Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 06:23 pm GMT

PDB ID	:	8OGI
Title	:	Structure of native human eosinophil peroxidase
Authors	:	Pfanzagl, V.; Obinger, C.
Deposited on	:	2023-03-20
Resolution	:	1.55 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 ⓘ 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 ⓘ) were used in the production of this report:

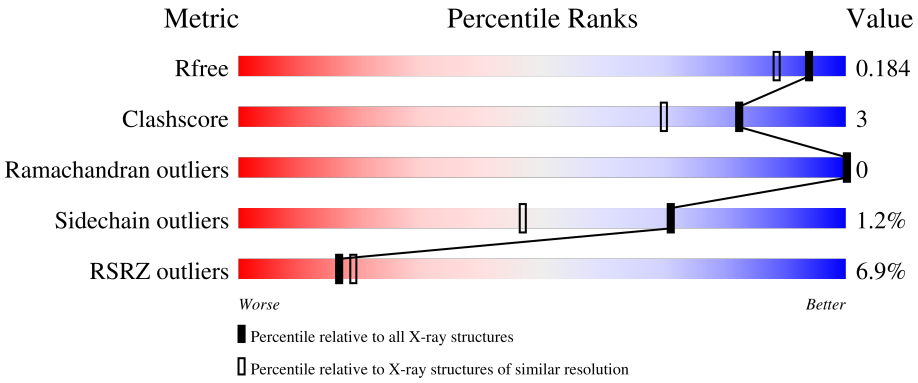
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.55 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	104	7% 91% 9%
2	B	465	7% 95% 5%
3	C	2	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	HEB	A	301	X	-	-	-
6	EDO	A	307	-	-	X	-
6	EDO	B	812	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 10322 atoms, of which 4922 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 Eosinophil peroxidase light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	104	1677	531	830	163	149	4	830	0	0

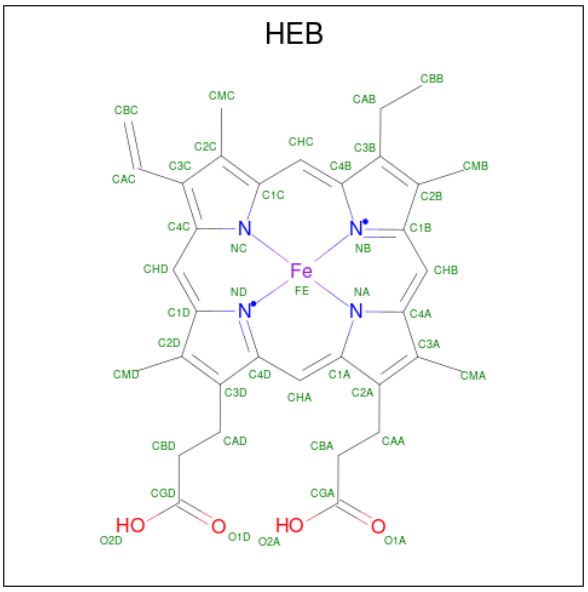
- Molecule 2 is a protein called Eosinophil peroxidase heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	465	7815	2439	3925	759	665	27	3925	15	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

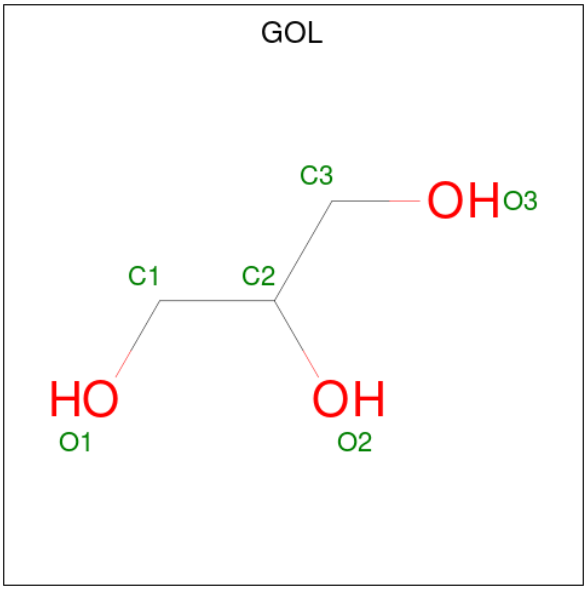
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	C	2	53	16	25	2	10	25	0	0

- Molecule 4 is HEME B/C (three-letter code: HEB) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	30	0
			73	34	1	30	4	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



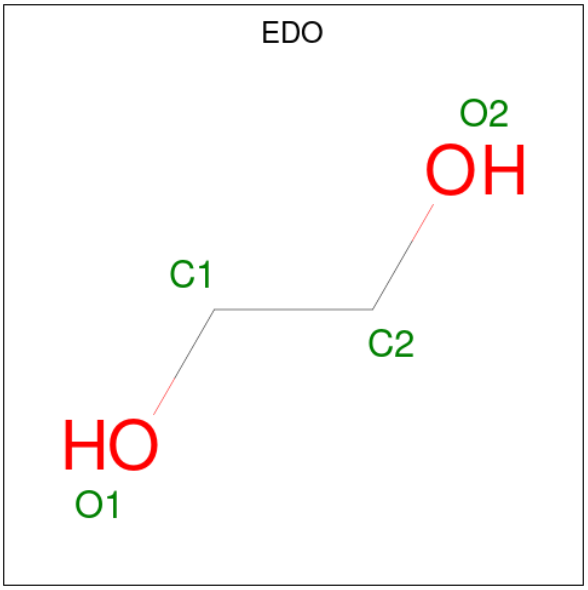
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	8	0
			14	3	8	3		
5	A	1	Total	C	H	O	8	0
			14	3	8	3		
5	B	1	Total	C	H	O	8	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

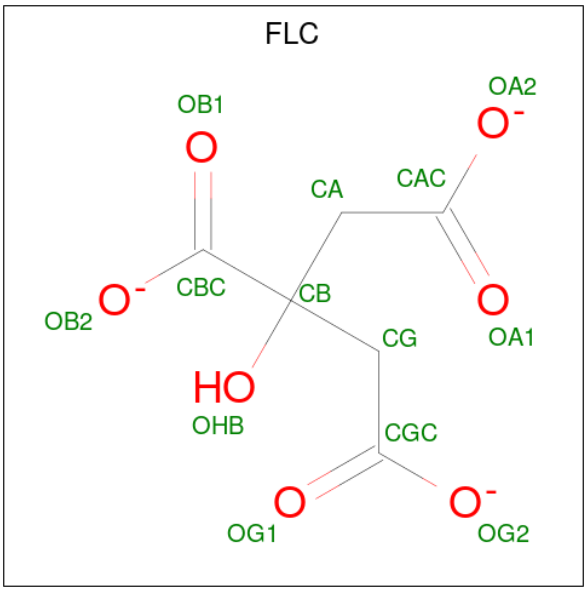
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H O 14 3 8 3	8	0
5	B	1	Total C H O 14 3 8 3	8	0
5	B	1	Total C H O 14 3 8 3	8	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 10 2 6 2	6	0
6	A	1	Total C H O 10 2 6 2	6	0
6	B	1	Total C H O 10 2 6 2	6	0
6	B	1	Total C H O 10 2 6 2	6	0
6	B	1	Total C H O 10 2 6 2	6	0

- Molecule 7 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

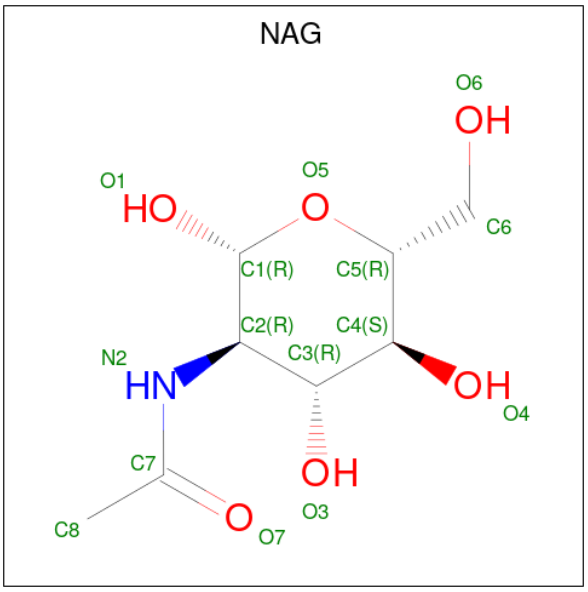


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 18 6 5 7	5	0
7	B	1	Total C H O 18 6 5 7	5	0
7	B	1	Total C H O 18 6 5 7	5	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

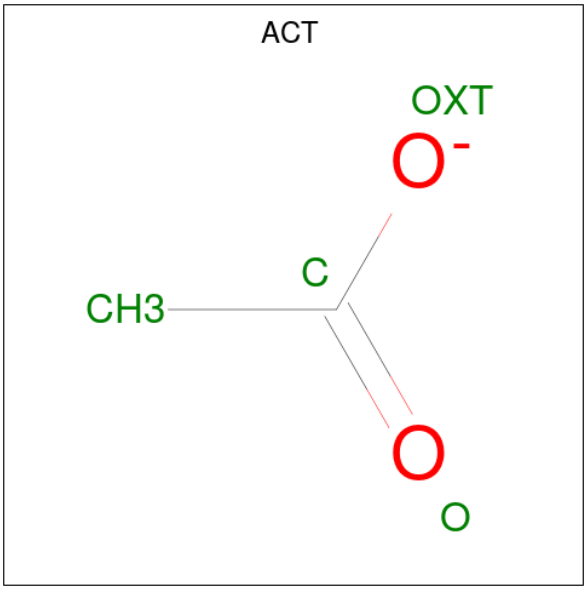
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0
8	B	1	Total Cl 1 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	3	0
			7	2	3	2		
10	B	1	Total	C	H	O	3	0
			7	2	3	2		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Ca 1 1	0	0

- Molecule 12 is water.

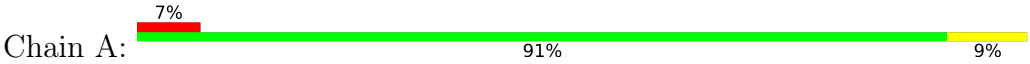
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	103	Total O 103 103	0	0
12	B	369	Total O 369 369	0	0

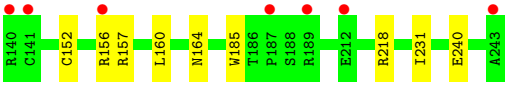
3 Residue-property plots (i)

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: Eosinophil peroxidase light chain

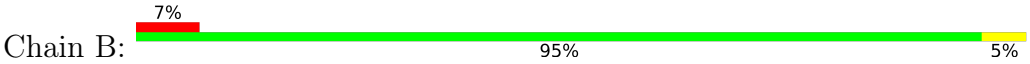
Chain A:

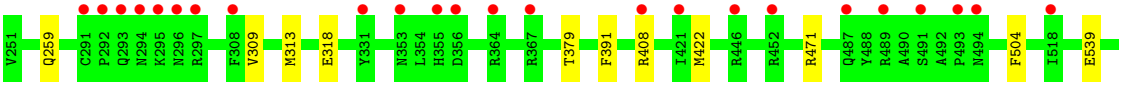




• Molecule 2: Eosinophil peroxidase heavy chain

Chain B:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.12Å 85.56Å 139.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.57 – 1.55 22.57 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (22.57-1.55) 98.8 (22.57-1.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.55Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.174 , 0.185 0.167 , 0.184	Depositor DCC
R_{free} test set	4700 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10322	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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: HEB, FLC, GOL, CL, NAG, ACT, EDO, CA

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	0.56	0/869	0.67	0/1174
2	B	0.52	0/3975	0.63	0/5367
All	All	0.53	0/4844	0.63	0/6541

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	847	830	830	7	0
2	B	3890	3925	3911	16	0
3	C	28	25	25	0	0
4	A	43	30	30	2	0
5	A	12	16	16	0	0
5	B	24	32	32	0	0
6	A	8	12	12	6	0
6	B	12	18	18	6	0
7	A	13	5	5	0	0
7	B	26	10	10	0	0
8	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1	0	0	1	0
9	B	14	13	13	0	0
10	B	8	6	6	0	0
11	B	1	0	0	0	0
12	A	103	0	0	0	0
12	B	369	0	0	1	0
All	All	5400	4922	4908	25	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 3.

All (25) 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)
4:A:301:HEB:HMC1	4:A:301:HEB:HBC1	1.67	0.75
4:A:301:HEB:HMB1	4:A:301:HEB:HBB3	1.82	0.60
2:B:597[B]:ASP:OD1	2:B:600:ARG:NH1	2.39	0.56
6:A:307:EDO:O1	6:B:812:EDO:H21	2.05	0.56
1:A:240:GLU:CG	6:A:307:EDO:H12	2.36	0.55
2:B:471:ARG:HH11	2:B:559:ASN:HD22	1.56	0.54
2:B:471:ARG:HH22	6:B:812:EDO:H22	1.73	0.53
2:B:259:GLN:NE2	12:B:902:HOH:O	2.42	0.52
6:A:307:EDO:H22	6:B:812:EDO:O2	2.09	0.52
6:A:307:EDO:H22	6:B:812:EDO:C2	2.40	0.51
2:B:471:ARG:HH11	2:B:559:ASN:ND2	2.08	0.50
2:B:539:GLU:HG2	8:B:806:CL:CL	2.47	0.50
2:B:471:ARG:NH2	6:B:812:EDO:H22	2.27	0.49
1:A:185:TRP:CH2	2:B:259:GLN:HG2	2.49	0.48
1:A:240:GLU:HG3	6:A:307:EDO:H12	1.95	0.48
6:A:307:EDO:H21	2:B:562:ARG:CZ	2.45	0.47
2:B:391:PHE:HD2	2:B:422[B]:MET:SD	2.38	0.46
2:B:686:ARG:NH2	2:B:703:ARG:NH1	2.64	0.45
1:A:157:ARG:CZ	1:A:160:LEU:HD11	2.47	0.44
1:A:231:ILE:HD11	2:B:309:VAL:HG13	1.99	0.44
1:A:164:ASN:OD1	2:B:318:GLU:OE2	2.36	0.44
2:B:379:THR:O	2:B:504:PHE:HA	2.18	0.43
2:B:471:ARG:HH22	6:B:812:EDO:C2	2.32	0.42
2:B:618:ALA:HB1	2:B:633:LEU:HG	2.00	0.42
1:A:218:ARG:O	1:A:218:ARG:HG3	2.19	0.42

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	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
2	B	478/465 (103%)	469 (98%)	9 (2%)	0	100	100
All	All	580/569 (102%)	569 (98%)	11 (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	90/90 (100%)	88 (98%)	2 (2%)	52	21
2	B	417/402 (104%)	413 (99%)	4 (1%)	76	55
All	All	507/492 (103%)	501 (99%)	6 (1%)	71	47

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	CYS
1	A	156	ARG
2	B	313	MET
2	B	408	ARG
2	B	635	CYS
2	B	696	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
2	B	259	GLN
2	B	559	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)

2 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	2,3	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	C	2	3	14,14,15	0.25	0	17,19,21	0.65	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	2,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

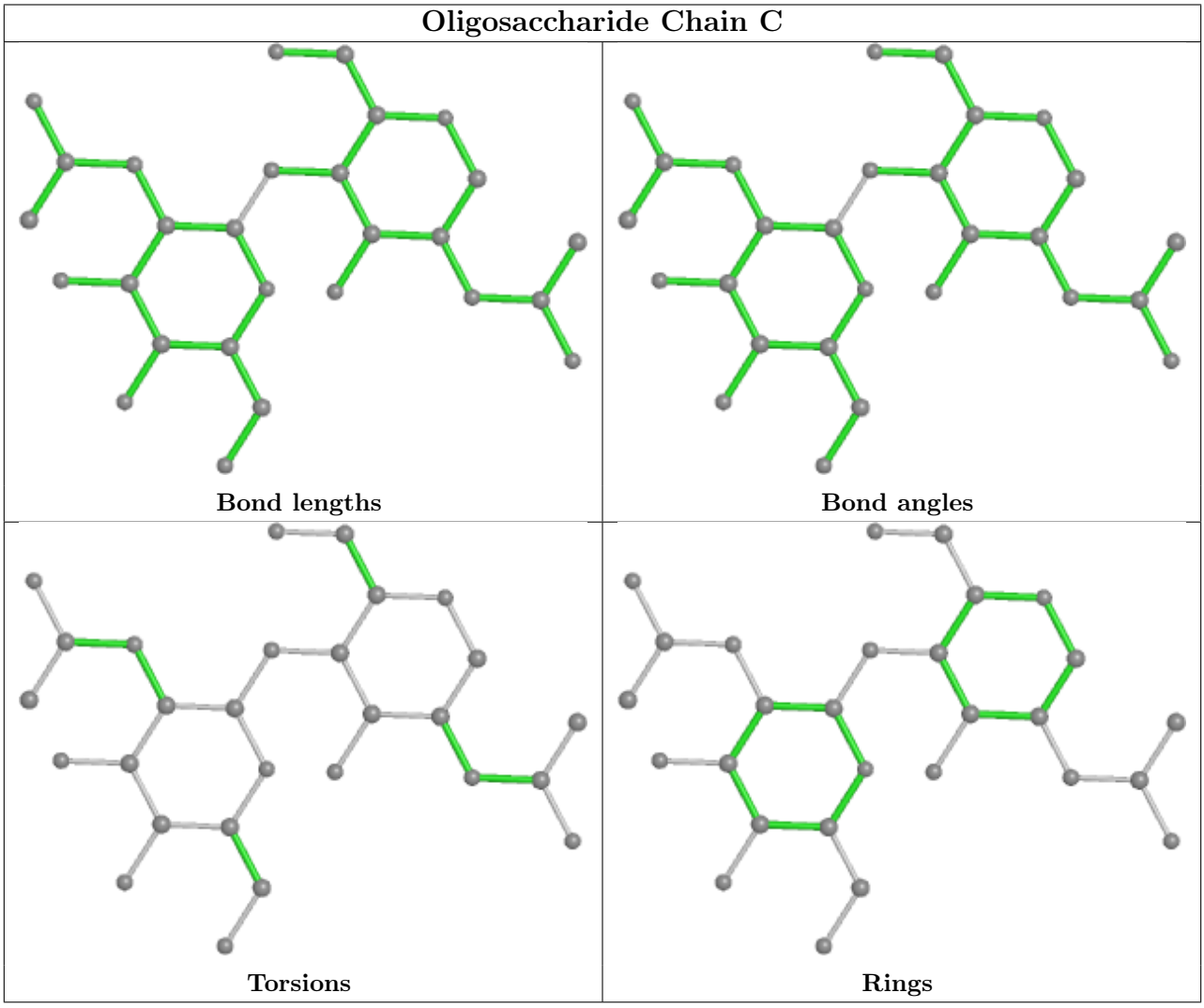
There are no chirality outliers.

There are no torsion outliers.

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)

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	A	303	-	3,3,3	0.55	0	2,2,2	0.14	0
6	EDO	B	809	-	3,3,3	0.53	0	2,2,2	0.20	0
7	FLC	B	804	-	12,12,12	1.00	0	17,17,17	1.56	3 (17%)
5	GOL	B	811	-	5,5,5	0.07	0	5,5,5	0.22	0
9	NAG	B	801	2	14,14,15	0.27	0	17,19,21	0.50	0
7	FLC	A	305	-	12,12,12	1.08	0	17,17,17	1.56	2 (11%)
10	ACT	B	802	-	3,3,3	0.98	0	3,3,3	1.34	0
7	FLC	B	813	-	12,12,12	1.05	0	17,17,17	1.40	2 (11%)
6	EDO	B	812	-	3,3,3	0.50	0	2,2,2	0.28	0
4	HEB	A	301	2,1	48,50,50	1.26	5 (10%)	55,82,82	1.05	4 (7%)
5	GOL	B	810	-	5,5,5	0.07	0	5,5,5	0.21	0
5	GOL	A	302	-	5,5,5	0.07	0	5,5,5	0.28	0
5	GOL	A	304	-	5,5,5	0.05	0	5,5,5	0.26	0
6	EDO	A	307	-	3,3,3	0.61	0	2,2,2	0.22	0
5	GOL	B	807	-	5,5,5	0.09	0	5,5,5	0.19	0
10	ACT	B	814	-	3,3,3	1.28	0	3,3,3	1.96	1 (33%)
5	GOL	B	803	-	5,5,5	0.07	0	5,5,5	0.19	0
6	EDO	B	808	-	3,3,3	0.50	0	2,2,2	0.21	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
6	EDO	A	303	-	-	1/1/1/1	-
6	EDO	B	809	-	-	1/1/1/1	-
7	FLC	B	804	-	-	6/16/16/16	-
5	GOL	B	811	-	-	2/4/4/4	-
9	NAG	B	801	2	-	0/6/23/26	0/1/1/1
7	FLC	A	305	-	-	0/16/16/16	-
7	FLC	B	813	-	-	1/16/16/16	-
6	EDO	B	812	-	-	1/1/1/1	-
4	HEB	A	301	2,1	1/1/8/8	6/12/54/54	-
5	GOL	B	810	-	-	0/4/4/4	-
5	GOL	A	302	-	-	0/4/4/4	-
5	GOL	A	304	-	-	0/4/4/4	-
6	EDO	A	307	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	807	-	-	0/4/4/4	-
5	GOL	B	803	-	-	0/4/4/4	-
6	EDO	B	808	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	HEB	C3C-C2C	-3.25	1.35	1.40
4	A	301	HEB	CBC-CAC	3.20	1.50	1.29
4	A	301	HEB	CHC-C4B	2.67	1.41	1.35
4	A	301	HEB	FE-NA	2.32	2.04	1.95
4	A	301	HEB	C4B-NB	-2.10	1.36	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	305	FLC	OB1-CBC-CB	-4.71	115.58	122.25
7	B	813	FLC	OB1-CBC-CB	-3.78	116.91	122.25
7	B	804	FLC	OB1-CBC-CB	-3.70	117.02	122.25
4	A	301	HEB	CAB-C3B-C4B	-3.01	120.91	124.81
10	B	814	ACT	OXT-C-O	2.84	132.54	122.05
4	A	301	HEB	CMC-C2C-C1C	-2.67	124.37	128.46
4	A	301	HEB	CMC-C2C-C3C	2.47	129.30	124.68
7	B	813	FLC	OB2-CBC-CB	2.47	117.34	113.05
7	A	305	FLC	OB2-CBC-CB	2.41	117.23	113.05
4	A	301	HEB	CAB-C3B-C2B	2.18	131.25	127.53
7	B	804	FLC	OG1-CGC-CG	-2.04	116.99	122.94
7	B	804	FLC	CG-CB-CBC	-2.02	105.76	110.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	301	HEB	NA

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	HEB	C4B-C3B-CAB-CBB
4	A	301	HEB	C2B-C3B-CAB-CBB
6	B	809	EDO	O1-C1-C2-O2
6	B	812	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	804	FLC	CA-CB-CBC-OB1
7	B	804	FLC	CA-CB-CBC-OB2
7	B	804	FLC	CG-CB-CBC-OB1
7	B	804	FLC	CG-CB-CBC-OB2
5	B	811	GOL	O1-C1-C2-O2
6	A	303	EDO	O1-C1-C2-O2
7	B	804	FLC	CB-CG-CGC-OG2
7	B	804	FLC	CB-CG-CGC-OG1
7	B	813	FLC	CAC-CA-CB-CBC
4	A	301	HEB	CAA-CBA-CGA-O2A
6	B	808	EDO	O1-C1-C2-O2
4	A	301	HEB	CAD-CBD-CGD-O2D
4	A	301	HEB	CAA-CBA-CGA-O1A
4	A	301	HEB	CAD-CBD-CGD-O1D
6	A	307	EDO	O1-C1-C2-O2
5	B	811	GOL	O1-C1-C2-C3

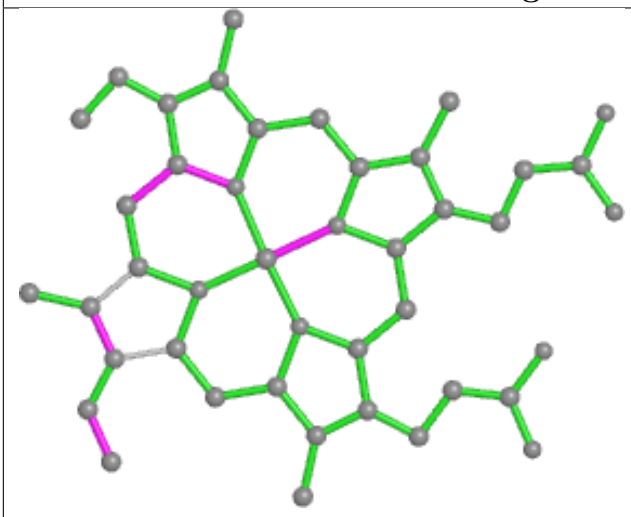
There are no ring outliers.

3 monomers are involved in 11 short contacts:

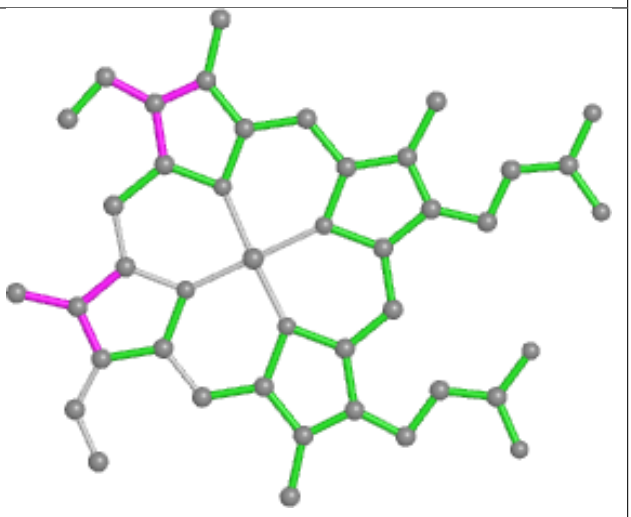
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	812	EDO	6	0
4	A	301	HEB	2	0
6	A	307	EDO	6	0

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.

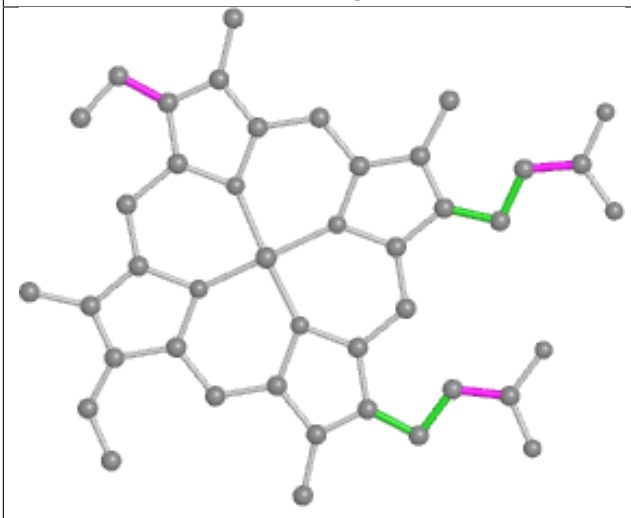
Ligand HEB A 301



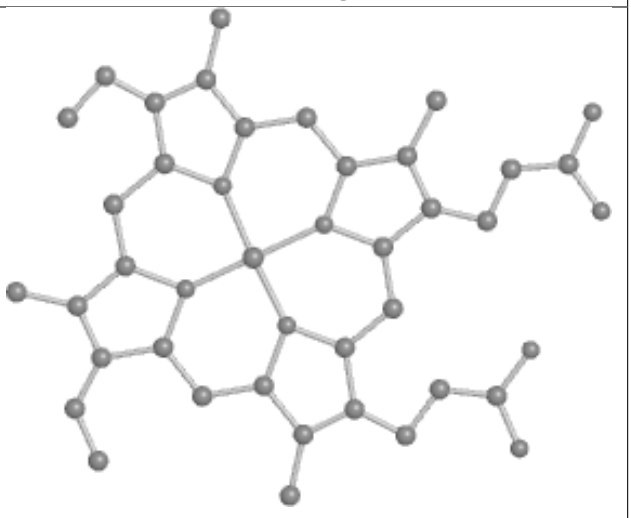
Bond lengths



Bond angles



Torsions



Rings

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	104/104 (100%)	0.22	7 (6%)	17	20	17, 22, 37, 54	0
2	B	465/465 (100%)	0.29	32 (6%)	16	19	15, 23, 41, 69	0
All	All	569/569 (100%)	0.28	39 (6%)	16	19	15, 23, 41, 69	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	493	PRO	10.9
2	B	294	ASN	10.8
2	B	293	GLN	10.7
2	B	296	ASN	9.9
2	B	292	PRO	9.5
2	B	291	CYS	8.2
1	A	140	ARG	6.8
2	B	355	HIS	6.7
2	B	295	LYS	6.0
1	A	187	PRO	5.3
2	B	655	ARG	4.6
2	B	356	ASP	4.6
2	B	696	ARG	4.5
1	A	156	ARG	3.7
2	B	494	ASN	3.6
2	B	367	ARG	3.6
2	B	491	SER	3.6
2	B	408	ARG	3.5
2	B	703	ARG	3.4
2	B	297	ARG	3.4
1	A	243	ALA	3.4
1	A	212	GLU	3.3
2	B	452	ARG	3.1
2	B	693	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	141	CYS	2.9
2	B	660	LYS	2.9
2	B	584	ARG	2.8
2	B	489	ARG	2.7
2	B	715	THR	2.6
2	B	446	ARG	2.5
2	B	308	PHE	2.4
2	B	518	ILE	2.4
2	B	487	GLN	2.4
2	B	364	ARG	2.3
2	B	331	TYR	2.3
2	B	353	ASN	2.3
2	B	421	ILE	2.2
1	A	189	ARG	2.2
2	B	616	ILE	2.1

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)

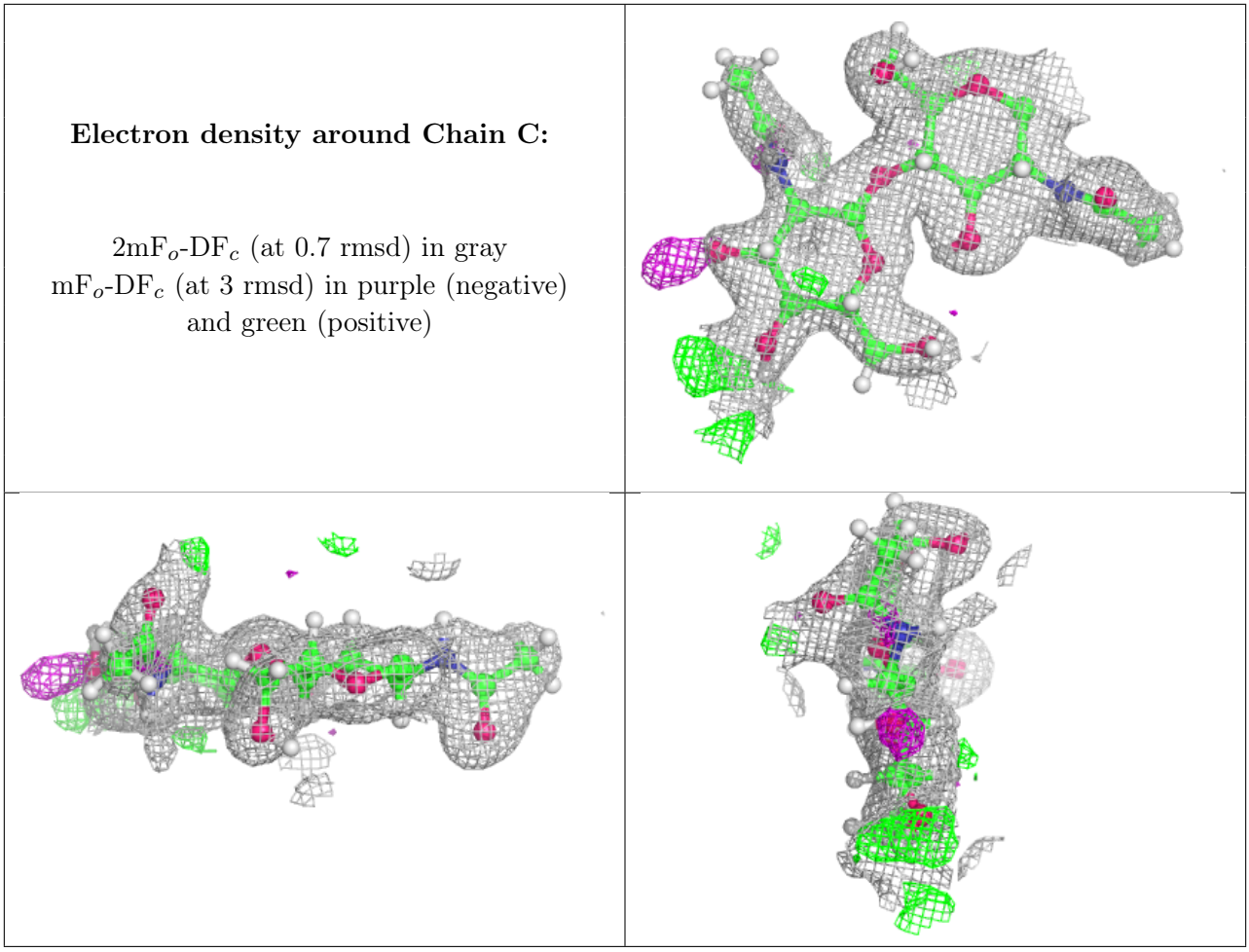
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	NAG	C	2	14/15	0.82	0.32	40,46,51,51	13
3	NAG	C	1	14/15	0.92	0.07	26,31,37,38	12

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)



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	EDO	B	812	4/4	0.47	0.26	43,43,44,45	6
6	EDO	B	809	4/4	0.54	0.15	54,56,57,57	6
7	FLC	A	305	13/13	0.59	0.23	38,42,47,47	5
7	FLC	B	813	13/13	0.60	0.26	69,71,72,72	5
5	GOL	B	810	6/6	0.61	0.18	53,55,57,58	8
5	GOL	A	304	6/6	0.62	0.25	62,63,66,66	8
5	GOL	A	302	6/6	0.66	0.22	42,43,44,44	8
5	GOL	B	811	6/6	0.67	0.23	65,67,68,68	8
6	EDO	B	808	4/4	0.69	0.16	52,53,55,55	6
10	ACT	B	802	4/4	0.69	0.20	44,45,48,48	3
9	NAG	B	801	14/15	0.74	0.22	40,46,51,51	13

Continued on next page...

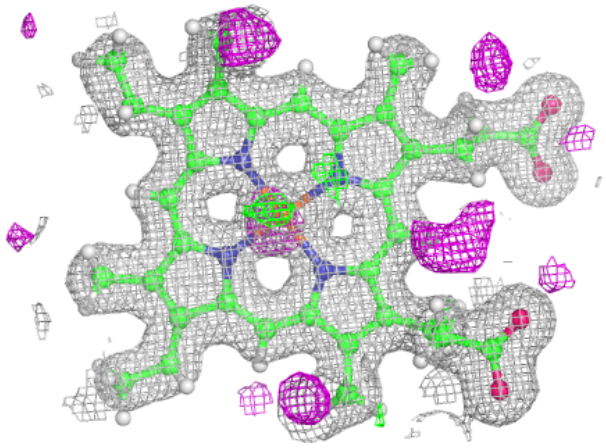
Continued from previous page...

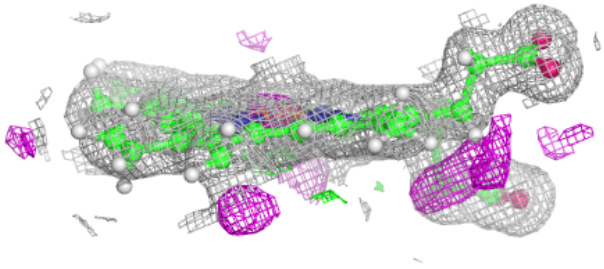
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	803	6/6	0.76	0.21	47,48,49,49	8
6	EDO	A	303	4/4	0.77	0.15	30,32,33,33	6
10	ACT	B	814	4/4	0.83	0.13	33,34,35,35	3
6	EDO	A	307	4/4	0.88	0.23	25,29,34,35	6
5	GOL	B	807	6/6	0.93	0.14	38,39,40,40	8
7	FLC	B	804	13/13	0.95	0.06	22,23,25,25	5
8	CL	B	806	1/1	0.98	0.04	27,27,27,27	1
4	HEB	A	301	43/43	0.98	0.07	14,16,19,21	30
8	CL	A	306	1/1	0.99	0.06	19,19,19,19	0
11	CA	B	805	1/1	1.00	0.08	17,17,17,17	0

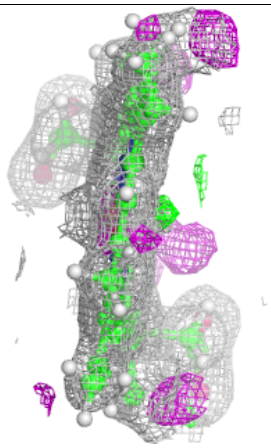
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEB A 301:

$2mF_o$-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

There are no such residues in this entry.