



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:11 PM UTC

PDB ID : 1T3I / pdb_00001t3i
Title : Structure of slr0077/SufS, the Essential Cysteine Desulfurase from *Synechocystis* PCC 6803
Authors : Tirupati, B.; Vey, J.L.; Drennan, C.L.; Bollinger Jr., J.M.
Deposited on : 2004-04-26
Resolution : 1.80 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

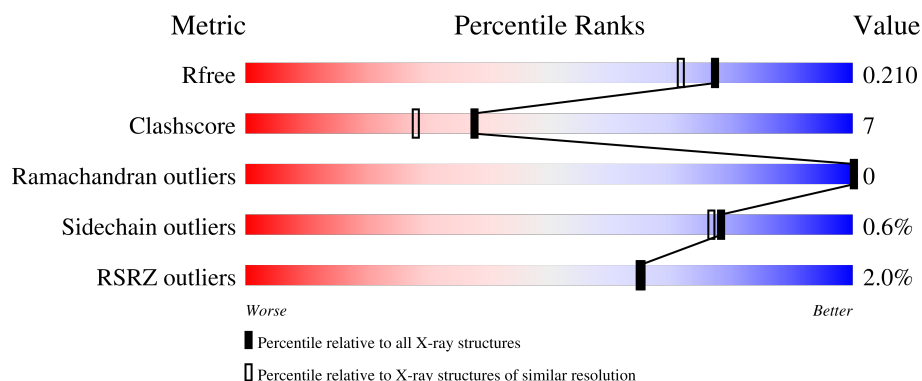
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

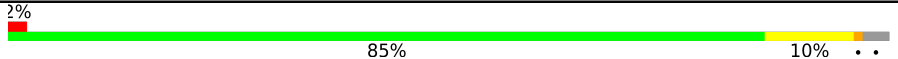
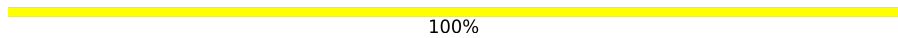
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	420	
1	B	420	
2	C	2	

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
3	PLP	B	601	-	X	-	-
4	GOL	B	604	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6858 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.

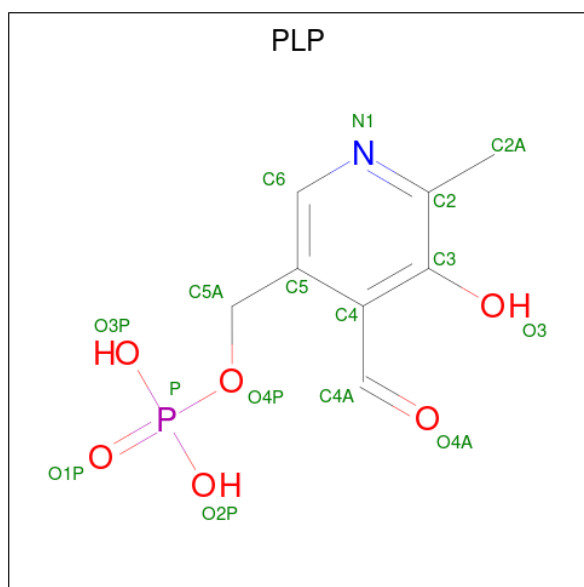
- Molecule 1 is a protein called Probable cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3099	1973	531	581	14			
1	B	405	Total	C	N	O	S	0	0	0
			3112	1982	535	581	14			

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-3-O-octanoyl-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			32	20	12			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

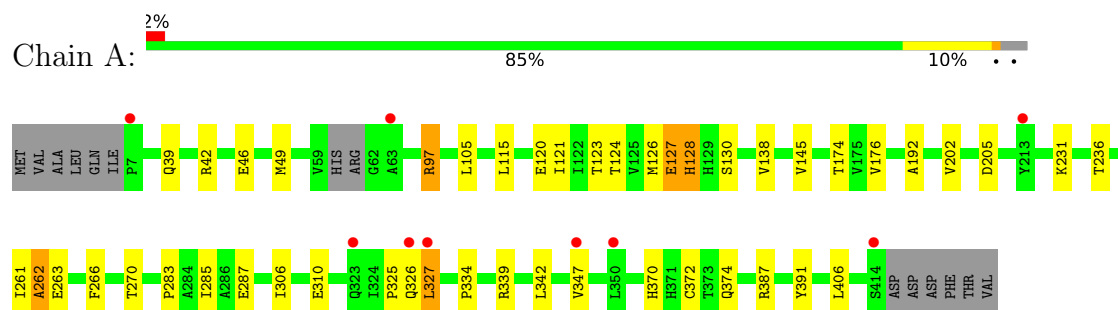
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	282	Total	O	0	0
			282	282		
5	B	291	Total	O	0	0
			291	291		

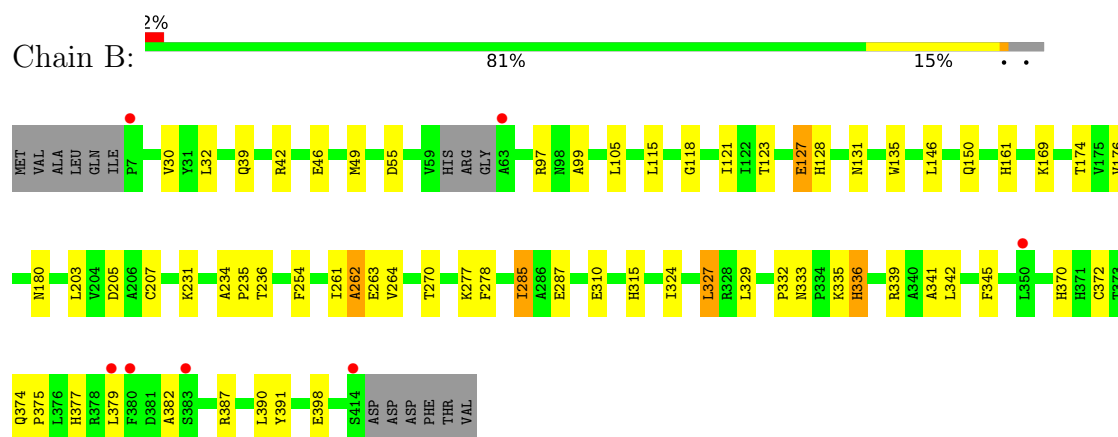
3 Residue-property plots

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: Probable cysteine desulfurase



- Molecule 1: Probable cysteine desulfurase



- Molecule 2: beta-D-fructofuranose-(2-1)-3-O-octanoyl-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.39Å 89.31Å 141.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.59 – 1.80 42.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.9 (42.59-1.80) 90.9 (42.59-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 1.79Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.191 , 0.216 0.186 , 0.210	Depositor DCC
R_{free} test set	9531 reflections (9.57%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6858	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: TU4, FRU, GOL, PLP

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	0.37	1/3174 (0.0%)	0.89	6/4329 (0.1%)
1	B	0.37	1/3187 (0.0%)	0.89	8/4343 (0.2%)
All	All	0.37	2/6361 (0.0%)	0.89	14/8672 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	LYS	CE-NZ	-6.15	1.30	1.49
1	A	231	LYS	CE-NZ	-5.36	1.33	1.49

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	ALA	N-CA-C	-7.51	102.95	112.93
1	B	336	HIS	N-CA-C	-7.34	102.25	112.45
1	A	327	LEU	N-CA-C	7.22	122.09	109.96
1	B	236	THR	N-CA-C	-7.12	101.13	110.53
1	A	262	ALA	N-CA-C	-7.02	103.59	112.93
1	A	236	THR	N-CA-C	-6.54	102.37	110.41
1	B	128	HIS	N-CA-C	-6.27	101.67	110.50
1	B	327	LEU	N-CA-C	6.10	120.01	110.32
1	A	127	GLU	N-CA-C	6.02	118.07	110.24
1	B	127	GLU	N-CA-C	5.78	117.75	110.24
1	A	285	ILE	N-CA-C	5.71	116.17	110.23
1	A	128	HIS	N-CA-C	-5.41	102.88	110.50
1	B	55	ASP	N-CA-C	5.37	120.69	113.72
1	B	285	ILE	N-CA-C	5.24	115.68	110.23

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	3099	0	2962	40	0
1	B	3112	0	2994	53	0
2	C	32	0	11	0	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
4	A	6	0	8	2	0
4	B	6	0	8	5	0
5	A	282	0	0	5	0
5	B	291	0	0	1	0
All	All	6858	0	5995	86	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 7.

All (86) 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:387:ARG:HH12	4:A:603:GOL:H31	1.23	1.03
1:A:128:HIS:HD2	1:A:130:SER:H	1.13	0.95
1:B:333:ASN:HD22	1:B:335:LYS:H	1.17	0.88
1:A:49:MET:HE3	1:B:49:MET:HE3	1.63	0.81
1:B:370:HIS:HD2	1:B:372:CYS:H	1.26	0.79
1:A:370:HIS:HD2	1:A:372:CYS:H	1.34	0.76
1:A:128:HIS:CD2	1:A:130:SER:H	2.04	0.73
1:A:387:ARG:NH1	4:A:603:GOL:H31	2.02	0.71
1:A:327:LEU:CD2	1:A:347:VAL:HG22	2.24	0.67
1:B:121:ILE:HB	1:B:146:LEU:HD23	1.75	0.67
1:B:131:ASN:ND2	1:B:135:TRP:HE1	1.91	0.67
1:B:150:GLN:HG2	1:B:161:HIS:ND1	2.12	0.64
1:B:387:ARG:HH12	4:B:604:GOL:H32	1.63	0.63
1:B:333:ASN:H	1:B:336:HIS:CD2	2.16	0.63
1:A:327:LEU:HD21	1:A:347:VAL:HG22	1.83	0.61
1:A:283:PRO:HB3	5:A:841:HOH:O	2.01	0.59
1:A:334:PRO:HG3	1:A:339:ARG:HD3	1.84	0.59
1:B:49:MET:HA	1:B:49:MET:HE2	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLU:H	1:A:287:GLU:CD	2.13	0.57
1:B:387:ARG:HH12	4:B:604:GOL:C3	2.18	0.56
1:B:234:ALA:HB1	1:B:235:PRO:HD2	1.88	0.55
1:B:370:HIS:HD2	1:B:372:CYS:N	2.00	0.55
1:B:387:ARG:HH22	4:B:604:GOL:H32	1.71	0.55
1:A:49:MET:HE3	1:B:49:MET:CE	2.35	0.55
1:B:105:LEU:C	1:B:105:LEU:HD23	2.33	0.54
1:A:370:HIS:HD2	1:A:372:CYS:N	2.04	0.53
1:B:32:LEU:HD22	1:B:390:LEU:HD23	1.91	0.53
1:B:176:VAL:HA	1:B:205:ASP:HB3	1.91	0.53
1:A:306:ILE:O	1:A:310:GLU:HG3	2.09	0.53
1:A:325:PRO:HG2	1:A:326:GLN:NE2	2.23	0.53
1:B:333:ASN:ND2	1:B:335:LYS:H	1.98	0.52
1:A:287:GLU:CD	1:A:287:GLU:N	2.67	0.52
1:B:180:ASN:HD22	4:B:604:GOL:H31	1.75	0.52
1:A:42:ARG:O	1:A:46:GLU:HG3	2.10	0.51
1:A:374:GLN:NE2	1:B:264:VAL:H	2.09	0.51
1:A:176:VAL:HA	1:A:205:ASP:HB3	1.93	0.50
1:B:374:GLN:HB3	1:B:375:PRO:HD3	1.93	0.50
1:A:120:GLU:HG2	1:A:145:VAL:CG2	2.42	0.50
1:A:192:ALA:HA	1:A:202:VAL:HG21	1.93	0.50
1:B:49:MET:HE2	1:B:49:MET:CA	2.42	0.50
1:B:287:GLU:CD	1:B:287:GLU:H	2.20	0.49
1:A:266:PHE:HE1	1:B:379:LEU:HD11	1.78	0.49
1:B:315:HIS:HD2	1:B:335:LYS:NZ	2.11	0.49
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.78	0.49
1:A:105:LEU:C	1:A:105:LEU:HD23	2.38	0.48
1:A:123:THR:OG1	1:A:127:GLU:HG3	2.13	0.48
1:B:42:ARG:O	1:B:46:GLU:HG3	2.13	0.48
1:B:370:HIS:CD2	1:B:372:CYS:H	2.17	0.47
1:A:49:MET:CE	1:B:49:MET:HE3	2.40	0.47
1:B:332:PRO:O	1:B:339:ARG:HD2	2.15	0.46
1:A:374:GLN:HE22	1:B:263:GLU:HA	1.80	0.46
5:A:853:HOH:O	1:B:370:HIS:HE1	1.98	0.46
1:A:261:ILE:C	1:A:261:ILE:HD12	2.40	0.46
1:A:327:LEU:HD11	1:A:406:LEU:HD21	1.98	0.46
1:B:30:VAL:HG13	1:B:398:GLU:HB3	1.97	0.46
5:A:874:HOH:O	1:B:285:ILE:HB	2.15	0.46
1:B:123:THR:OG1	1:B:127:GLU:HG3	2.16	0.45
1:B:342:LEU:C	1:B:342:LEU:HD12	2.41	0.45
1:B:254:PHE:HB3	5:B:647:HOH:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLU:CD	1:B:287:GLU:N	2.75	0.45
1:A:342:LEU:C	1:A:342:LEU:HD12	2.42	0.45
1:A:174:THR:O	1:A:174:THR:HG23	2.17	0.45
1:A:370:HIS:CD2	1:A:372:CYS:H	2.24	0.45
1:B:99:ALA:CB	1:B:207:CYS:SG	3.04	0.45
1:B:387:ARG:NH1	4:B:604:GOL:H32	2.31	0.44
1:A:115:LEU:HD12	1:A:138:VAL:HG11	2.00	0.44
1:A:49:MET:HG2	1:B:49:MET:CE	2.48	0.44
1:A:262:ALA:HB3	1:A:270:THR:OG1	2.18	0.44
1:B:150:GLN:HG2	1:B:161:HIS:CG	2.53	0.44
1:B:203:LEU:HD23	1:B:203:LEU:C	2.42	0.44
1:B:324:ILE:HB	1:B:327:LEU:HD22	1.99	0.44
1:A:39:GLN:HA	1:A:39:GLN:OE1	2.18	0.43
1:B:329:LEU:HD23	1:B:345:PHE:HB3	2.00	0.43
1:A:49:MET:HA	1:A:49:MET:HE2	2.00	0.43
5:A:684:HOH:O	1:B:97:ARG:HG3	2.18	0.43
1:B:261:ILE:C	1:B:261:ILE:HD12	2.43	0.43
1:A:124:THR:OG1	1:A:126:MET:HG2	2.19	0.42
1:B:277:LYS:HD2	1:B:278:PHE:CE1	2.55	0.42
1:B:377:HIS:HB3	1:B:382:ALA:O	2.20	0.42
1:B:39:GLN:OE1	1:B:39:GLN:HA	2.19	0.42
1:B:262:ALA:HB3	1:B:270:THR:OG1	2.21	0.41
1:A:263:GLU:HG2	5:A:815:HOH:O	2.21	0.41
1:B:174:THR:O	1:B:174:THR:HG23	2.21	0.40
1:A:115:LEU:HD13	1:A:121:ILE:HD11	2.03	0.40
1:B:118:GLY:O	1:B:169:LYS:HE3	2.21	0.40
1:B:310:GLU:HB3	1:B:341:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	402/420 (96%)	392 (98%)	10 (2%)	0	100	100
1	B	401/420 (96%)	390 (97%)	11 (3%)	0	100	100
All	All	803/840 (96%)	782 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	317/345 (92%)	315 (99%)	2 (1%)	78	77
1	B	320/345 (93%)	318 (99%)	2 (1%)	78	77
All	All	637/690 (92%)	633 (99%)	4 (1%)	78	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	391	TYR
1	B	115	LEU
1	B	391	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	56	ASN
1	A	86	ASN
1	A	114	ASN
1	A	128	HIS
1	A	150	GLN
1	A	154	GLN
1	A	218	GLN
1	A	305	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	323	GLN
1	A	370	HIS
1	A	374	GLN
1	B	25	ASN
1	B	50	HIS
1	B	58	ASN
1	B	114	ASN
1	B	131	ASN
1	B	268	HIS
1	B	315	HIS
1	B	333	ASN
1	B	336	HIS
1	B	370	HIS
1	B	404	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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$
2	TU4	C	1	2	20,20,21	2.09	7 (35%)	24,25,27	1.74	4 (16%)
2	FRU	C	2	2	11,12,12	4.29	4 (36%)	10,18,18	1.00	1 (10%)

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	TU4	C	1	2	-	2/13/30/33	0/1/1/1
2	FRU	C	2	2	-	1/5/24/24	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	FRU	O2-C2	9.44	1.57	1.40
2	C	2	FRU	O5-C5	7.09	1.59	1.43
2	C	2	FRU	O3-C3	5.53	1.53	1.42
2	C	2	FRU	O5-C2	5.11	1.51	1.43
2	C	1	TU4	C4-C5	4.75	1.63	1.53
2	C	1	TU4	C2-C3	4.55	1.62	1.52
2	C	1	TU4	O7-C13	3.19	1.32	1.22
2	C	1	TU4	O5-C5	3.09	1.49	1.43
2	C	1	TU4	O6-C6	2.57	1.53	1.42
2	C	1	TU4	O3-C3	2.56	1.48	1.44
2	C	1	TU4	O3-C13	-2.04	1.28	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	TU4	C3-O3-C13	5.59	126.69	117.59
2	C	1	TU4	C1-O5-C5	2.71	115.82	112.19
2	C	1	TU4	O4-C4-C3	-2.39	103.82	109.94
2	C	2	FRU	O6-C6-C5	-2.35	103.33	111.33
2	C	1	TU4	O3-C13-C7	-2.04	107.07	111.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

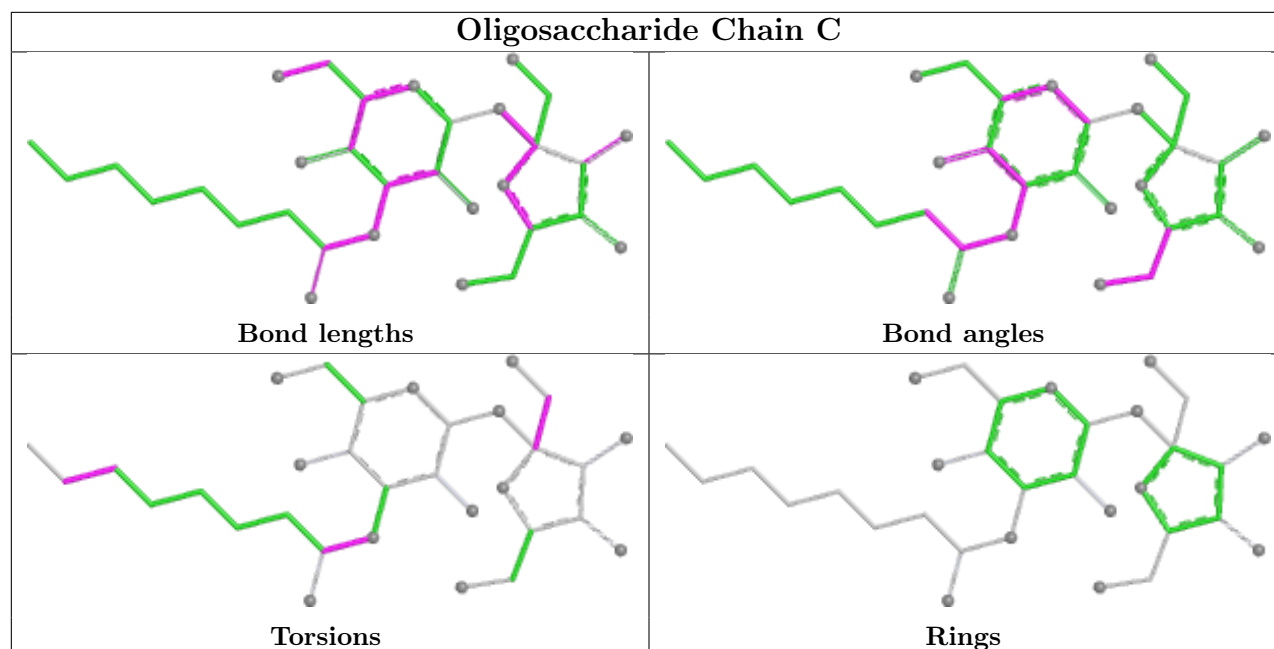
Mol	Chain	Res	Type	Atoms
2	C	1	TU4	O7-C13-O3-C3
2	C	1	TU4	C10-C11-C12-C31
2	C	2	FRU	O1-C1-C2-C3

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	A	600	1	15,15,16	4.59	9 (60%)	21,22,23	3.07	8 (38%)
4	GOL	B	604	-	5,5,5	1.43	0	5,5,5	1.03	0
3	PLP	B	601	1	15,15,16	4.61	9 (60%)	21,22,23	2.96	9 (42%)
4	GOL	A	603	-	5,5,5	1.65	2 (40%)	5,5,5	0.97	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	PLP	A	600	1	-	0/6/6/8	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	604	-	-	4/4/4/4	-
3	PLP	B	601	1	-	0/6/6/8	0/1/1/1
4	GOL	A	603	-	-	2/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	PLP	C3-C2	8.48	1.49	1.41
3	B	601	PLP	C6-N1	8.07	1.50	1.34
3	B	601	PLP	O4P-C5A	-8.04	1.15	1.44
3	B	601	PLP	C5-C4	7.48	1.49	1.40
3	A	600	PLP	O4P-C5A	-7.47	1.17	1.44
3	B	601	PLP	C2-N1	6.87	1.46	1.33
3	A	600	PLP	C5-C4	6.52	1.47	1.40
3	A	600	PLP	C2-N1	6.37	1.45	1.33
3	A	600	PLP	C6-C5	6.35	1.50	1.37
3	B	601	PLP	C3-C2	5.87	1.47	1.41
3	A	600	PLP	C6-N1	5.63	1.45	1.34
3	B	601	PLP	C6-C5	5.36	1.48	1.37
3	A	600	PLP	C3-C4	3.44	1.46	1.40
3	A	600	PLP	O3-C3	-2.67	1.30	1.36
3	B	601	PLP	P-O2P	-2.52	1.45	1.54
3	B	601	PLP	C3-C4	2.25	1.44	1.40
3	A	600	PLP	P-O2P	-2.09	1.47	1.54
3	B	601	PLP	O3-C3	-2.03	1.32	1.36
4	A	603	GOL	C1-C2	2.02	1.59	1.51
4	A	603	GOL	O1-C1	2.02	1.50	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	PLP	O4P-C5A-C5	11.26	130.47	109.36
3	B	601	PLP	O4P-C5A-C5	10.47	128.98	109.36
3	A	600	PLP	C2A-C2-C3	4.54	126.11	120.80
3	B	601	PLP	C2A-C2-C3	4.05	125.54	120.80
3	B	601	PLP	O4P-P-O1P	-3.64	96.59	106.44
3	A	600	PLP	C3-C2-N1	-2.89	117.31	120.96
3	B	601	PLP	C4-C3-C2	2.81	124.08	119.89
3	A	600	PLP	O4P-P-O1P	-2.70	99.14	106.44
3	B	601	PLP	C5-C6-N1	-2.50	119.76	123.83
3	B	601	PLP	C5A-C5-C4	-2.47	117.75	122.64
3	A	600	PLP	C5A-C5-C4	-2.38	117.94	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	PLP	C3-C2-N1	-2.37	117.97	120.96
3	A	600	PLP	C5-C6-N1	-2.30	120.10	123.83
3	B	601	PLP	O2P-P-O4P	2.26	112.56	106.67
3	A	600	PLP	O2P-P-O4P	2.07	112.06	106.67
3	A	600	PLP	C4-C3-C2	2.05	122.94	119.89
3	B	601	PLP	C5A-C5-C6	2.03	122.67	119.36

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	GOL	C1-C2-C3-O3
4	B	604	GOL	C1-C2-C3-O3
4	B	604	GOL	O2-C2-C3-O3
4	B	604	GOL	O1-C1-C2-C3
4	A	603	GOL	O2-C2-C3-O3
4	B	604	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	GOL	5	0
4	A	603	GOL	2	0

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	406/420 (96%)	0.05	9 (2%) 62 62	19, 26, 36, 45	0
1	B	405/420 (96%)	0.03	7 (1%) 69 69	19, 26, 36, 44	0
All	All	811/840 (96%)	0.04	16 (1%) 65 65	19, 26, 36, 45	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	ALA	6.1
1	A	7	PRO	4.1
1	A	63	ALA	4.1
1	A	213	TYR	4.0
1	B	414	SER	4.0
1	B	379	LEU	3.3
1	A	414	SER	2.7
1	B	383	SER	2.7
1	B	350	LEU	2.7
1	B	380	PHE	2.6
1	A	327	LEU	2.5
1	A	350	LEU	2.4
1	A	323	GLN	2.4
1	A	326	GLN	2.3
1	B	7	PRO	2.3
1	A	347	VAL	2.0

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

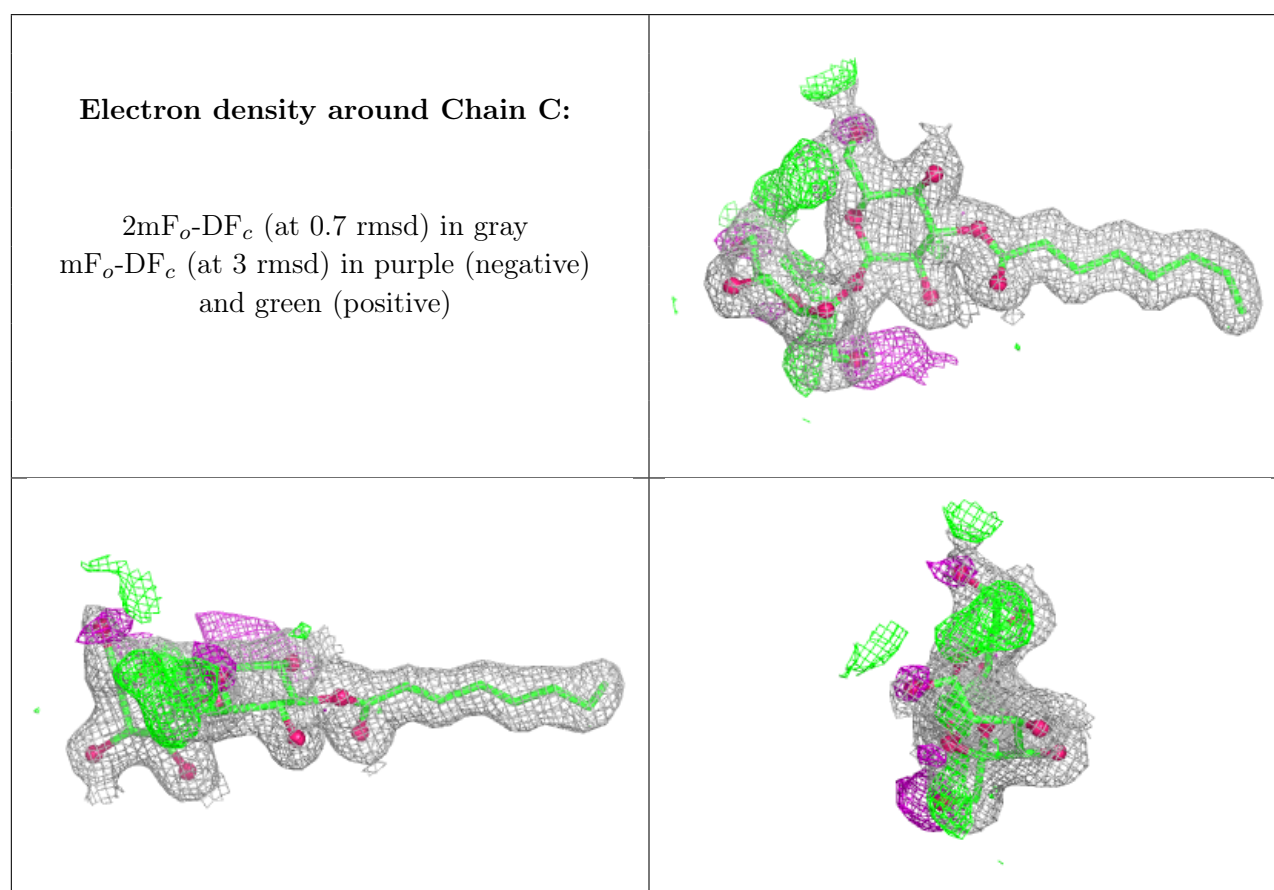
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	FRU	C	2	12/12	0.84	0.13	26,29,35,38	0
2	TU4	C	1	20/21	0.93	0.09	21,23,28,31	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.



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($\text{\AA}^2$)	Q<0.9
4	GOL	B	604	6/6	0.82	0.18	41,47,49,49	0
4	GOL	A	603	6/6	0.84	0.17	45,47,47,48	0
3	PLP	A	600	15/16	0.94	0.09	20,27,30,32	0
3	PLP	B	601	15/16	0.96	0.09	24,26,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.