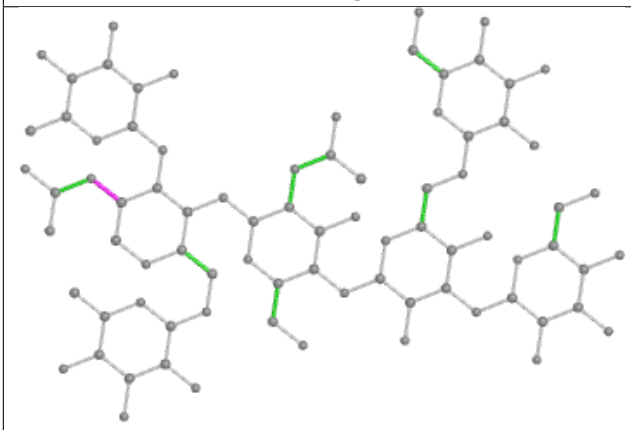
Oligosaccharide Chain C



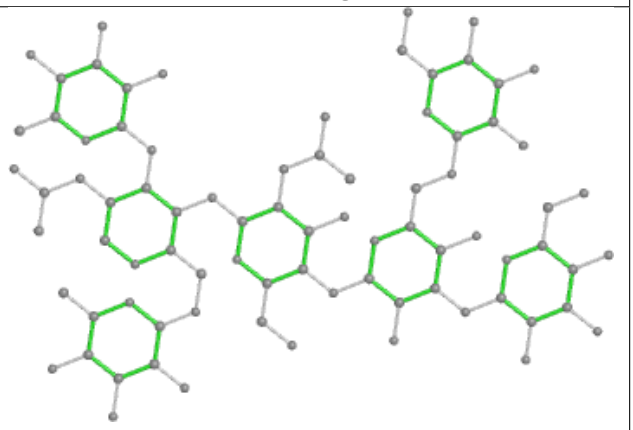
Bond lengths



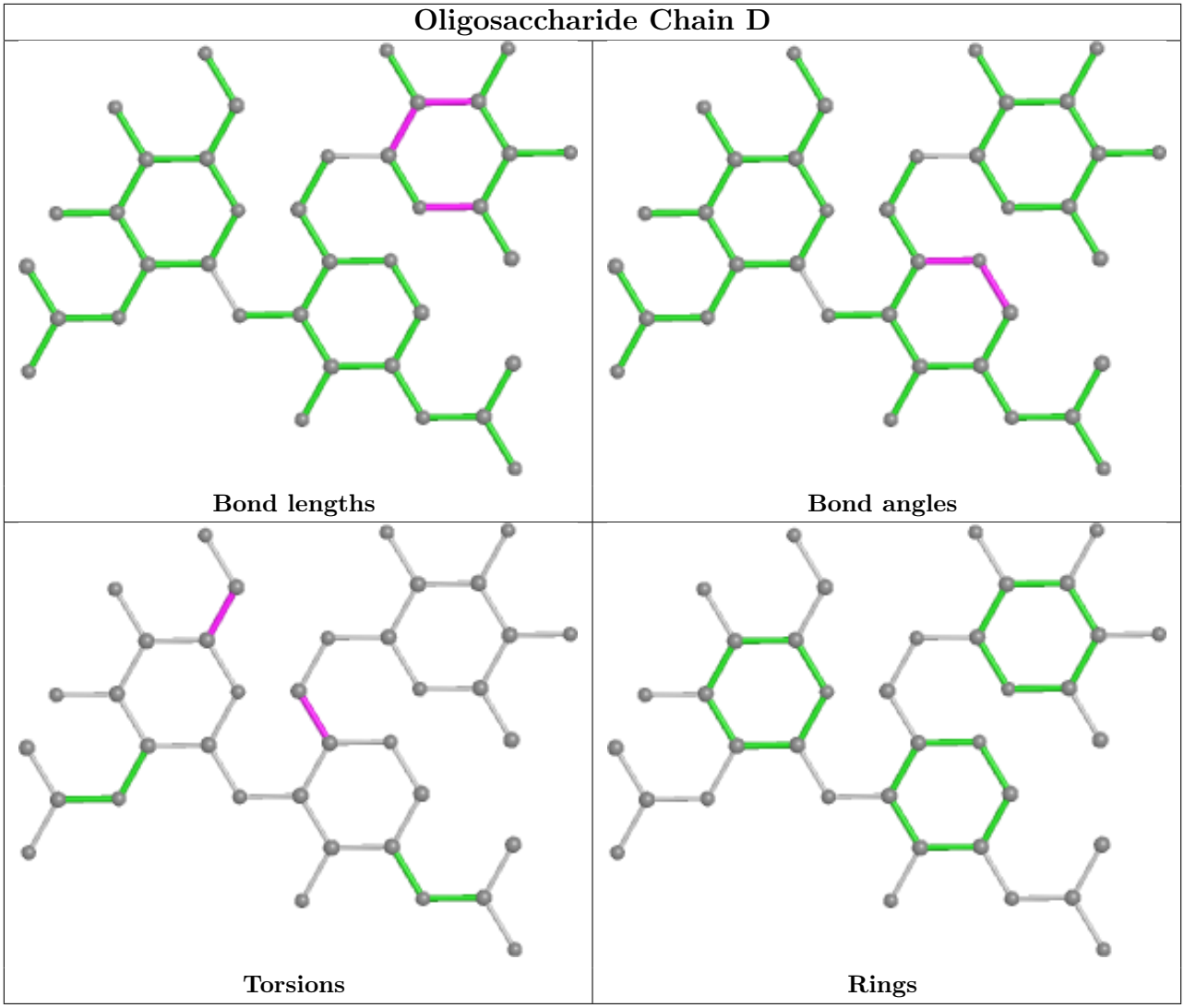
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
5	EDO	A	1204	-	3,3,3	0.50	0	2,2,2	0.32	0
5	EDO	A	1207	-	3,3,3	0.49	0	2,2,2	0.43	0
5	EDO	A	1211	-	3,3,3	0.49	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	PIE	A	1212	-	57,57,57	0.31	0	67,69,69	0.53	0
5	EDO	A	1210	-	3,3,3	0.57	0	2,2,2	0.16	0
8	6UL	A	1205	-	31,31,41	0.35	0	31,31,41	0.43	0
5	EDO	A	1201	-	3,3,3	0.42	0	2,2,2	0.44	0
5	EDO	A	1208	-	3,3,3	0.45	0	2,2,2	0.38	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
5	EDO	A	1204	-	-	0/1/1/1	-
5	EDO	A	1207	-	-	0/1/1/1	-
5	EDO	A	1211	-	-	1/1/1/1	-
10	PIE	A	1212	-	-	14/52/76/76	0/1/1/1
5	EDO	A	1210	-	-	0/1/1/1	-
8	6UL	A	1205	-	-	13/30/30/40	-
5	EDO	A	1201	-	-	0/1/1/1	-
5	EDO	A	1208	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1212	PIE	C1-O11-P-O12
10	A	1212	PIE	C1-O11-P-O13
10	A	1212	PIE	C4'-C5'-O14-P
10	A	1212	PIE	C6'-C5'-O14-P
10	A	1212	PIE	C1-O11-P-O14
8	A	1205	6UL	CBB-CBC-CBD-CBE
8	A	1205	6UL	CBK-CBL-CBM-CAW
10	A	1212	PIE	C41-C42-C43-C44
8	A	1205	6UL	CBI-CBJ-CBK-CBL
8	A	1205	6UL	CAX-CAY-CAZ-CBA
8	A	1205	6UL	CBF-CBG-CBH-CBI
10	A	1212	PIE	C21-C22-C23-C24
10	A	1212	PIE	C32-C33-C34-C35

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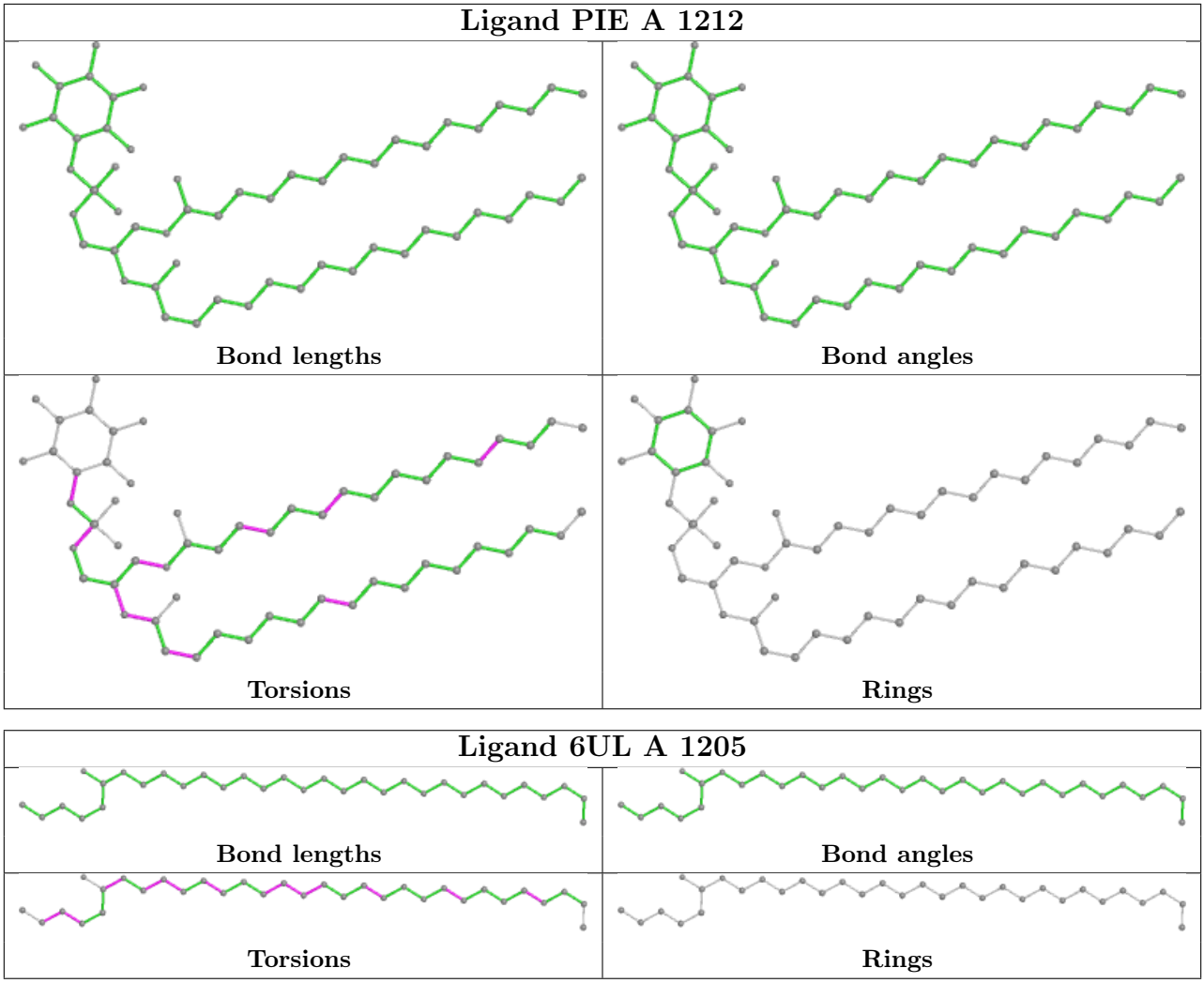
Mol	Chain	Res	Type	Atoms
8	A	1205	6UL	CAT-CAU-CAV-CAW
5	A	1208	EDO	O1-C1-C2-O2
10	A	1212	PIE	C2-C3-O31-C31
8	A	1205	6UL	CAK-CAL-CAM-CAN
10	A	1212	PIE	C35-C36-C37-C38
8	A	1205	6UL	OAQ-CAR-CAS-CAT
8	A	1205	6UL	CAL-CAM-CAN-CAO
10	A	1212	PIE	C3-C2-O21-C21
10	A	1212	PIE	C27-C28-C29-C47
10	A	1212	PIE	C22-C21-O21-C2
8	A	1205	6UL	CAR-CAS-CAT-CAU
8	A	1205	6UL	OBO-CAP-OAQ-CAR
10	A	1212	PIE	O22-C21-O21-C2
8	A	1205	6UL	CBJ-CBK-CBL-CBM
8	A	1205	6UL	CAO-CAP-OAQ-CAR
5	A	1211	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1211	EDO	1	0
10	A	1212	PIE	4	0
5	A	1210	EDO	1	0
8	A	1205	6UL	4	0
5	A	1201	EDO	1	0
5	A	1208	EDO	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.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	281/300 (93%)	-0.03	7 (2%)	57	60	14, 25, 50, 77	0
2	B	100/101 (99%)	0.09	1 (1%)	82	84	17, 34, 58, 72	0
All	All	381/401 (95%)	0.00	8 (2%)	63	66	14, 27, 53, 77	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	PRO	5.0
1	A	194	GLY	4.3
2	B	1	PRO	4.3
1	A	284	ASP	4.2
1	A	197	PRO	3.6
1	A	283	ASN	2.5
1	A	199	PRO	2.3
1	A	200	GLY	2.0

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
4	FUC	D	3	10/11	0.74	0.41	69,81,86,92	0

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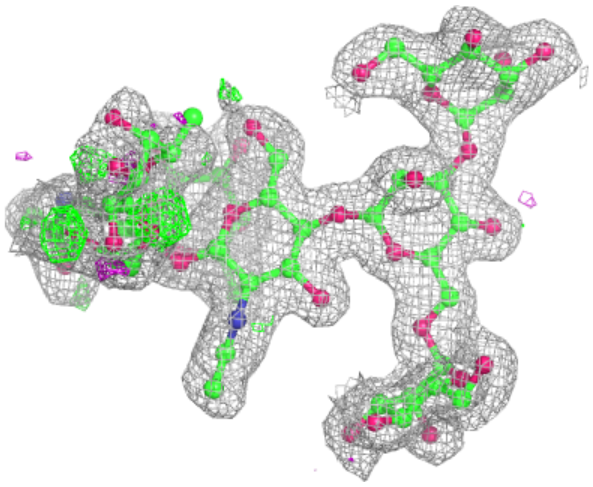
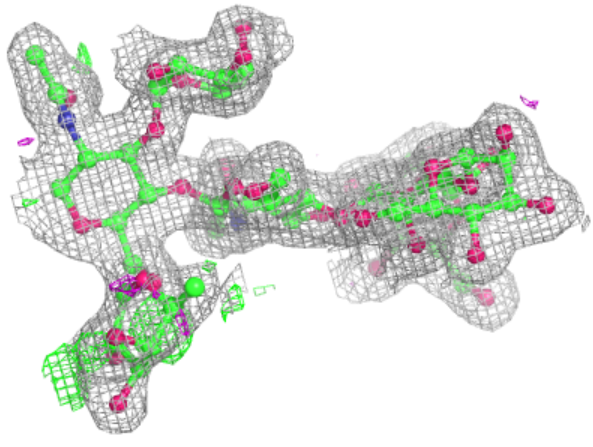
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	D	2	14/15	0.76	0.27	86,92,100,109	0
4	NAG	D	1	14/15	0.78	0.17	47,56,75,81	0
3	FUC	C	7	10/11	0.81	0.23	31,41,50,52	0
3	FUC	C	6	10/11	0.92	0.12	26,30,38,42	0
3	MAN	C	5	11/12	0.95	0.11	20,23,25,26	0
3	NAG	C	1	14/15	0.96	0.09	15,20,26,29	0
3	NAG	C	2	14/15	0.96	0.10	20,25,30,33	0
3	BMA	C	3	11/12	0.97	0.06	19,23,26,26	0
3	MAN	C	4	11/12	0.97	0.10	26,29,33,36	0

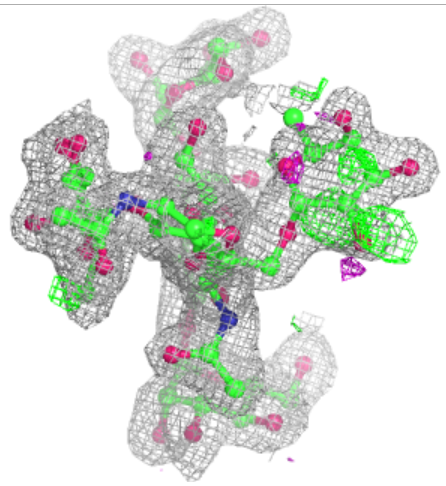
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

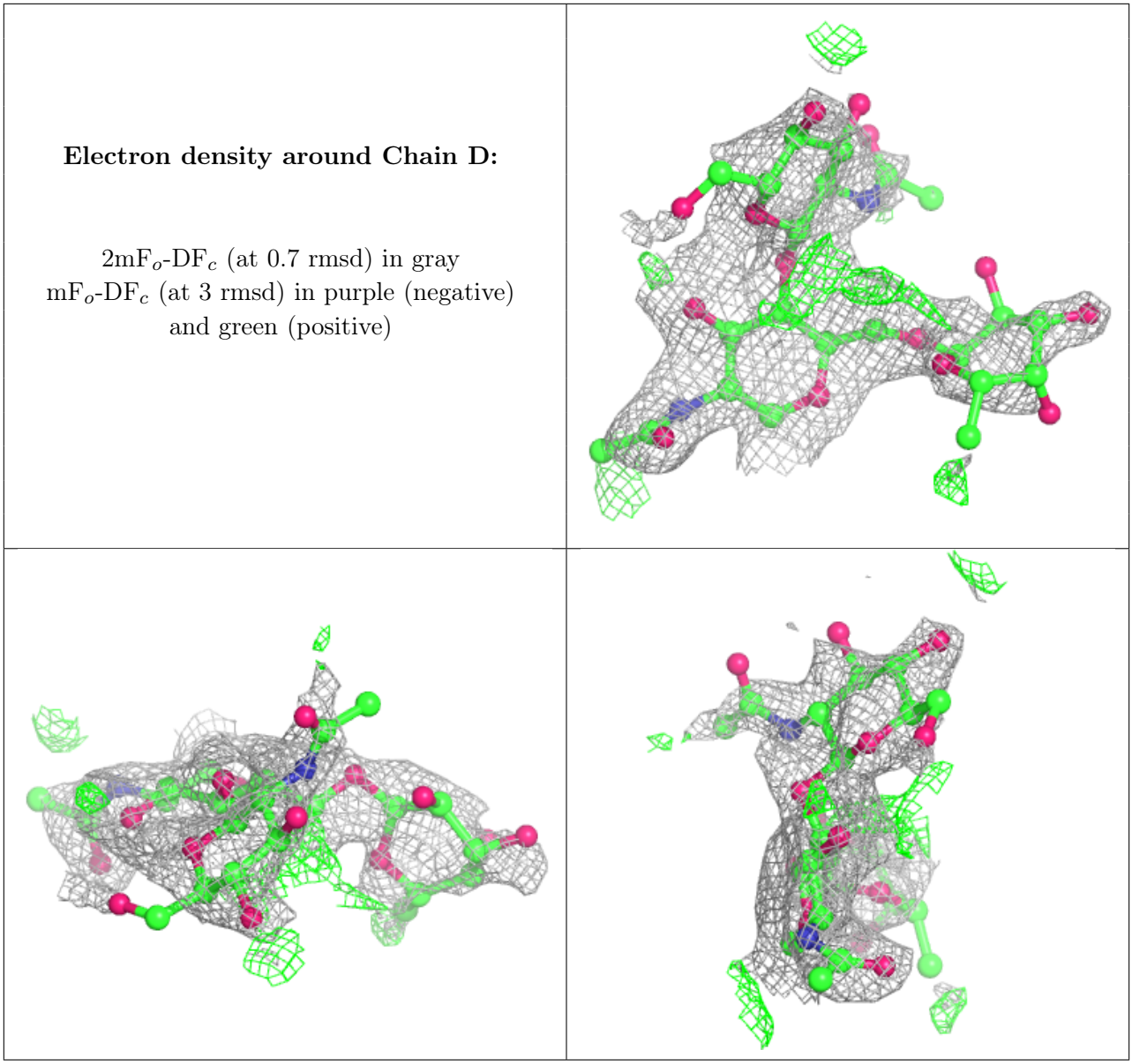






Electron density around Chain D:

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



6.4 Ligands

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	EDO	A	1211	4/4	0.72	0.20	72,74,74,74	0
7	NA	A	1216	1/1	0.72	0.25	64,64,64,64	0
10	PIE	A	1212	57/57	0.73	0.30	27,50,88,97	0
5	EDO	A	1210	4/4	0.83	0.29	36,43,44,45	0
5	EDO	A	1208	4/4	0.86	0.39	36,41,54,64	0

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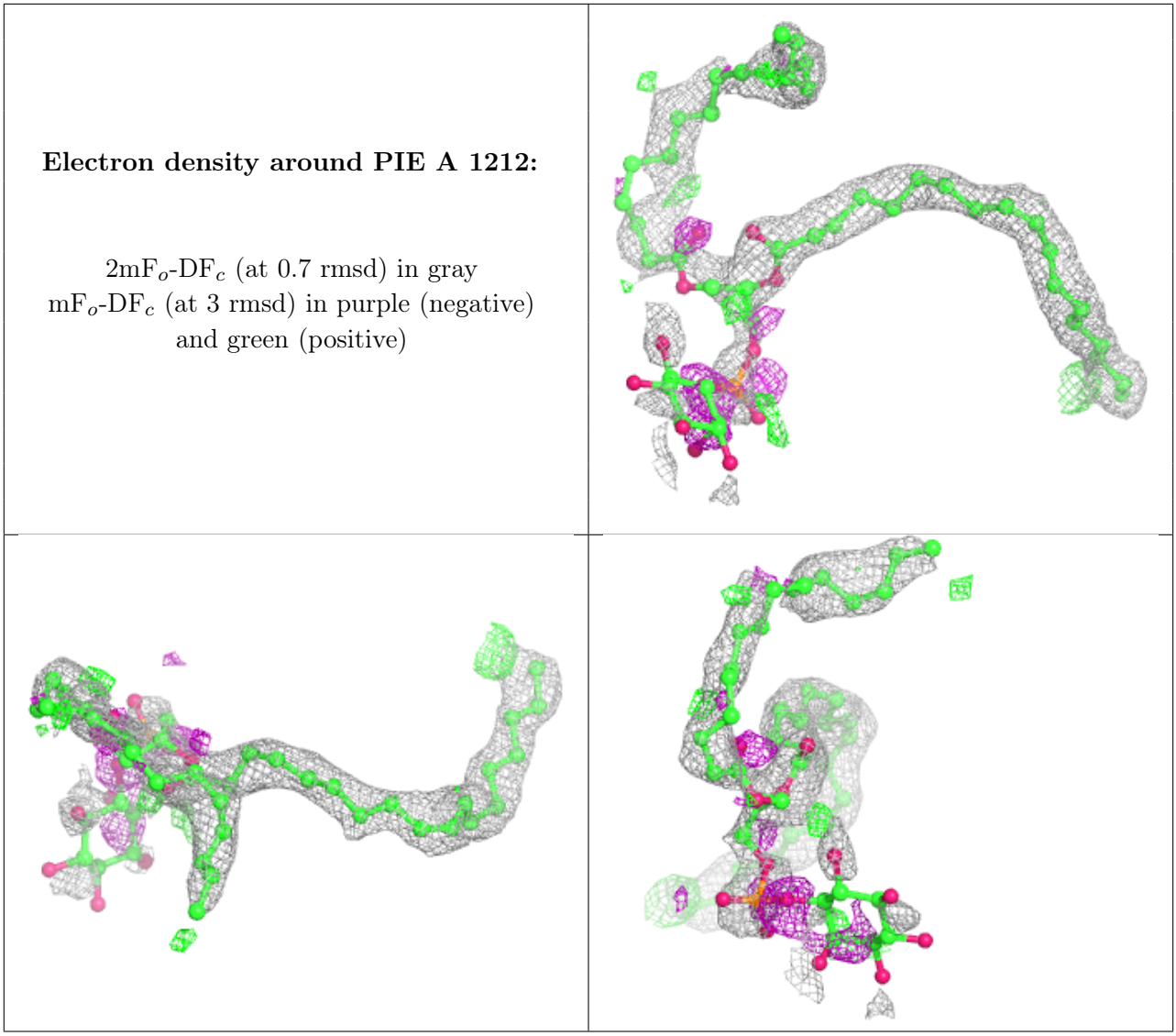
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	6UL	A	1205	32/42	0.87	0.17	27,37,43,45	0
5	EDO	A	1207	4/4	0.88	0.15	44,48,50,54	0
5	EDO	A	1204	4/4	0.89	0.15	38,43,50,51	0
5	EDO	A	1201	4/4	0.93	0.18	14,25,33,36	0
7	NA	A	1203	1/1	0.96	0.14	35,35,35,35	0
9	IOD	A	1209	1/1	0.96	0.36	126,126,126,126	0
6	CL	B	202	1/1	0.96	0.14	29,29,29,29	0
6	CL	B	201	1/1	0.97	0.25	19,19,19,19	0
6	CL	A	1215	1/1	0.98	0.13	26,26,26,26	0
6	CL	A	1202	1/1	0.98	0.04	33,33,33,33	0
6	CL	A	1213	1/1	0.98	0.13	35,35,35,35	0
6	CL	A	1214	1/1	0.98	0.19	19,19,19,19	0
9	IOD	A	1206	1/1	1.00	0.08	22,22,22,22	1

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.

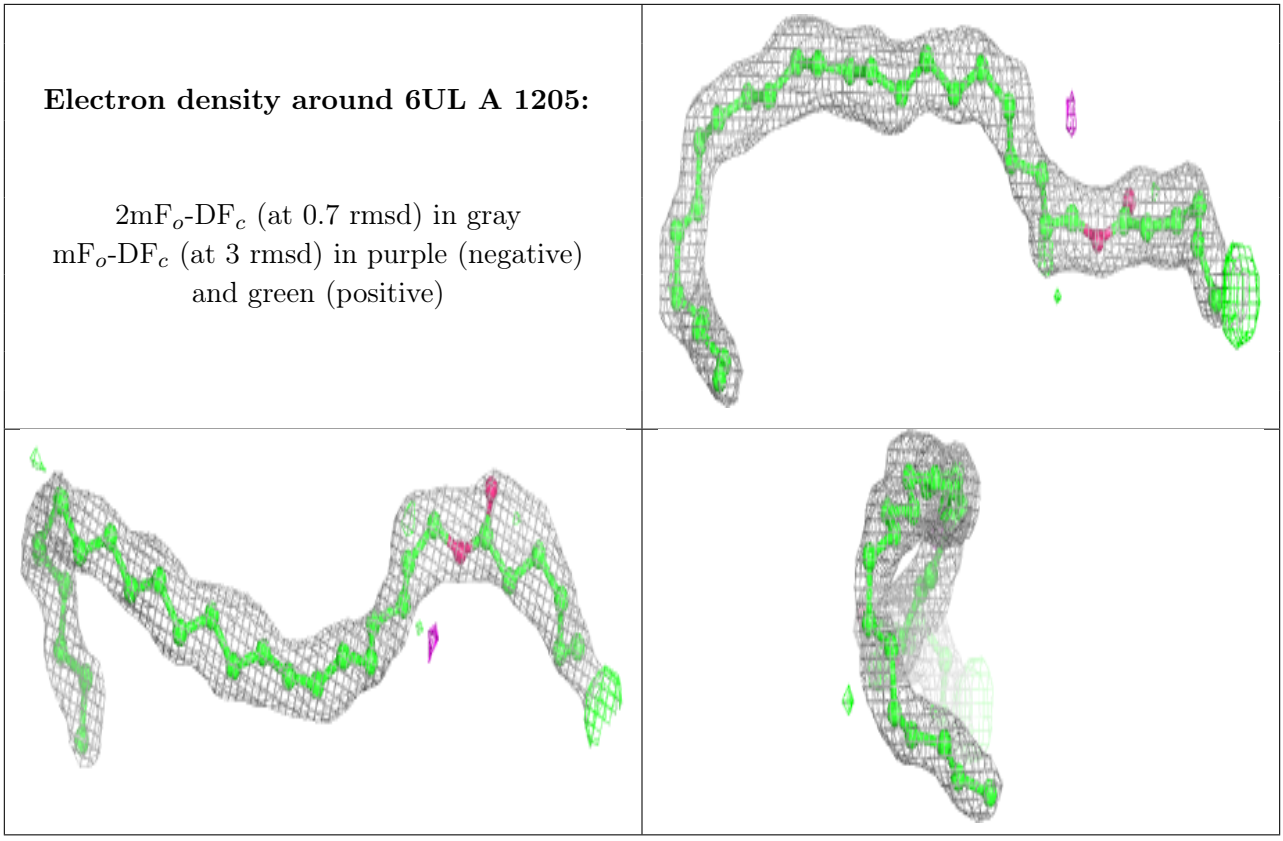
Electron density around PIE A 1212:

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



Electron density around 6UL A 1205:

$2mF_o$-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.