Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 01:58 AM EDT

PDB ID	:	4EWS
Title	:	Crystal structure of cholesteryl ester transfer protein in complex with inhibitors
Authors	:	Liu, S.; Qiu, X.
Deposited on	:	2012-04-27
Resolution	:	2.59 Å(reported)

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

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

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

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

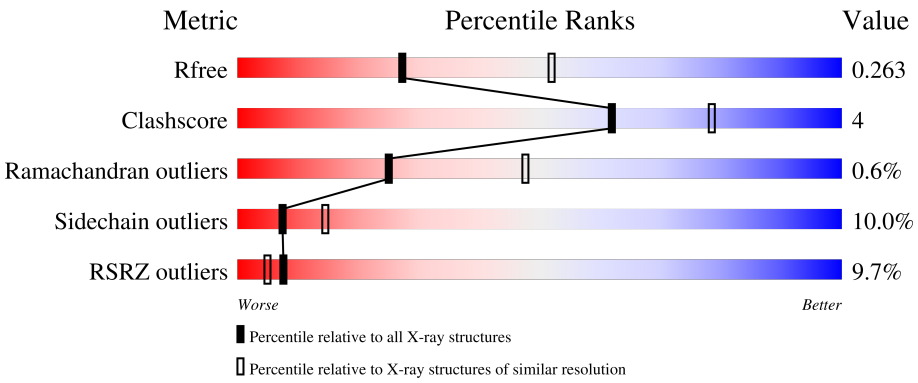
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	476	10% 78% 20% ••
2	B	4	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
2	MAN	B	3	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4044 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.

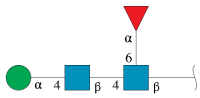
- Molecule 1 is a protein called CETP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3712	2390	603	702	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

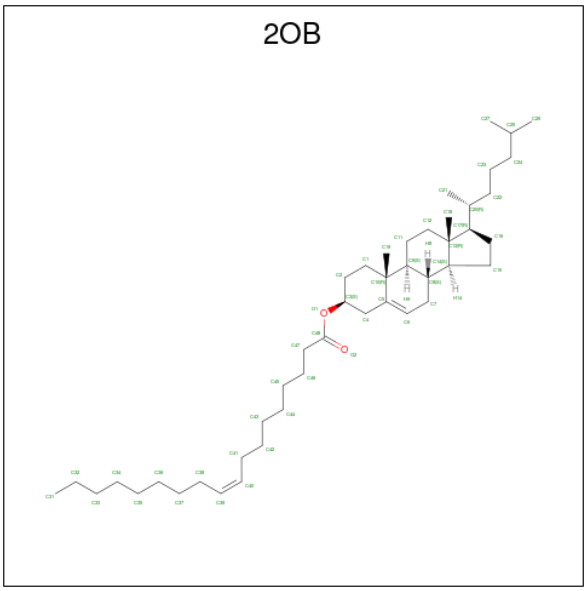
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	engineered mutation	UNP P11597
A	88	ASP	ASN	engineered mutation	UNP P11597
A	131	ALA	CYS	engineered mutation	UNP P11597
A	240	ASP	ASN	engineered mutation	UNP P11597
A	341	ASP	ASN	engineered mutation	UNP P11597
A	405	ILE	VAL	engineered mutation	UNP P11597

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



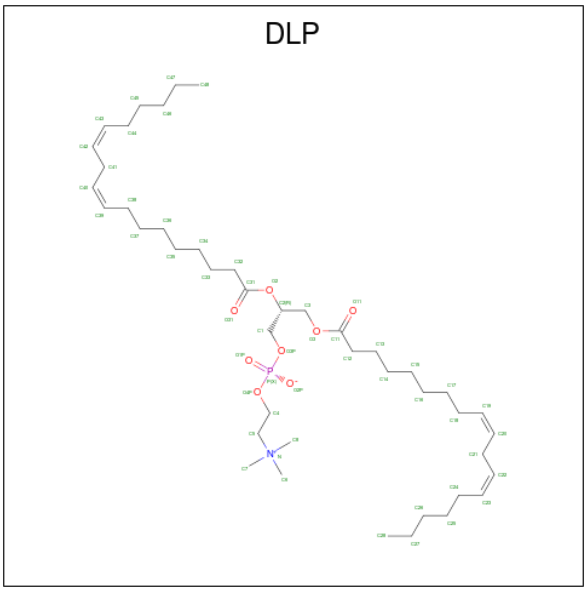
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	49	28	2	19	0	0	0

- Molecule 3 is CHOLESTERYL OLEATE (three-letter code: 2OB) (formula: $C_{45}H_{78}O_2$).



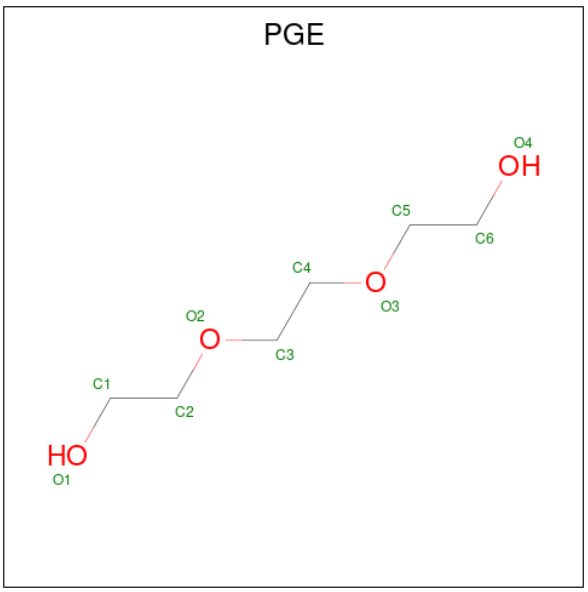
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	39	37	2	0	0
			Total	C	O		
3	A	1	47	45	2	0	0

- Molecule 4 is 1,2-DILINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: DLP) (formula: $C_{44}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	54	44	1	8	1	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

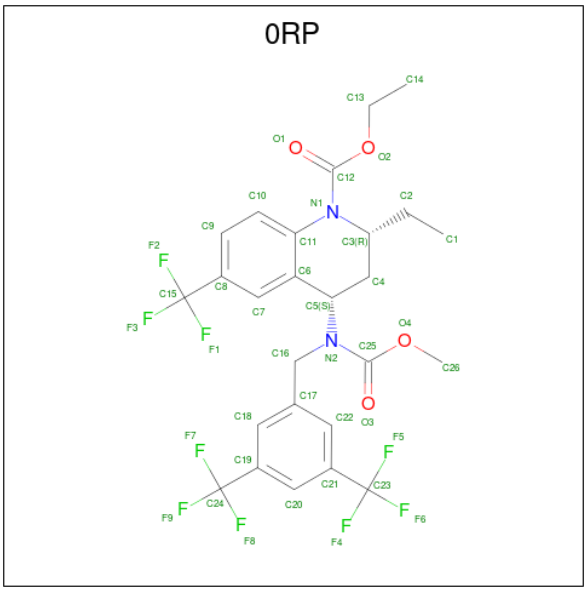


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	10	6	4	0	0
			Total	C	O		
5	A	1	10	6	4	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	A	1	1	1	0	0

- Molecule 7 is ethyl (2R,4S)-4-{[3,5-bis(trifluoromethyl)benzyl](methoxycarbonyl)amino}-2-ethyl-6-(trifluoromethyl)-3,4-dihydroquinoline-1(2H)-carboxylate (three-letter code: 0RP) (formula: $C_{26}H_{25}F_9N_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
7	A	1	41	26	9	2	4	0	0

- Molecule 8 is water.

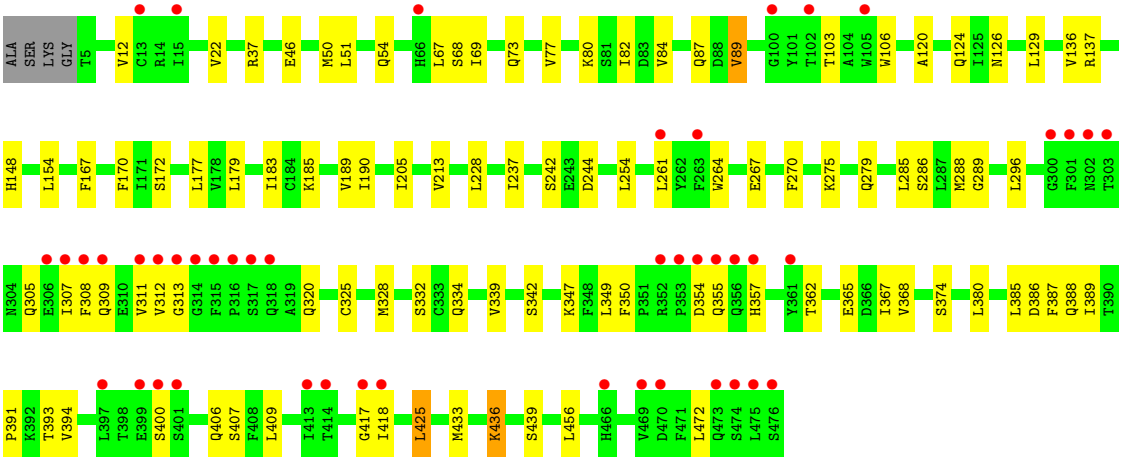
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	81	81	81	0	0

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.

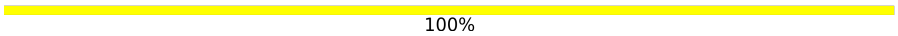
• Molecule 1: CETP

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.60Å 69.32Å 188.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.75 – 2.59 28.58 – 2.59	Depositor EDS
% Data completeness (in resolution range)	78.9 (28.75-2.59) 79.0 (28.58-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.213 , 0.259 0.218 , 0.263	Depositor DCC
R_{free} test set	1148 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4044	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: MAN, FUC, CL, DLP, 2OB, PGE, 0RP, 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	0.45	0/3790	0.73	0/5138

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 (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	3712	0	3724	34	0
2	B	49	0	43	0	0
3	A	86	0	138	3	0
4	A	54	0	80	2	0
5	A	20	0	28	0	0
6	A	1	0	0	0	0
7	A	41	0	25	1	0
8	A	81	0	0	0	0
All	All	4044	0	4038	35	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 4.

All (35) 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:285:LEU:HB2	4:A:503:DLP:H142	1.75	0.68
1:A:46:GLU:HG2	1:A:54:GLN:HE21	1.62	0.65
1:A:124:GLN:HE21	1:A:126:ASN:HD21	1.46	0.63
1:A:37:ARG:HD3	1:A:190:ILE:HD11	1.85	0.57
1:A:311:VAL:C	1:A:313:GLY:HA3	2.25	0.57
1:A:179:LEU:O	1:A:183:ILE:HG12	2.05	0.57
1:A:365:GLU:HB3	1:A:391:PRO:HA	1.89	0.53
1:A:312:VAL:N	1:A:313:GLY:HA3	2.24	0.53
1:A:82:ILE:HD11	1:A:129:LEU:HD11	1.92	0.52
1:A:275:LYS:HA	1:A:328:MET:HG3	1.93	0.50
1:A:433:MET:CE	3:A:502:2OB:H262	2.45	0.47
1:A:205:ILE:HG12	1:A:436:LYS:HB3	1.96	0.47
1:A:312:VAL:HG12	1:A:350:PHE:CE2	2.51	0.46
1:A:325:CYS:SG	4:A:503:DLP:H20	2.56	0.46
1:A:54:GLN:HB2	1:A:103:THR:HG23	1.97	0.45
1:A:77:VAL:HG12	1:A:80:LYS:HB3	1.99	0.45
1:A:354:ASP:HB3	1:A:357:HIS:CD2	2.52	0.45
1:A:167:PHE:O	1:A:172:SER:HB2	2.17	0.44
1:A:296:LEU:HD22	1:A:308:PHE:HE2	1.83	0.44
1:A:367:ILE:HG12	1:A:389:ILE:HG12	1.98	0.44
1:A:12:VAL:HB	1:A:264:TRP:HB3	2.00	0.43
1:A:261:LEU:HD21	7:A:507:0RP:H4	2.00	0.43
1:A:288:MET:SD	1:A:320:GLN:HG2	2.59	0.42
1:A:417:GLY:HA2	3:A:502:2OB:H361	2.01	0.42
1:A:120:ALA:HB3	1:A:148:HIS:HB2	2.02	0.42
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.94	0.42
1:A:394:VAL:HG11	1:A:406:GLN:HG3	2.02	0.42
1:A:69:ILE:HG13	1:A:89:VAL:HB	2.02	0.41
3:A:501:2OB:H212	3:A:501:2OB:H121	2.03	0.41
1:A:368:VAL:O	1:A:387:PHE:HA	2.20	0.41
1:A:305:GLN:O	1:A:309:GLN:HG2	2.21	0.40
1:A:237:ILE:HG12	1:A:242:SER:HB3	2.04	0.40
1:A:389:ILE:HD11	1:A:418:ILE:HD11	2.03	0.40
1:A:347:LYS:HG2	1:A:362:THR:HG22	2.03	0.40
1:A:267:GLU:HA	1:A:270:PHE:HD1	1.87	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	470/476 (99%)	442 (94%)	25 (5%)	3 (1%)	25 47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	GLY
1	A	170	PHE
1	A	355	GLN

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	422/424 (100%)	380 (90%)	42 (10%)	7 14

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	50	MET
1	A	51	LEU
1	A	67	LEU
1	A	68	SER
1	A	73	GLN
1	A	84	VAL
1	A	87	GLN

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Mol	Chain	Res	Type
1	A	89	VAL
1	A	106	TRP
1	A	136	VAL
1	A	137	ARG
1	A	154	LEU
1	A	177	LEU
1	A	185	LYS
1	A	189	VAL
1	A	213	VAL
1	A	228	LEU
1	A	244	ASP
1	A	254	LEU
1	A	279	GLN
1	A	286	SER
1	A	307	ILE
1	A	332	SER
1	A	334	GLN
1	A	339	VAL
1	A	342	SER
1	A	349	LEU
1	A	374	SER
1	A	380	LEU
1	A	385	LEU
1	A	386	ASP
1	A	388	GLN
1	A	393	THR
1	A	400	SER
1	A	407	SER
1	A	409	LEU
1	A	425	LEU
1	A	436	LYS
1	A	439	SER
1	A	456	LEU
1	A	472	LEU

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

Mol	Chain	Res	Type
1	A	54	GLN
1	A	87	GLN
1	A	126	ASN
1	A	192	ASN

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Mol	Chain	Res	Type
1	A	279	GLN
1	A	357	HIS

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)

4 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	NAG	B	1	1,2	14,14,15	0.28	0	17,19,21	0.72	1 (5%)
2	NAG	B	2	2	14,14,15	0.27	0	17,19,21	0.92	2 (11%)
2	MAN	B	3	2	11,11,12	0.49	0	15,15,17	1.37	1 (6%)
2	FUC	B	4	2	10,10,11	0.41	0	14,14,16	1.15	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	0/2/19/22	1/1/1/1
2	FUC	B	4	2	-	-	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	MAN	C1-O5-C5	4.69	118.54	112.19
2	B	4	FUC	C1-O5-C5	3.05	119.70	112.78
2	B	1	NAG	O5-C1-C2	-2.30	107.65	111.29
2	B	2	NAG	C1-O5-C5	2.26	115.25	112.19
2	B	4	FUC	C1-C2-C3	2.16	112.33	109.67
2	B	2	NAG	C1-C2-N2	2.15	114.17	110.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

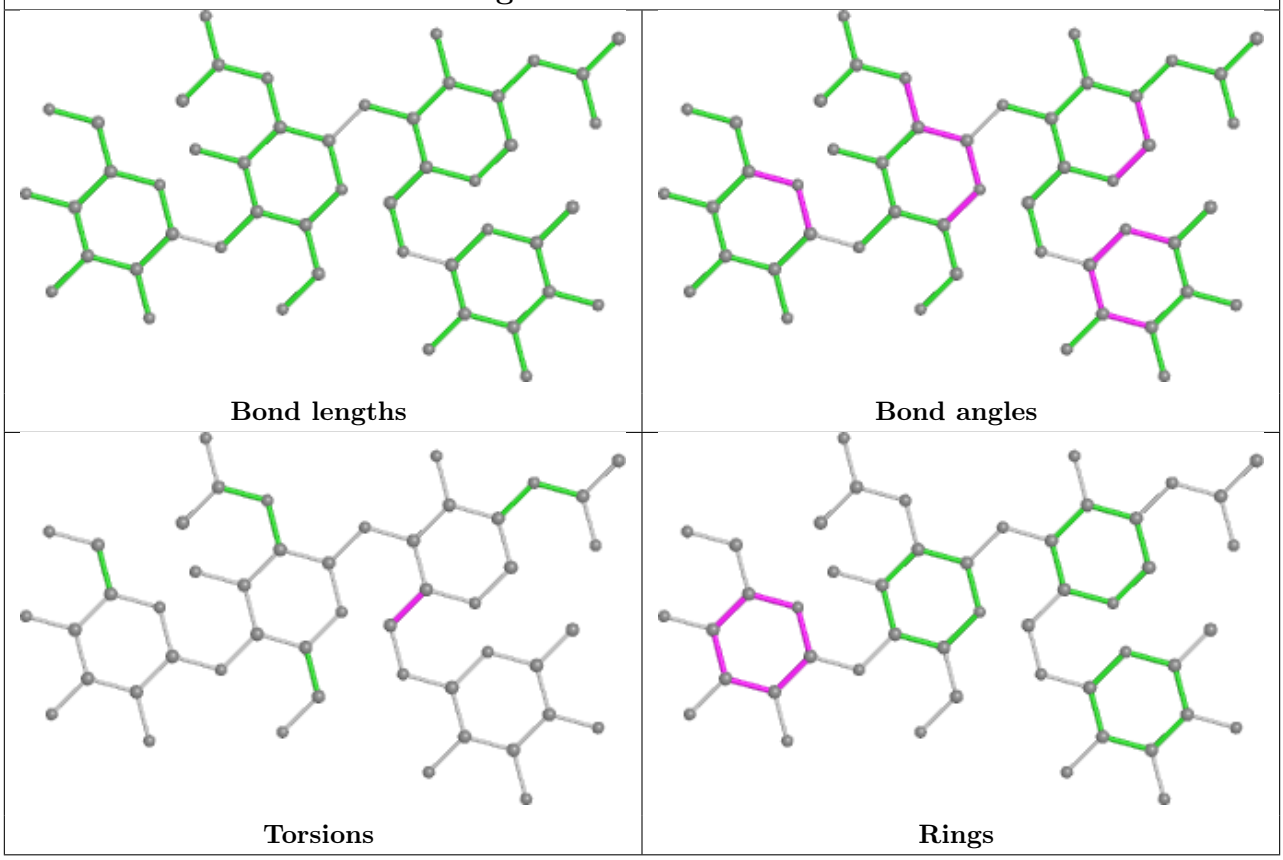
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	MAN	C1-C2-C3-C4-C5-O5

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.

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
5	PGE	A	504	-	9,9,9	0.51	0	8,8,8	0.20	0
7	0RP	A	507	-	43,43,43	1.53	6 (13%)	58,66,66	1.50	11 (18%)
3	2OB	A	501	-	42,42,50	0.66	1 (2%)	60,60,68	0.44	0
3	2OB	A	502	-	50,50,50	0.76	1 (2%)	68,68,68	1.44	11 (16%)
4	DLP	A	503	-	53,53,53	1.63	5 (9%)	59,61,61	1.08	6 (10%)
5	PGE	A	505	-	9,9,9	0.61	0	8,8,8	0.36	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	PGE	A	504	-	-	3/7/7/7	-
7	0RP	A	507	-	-	2/41/57/57	0/3/3/3
3	2OB	A	501	-	-	1/23/81/89	0/4/4/4
3	2OB	A	502	-	-	16/31/89/89	0/4/4/4
4	DLP	A	503	-	-	26/57/57/57	-
5	PGE	A	505	-	-	4/7/7/7	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	DLP	P-O1P	8.14	1.79	1.50
7	A	507	0RP	C12-N1	5.78	1.45	1.37
4	A	503	DLP	O3-C11	4.34	1.46	1.33
3	A	502	2OB	O1-C48	4.27	1.46	1.34
4	A	503	DLP	O2-C31	4.21	1.46	1.34
4	A	503	DLP	C43-C42	3.75	1.53	1.31
3	A	501	2OB	C39-C40	3.62	1.53	1.28
4	A	503	DLP	C23-C22	3.59	1.52	1.31
7	A	507	0RP	C10-C11	3.11	1.44	1.39
7	A	507	0RP	C25-N2	2.87	1.39	1.35
7	A	507	0RP	C4-C5	2.11	1.55	1.53
7	A	507	0RP	O3-C25	2.10	1.24	1.21
7	A	507	0RP	C4-C3	2.08	1.57	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	2OB	C4-C5-C10	4.12	121.89	116.42
3	A	502	2OB	C4-C5-C6	-3.72	115.25	120.61
7	A	507	0RP	O4-C25-N2	3.66	115.27	111.64
3	A	502	2OB	O1-C48-C47	3.65	119.38	111.50
7	A	507	0RP	O2-C12-N1	3.58	116.44	111.07
4	A	503	DLP	O3-C11-C12	3.49	122.87	111.91
7	A	507	0RP	C11-C6-C5	-3.41	114.95	120.78
3	A	502	2OB	C15-C14-C13	3.27	107.78	103.84
7	A	507	0RP	O2-C12-O1	-3.18	119.36	124.78
3	A	502	2OB	C21-C20-C22	-2.96	105.72	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	2OB	C13-C17-C20	2.81	123.89	119.49
7	A	507	0RP	C7-C6-C5	2.75	123.52	119.39
7	A	507	0RP	C8-C7-C6	-2.69	119.77	122.59
4	A	503	DLP	O2-C31-C32	2.69	117.29	111.50
4	A	503	DLP	O2-C2-C3	2.68	118.10	108.40
4	A	503	DLP	C3-O3-C11	2.66	126.97	117.12
7	A	507	0RP	C4-C5-C6	-2.63	106.85	110.10
7	A	507	0RP	C26-O4-C25	2.59	118.33	115.34
3	A	502	2OB	C16-C17-C20	2.45	115.94	112.15
3	A	502	2OB	C11-C9-C8	2.42	115.23	111.75
7	A	507	0RP	C7-C6-C11	2.35	121.48	118.82
4	A	503	DLP	O3-C11-O11	-2.34	117.69	123.59
3	A	502	2OB	C13-C14-C8	2.28	117.76	114.38
3	A	502	2OB	C14-C13-C17	-2.10	97.59	100.07
7	A	507	0RP	C4-C3-C2	-2.08	107.32	113.25
3	A	502	2OB	C11-C9-C10	2.05	115.78	113.08
7	A	507	0RP	C4-C5-N2	2.05	115.07	112.03
4	A	503	DLP	C24-C23-C22	-2.02	109.25	124.73

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	DLP	O4P-C4-C5-N
4	A	503	DLP	C12-C11-O3-C3
4	A	503	DLP	O11-C11-O3-C3
4	A	503	DLP	C19-C20-C21-C22
4	A	503	DLP	C21-C22-C23-C24
4	A	503	DLP	C41-C42-C43-C44
3	A	502	2OB	C17-C20-C22-C23
3	A	502	2OB	C21-C20-C22-C23
5	A	504	PGE	O3-C5-C6-O4
3	A	502	2OB	C41-C42-C43-C44
4	A	503	DLP	C35-C36-C37-C38
3	A	502	2OB	C34-C35-C36-C37
3	A	502	2OB	C33-C34-C35-C36
5	A	504	PGE	O2-C3-C4-O3
3	A	502	2OB	C32-C33-C34-C35
4	A	503	DLP	C31-C32-C33-C34
4	A	503	DLP	C14-C15-C16-C17
4	A	503	DLP	C34-C35-C36-C37
4	A	503	DLP	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
5	A	505	PGE	O3-C5-C6-O4
4	A	503	DLP	C13-C14-C15-C16
3	A	502	2OB	C44-C45-C46-C47
4	A	503	DLP	C23-C24-C25-C26
4	A	503	DLP	C36-C37-C38-C39
3	A	502	2OB	C23-C24-C25-C27
3	A	502	2OB	C42-C43-C44-C45
3	A	502	2OB	C23-C24-C25-C26
3	A	502	2OB	C40-C41-C42-C43
4	A	503	DLP	C45-C46-C47-C48
3	A	502	2OB	C31-C32-C33-C34
5	A	505	PGE	O2-C3-C4-O3
4	A	503	DLP	C25-C26-C27-C28
7	A	507	0RP	C4-C5-N2-C25
3	A	501	2OB	C43-C44-C45-C46
5	A	505	PGE	C4-C3-O2-C2
5	A	504	PGE	C4-C3-O2-C2
4	A	503	DLP	O3P-C1-C2-O2
5	A	505	PGE	C1-C2-O2-C3
4	A	503	DLP	C1-C2-C3-O3
4	A	503	DLP	C3-C2-O2-C31
3	A	502	2OB	C13-C17-C20-C21
3	A	502	2OB	C13-C17-C20-C22
4	A	503	DLP	O2-C2-C3-O3
3	A	502	2OB	C37-C38-C39-C40
7	A	507	0RP	C14-C13-O2-C12
4	A	503	DLP	O3-C11-C12-C13
4	A	503	DLP	O3P-C1-C2-C3
4	A	503	DLP	C22-C23-C24-C25
3	A	502	2OB	C39-C40-C41-C42
4	A	503	DLP	C1-O3P-P-O1P
4	A	503	DLP	O11-C11-C12-C13
4	A	503	DLP	C16-C17-C18-C19

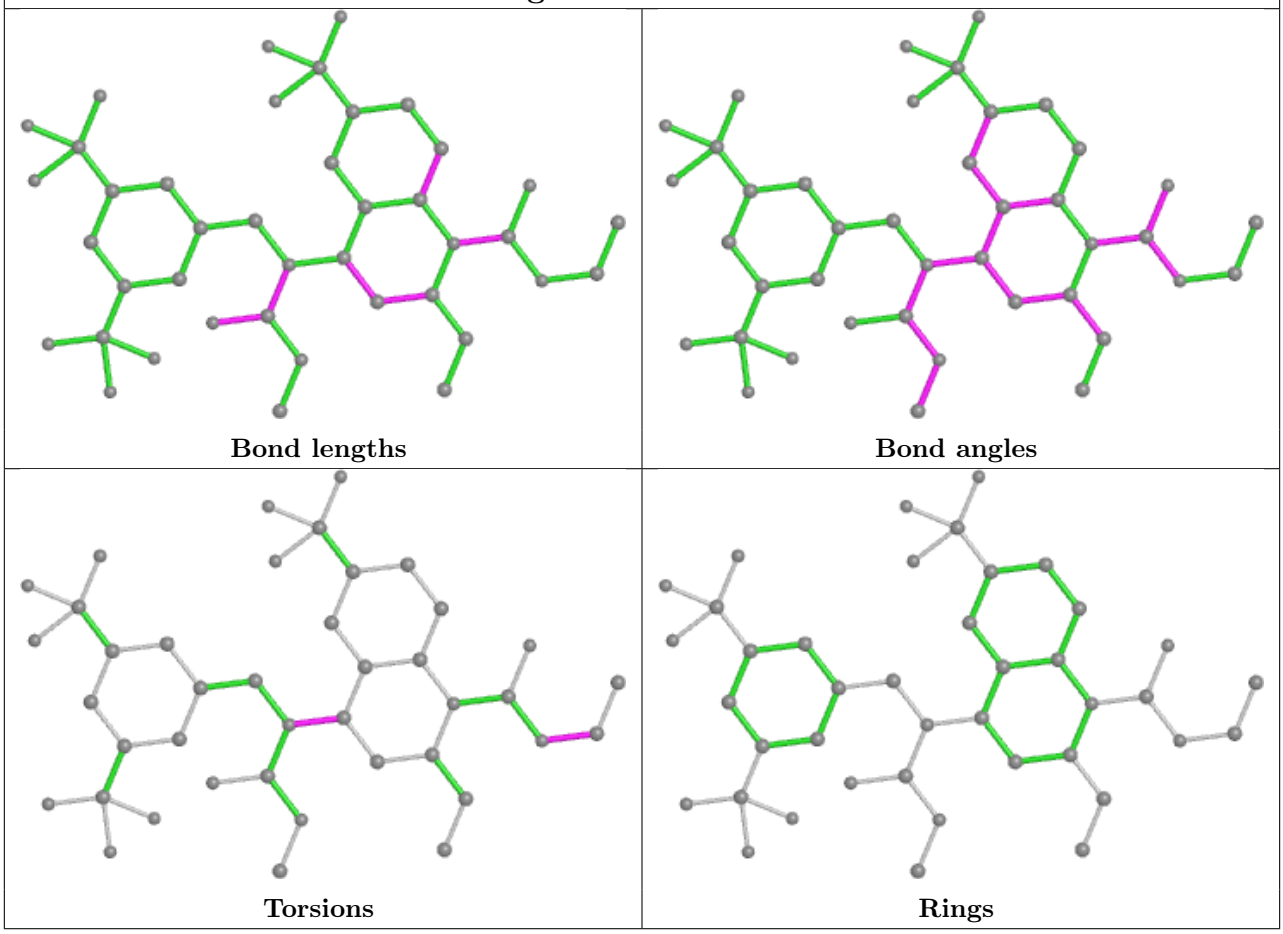
There are no ring outliers.

4 monomers are involved in 6 short contacts:

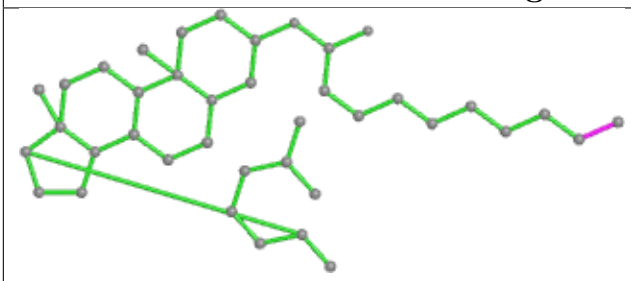
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	507	0RP	1	0
3	A	501	2OB	1	0
3	A	502	2OB	2	0
4	A	503	DLP	2	0

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.

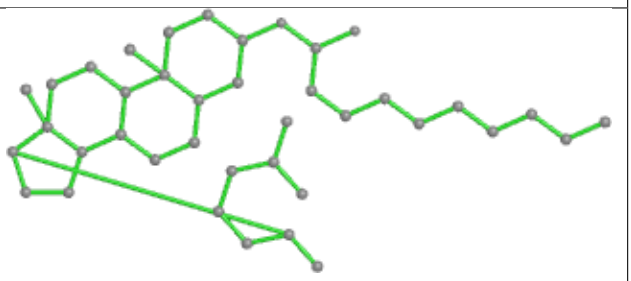
Ligand 0RP A 507



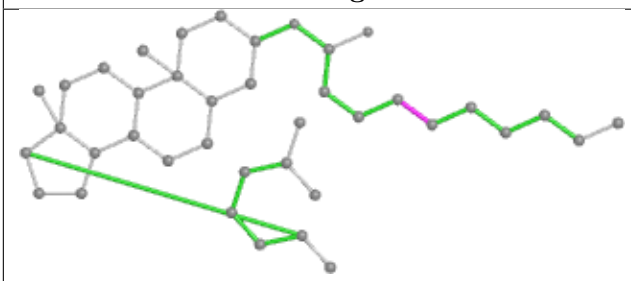
Ligand 2OB A 501



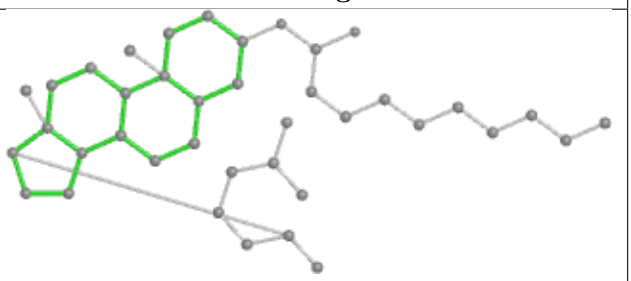
Bond lengths



Bond angles

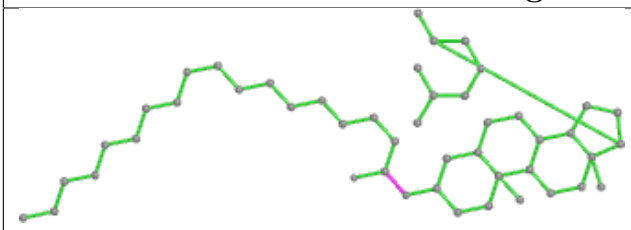


Torsions

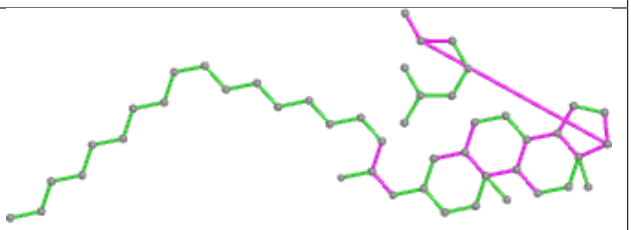


Rings

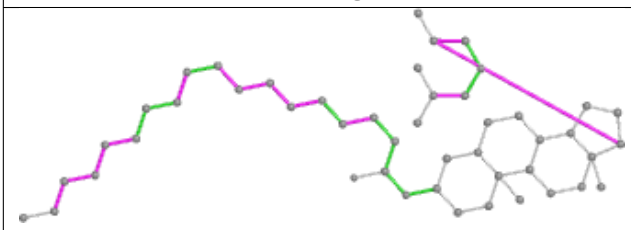
Ligand 2OB A 502



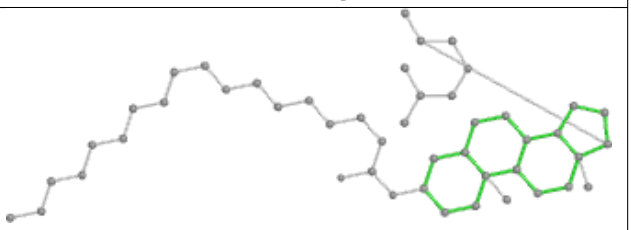
Bond lengths



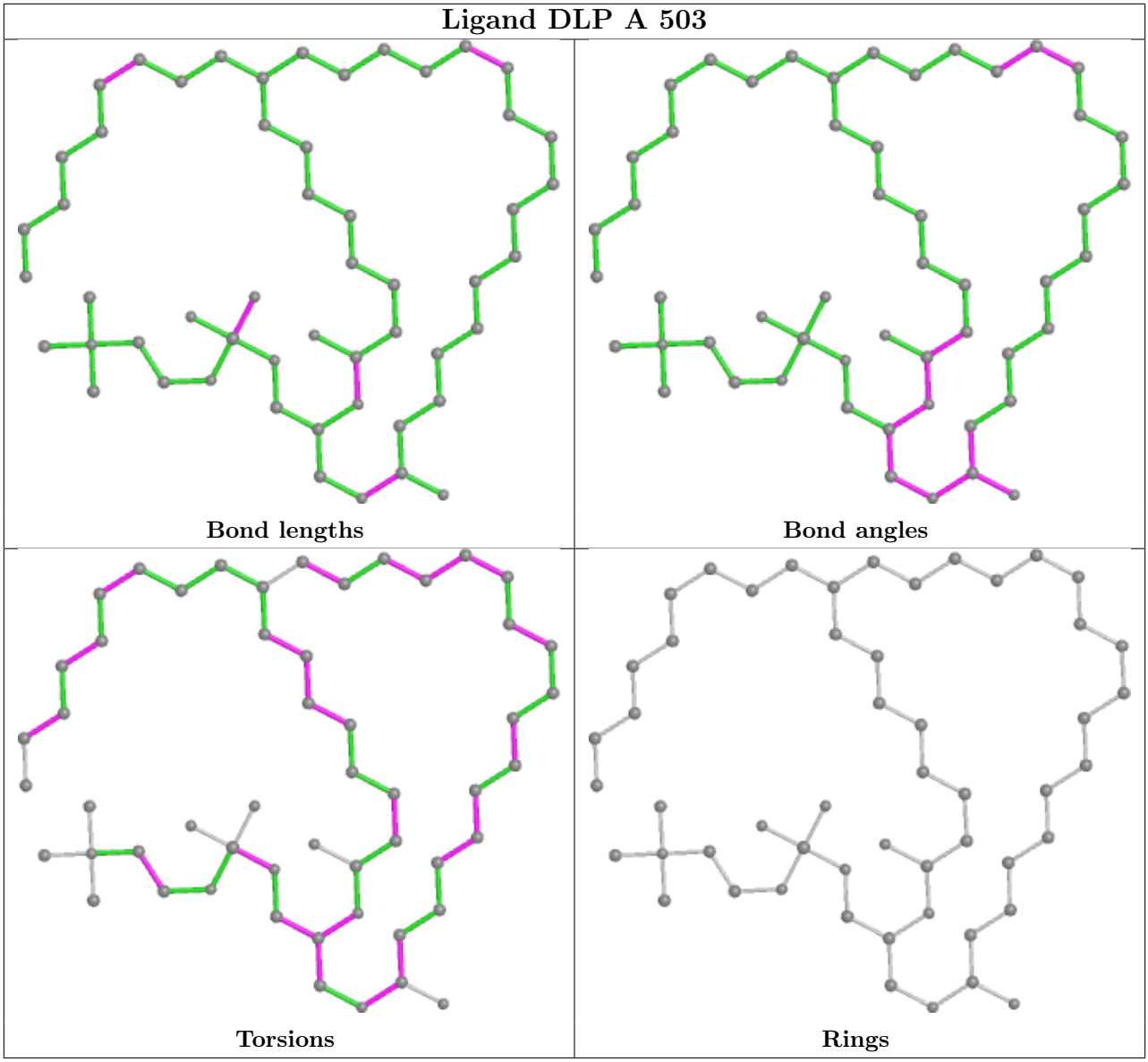
Bond angles



Torsions



Rings



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	472/476 (99%)	0.36	46 (9%) 7 5	51, 75, 141, 173	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	HIS	8.4
1	A	312	VAL	8.3
1	A	476	SER	7.2
1	A	308	PHE	6.1
1	A	315	PHE	5.8
1	A	314	GLY	5.7
1	A	313	GLY	5.5
1	A	301	PHE	5.2
1	A	302	ASN	4.9
1	A	311	VAL	4.8
1	A	399	GLU	4.6
1	A	263	PHE	4.4
1	A	354	ASP	4.1
1	A	300	GLY	4.1
1	A	466	HIS	4.1
1	A	317	SER	3.8
1	A	353	PRO	3.5
1	A	307	ILE	3.4
1	A	397	LEU	3.3
1	A	355	GLN	3.3
1	A	105	TRP	3.0
1	A	469	VAL	2.9
1	A	316	PRO	2.9
1	A	13	CYS	2.9
1	A	475	LEU	2.8
1	A	400	SER	2.8
1	A	15	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	303	THR	2.7
1	A	401	SER	2.6
1	A	318	GLN	2.5
1	A	417	GLY	2.4
1	A	414	THR	2.4
1	A	102	THR	2.3
1	A	470	ASP	2.3
1	A	66	HIS	2.2
1	A	306	GLU	2.2
1	A	361	TYR	2.2
1	A	413	ILE	2.2
1	A	309	GLN	2.2
1	A	418	ILE	2.1
1	A	473	GLN	2.1
1	A	474	SER	2.1
1	A	261	LEU	2.1
1	A	352	ARG	2.1
1	A	356	GLN	2.1
1	A	100	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

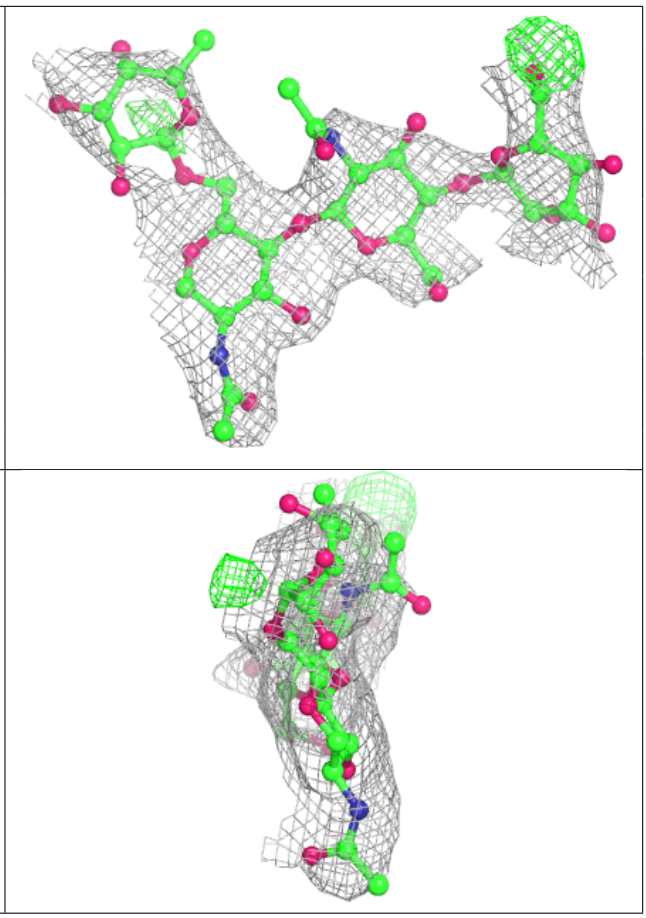
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	B	3	11/12	0.60	0.42	161,162,163,164	0
2	NAG	B	2	14/15	0.86	0.47	145,150,153,157	0
2	NAG	B	1	14/15	0.86	0.30	124,127,133,139	0
2	FUC	B	4	10/11	0.86	0.39	135,137,138,138	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)

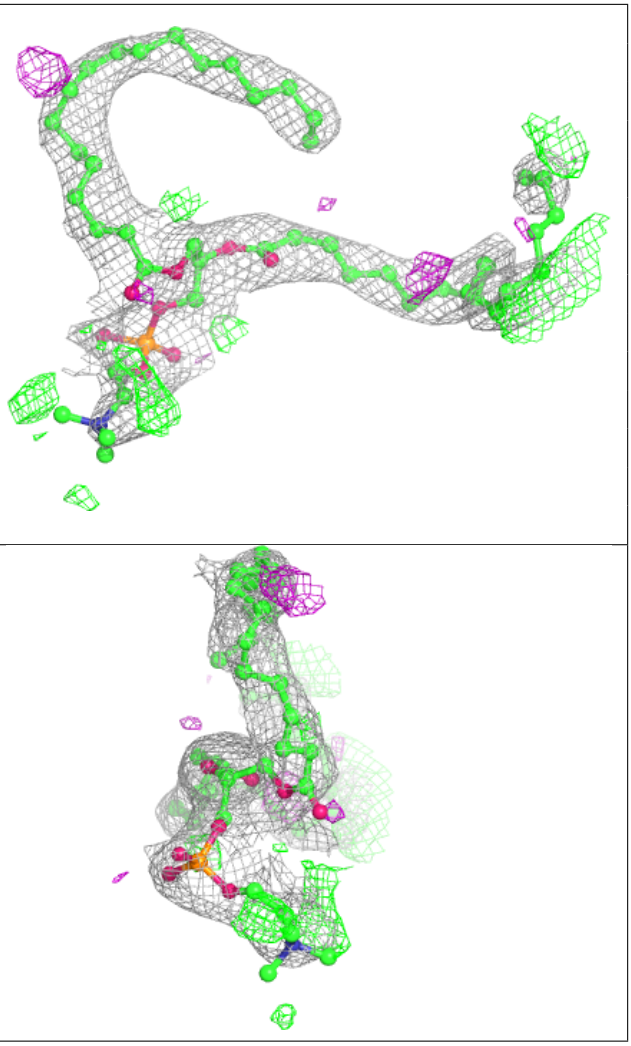
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DLP	A	503	54/54	0.79	0.26	64,86,137,138	0
5	PGE	A	504	10/10	0.85	0.18	77,80,82,82	0
5	PGE	A	505	10/10	0.89	0.33	72,74,75,75	0
3	2OB	A	501	39/47	0.93	0.40	51,64,77,79	0
3	2OB	A	502	47/47	0.94	0.24	51,58,90,96	0
7	0RP	A	507	41/41	0.95	0.24	52,62,71,84	0
6	CL	A	506	1/1	0.98	0.10	64,64,64,64	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.

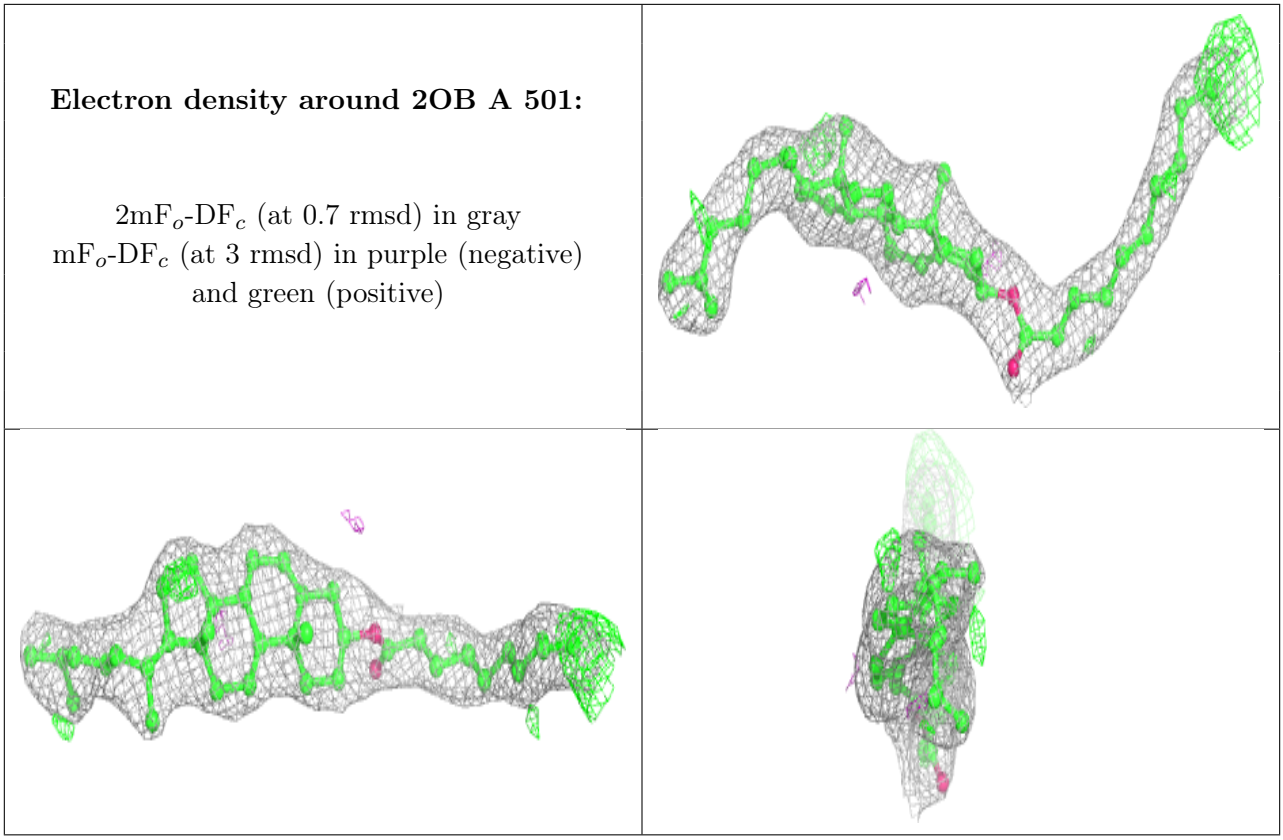
Electron density around DLP A 503:

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



Electron density around 2OB A 501:

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



Electron density around 2OB A 502:

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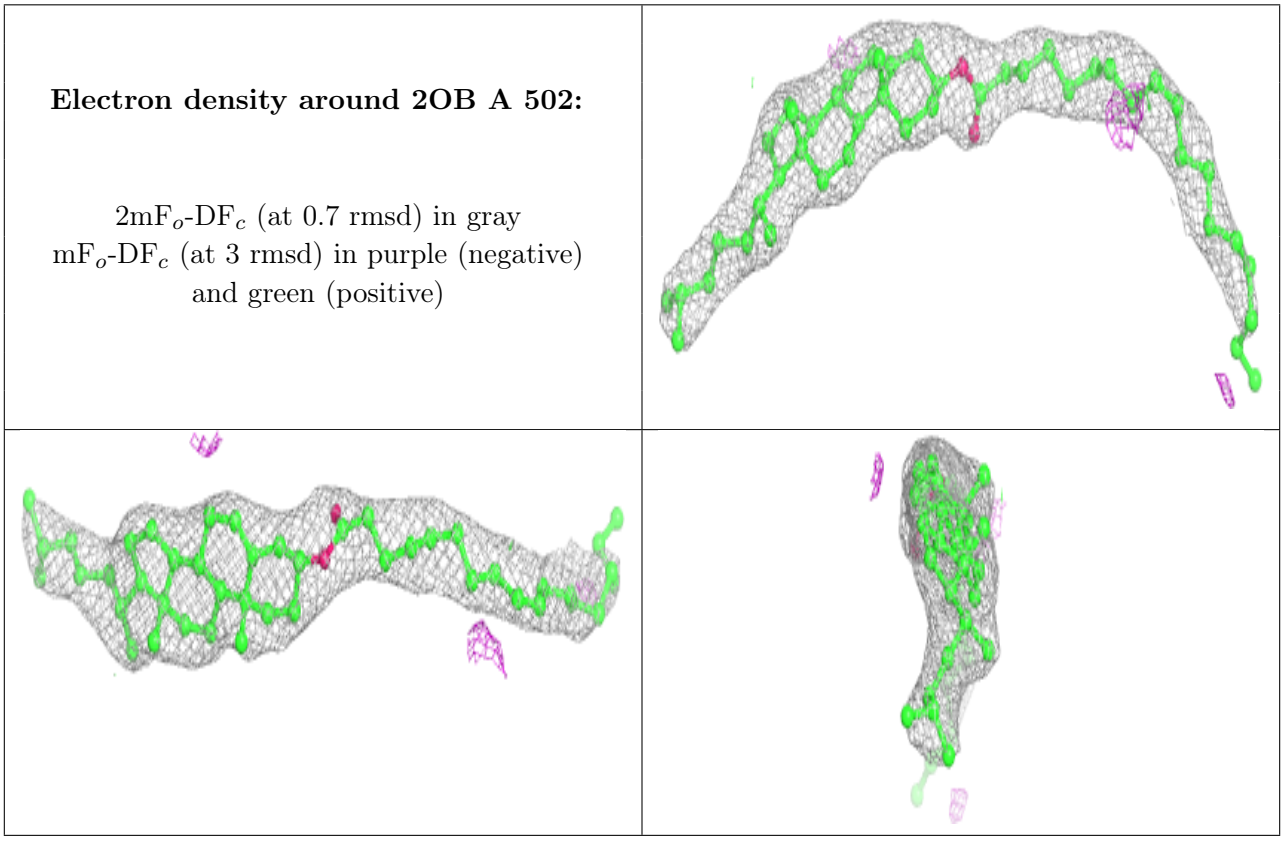
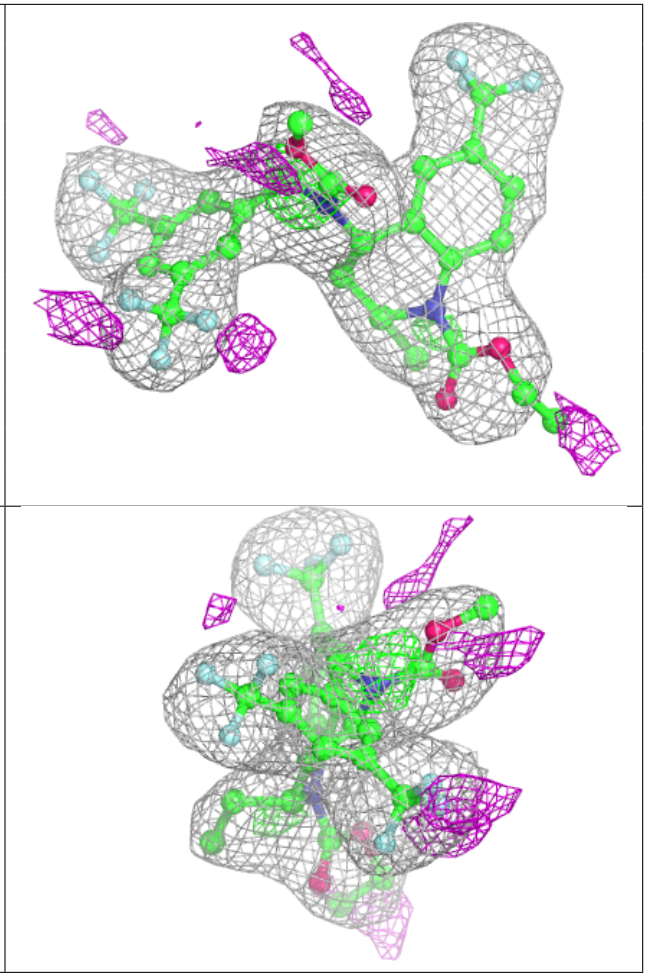
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 0RP A 507:

$2mF_o$-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.