



Full wwPDB X-ray Structure Validation Report i

Oct 3, 2023 – 02:31 PM JST

PDB ID : 8H2W
Title : Cellobextrin phosphorylase from Clostridium thermocellum mutant - all cysteine residues were substituted with serines
Authors : Kuga, T.; Sunagawa, N.; Igarashi, K.
Deposited on : 2022-10-07
Resolution : 1.21 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 ①) were used in the production of this report:

MolProbitiy : 4.02b-467
Xtrige (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

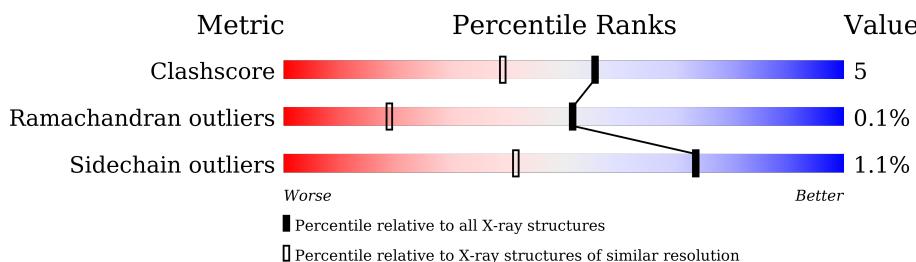
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1294 (1.24-1.20)
Ramachandran outliers	138981	1251 (1.24-1.20)
Sidechain outliers	138945	1250 (1.24-1.20)

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	BGC	D	1	-	-	X	-
3	ACT	B	1002	-	-	X	-
5	SO4	A	1007	-	-	X	-
6	PEG	A	1008	-	-	X	-
7	GOL	B	1018	-	-	X	-
7	GOL	B	1019	-	-	X	-

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 34642 atoms, of which 15434 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 Cellobextrin phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	984	15858	5311	7533	1393	1596	25	177	55	0
1	B	984	16079	5395	7607	1425	1628	24	188	71	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q93HT8
A	2	GLY	-	expression tag	UNP Q93HT8
A	65	SER	CYS	engineered mutation	UNP Q93HT8
A	81	SER	CYS	engineered mutation	UNP Q93HT8
A	226	SER	CYS	engineered mutation	UNP Q93HT8
A	230	SER	CYS	engineered mutation	UNP Q93HT8
A	241	SER	CYS	engineered mutation	UNP Q93HT8
A	354	SER	CYS	engineered mutation	UNP Q93HT8
A	373	SER	CYS	engineered mutation	UNP Q93HT8
A	607	SER	CYS	engineered mutation	UNP Q93HT8
A	626	SER	CYS	engineered mutation	UNP Q93HT8
A	630	ASP	ALA	engineered mutation	UNP Q93HT8
A	873	SER	CYS	engineered mutation	UNP Q93HT8
A	935	SER	CYS	engineered mutation	UNP Q93HT8
A	986	LEU	-	expression tag	UNP Q93HT8
A	987	GLU	-	expression tag	UNP Q93HT8
A	988	HIS	-	expression tag	UNP Q93HT8
A	989	HIS	-	expression tag	UNP Q93HT8
A	990	HIS	-	expression tag	UNP Q93HT8
A	991	HIS	-	expression tag	UNP Q93HT8
A	992	HIS	-	expression tag	UNP Q93HT8
A	993	HIS	-	expression tag	UNP Q93HT8
B	1	MET	-	initiating methionine	UNP Q93HT8
B	2	GLY	-	expression tag	UNP Q93HT8
B	65	SER	CYS	engineered mutation	UNP Q93HT8

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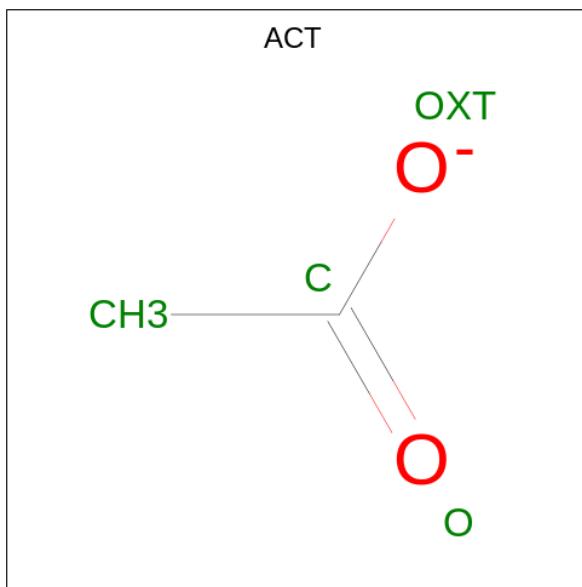
Chain	Residue	Modelled	Actual	Comment	Reference
B	81	SER	CYS	engineered mutation	UNP Q93HT8
B	226	SER	CYS	engineered mutation	UNP Q93HT8
B	230	SER	CYS	engineered mutation	UNP Q93HT8
B	241	SER	CYS	engineered mutation	UNP Q93HT8
B	354	SER	CYS	engineered mutation	UNP Q93HT8
B	373	SER	CYS	engineered mutation	UNP Q93HT8
B	607	SER	CYS	engineered mutation	UNP Q93HT8
B	626	SER	CYS	engineered mutation	UNP Q93HT8
B	630	ASP	ALA	engineered mutation	UNP Q93HT8
B	873	SER	CYS	engineered mutation	UNP Q93HT8
B	935	SER	CYS	engineered mutation	UNP Q93HT8
B	986	LEU	-	expression tag	UNP Q93HT8
B	987	GLU	-	expression tag	UNP Q93HT8
B	988	HIS	-	expression tag	UNP Q93HT8
B	989	HIS	-	expression tag	UNP Q93HT8
B	990	HIS	-	expression tag	UNP Q93HT8
B	991	HIS	-	expression tag	UNP Q93HT8
B	992	HIS	-	expression tag	UNP Q93HT8
B	993	HIS	-	expression tag	UNP Q93HT8

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



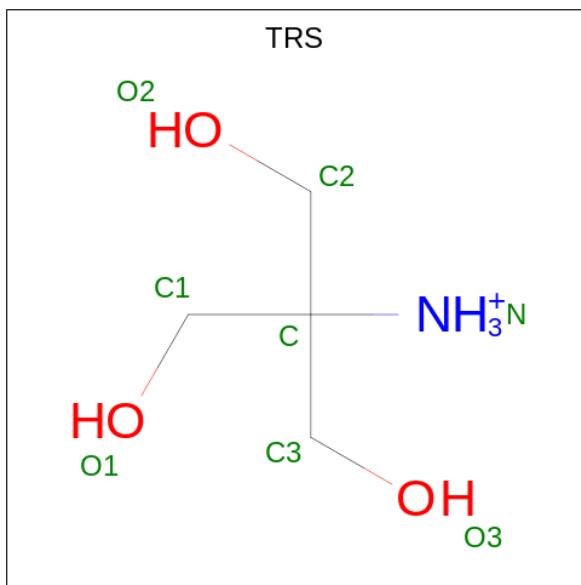
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	3	Total C O 34 18 16	0	0	0
2	D	3	Total C O 34 18 16	0	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



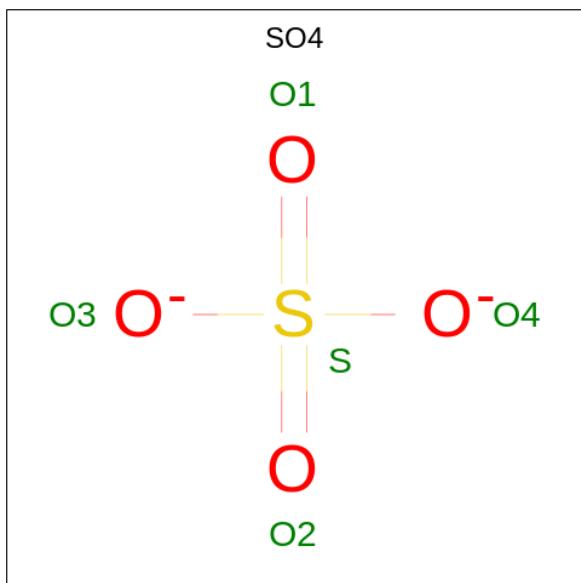
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	H	O	
			7	2	3	2	
3	A	1	Total	C	H	O	
			7	2	3	2	
3	A	1	Total	C	H	O	
			7	2	3	2	
3	A	1	Total	C	H	O	
			7	2	3	2	
3	A	1	Total	C	H	O	
			7	2	3	2	
3	B	1	Total	C	H	O	
			7	2	3	2	
3	B	1	Total	C	H	O	
			7	2	3	2	
3	B	1	Total	C	H	O	
			7	2	3	2	

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



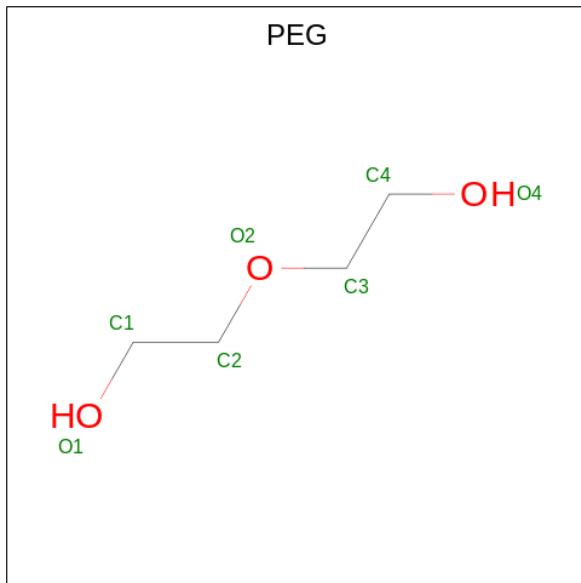
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	20	4	12	1	3	0	0
4	B	1	20	4	12	1	3	0	0
4	B	1	20	4	12	1	3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



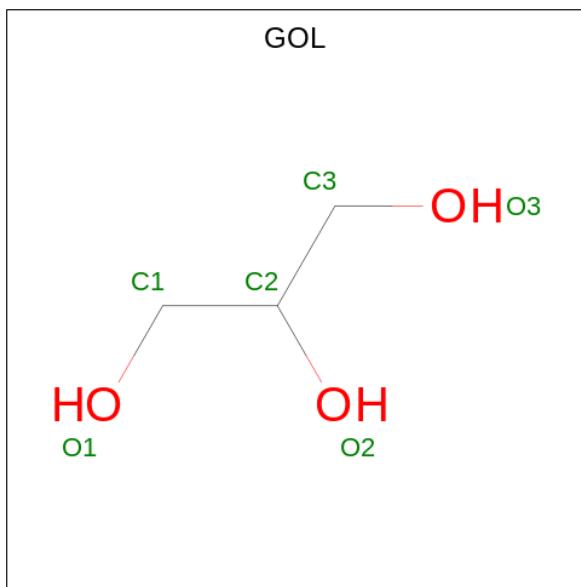
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 17 4 10 3	0	0
6	A	1	Total C H O 17 4 10 3	0	0
6	A	1	Total C H O 17 4 10 3	0	0
6	B	1	Total C H O 17 4 10 3	0	0
6	B	1	Total C H O 17 4 10 3	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Cl 2 2	0	0
8	B	3	Total Cl 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1053	Total O 1053 1053	0	0
9	B	1046	Total O 1046 1046	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.21Å 88.78Å 88.76Å 98.58° 110.55° 110.56°	Depositor
Resolution (Å)	43.82 – 1.21	Depositor
% Data completeness (in resolution range)	94.3 (43.82-1.21)	Depositor
R _{merge}	0.04	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.40 (at 1.21Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R _{free}	0.143 , 0.163	Depositor
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.065	Xtriage
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.447 for -h,-l,-k	Xtriage
Total number of atoms	34642	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [\(i\)](#)

4.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CL, ACT, TRS, SO4, BGC, GOL

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	0.41	0/8503	0.68	2/11495 (0.0%)
1	B	0.42	0/8651	0.69	1/11689 (0.0%)
All	All	0.42	0/17154	0.68	3/23184 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	485	MET	CB-CG-SD	-5.58	95.67	112.40
1	A	485	MET	CB-CG-SD	-5.41	96.17	112.40
1	A	339	MET	CA-CB-CG	5.06	121.90	113.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	797	ALA	Peptide
1	A	798	ASN	Peptide
1	B	412	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	B	503	GLU	Mainchain

4.2 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	8325	7533	8157	69	0
1	B	8472	7607	8277	100	0
2	C	34	0	30	4	0
2	D	34	0	30	6	0
3	A	20	15	15	2	0
3	B	12	9	9	9	0
4	A	8	12	12	2	0
4	B	16	24	24	5	0
5	A	5	0	0	3	0
5	B	5	0	0	0	0
6	A	21	30	30	8	0
6	B	14	20	20	0	0
7	A	66	88	87	5	0
7	B	72	96	95	19	0
8	A	2	0	0	0	0
8	B	3	0	0	0	0
9	A	1053	0	0	11	0
9	B	1046	0	0	13	0
All	All	19208	15434	16786	172	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (172) 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:956:GLU:OE1	1:A:963:LYS:NZ	1.87	1.07
1:B:632:ASN:HD21	7:B:1019:GOL:H11	1.38	0.89
1:B:772:VAL:HG12	1:B:776[A]:LYS:HE2	1.57	0.86
1:A:954[B]:GLU:CG	1:A:985:LYS:HD2	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296[B]:PHE:O	3:B:1002:ACT:H3	1.76	0.84
1:A:776:LYS:HD2	1:A:842:GLU:OE2	1.79	0.81
1:A:502:ARG:HH12	6:A:1008:PEG:H21	1.46	0.80
1:A:954[B]:GLU:HG2	1:A:985:LYS:HD2	1.62	0.80
1:B:296[A]:PHE:O	3:B:1002:ACT:H3	1.85	0.76
1:B:165[B]:VAL:HG13	1:B:489:PHE:CE2	2.20	0.76
1:A:296[B]:PHE:CG	1:B:296[B]:PHE:HE2	2.03	0.76
1:B:255[B]:LYS:HE2	1:B:433:TYR:CE1	2.22	0.74
1:A:494:LYS:HE3	3:B:1002:ACT:H2	1.69	0.74
1:B:776[A]:LYS:CE	1:B:842:GLU:OE2	2.39	0.71
1:B:910[B]:ARG:NH1	9:B:1101:HOH:O	2.22	0.71
1:B:502:ARG:HH12	7:B:1012:GOL:H31	1.56	0.71
5:A:1007:SO4:O1	9:A:1101:HOH:O	2.08	0.70
1:B:299:VAL:N	3:B:1002:ACT:OXT	2.25	0.70
1:B:925[A]:GLN:OE1	1:B:942[A]:THR:HG22	1.94	0.66
1:A:296[B]:PHE:CD1	1:B:296[B]:PHE:CE2	2.84	0.66
1:B:804[A]:HIS:HE1	2:D:1:BGC:H6C1	1.61	0.65
1:B:704:ASP:HB3	9:B:1930:HOH:O	1.96	0.64
1:A:330:PHE:HZ	2:D:1:BGC:H1	1.63	0.63
1:A:296[B]:PHE:CD1	1:B:296[B]:PHE:HE2	2.15	0.62
1:B:330:PHE:HZ	2:C:1:BGC:H1	1.64	0.62
1:A:378:LYS:CE	4:B:1004:TRS:H22	2.30	0.62
1:A:925[A]:GLN:OE1	1:A:942[A]:THR:HG22	2.00	0.62
1:B:773:ASP:HA	1:B:776[A]:LYS:HE3	1.81	0.61
1:B:12:LYS:N	1:B:12:LYS:HD3	2.14	0.61
1:B:786[B]:ARG:NH1	9:B:1107:HOH:O	2.35	0.60
1:A:798:ASN:OD1	1:A:798:ASN:O	2.20	0.59
1:A:494:LYS:HB2	3:B:1002:ACT:H2	1.84	0.59
1:B:641:LYS:HD3	9:B:1892:HOH:O	2.01	0.59
1:B:797:ALA:O	1:B:800:THR:N	2.36	0.59
1:A:428:ASP:OD1	4:A:1003:TRS:H11	2.04	0.58
1:B:428[A]:ASP:OD2	1:B:432[A]:ARG:NH1	2.34	0.58
1:A:333:ASP:OD2	3:A:1001:ACT:H1	2.03	0.58
1:B:165[B]:VAL:HG13	1:B:489:PHE:CZ	2.39	0.58
1:B:632:ASN:ND2	7:B:1019:GOL:H11	2.15	0.58
1:A:730[B]:THR:HG23	1:A:731:TYR:HD1	1.69	0.58
1:A:954[A]:GLU:HB3	1:A:985:LYS:HD2	1.85	0.57
1:B:547:VAL:HA	7:B:1017:GOL:H12	1.86	0.57
1:A:776:LYS:CD	1:A:842:GLU:OE2	2.51	0.57
1:A:296[B]:PHE:CG	1:B:296[B]:PHE:CE2	2.91	0.56
1:B:106:ASN:OD1	1:B:110[B]:LYS:HE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890[B]:SER:HB2	5:A:1007:SO4:O1	2.06	0.56
1:B:326:TYR:HA	7:B:1009:GOL:C3	2.35	0.56
1:B:299:VAL:HB	3:B:1002:ACT:OXT	2.07	0.55
1:A:296[B]:PHE:CD2	1:B:296[B]:PHE:HE2	2.24	0.55
1:B:326:TYR:HA	7:B:1009:GOL:H32	1.87	0.55
1:A:313:ASN:HB2	4:A:1003:TRS:O1	2.07	0.54
1:A:497[B]:ARG:NH2	9:A:1109:HOH:O	2.40	0.54
1:B:761[B]:ASP:OD1	1:B:833[B]:LYS:NZ	2.41	0.54
1:A:296[B]:PHE:CD1	1:B:187:PHE:HB3	2.43	0.54
1:B:502:ARG:HH12	7:B:1012:GOL:C3	2.19	0.54
1:B:772:VAL:HG12	1:B:776[A]:LYS:CE	2.32	0.54
1:A:494:LYS:CE	3:B:1002:ACT:H2	2.37	0.53
1:B:661:ASP:OD1	7:B:1019:GOL:H12	2.09	0.53
1:B:521:ASP:O	1:B:525[A]:GLU:HG3	2.09	0.53
1:B:776[A]:LYS:HD3	1:B:842:GLU:OE2	2.07	0.53
1:B:299:VAL:H	3:B:1002:ACT:C	2.21	0.53
1:A:547:VAL:HA	7:A:1011:GOL:H2	1.91	0.53
1:B:293:HIS:O	1:B:296[B]:PHE:HD1	1.92	0.53
1:B:804[A]:HIS:CE1	2:D:1:BGC:H6C1	2.42	0.53
1:A:954[B]:GLU:HG3	1:A:985:LYS:HD2	1.89	0.52
1:B:255[B]:LYS:HB3	1:B:255[B]:LYS:NZ	2.23	0.52
1:A:296[B]:PHE:CE1	1:B:296[B]:PHE:CE2	2.97	0.52
1:B:295:ILE:O	3:B:1002:ACT:H1	2.10	0.52
1:A:351:GLN:HG2	9:A:1102:HOH:O	2.11	0.51
1:B:797:ALA:O	1:B:799:ASP:N	2.44	0.51
1:B:107[B]:LYS:HE3	9:B:1177:HOH:O	2.10	0.51
1:B:255[A]:LYS:HE3	1:B:433:TYR:CE1	2.46	0.51
1:A:797:ALA:O	1:A:799:ASP:N	2.45	0.50
7:B:1020:GOL:O1	7:B:1020:GOL:O3	2.25	0.50
1:A:27:ILE:HD12	1:A:83[A]:VAL:CG1	2.42	0.50
1:A:786[B]:ARG:NH2	9:A:1119:HOH:O	2.45	0.49
1:B:956:GLU:OE1	1:B:963[A]:LYS:NZ	2.45	0.49
1:B:133:LEU:HD12	1:B:224:ALA:HB1	1.95	0.49
1:B:533:ASN:OD1	7:B:1017:GOL:H11	2.13	0.48
1:A:925[B]:GLN:HE21	1:A:927:ASN:HD21	1.61	0.48
1:B:776[A]:LYS:HE2	1:B:842:GLU:OE2	2.11	0.48
1:B:700[B]:LYS:NZ	9:B:1116:HOH:O	2.46	0.48
1:B:107[A]:LYS:HE2	9:B:1177:HOH:O	2.13	0.48
1:B:255[B]:LYS:HE2	1:B:433:TYR:CD1	2.48	0.48
1:A:797:ALA:HB1	1:A:800:THR:CG2	2.43	0.48
1:B:772:VAL:O	1:B:776[A]:LYS:HE3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1008:PEG:H12	9:A:1128:HOH:O	2.14	0.48
1:B:351[B]:GLN:HB3	9:B:1172:HOH:O	2.13	0.48
1:A:766[B]:GLU:HG3	9:A:1795:HOH:O	2.14	0.47
1:B:776[A]:LYS:CD	1:B:842:GLU:OE2	2.62	0.47
1:B:776[A]:LYS:NZ	1:B:842:GLU:OE2	2.47	0.47
1:A:133:LEU:HD12	1:A:224:ALA:HB1	1.96	0.47
1:A:502:ARG:NH1	6:A:1008:PEG:H21	2.24	0.47
1:B:12:LYS:N	1:B:12:LYS:CD	2.77	0.47
1:B:441[A]:GLU:OE1	7:B:1013:GOL:H31	2.14	0.47
1:A:502:ARG:HH12	6:A:1008:PEG:C2	2.22	0.47
1:B:296[B]:PHE:CD1	1:B:296[B]:PHE:N	2.82	0.47
1:A:68:SER:O	1:A:72:LYS:HG2	2.15	0.47
1:A:533:ASN:ND2	7:A:1011:GOL:H32	2.31	0.46
1:B:351[A]:GLN:HG2	9:B:1111:HOH:O	2.13	0.46
1:B:817[B]:LYS:HE3	1:B:874:THR:O	2.14	0.46
1:B:910[B]:ARG:NH1	9:B:1122:HOH:O	2.48	0.46
1:A:811:GLU:OE2	7:A:1019:GOL:H11	2.15	0.46
1:A:22:LYS:HZ1	6:A:1009:PEG:H21	1.80	0.46
1:B:465[A]:LYS:HE3	1:B:465[A]:LYS:HB2	1.59	0.46
1:A:797:ALA:HB1	1:A:800:THR:HG23	1.98	0.46
1:A:862:ASN:ND2	1:A:865:GLN:HB3	2.30	0.46
7:A:1017:GOL:H2	9:A:1470:HOH:O	2.14	0.46
1:B:660:SER:HB2	7:B:1019:GOL:C3	2.45	0.46
1:A:489[B]:PHE:HE1	9:A:1108:HOH:O	1.97	0.46
1:B:452[A]:GLU:HG2	1:B:473[A]:ARG:HH12	1.81	0.46
1:B:465[A]:LYS:HE3	9:B:1858:HOH:O	2.15	0.46
1:B:95:ASP:OD1	1:B:97:GLN:HG3	2.16	0.45
1:B:117:LYS:NZ	9:B:1109:HOH:O	2.39	0.45
1:A:890[A]:SER:HB2	5:A:1007:SO4:O1	2.16	0.45
1:A:330:PHE:HZ	2:D:1:BGC:C1	2.29	0.45
1:B:301:TYR:CE1	2:C:2:BGC:H5	2.52	0.45
1:A:964:ILE:HD12	1:A:966:ASN:O	2.17	0.45
1:A:338[A]:THR:HG21	1:A:431:LEU:HD21	1.99	0.44
1:A:959:VAL:HG21	1:A:969[B]:ILE:HD12	1.99	0.44
3:A:1002:ACT:H1	9:A:1636:HOH:O	2.17	0.44
1:B:255[A]:LYS:HB2	1:B:255[A]:LYS:HE2	1.61	0.44
1:A:708:LYS:HE3	1:A:709:HIS:CE1	2.52	0.44
1:B:35:ALA:HB1	1:B:45[B]:VAL:CG2	2.47	0.44
1:A:625:ASP:CG	6:A:1008:PEG:H11	2.38	0.44
1:A:18:LEU:HD23	1:A:45:VAL:HG13	1.98	0.44
1:B:293:HIS:O	1:B:296[B]:PHE:CD1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:ASP:CG	7:B:1012:GOL:H2	2.39	0.43
1:B:641:LYS:HE2	1:B:645:GLU:OE2	2.17	0.43
1:A:296[B]:PHE:CD1	1:B:187:PHE:CB	3.01	0.43
1:B:862:ASN:ND2	1:B:865:GLN:HB3	2.34	0.43
1:A:378:LYS:HE3	4:B:1004:TRS:H22	2.00	0.43
1:A:648:LYS:HD3	1:A:649[B]:LYS:NZ	2.33	0.43
1:B:402:ILE:HD12	7:B:1014:GOL:H12	2.01	0.43
2:D:1:BGC:O6	2:D:1:BGC:O4	2.36	0.43
1:B:566:TYR:CZ	1:B:570:ILE:HG13	2.54	0.43
1:B:808:GLY:O	1:B:878:ASN:HA	2.19	0.43
1:B:36[A]:VAL:HG12	4:B:1004:TRS:O2	2.19	0.42
1:A:641:LYS:HE2	1:A:645:GLU:OE2	2.19	0.42
1:B:910[B]:ARG:CZ	9:B:1122:HOH:O	2.68	0.42
1:A:330:PHE:CZ	2:D:1:BGC:H1	2.49	0.42
1:B:349[B]:PHE:HB3	1:B:350:PRO:HD2	2.00	0.42
1:B:959:VAL:HG21	1:B:969[B]:ILE:HD12	2.01	0.42
1:A:804:HIS:HE1	2:C:1:BGC:H6C1	1.85	0.42
1:B:956:GLU:HG3	1:B:985:LYS:HE3	2.02	0.42
6:A:1010:PEG:C4	7:A:1018:GOL:H31	2.50	0.42
1:B:715:PHE:CD1	1:B:771:MET:HG2	2.54	0.42
1:A:80:VAL:HG12	1:A:93:LEU:CD2	2.49	0.41
1:A:482:GLN:CG	1:A:889[B]:LEU:HD12	2.50	0.41
1:B:349[B]:PHE:HB3	1:B:350:PRO:CD	2.50	0.41
1:A:38:THR:HG21	9:A:1125:HOH:O	2.19	0.41
1:B:165[B]:VAL:HG21	1:B:194:ASN:OD1	2.20	0.41
1:B:255[A]:LYS:HE3	1:B:433:TYR:CZ	2.55	0.41
1:B:547:VAL:CA	7:B:1017:GOL:H12	2.48	0.41
1:A:554:TYR:CZ	6:A:1008:PEG:H22	2.55	0.41
1:B:873[C]:SER:O	1:B:888:LEU:O	2.38	0.41
1:A:766[B]:GLU:HG2	9:A:1195:HOH:O	2.20	0.41
1:B:330:PHE:HZ	2:C:1:BGC:C1	2.32	0.41
1:B:700[B]:LYS:HG3	1:B:701[B]:GLU:N	2.35	0.41
1:A:925[B]:GLN:HA	1:A:941:ILE:O	2.21	0.40
1:B:811[B]:GLU:OE2	4:B:1001:TRS:C3	2.69	0.40
1:B:56:PRO:HB3	4:B:1004:TRS:N	2.36	0.40
1:B:22:LYS:NZ	1:B:94:GLU:OE1	2.51	0.40
1:B:88:LYS:CE	1:B:103:GLU:OE2	2.70	0.40
1:B:165[B]:VAL:HG23	1:B:173:SER:H	1.87	0.40
1:A:165[B]:VAL:HG21	1:A:194:ASN:OD1	2.22	0.40
1:A:566:TYR:CZ	1:A:570:ILE:HG13	2.56	0.40
1:A:690:GLN:O	1:A:694[A]:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [\(i\)](#)

4.3.1 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	1039/993 (105%)	1011 (97%)	27 (3%)	1 (0%)	51 19
1	B	1054/993 (106%)	1023 (97%)	30 (3%)	1 (0%)	51 19
All	All	2093/1986 (105%)	2034 (97%)	57 (3%)	2 (0%)	51 19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	798	ASN
1	A	799	ASP

4.3.2 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	906/859 (106%)	897 (99%)	9 (1%)	76 47
1	B	922/859 (107%)	908 (98%)	14 (2%)	65 30
All	All	1828/1718 (106%)	1805 (99%)	23 (1%)	73 34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS

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Mol	Chain	Res	Type
1	A	163	LYS
1	A	232	ARG
1	A	314	ASP
1	A	653	LYS
1	A	693	GLN
1	A	715	PHE
1	A	890[A]	SER
1	A	890[B]	SER
1	B	12	LYS
1	B	43	LYS
1	B	125	GLU
1	B	163	LYS
1	B	174	PHE
1	B	232	ARG
1	B	314[A]	ASP
1	B	314[B]	ASP
1	B	715	PHE
1	B	766[A]	GLU
1	B	766[B]	GLU
1	B	890[A]	SER
1	B	890[B]	SER
1	B	931	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	818	HIS
1	A	927	ASN
1	B	220	ASN
1	B	927	ASN

4.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

4.5 Carbohydrates [\(i\)](#)

6 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

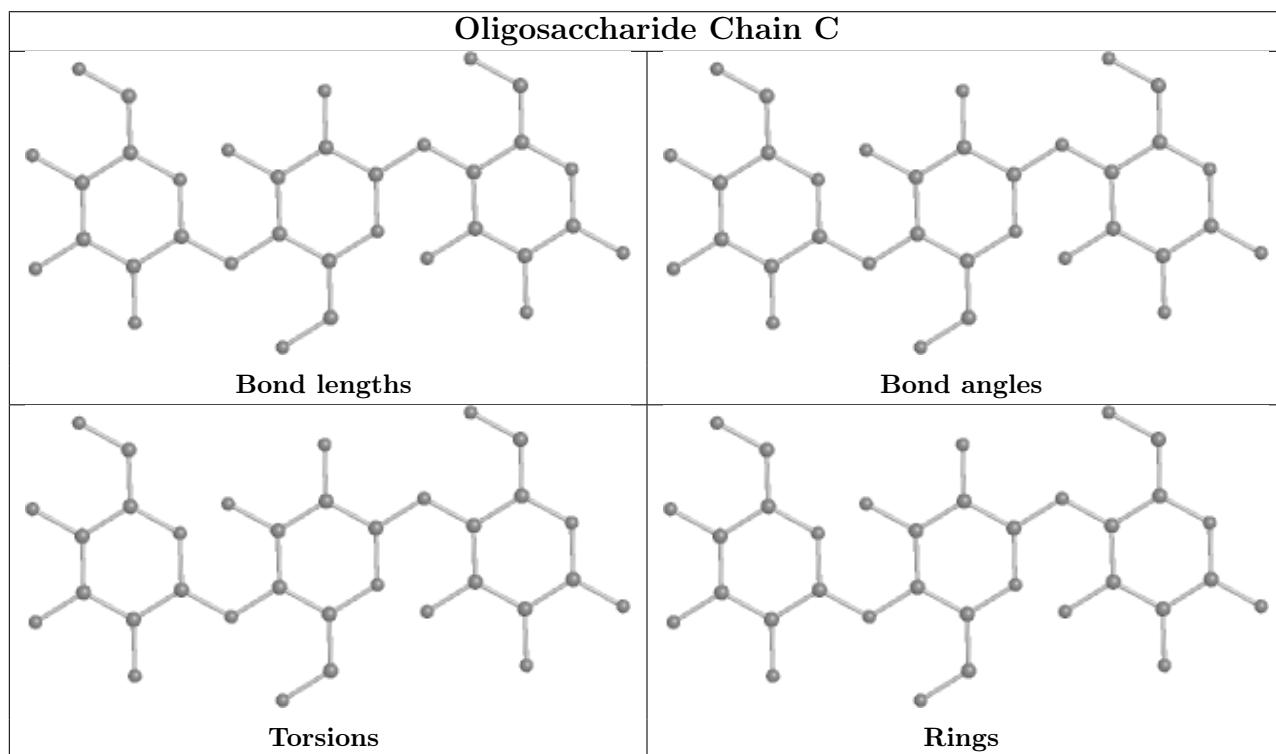
There are no chirality outliers.

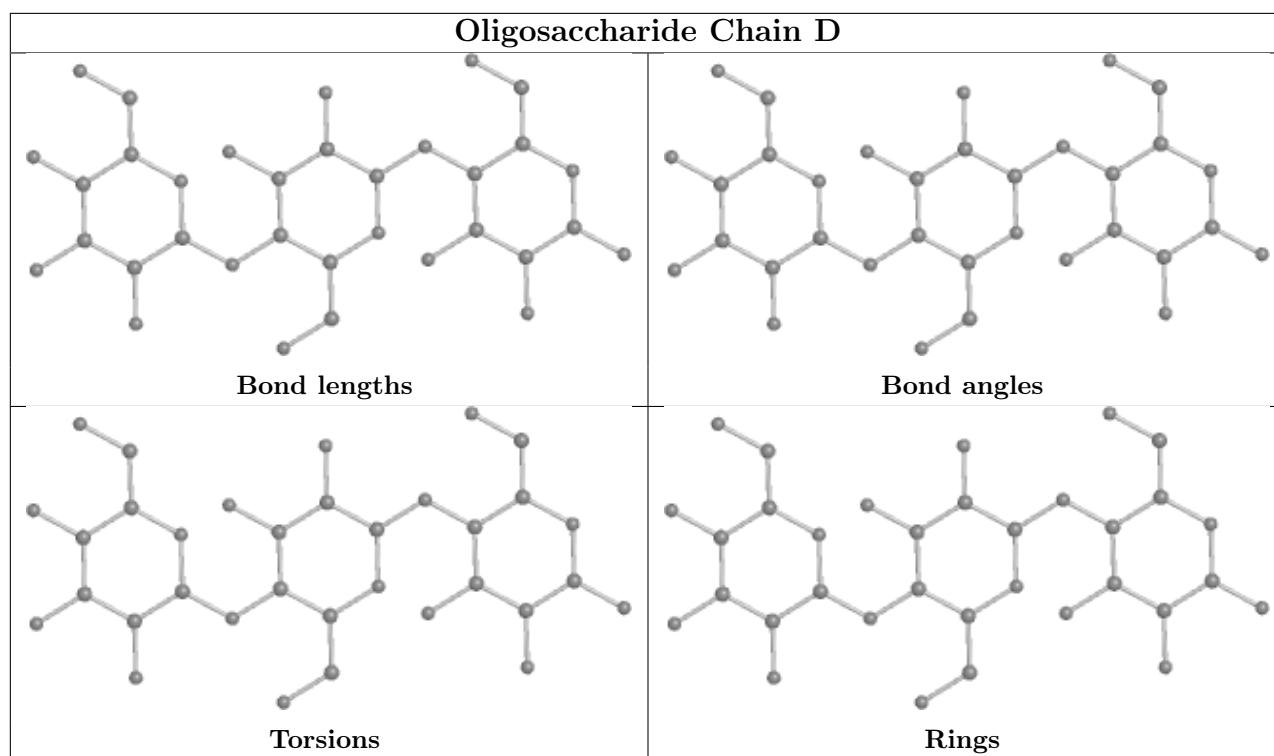
There are no torsion outliers.

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.





4.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 5 are monoatomic - leaving 41 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

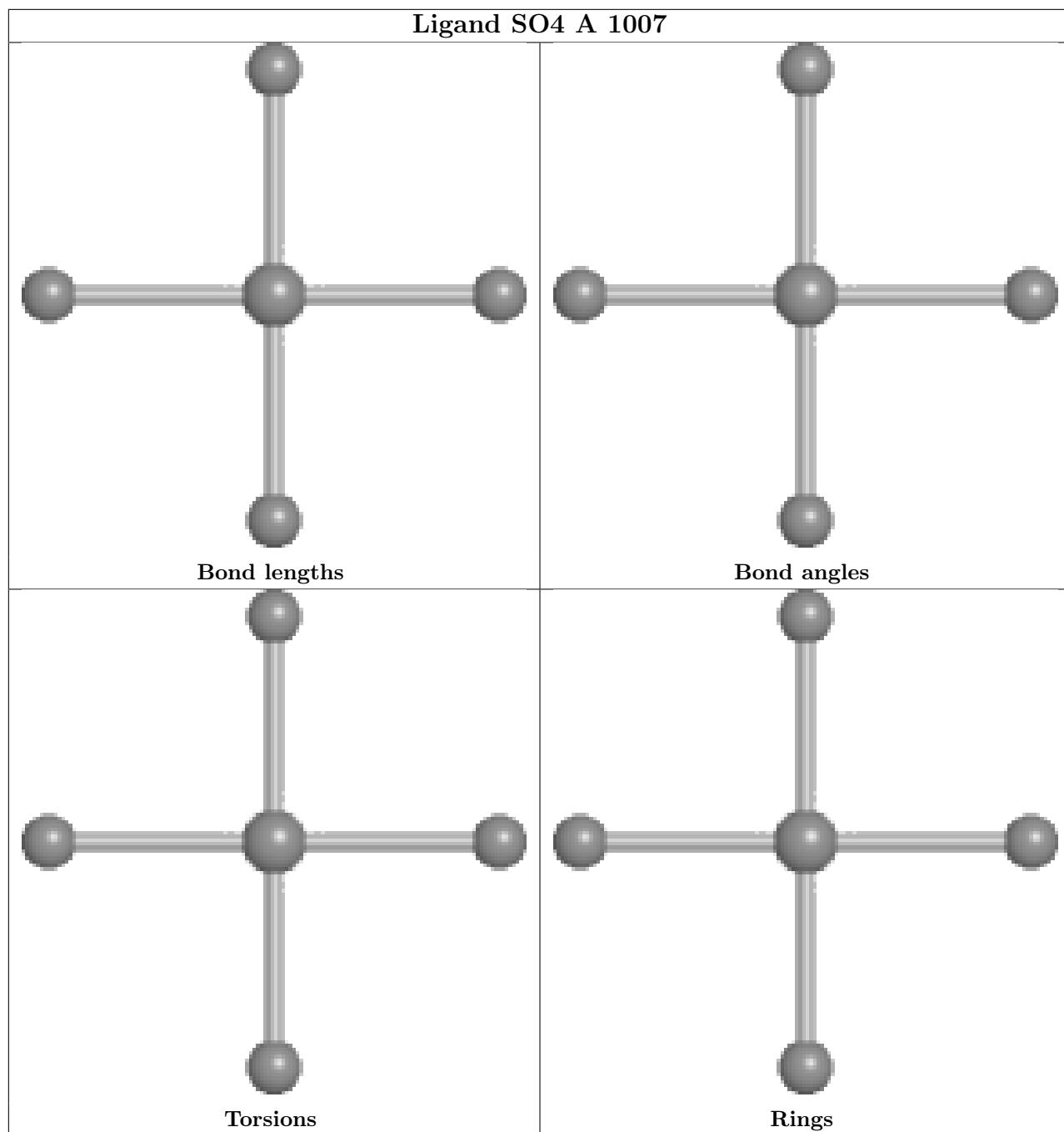
There are no chirality outliers.

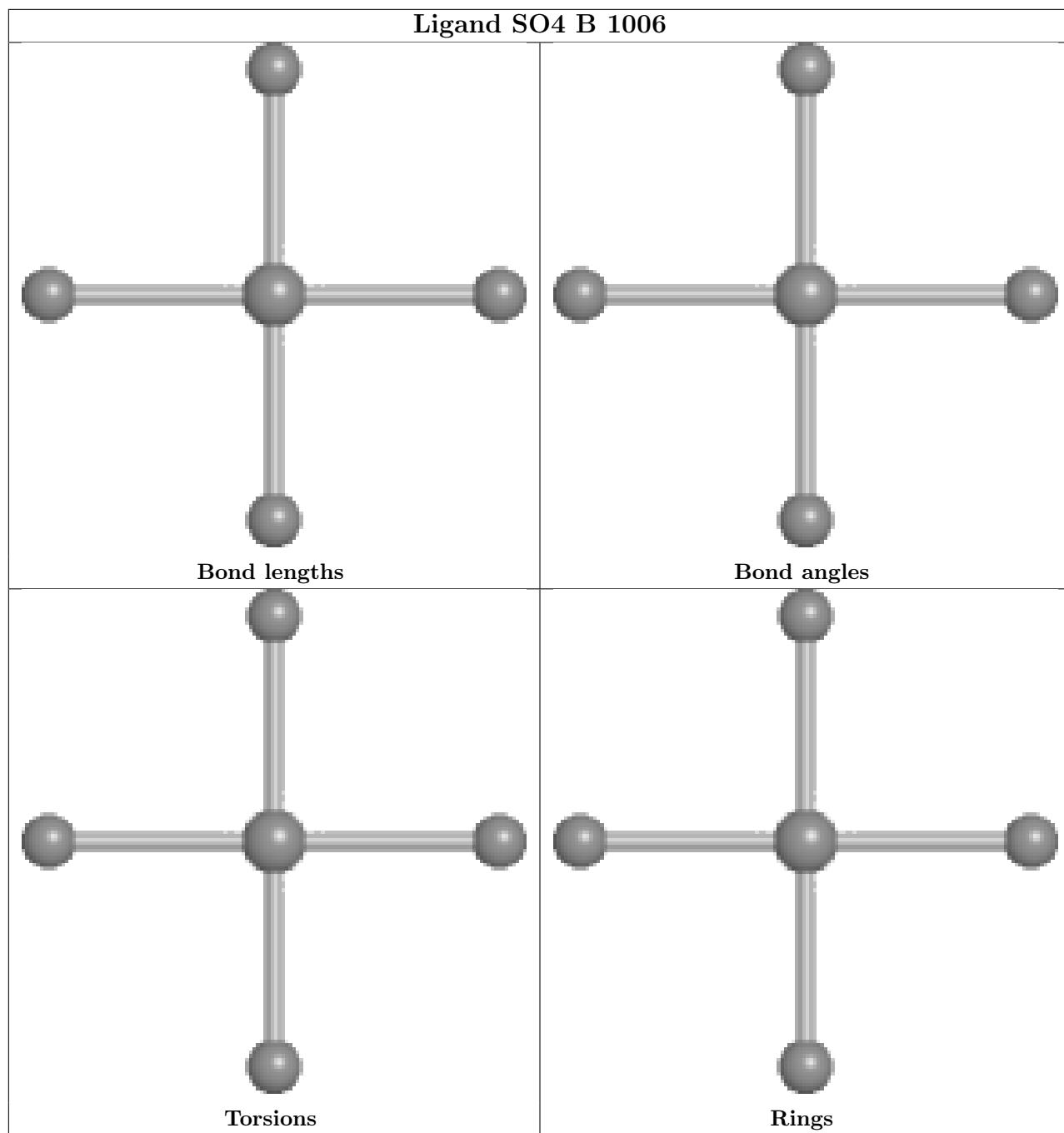
There are no torsion outliers.

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 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 than 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.





4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

5 Fit of model and data [\(i\)](#)

5.1 Protein, DNA and RNA chains [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

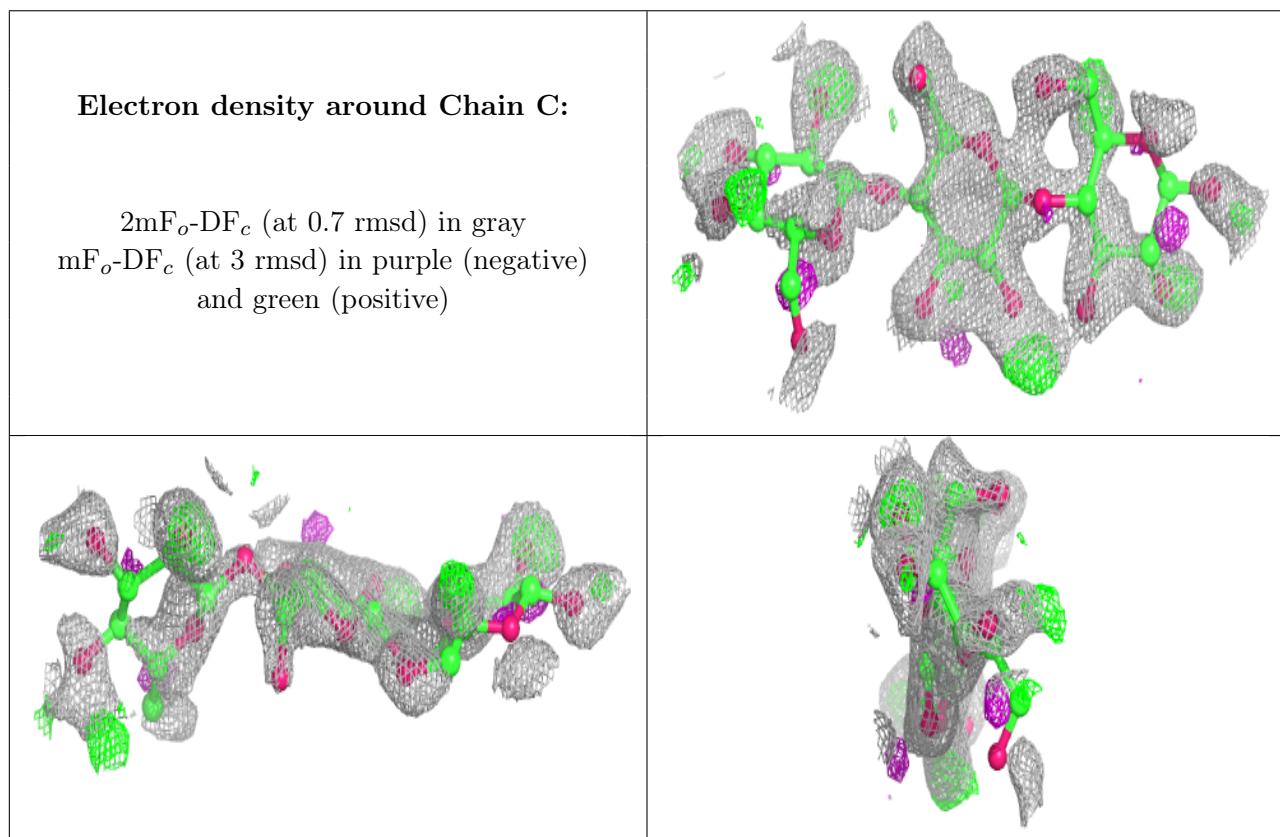
5.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

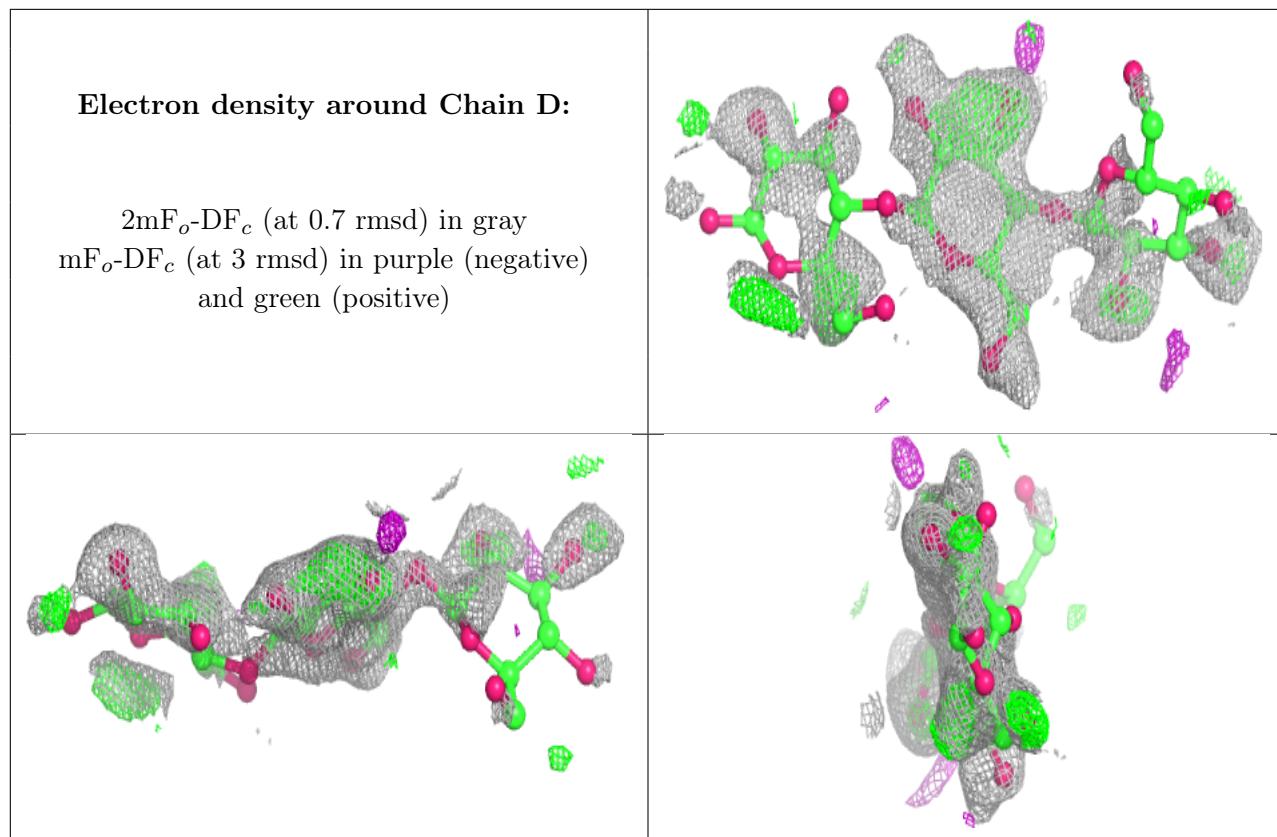
EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

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.

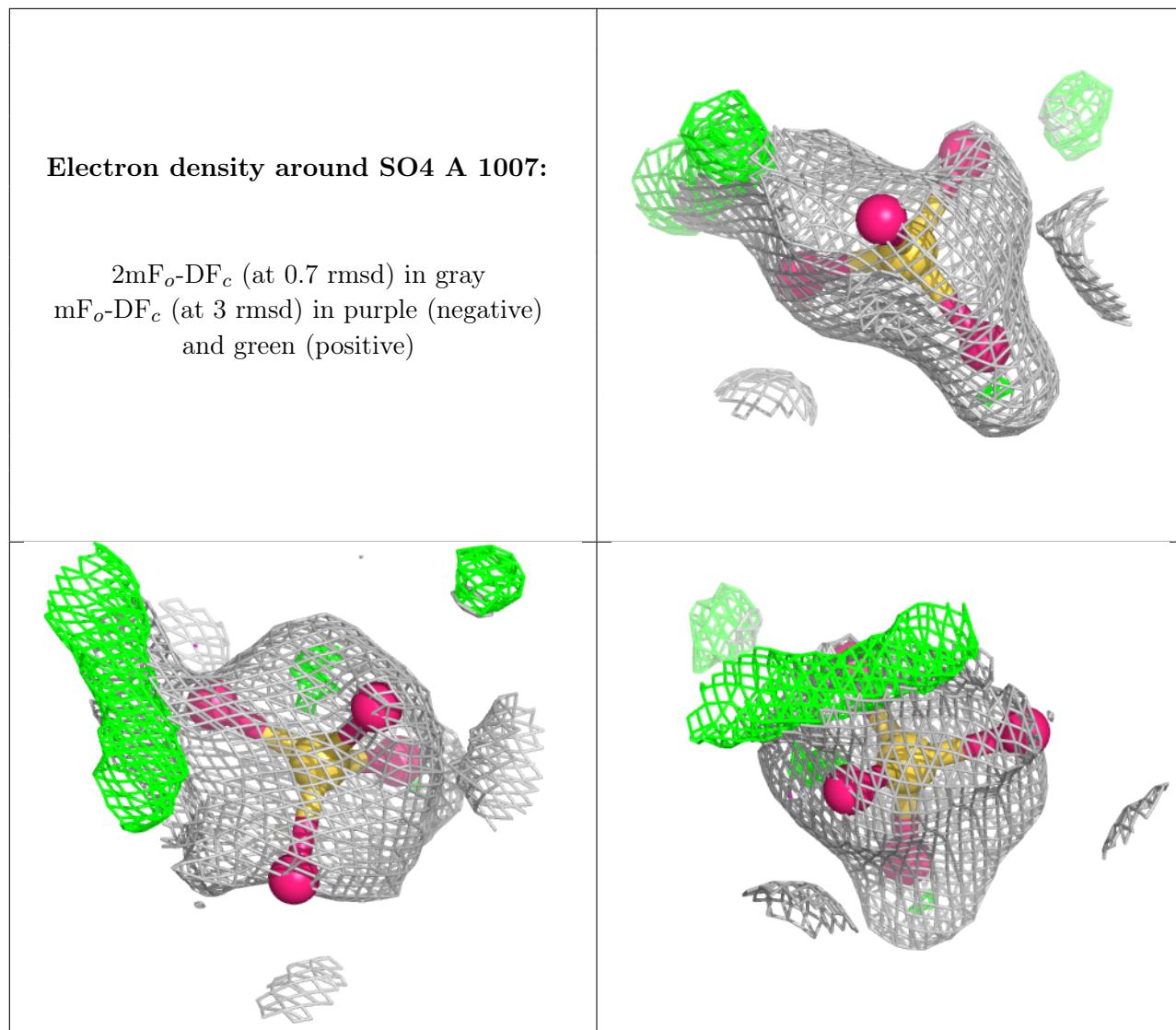


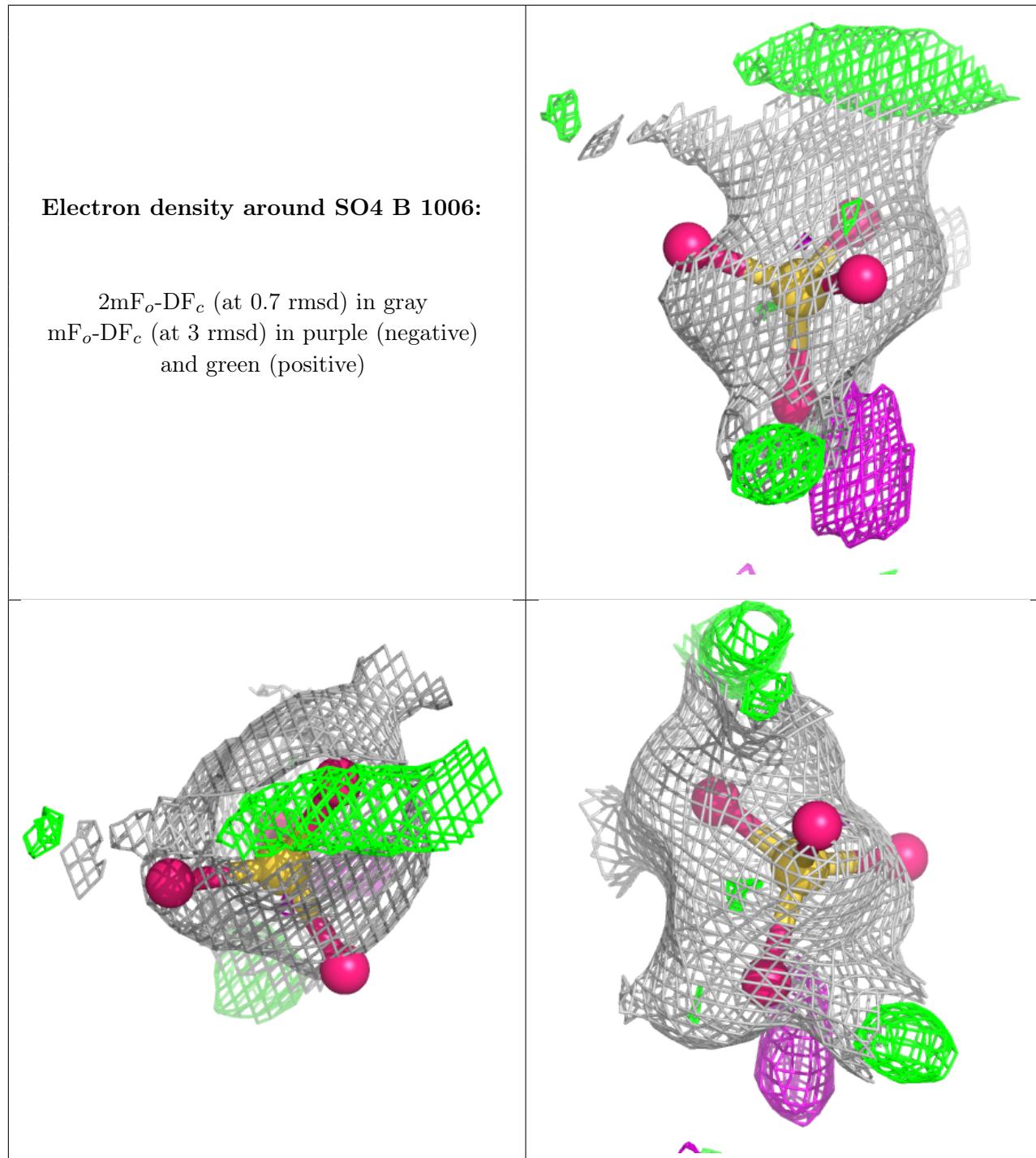


5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

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.





5.5 Other polymers [\(i\)](#)

EDS failed to run properly - this section is therefore empty.