



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:10 PM UTC

PDB ID : 3LJF / pdb_00003ljf
Title : The X-ray structure of iron superoxide dismutase from *Pseudoalteromonas haloplanktis* (crystal form II)
Authors : Merlino, A.; Russo Krauss, I.; Rossi, B.; Conte, M.; Vergara, A.; Sica, F.
Deposited on : 2010-01-26
Resolution : 2.10 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

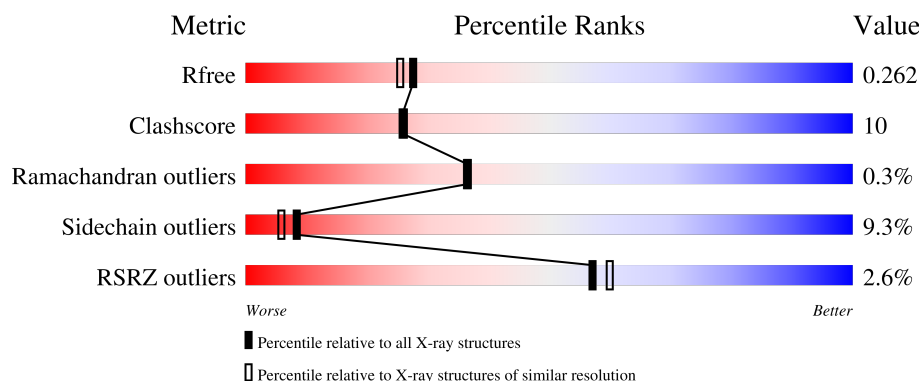
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	192	5% 78% 17% 5%
1	B	192	73% 21%
1	C	192	5% 74% 19% 6%
1	D	192	4% 67% 25% 7%
2	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 50% 50%
2	H	2	 50% 50%

2 Entry composition

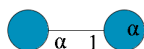
There are 4 unique types of molecules in this entry. The entry contains 6672 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 iron superoxide dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1511	974	249	287	1			
1	C	192	Total	C	N	O	S	0	0	0
			1511	974	249	287	1			
1	B	192	Total	C	N	O	S	0	0	0
			1511	974	249	287	1			
1	D	192	Total	C	N	O	S	0	0	0
			1511	974	249	287	1			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Fe 1	0	0
3	D	1	Total 1	Fe 1	0	0

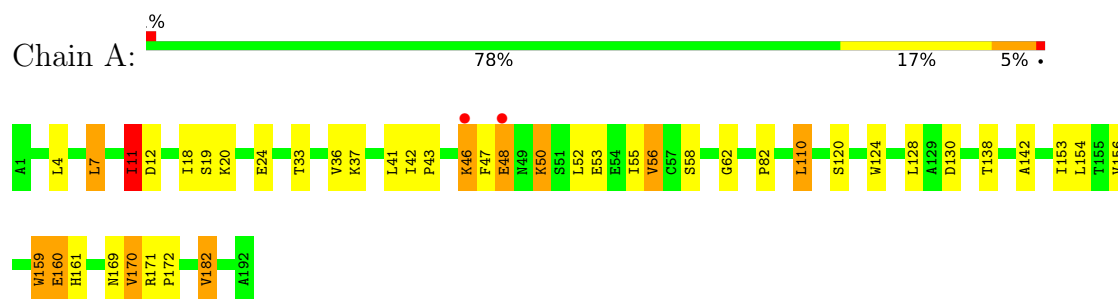
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total 141	O 141	0	0
4	C	117	Total 117	O 117	0	0
4	B	150	Total 150	O 150	0	0
4	D	124	Total 124	O 124	0	0

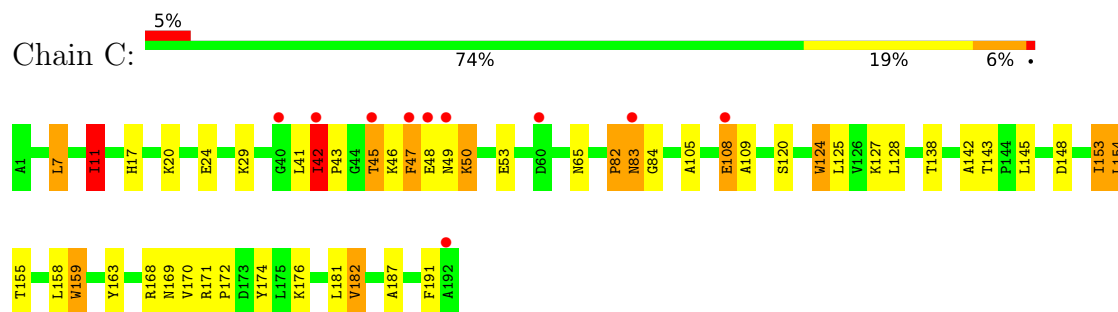
3 Residue-property plots [i](#)

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.

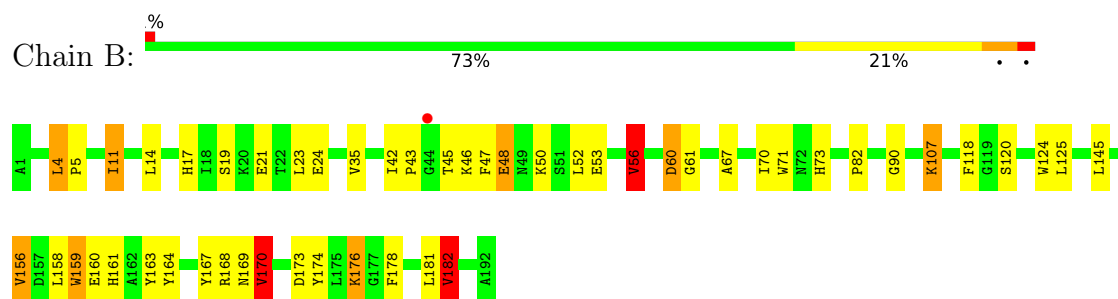
- Molecule 1: iron superoxide dismutase



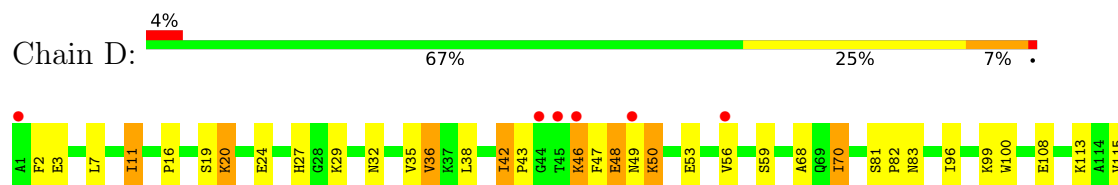
- Molecule 1: iron superoxide dismutase



- Molecule 1: iron superoxide dismutase



- Molecule 1: iron superoxide dismutase





- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain E:  100%



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain F:  100%



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain G:  50%



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain H:  50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.48Å 103.78Å 90.25Å 90.00° 103.81° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.10) 94.6 (30.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.248 0.206 , 0.262	Depositor DCC
R_{free} test set	5237 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6672	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0092e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, GLC

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	1.11	2/1560 (0.1%)	1.26	19/2134 (0.9%)
1	B	1.13	5/1560 (0.3%)	1.27	19/2134 (0.9%)
1	C	1.08	2/1560 (0.1%)	1.27	19/2134 (0.9%)
1	D	1.06	2/1560 (0.1%)	1.28	21/2134 (1.0%)
All	All	1.10	11/6240 (0.2%)	1.27	78/8536 (0.9%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	96	ILE	CA-CB	6.80	1.63	1.54
1	B	170	VAL	CA-CB	5.92	1.60	1.53
1	B	161	HIS	CD2-NE2	5.44	1.43	1.37
1	B	56	VAL	CA-CB	5.40	1.61	1.54
1	C	11	ILE	CA-CB	5.39	1.62	1.54
1	B	73	HIS	ND1-CE1	5.36	1.38	1.32
1	B	156	VAL	CA-CB	5.19	1.60	1.54
1	A	153	ILE	CA-CB	5.17	1.60	1.55
1	A	161	HIS	CD2-NE2	5.16	1.43	1.37
1	D	170	VAL	CA-CB	5.16	1.59	1.53
1	C	153	ILE	CA-CB	5.06	1.60	1.55

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	PRO	N-CA-C	-9.83	96.67	111.41
1	C	84	GLY	N-CA-C	-9.74	98.53	112.55
1	A	159	TRP	N-CA-C	-9.18	97.86	110.35
1	B	170	VAL	N-CA-C	8.15	118.36	106.55
1	B	182	VAL	CB-CA-C	-7.86	98.40	111.29
1	D	159	TRP	N-CA-C	-7.60	100.01	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	170	VAL	N-CA-C	7.36	117.23	106.55
1	B	125	LEU	N-CA-C	-7.31	97.33	109.24
1	A	50	LYS	N-CA-C	7.24	119.92	110.43
1	C	170	VAL	N-CA-C	7.21	117.01	106.55
1	A	182	VAL	CB-CA-C	-7.11	100.48	111.71
1	A	19	SER	N-CA-C	7.06	119.86	110.53
1	C	41	LEU	CA-C-N	7.06	124.69	120.24
1	C	41	LEU	C-N-CA	7.06	124.69	120.24
1	A	169	ASN	CA-C-N	-6.96	114.32	122.95
1	A	169	ASN	C-N-CA	-6.96	114.32	122.95
1	B	164	TYR	N-CA-C	6.79	118.68	111.28
1	B	176	LYS	N-CA-C	-6.77	103.90	111.28
1	C	83	ASN	N-CA-C	6.73	120.78	111.90
1	B	159	TRP	N-CA-C	-6.65	101.31	110.35
1	B	82	PRO	N-CA-C	-6.61	105.90	114.03
1	D	47	PHE	N-CA-C	6.58	121.05	112.89
1	C	182	VAL	CB-CA-C	-6.53	100.58	111.29
1	D	164	TYR	N-CA-C	6.35	118.20	111.28
1	D	124	TRP	N-CA-C	6.34	119.80	109.59
1	B	4	LEU	CA-C-N	-6.31	113.78	120.03
1	B	4	LEU	C-N-CA	-6.31	113.78	120.03
1	D	117	ASN	N-CA-C	-6.30	98.90	108.67
1	A	182	VAL	N-CA-CB	6.26	118.31	110.05
1	D	42	ILE	CA-C-N	-6.18	113.31	119.93
1	D	42	ILE	C-N-CA	-6.18	113.31	119.93
1	D	171	ARG	CA-C-N	-6.07	112.60	119.28
1	D	171	ARG	C-N-CA	-6.07	112.60	119.28
1	A	160	GLU	N-CA-C	6.04	118.65	111.71
1	C	168	ARG	CB-CA-C	-6.03	109.60	116.54
1	D	125	LEU	N-CA-C	-5.98	99.53	109.46
1	A	4	LEU	CA-C-N	-5.97	114.46	120.31
1	A	4	LEU	C-N-CA	-5.97	114.46	120.31
1	D	19	SER	N-CA-C	5.97	118.47	110.35
1	A	170	VAL	N-CA-C	5.96	115.95	106.88
1	B	45	THR	N-CA-C	5.95	117.72	110.41
1	B	168	ARG	CB-CA-C	-5.93	109.72	116.54
1	D	82	PRO	N-CA-C	-5.81	106.48	113.98
1	B	118	PHE	N-CA-C	5.75	118.59	109.96
1	A	18	ILE	N-CA-C	-5.75	99.22	107.78
1	C	7	LEU	N-CA-C	-5.66	102.64	109.83
1	B	19	SER	N-CA-C	5.64	117.98	110.53
1	A	124	TRP	N-CA-C	5.64	118.67	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	GLU	N-CA-C	5.63	117.86	111.11
1	B	124	TRP	N-CA-C	5.60	118.86	109.95
1	C	42	ILE	N-CA-C	5.59	120.71	112.61
1	C	124	TRP	N-CA-C	5.50	118.36	109.40
1	A	82	PRO	N-CA-C	-5.44	107.34	114.03
1	B	90	GLY	N-CA-C	5.38	120.87	111.78
1	D	143	THR	CA-C-N	-5.34	113.16	119.84
1	D	143	THR	C-N-CA	-5.34	113.16	119.84
1	A	11	ILE	CB-CA-C	-5.33	101.61	111.79
1	C	82	PRO	CA-C-N	-5.31	114.27	122.08
1	C	82	PRO	C-N-CA	-5.31	114.27	122.08
1	C	125	LEU	N-CA-C	-5.26	100.16	108.73
1	B	169	ASN	CA-C-N	-5.21	116.23	122.22
1	B	169	ASN	C-N-CA	-5.21	116.23	122.22
1	A	62	GLY	N-CA-C	5.21	120.06	113.24
1	B	42	ILE	N-CA-C	5.20	120.12	108.88
1	C	169	ASN	CA-C-N	-5.19	116.25	122.22
1	C	169	ASN	C-N-CA	-5.19	116.25	122.22
1	D	145	LEU	N-CA-C	-5.19	105.75	111.71
1	A	41	LEU	N-CA-C	5.18	119.66	113.23
1	C	159	TRP	N-CA-C	-5.16	102.74	110.23
1	D	176	LYS	N-CA-C	-5.16	105.55	111.07
1	D	70	ILE	CB-CA-C	-5.16	105.18	112.14
1	D	146	THR	N-CA-C	5.14	119.53	113.16
1	A	7	LEU	N-CA-C	-5.14	103.31	109.83
1	D	2	PHE	N-CA-C	-5.12	100.68	108.76
1	B	73	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
1	D	182	VAL	CB-CA-C	-5.06	103.00	111.29
1	C	50	LYS	N-CA-C	5.04	121.53	110.80
1	C	42	ILE	CB-CA-C	-5.03	109.02	114.35

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	1511	0	1419	26	0
1	B	1511	0	1419	23	0
1	C	1511	0	1419	31	0
1	D	1511	0	1419	35	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	141	0	0	0	0
4	B	150	0	0	5	0
4	C	117	0	0	7	0
4	D	124	0	0	3	0
All	All	6672	0	5760	113	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 10.

All (113) 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:B:67:ALA:HB3	4:B:5421:HOH:O	1.76	0.83
1:D:20:LYS:O	1:D:24:GLU:HG3	1.81	0.80
1:A:47:PHE:HA	1:A:50:LYS:HD2	1.63	0.80
1:C:20:LYS:O	1:C:24:GLU:HG3	1.81	0.80
1:D:49:ASN:HB2	4:D:5178:HOH:O	1.87	0.75
1:A:52:LEU:O	1:A:56:VAL:HG12	1.89	0.71
1:D:153:ILE:HD11	1:D:187:ALA:HB1	1.74	0.69
1:D:108:GLU:HG3	4:D:5320:HOH:O	1.91	0.69
1:A:46:LYS:HE2	1:A:46:LYS:HA	1.75	0.69
1:D:56:VAL:HG21	1:D:145:LEU:CD1	2.22	0.67
1:B:107:LYS:NZ	4:B:5298:HOH:O	2.23	0.66
1:C:42:ILE:HD12	1:C:43:PRO:HD3	1.79	0.65
1:C:42:ILE:CG1	1:C:43:PRO:HD3	2.28	0.63
1:C:42:ILE:CD1	1:C:43:PRO:HD3	2.28	0.63
1:D:32:ASN:O	1:D:36:VAL:HG13	1.99	0.63
1:D:147:ASP:HB2	1:D:150:VAL:HG21	1.81	0.63
1:A:46:LYS:O	1:A:46:LYS:HG3	1.97	0.63
1:D:150:VAL:HG23	1:D:150:VAL:O	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:VAL:HG21	1:D:145:LEU:HD12	1.84	0.60
1:A:20:LYS:O	1:A:24:GLU:HG3	2.02	0.60
1:C:42:ILE:HG13	1:C:43:PRO:HD3	1.82	0.60
1:C:11:ILE:HD13	1:C:20:LYS:HE3	1.83	0.60
1:D:120:SER:HB3	1:D:159:TRP:CD2	2.37	0.59
1:D:46:LYS:O	4:D:5178:HOH:O	2.17	0.58
1:C:83:ASN:HA	4:C:5428:HOH:O	2.04	0.58
1:C:45:THR:HA	4:C:5331:HOH:O	2.04	0.57
1:B:120:SER:HB3	1:B:159:TRP:CE2	2.40	0.57
1:D:53:GLU:HA	1:D:56:VAL:HG22	1.89	0.55
1:D:147:ASP:O	1:D:150:VAL:HG22	2.06	0.55
1:C:120:SER:HB3	1:C:159:TRP:CE2	2.41	0.55
1:B:47:PHE:HA	1:B:50:LYS:HD2	1.89	0.55
1:C:105:ALA:HA	1:C:108:GLU:OE1	2.07	0.55
1:D:153:ILE:HD12	1:D:187:ALA:HA	1.89	0.55
1:C:42:ILE:HD12	1:C:43:PRO:CD	2.38	0.54
1:D:147:ASP:HB2	1:D:150:VAL:CG2	2.37	0.54
1:A:42:ILE:CG1	1:A:43:PRO:HD3	2.39	0.53
1:B:120:SER:HB3	1:B:159:TRP:CD2	2.43	0.53
1:D:126:VAL:HA	1:D:153:ILE:HG23	1.91	0.53
1:A:120:SER:HB3	1:A:159:TRP:CE2	2.44	0.53
1:D:150:VAL:O	1:D:150:VAL:CG2	2.57	0.52
1:A:42:ILE:HG12	1:A:43:PRO:HD3	1.92	0.51
1:A:50:LYS:NZ	1:A:58:SER:OG	2.43	0.51
1:A:33:THR:HA	1:A:36:VAL:HG22	1.94	0.50
1:D:53:GLU:O	1:D:56:VAL:HG22	2.11	0.50
1:D:46:LYS:HE2	1:D:50:LYS:HE3	1.94	0.50
1:A:11:ILE:HD13	1:A:20:LYS:HE3	1.94	0.50
1:A:120:SER:HB3	1:A:159:TRP:CD2	2.47	0.49
1:B:170:VAL:HG22	1:B:173:ASP:HB2	1.93	0.49
1:C:11:ILE:HD13	1:C:20:LYS:CE	2.43	0.49
1:C:108:GLU:HG2	1:C:109:ALA:N	2.25	0.49
1:B:11:ILE:O	1:B:23:LEU:HD12	2.13	0.49
1:D:99:LYS:HG3	1:D:100:TRP:CD2	2.48	0.49
1:A:46:LYS:HE2	1:A:46:LYS:CA	2.42	0.48
1:A:11:ILE:HD12	1:A:12:ASP:N	2.29	0.48
1:B:35:VAL:HA	1:B:70:ILE:HD11	1.96	0.48
1:A:138:THR:HB	1:A:142:ALA:HB3	1.97	0.47
1:B:53:GLU:HB2	4:B:5168:HOH:O	2.15	0.47
1:D:120:SER:HB3	1:D:159:TRP:CE2	2.50	0.47
1:D:128:LEU:HD22	1:D:134:ASP:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:VAL:HA	1:D:70:ILE:HD11	1.95	0.47
1:C:53:GLU:HG3	4:C:5310:HOH:O	2.13	0.46
1:B:71:TRP:CE2	1:B:145:LEU:HD22	2.50	0.46
1:A:46:LYS:O	1:A:46:LYS:CG	2.61	0.46
1:C:153:ILE:O	1:C:154:LEU:HD13	2.15	0.46
1:B:53:GLU:HG2	1:B:145:LEU:HD21	1.97	0.46
1:D:11:ILE:HG13	1:D:20:LYS:HD2	1.98	0.46
1:D:7:LEU:HD13	1:D:27:HIS:CD2	2.51	0.46
1:C:45:THR:CA	4:C:5331:HOH:O	2.63	0.45
1:D:42:ILE:N	1:D:43:PRO:CD	2.79	0.45
1:B:52:LEU:O	1:B:56:VAL:HG12	2.17	0.45
1:A:11:ILE:H	1:A:11:ILE:HG13	1.60	0.45
1:C:124:TRP:CE3	1:C:155:THR:HB	2.52	0.45
1:D:48:GLU:O	1:D:48:GLU:HG3	2.16	0.45
1:B:17:HIS:HB2	1:B:181:LEU:HD11	1.99	0.44
1:C:42:ILE:HG13	1:C:42:ILE:H	1.49	0.44
1:B:160:GLU:HG3	4:B:5409:HOH:O	2.17	0.44
1:A:36:VAL:HG23	1:A:37:LYS:N	2.33	0.44
1:A:7:LEU:HD12	1:A:7:LEU:HA	1.89	0.44
1:C:82:PRO:O	1:C:83:ASN:CG	2.61	0.44
1:B:167:TYR:CD1	1:B:173:ASP:HB3	2.53	0.44
1:C:45:THR:HB	4:C:5331:HOH:O	2.17	0.43
1:C:47:PHE:C	1:C:49:ASN:N	2.75	0.43
1:C:127:LYS:HD3	1:C:191:PHE:CE2	2.53	0.43
1:D:38:LEU:O	1:D:42:ILE:HG12	2.18	0.43
1:C:65:ASN:HB3	1:D:118:PHE:CZ	2.54	0.43
1:A:160:GLU:HB2	1:B:160:GLU:HB2	2.01	0.43
1:C:163:TYR:HB3	1:C:174:TYR:CD1	2.54	0.42
1:A:46:LYS:C	1:A:48:GLU:H	2.26	0.42
1:B:178:PHE:CZ	1:B:182:VAL:HG13	2.55	0.42
1:B:43:PRO:HA	1:B:48:GLU:OE2	2.19	0.42
1:A:47:PHE:HB3	1:A:55:ILE:HG12	2.02	0.42
1:C:42:ILE:HD13	4:C:5426:HOH:O	2.20	0.42
1:C:138:THR:HB	1:C:142:ALA:HB3	2.02	0.42
1:B:21:GLU:HA	1:B:24:GLU:HG2	2.02	0.42
1:B:60:ASP:HB2	4:B:1741:HOH:O	2.20	0.42
1:C:171:ARG:N	1:C:172:PRO:CD	2.83	0.41
1:D:42:ILE:O	1:D:43:PRO:C	2.61	0.41
1:D:125:LEU:HD23	1:D:153:ILE:CG1	2.49	0.41
1:C:82:PRO:O	1:C:83:ASN:OD1	2.38	0.41
1:C:154:LEU:CD1	1:C:187:ALA:HB2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:VAL:HG23	1:D:116:ASN:ND2	2.36	0.41
1:A:171:ARG:N	1:A:172:PRO:CD	2.82	0.41
1:C:42:ILE:CD1	4:C:5426:HOH:O	2.68	0.41
1:B:14:LEU:HD22	1:B:181:LEU:HD22	2.01	0.41
1:B:163:TYR:HB3	1:B:174:TYR:CD1	2.56	0.41
1:A:110:LEU:CD1	1:A:110:LEU:C	2.94	0.41
1:C:17:HIS:HB2	1:C:181:LEU:HD11	2.03	0.41
1:B:4:LEU:HD12	1:B:5:PRO:HD2	2.03	0.41
1:A:130:ASP:OD1	1:A:130:ASP:C	2.63	0.41
1:D:81:SER:C	1:D:83:ASN:N	2.78	0.41
1:A:110:LEU:C	1:A:110:LEU:HD12	2.46	0.40
1:D:145:LEU:HD22	1:D:145:LEU:O	2.21	0.40
1:D:68:ALA:HB3	1:D:141:ALA:HB1	2.04	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	190/192 (99%)	185 (97%)	5 (3%)	0	100	100
1	B	190/192 (99%)	183 (96%)	6 (3%)	1 (0%)	24	22
1	C	190/192 (99%)	180 (95%)	9 (5%)	1 (0%)	24	22
1	D	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
All	All	760/768 (99%)	731 (96%)	27 (4%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	GLY
1	C	47	PHE

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	158/158 (100%)	148 (94%)	10 (6%)	16	14
1	B	158/158 (100%)	147 (93%)	11 (7%)	14	11
1	C	158/158 (100%)	141 (89%)	17 (11%)	6	4
1	D	158/158 (100%)	137 (87%)	21 (13%)	4	2
All	All	632/632 (100%)	573 (91%)	59 (9%)	8	6

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	46	LYS
1	A	53	GLU
1	A	56	VAL
1	A	110	LEU
1	A	128	LEU
1	A	154	LEU
1	A	156	VAL
1	A	170	VAL
1	A	182	VAL
1	C	7	LEU
1	C	11	ILE
1	C	29	LYS
1	C	42	ILE
1	C	45	THR
1	C	46	LYS
1	C	48	GLU
1	C	50	LYS
1	C	108	GLU
1	C	128	LEU
1	C	143	THR
1	C	145	LEU
1	C	148	ASP
1	C	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	158	LEU
1	C	176	LYS
1	C	182	VAL
1	B	11	ILE
1	B	46	LYS
1	B	48	GLU
1	B	56	VAL
1	B	60	ASP
1	B	107	LYS
1	B	156	VAL
1	B	158	LEU
1	B	170	VAL
1	B	176	LYS
1	B	182	VAL
1	D	3	GLU
1	D	11	ILE
1	D	16	PRO
1	D	20	LYS
1	D	29	LYS
1	D	36	VAL
1	D	46	LYS
1	D	48	GLU
1	D	50	LYS
1	D	59	SER
1	D	113	LYS
1	D	128	LEU
1	D	139	SER
1	D	145	LEU
1	D	148	ASP
1	D	153	ILE
1	D	154	LEU
1	D	155	THR
1	D	158	LEU
1	D	176	LYS
1	D	182	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	C	32	ASN
1	C	65	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	65	ASN
1	D	32	ASN
1	D	49	ASN
1	D	78	ASN
1	D	116	ASN

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 ⓘ

8 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	GLC	E	1	2	11,11,12	0.31	0	15,15,17	0.83	0
2	GLC	E	2	2	12,12,12	0.53	0	17,17,17	0.68	0
2	GLC	F	1	2	11,11,12	0.27	0	15,15,17	0.78	0
2	GLC	F	2	2	12,12,12	0.48	0	17,17,17	0.79	0
2	GLC	G	1	2	11,11,12	0.28	0	15,15,17	0.82	0
2	GLC	G	2	2	12,12,12	0.51	0	17,17,17	0.69	1 (5%)
2	GLC	H	1	2	11,11,12	0.28	0	15,15,17	0.93	1 (6%)
2	GLC	H	2	2	12,12,12	0.54	0	17,17,17	0.74	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
2	GLC	E	1	2	-	0/2/19/22	0/1/1/1
2	GLC	E	2	2	-	0/2/22/22	0/1/1/1
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	GLC	F	2	2	-	0/2/22/22	0/1/1/1
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	GLC	G	2	2	-	0/2/22/22	0/1/1/1
2	GLC	H	1	2	-	0/2/19/22	0/1/1/1
2	GLC	H	2	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	GLC	C6-C5-C4	-2.07	107.94	113.02
2	H	1	GLC	C6-C5-C4	-2.01	108.09	113.02

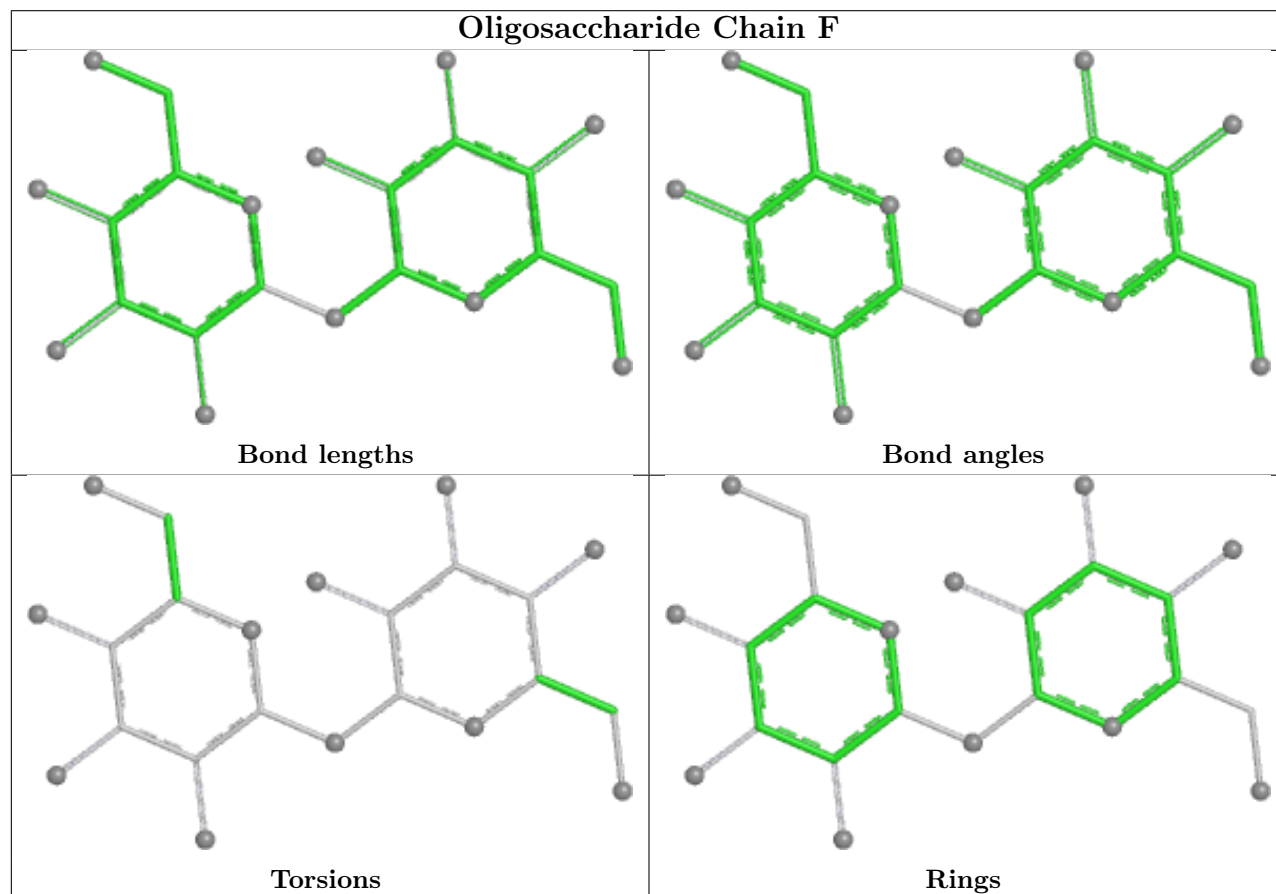
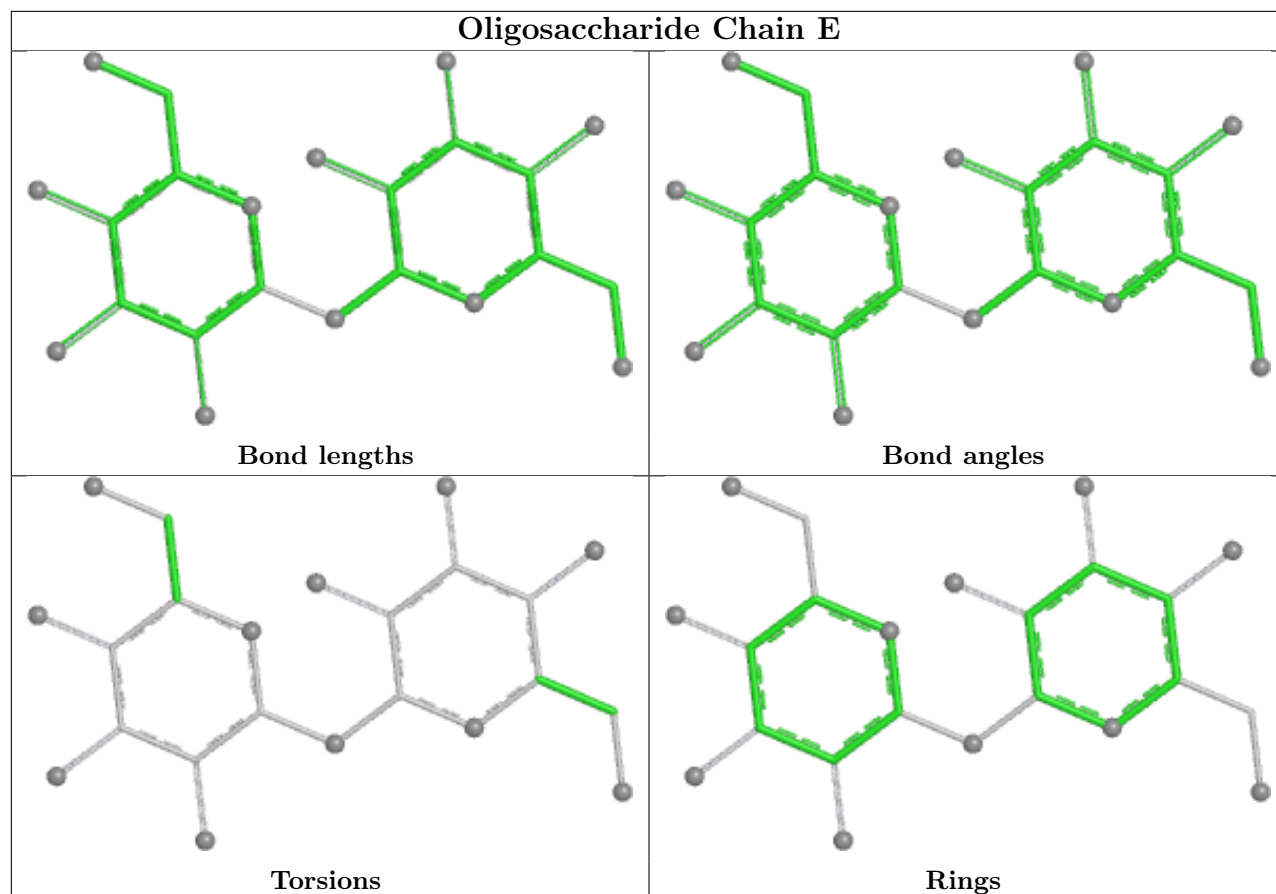
There are no chirality outliers.

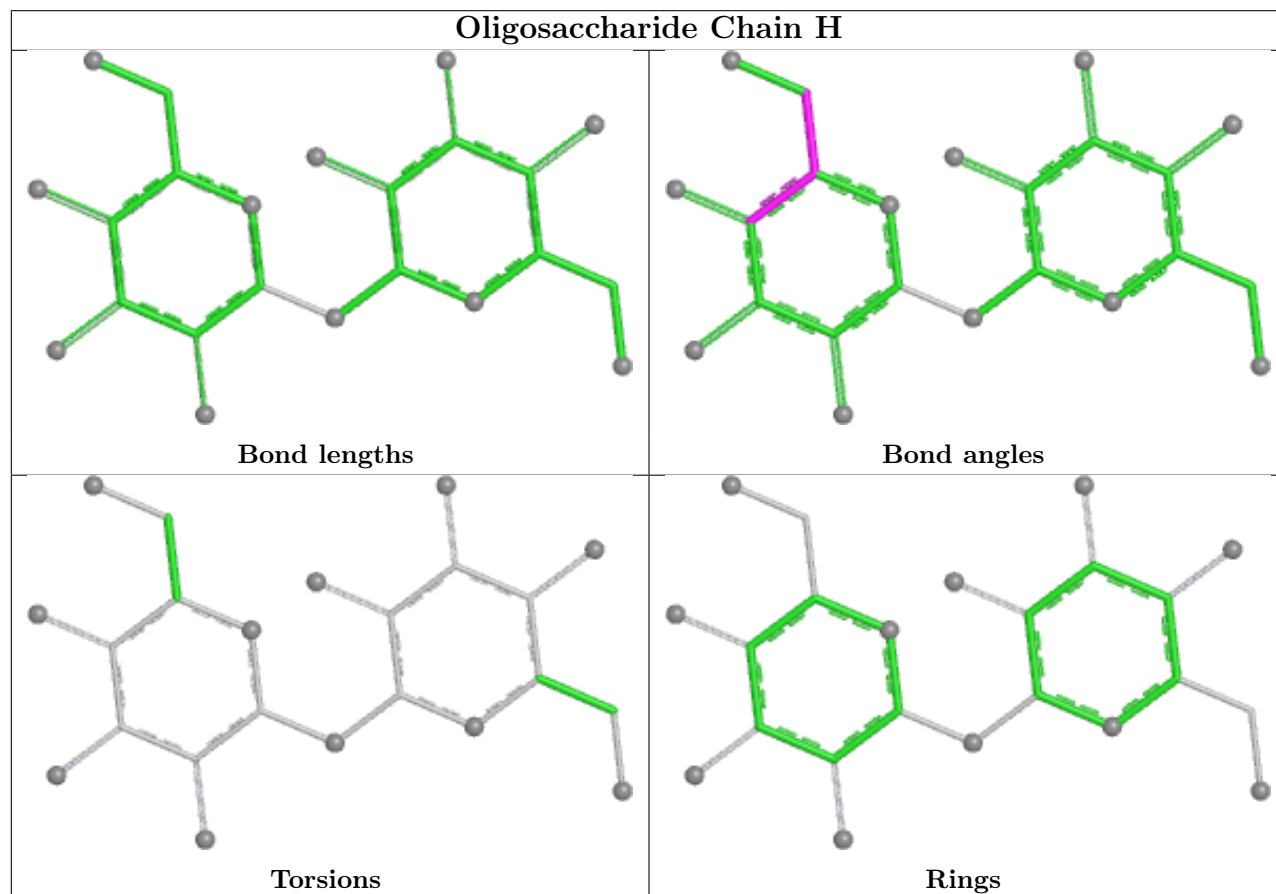
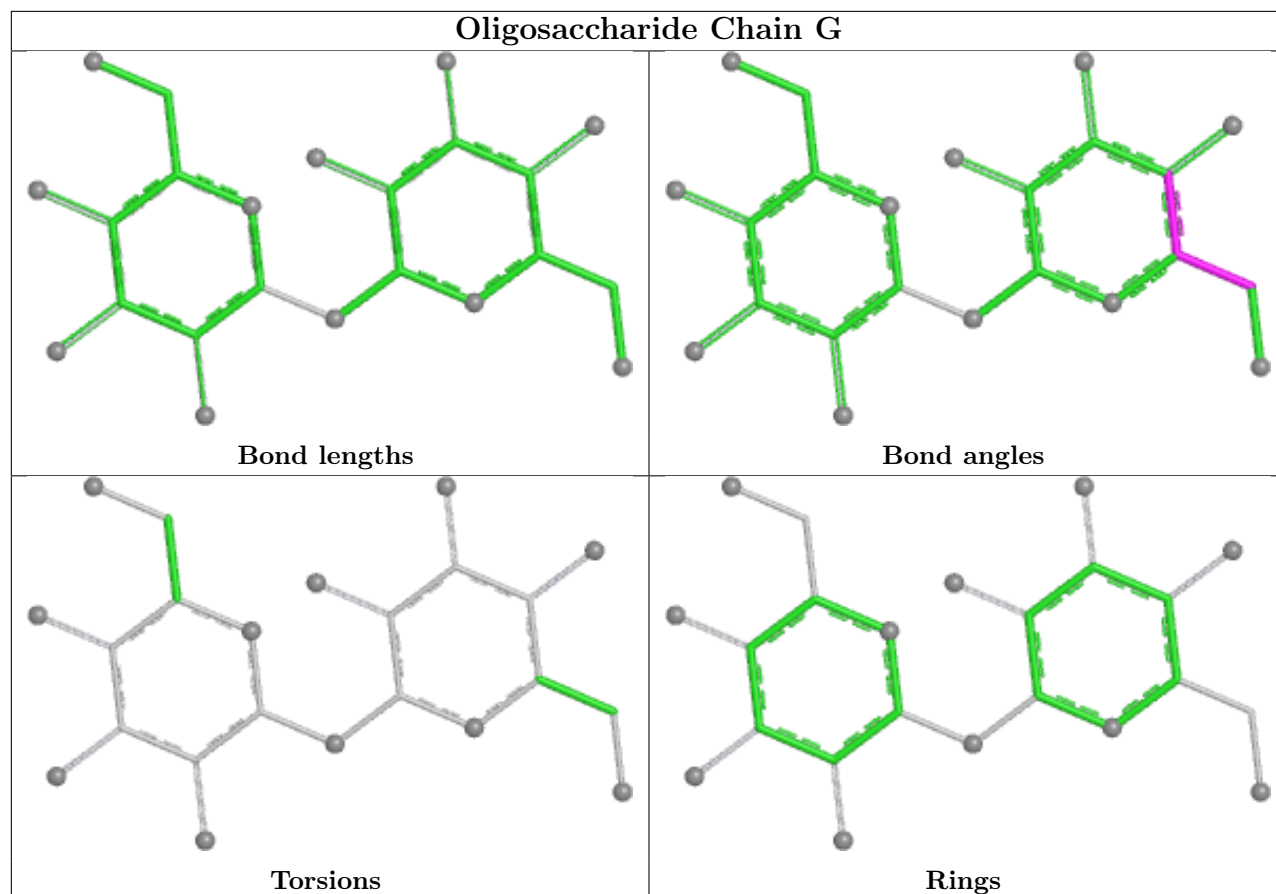
There are no torsion outliers.

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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 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.

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, 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	192/192 (100%)	-0.23	2 (1%) 79 81	12, 19, 32, 50	0
1	B	192/192 (100%)	-0.28	1 (0%) 87 88	12, 19, 30, 41	0
1	C	192/192 (100%)	-0.01	10 (5%) 33 35	13, 21, 37, 58	0
1	D	192/192 (100%)	-0.00	7 (3%) 46 48	14, 22, 39, 51	0
All	All	768/768 (100%)	-0.13	20 (2%) 57 60	12, 20, 36, 58	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	45	THR	3.8
1	A	48	GLU	3.5
1	C	48	GLU	3.5
1	C	49	ASN	3.5
1	D	44	GLY	3.4
1	C	83	ASN	3.0
1	D	1	ALA	2.6
1	D	46	LYS	2.5
1	B	44	GLY	2.5
1	C	47	PHE	2.5
1	A	46	LYS	2.4
1	C	108	GLU	2.3
1	D	192	ALA	2.2
1	C	42	ILE	2.1
1	D	56	VAL	2.1
1	D	49	ASN	2.1
1	D	45	THR	2.1
1	C	40	GLY	2.1
1	C	192	ALA	2.1
1	C	60	ASP	2.0

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

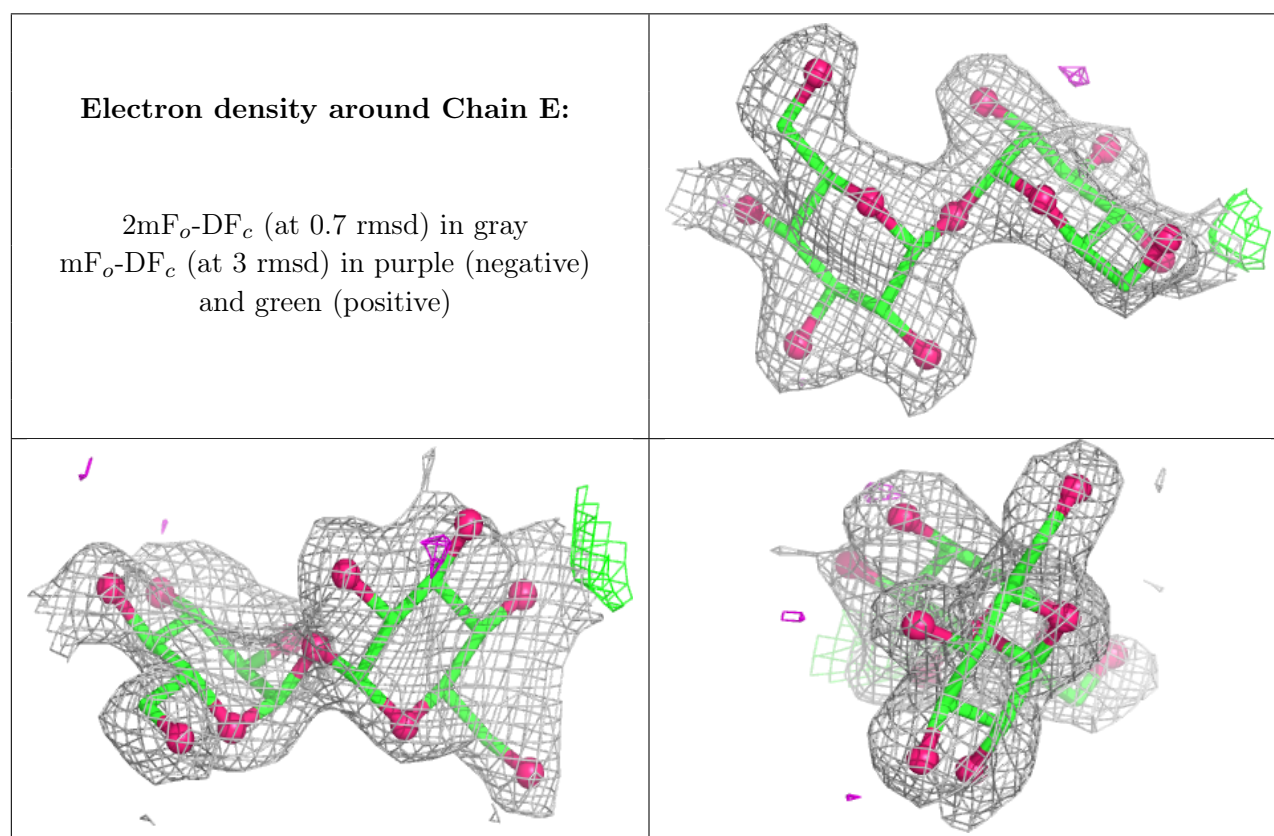
There are no non-standard protein/DNA/RNA residues in this entry.

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.

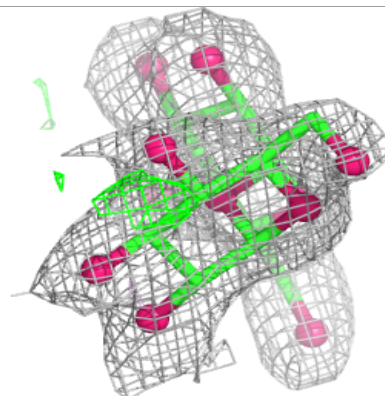
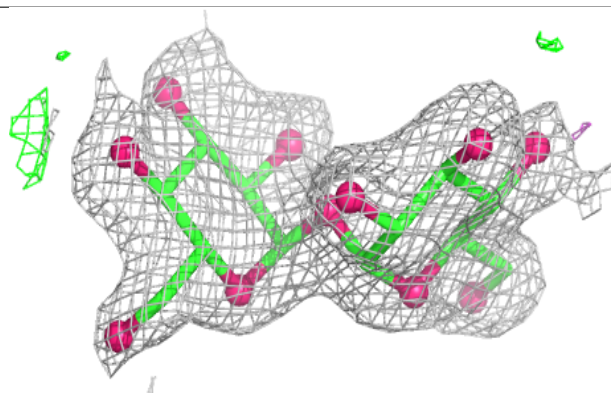
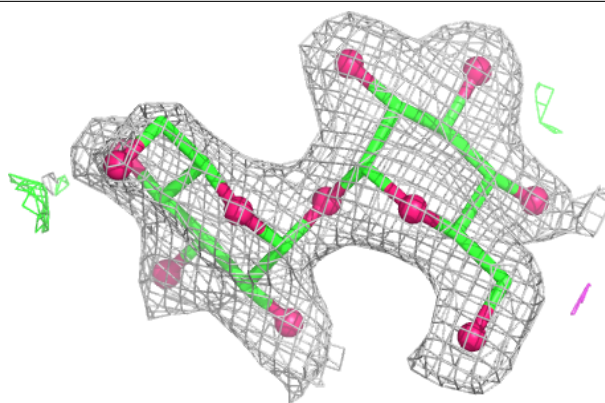
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	H	2	12/12	0.81	0.13	37,40,42,45	0
2	GLC	E	1	11/12	0.82	0.12	37,41,43,44	0
2	GLC	H	1	11/12	0.85	0.10	47,48,50,51	0
2	GLC	G	1	11/12	0.88	0.10	38,38,40,41	0
2	GLC	E	2	12/12	0.88	0.10	28,31,34,36	0
2	GLC	F	1	11/12	0.88	0.09	41,43,44,47	0
2	GLC	G	2	12/12	0.89	0.09	31,33,35,36	0
2	GLC	F	2	12/12	0.92	0.08	26,29,34,37	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.

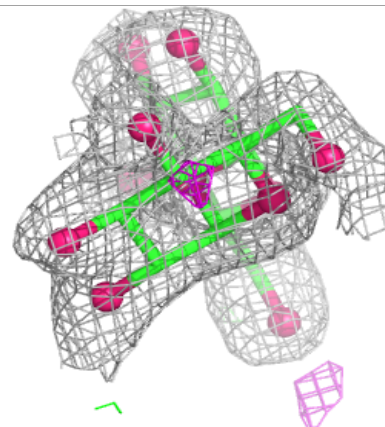
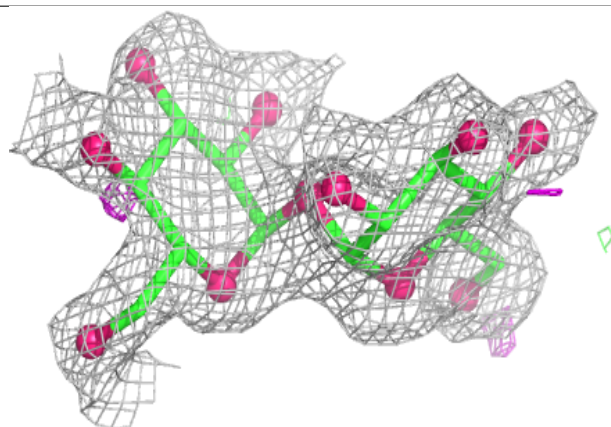
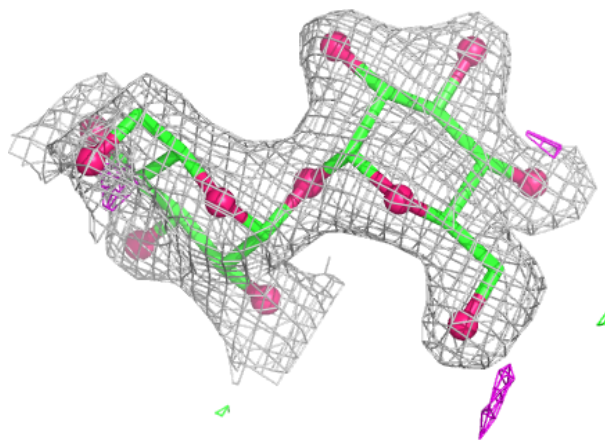


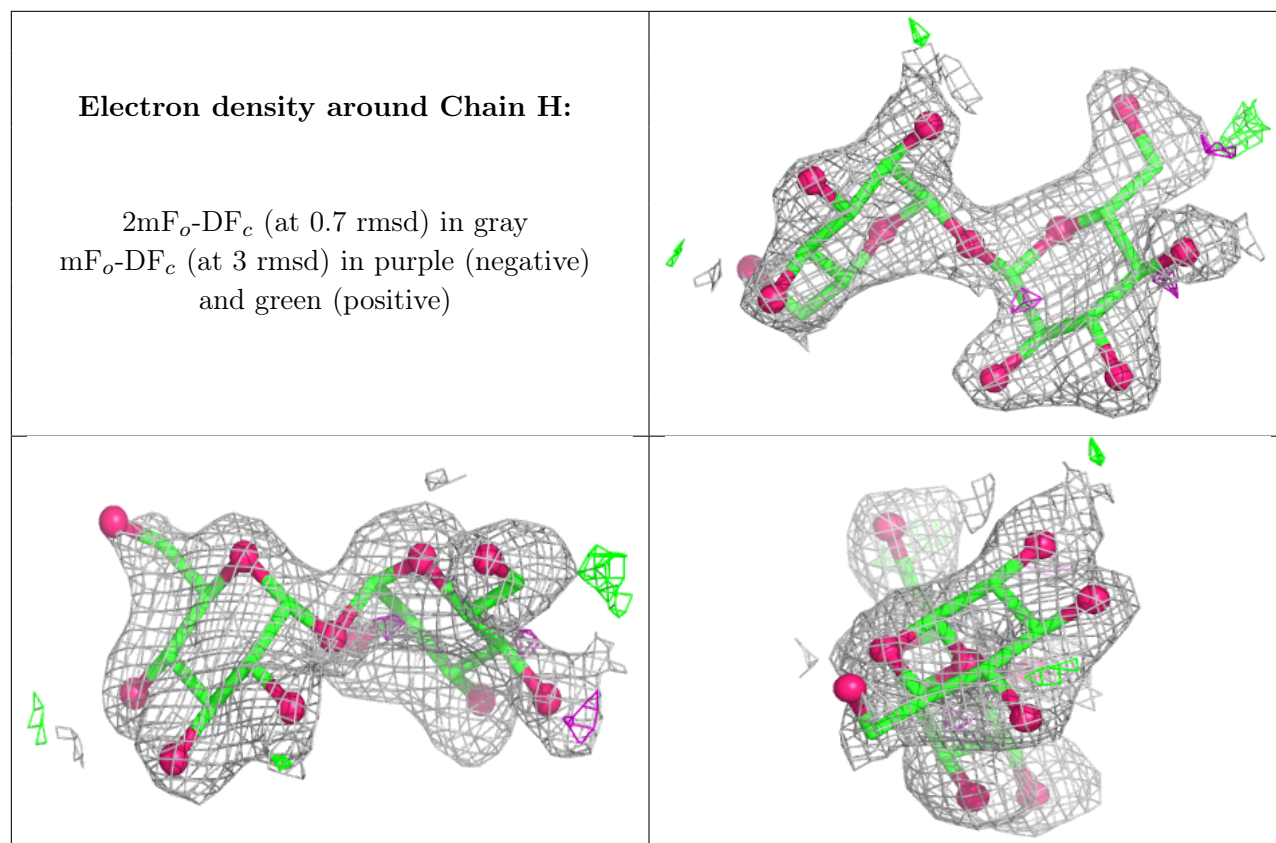
Electron density around Chain F:

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

**Electron density around Chain G:**

$2mF_o - DF_c$ (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($\text{\AA}^2$)	Q<0.9
3	FE	C	5002	1/1	0.99	0.04	18,18,18,18	0
3	FE	D	5003	1/1	0.99	0.04	17,17,17,17	0
3	FE	B	5001	1/1	1.00	0.02	16,16,16,16	0
3	FE	A	5000	1/1	1.00	0.04	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.