



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 03:38 AM EST

PDB ID : 4IRL
Title : X-ray structure of the CARD domain of zebrafish GBP-NLRP1 like protein
Authors : Jin, T.; Huang, M.; Smith, P.; Xiao, T.
Deposited on : 2013-01-15
Resolution : 1.47 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

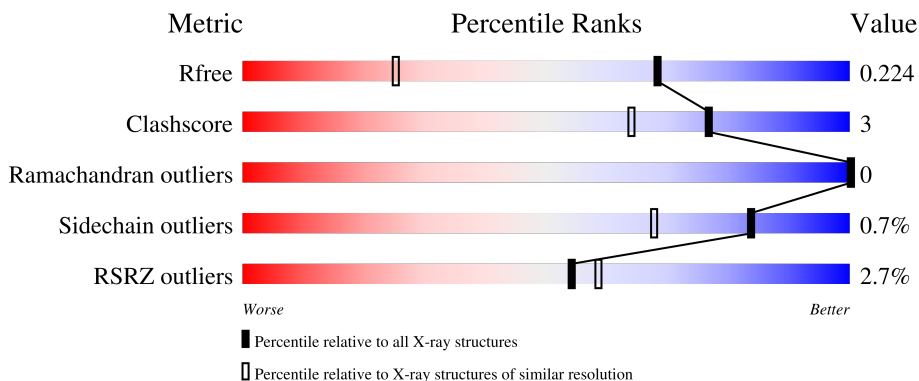
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

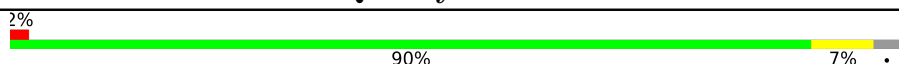
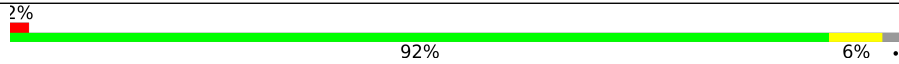
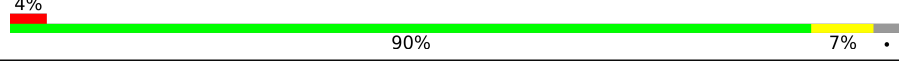
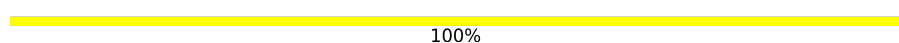

The reported resolution of this entry is 1.47 Å.

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.



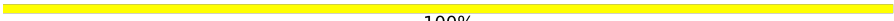
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	476	 2% 90% 7%
1	B	476	 2% 92% 6%
1	C	476	 4% 90% 7%
2	D	4	 100%
2	E	4	 100%

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Mol	Chain	Length	Quality of chain
2	F	4	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	503	-	-	X	-
4	EDO	B	504	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12984 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 Maltose-binding periplasmic protein, Novel protein similar to vertebrate guanylate binding protein family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	462	Total 3649	C 2346	N 601	O 690	S 12	0	16	0
1	B	463	Total 3614	C 2315	N 597	O 690	S 12	0	7	0
1	C	462	Total 3600	C 2304	N 599	O 685	S 12	0	6	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P0AEX9
A	83	ALA	ASP	conflict	UNP P0AEX9
A	84	ALA	LYS	conflict	UNP P0AEX9
A	173	ALA	GLU	conflict	UNP P0AEX9
A	174	ALA	ASN	conflict	UNP P0AEX9
A	240	ALA	LYS	conflict	UNP P0AEX9
A	360	ALA	-	linker	UNP B0V1H4
A	361	ALA	-	linker	UNP B0V1H4
A	362	LEU	-	linker	UNP B0V1H4
A	363	ALA	-	linker	UNP B0V1H4
A	364	ALA	-	linker	UNP B0V1H4
A	365	ALA	-	linker	UNP B0V1H4
A	366	GLN	-	linker	UNP B0V1H4
A	367	THR	-	linker	UNP B0V1H4
A	368	ASN	-	linker	UNP B0V1H4
A	369	ALA	-	linker	UNP B0V1H4
A	370	ALA	-	linker	UNP B0V1H4
A	371	ARG	-	linker	UNP B0V1H4
A	372	ALA	-	linker	UNP B0V1H4
A	373	ALA	-	linker	UNP B0V1H4
A	374	ALA	-	linker	UNP B0V1H4
A	375	ALA	-	linker	UNP B0V1H4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	412	SER	ASN	conflict	UNP B0V1H4
A	416	TYR	ASN	conflict	UNP B0V1H4
A	469	LEU	-	expression tag	UNP B0V1H4
A	470	GLU	-	expression tag	UNP B0V1H4
A	471	HIS	-	expression tag	UNP B0V1H4
A	472	HIS	-	expression tag	UNP B0V1H4
A	473	HIS	-	expression tag	UNP B0V1H4
A	474	HIS	-	expression tag	UNP B0V1H4
A	475	HIS	-	expression tag	UNP B0V1H4
A	476	HIS	-	expression tag	UNP B0V1H4
B	1	MET	-	expression tag	UNP P0AEX9
B	83	ALA	ASP	conflict	UNP P0AEX9
B	84	ALA	LYS	conflict	UNP P0AEX9
B	173	ALA	GLU	conflict	UNP P0AEX9
B	174	ALA	ASN	conflict	UNP P0AEX9
B	240	ALA	LYS	conflict	UNP P0AEX9
B	360	ALA	-	linker	UNP B0V1H4
B	361	ALA	-	linker	UNP B0V1H4
B	362	LEU	-	linker	UNP B0V1H4
B	363	ALA	-	linker	UNP B0V1H4
B	364	ALA	-	linker	UNP B0V1H4
B	365	ALA	-	linker	UNP B0V1H4
B	366	GLN	-	linker	UNP B0V1H4
B	367	THR	-	linker	UNP B0V1H4
B	368	ASN	-	linker	UNP B0V1H4
B	369	ALA	-	linker	UNP B0V1H4
B	370	ALA	-	linker	UNP B0V1H4
B	371	ARG	-	linker	UNP B0V1H4
B	372	ALA	-	linker	UNP B0V1H4
B	373	ALA	-	linker	UNP B0V1H4
B	374	ALA	-	linker	UNP B0V1H4
B	375	ALA	-	linker	UNP B0V1H4
B	412	SER	ASN	conflict	UNP B0V1H4
B	416	TYR	ASN	conflict	UNP B0V1H4
B	469	LEU	-	expression tag	UNP B0V1H4
B	470	GLU	-	expression tag	UNP B0V1H4
B	471	HIS	-	expression tag	UNP B0V1H4
B	472	HIS	-	expression tag	UNP B0V1H4
B	473	HIS	-	expression tag	UNP B0V1H4
B	474	HIS	-	expression tag	UNP B0V1H4
B	475	HIS	-	expression tag	UNP B0V1H4
B	476	HIS	-	expression tag	UNP B0V1H4

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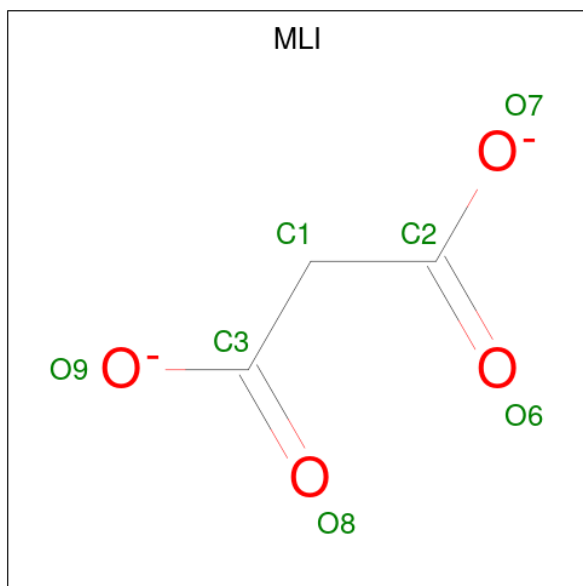
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	expression tag	UNP P0AEX9
C	83	ALA	ASP	conflict	UNP P0AEX9
C	84	ALA	LYS	conflict	UNP P0AEX9
C	173	ALA	GLU	conflict	UNP P0AEX9
C	174	ALA	ASN	conflict	UNP P0AEX9
C	240	ALA	LYS	conflict	UNP P0AEX9
C	360	ALA	-	linker	UNP B0V1H4
C	361	ALA	-	linker	UNP B0V1H4
C	362	LEU	-	linker	UNP B0V1H4
C	363	ALA	-	linker	UNP B0V1H4
C	364	ALA	-	linker	UNP B0V1H4
C	365	ALA	-	linker	UNP B0V1H4
C	366	GLN	-	linker	UNP B0V1H4
C	367	THR	-	linker	UNP B0V1H4
C	368	ASN	-	linker	UNP B0V1H4
C	369	ALA	-	linker	UNP B0V1H4
C	370	ALA	-	linker	UNP B0V1H4
C	371	ARG	-	linker	UNP B0V1H4
C	372	ALA	-	linker	UNP B0V1H4
C	373	ALA	-	linker	UNP B0V1H4
C	374	ALA	-	linker	UNP B0V1H4
C	375	ALA	-	linker	UNP B0V1H4
C	412	SER	ASN	conflict	UNP B0V1H4
C	416	TYR	ASN	conflict	UNP B0V1H4
C	469	LEU	-	expression tag	UNP B0V1H4
C	470	GLU	-	expression tag	UNP B0V1H4
C	471	HIS	-	expression tag	UNP B0V1H4
C	472	HIS	-	expression tag	UNP B0V1H4
C	473	HIS	-	expression tag	UNP B0V1H4
C	474	HIS	-	expression tag	UNP B0V1H4
C	475	HIS	-	expression tag	UNP B0V1H4
C	476	HIS	-	expression tag	UNP B0V1H4

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	4	Total	C	O	0	0	0
			45	24	21			
2	E	4	Total	C	O	0	0	0
			45	24	21			
2	F	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



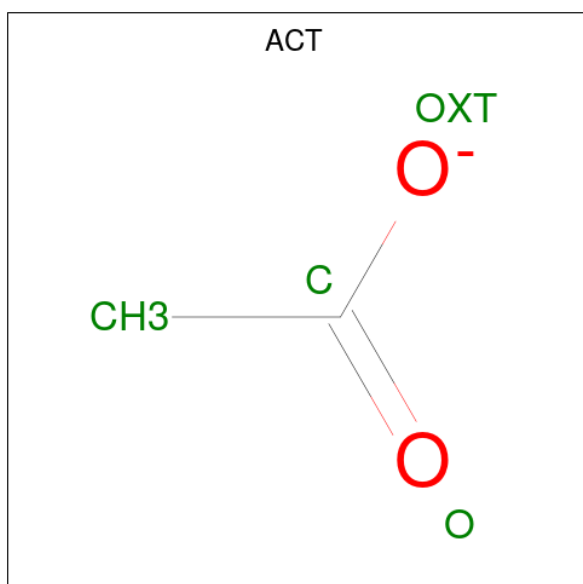
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	B	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2^-$).

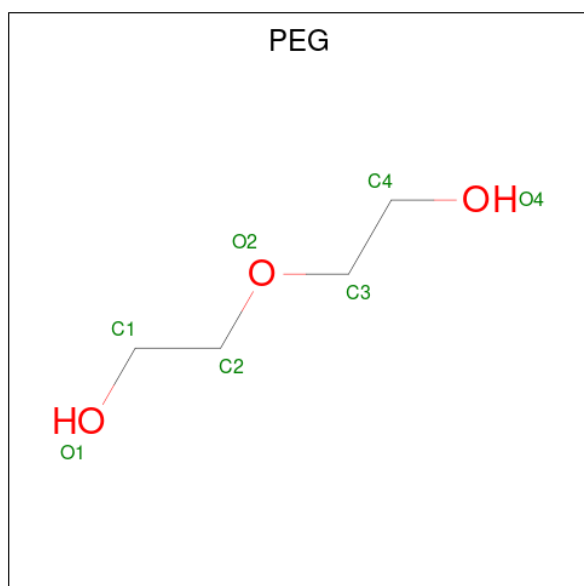


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	2	Total	Na	0	0
			2	2		
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	669	Total 669	O 669	0	0
8	B	626	Total 626	O 626	0	0
8	C	627	Total 627	O 627	0	0

Chain D:  100%

GLC1
GLC2
GLC3
GLC4

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  100%

GLC1
GLC2
GLC3
GLC4

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  100%

GLC1
GLC2
GLC3
GLC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.75Å 124.75Å 178.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.43 – 1.47 29.43 – 1.47	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.43-1.47) 95.6 (29.43-1.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.47Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1217)	Depositor
R, R_{free}	0.188 , 0.224 0.189 , 0.224	Depositor DCC
R_{free} test set	11934 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtrriage
Anisotropy	0.183	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12984	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.56 % 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 3.0569e-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: MLI, EDO, NA, PEG, ACT, 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	0.50	0/3776	0.61	0/5118
1	B	0.50	0/3714	0.60	0/5036
1	C	0.48	0/3697	0.58	1/5011 (0.0%)
All	All	0.49	0/11187	0.60	1/15165 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	317	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3649	0	3685	25	0
1	B	3614	0	3604	20	0
1	C	3600	0	3593	21	0
2	D	45	0	39	0	0
2	E	45	0	39	0	0
2	F	45	0	39	0	0
3	A	7	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	2	0	0
3	C	7	0	2	0	0
4	A	4	0	6	4	0
4	B	12	0	18	5	0
4	C	4	0	6	0	0
5	A	4	0	3	1	0
5	B	4	0	3	1	0
5	C	4	0	3	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
7	C	7	0	10	0	0
8	A	669	0	0	6	0
8	B	626	0	0	5	0
8	C	627	0	0	6	0
All	All	12984	0	11054	66	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 (66) 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:92:PRO:HA	4:B:504:EDO:H21	1.65	0.77
4:A:503:EDO:H12	8:A:776:HOH:O	1.89	0.73
1:B:385:ASP:OD2	1:B:460:ARG:NH2	2.22	0.72
1:B:382[B]:LEU:HD23	1:B:457:LEU:HB3	1.72	0.70
1:A:237:ASP:O	5:A:504:ACT:H1	1.93	0.69
1:A:382[B]:LEU:HD23	1:A:457:LEU:HB3	1.75	0.68
1:B:237:ASP:O	5:B:506:ACT:H1	1.94	0.68
1:A:336:GLN:NE2	8:A:1218:HOH:O	2.27	0.66
1:C:410:LEU:HD11	1:C:429:ARG:HB2	1.77	0.66
1:A:89:LYS:HD3	4:A:503:EDO:H21	1.78	0.65
1:C:314:LYS:NZ	8:C:1223:HOH:O	2.30	0.63
1:A:382[A]:LEU:HD13	1:A:457:LEU:HB3	1.81	0.63
1:A:26:LYS:NZ	8:A:1230:HOH:O	2.25	0.61
1:A:287:THR:HG22	4:A:503:EDO:H11	1.83	0.59
1:C:237:ASP:O	5:C:505:ACT:H1	2.02	0.59
1:B:461:HIS:ND1	8:B:848:HOH:O	2.32	0.58
1:C:385:ASP:OD2	1:C:460:ARG:NH2	2.36	0.58
1:A:68:PHE:HB3	1:A:105[B]:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368[B]:ASN:ND2	8:A:679:HOH:O	2.37	0.57
1:C:7:LYS:NZ	8:C:1141:HOH:O	2.27	0.55
1:A:43:LYS:NZ	8:A:829:HOH:O	2.40	0.54
1:B:443:TYR:OH	1:B:458:GLU:OE1	2.22	0.53
4:B:504:EDO:H22	8:C:1164:HOH:O	2.08	0.53
1:A:80:ILE:HG22	1:A:82:PRO:HD3	1.91	0.52
1:C:7:LYS:HD2	8:C:1100:HOH:O	2.10	0.52
1:C:80:ILE:HG22	1:C:82:PRO:HD3	1.92	0.51
1:A:429:ARG:NH2	1:A:432:ASP:OD2	2.42	0.51
1:A:399:SER:O	1:A:403:GLU:HG2	2.12	0.49
1:B:92:PRO:CA	4:B:504:EDO:H21	2.39	0.49
1:A:287:THR:HG22	4:A:503:EDO:C1	2.43	0.49
1:B:95:TRP:CD1	4:B:504:EDO:H12	2.47	0.49
1:A:130:TRP:CD1	1:A:249:PRO:HB2	2.49	0.47
1:B:173:ALA:O	8:B:1080:HOH:O	2.20	0.47
1:A:46:GLU:OE2	1:A:342:TYR:OH	2.22	0.47
1:A:103:LYS:HE3	1:B:404:ARG:NH2	2.29	0.47
1:C:382:LEU:HD21	1:C:461:HIS:HB2	1.97	0.47
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.51	0.46
1:C:234[A]:SER:OG	1:C:299:PRO:HD3	2.15	0.46
1:B:382[B]:LEU:CD2	1:B:457:LEU:HB3	2.42	0.45
1:A:34:ILE:HG13	1:A:276:LEU:HD13	1.97	0.45
1:B:359[A]:ASP:OD2	8:B:979:HOH:O	2.21	0.45
1:C:103:LYS:NZ	8:C:903:HOH:O	2.38	0.44
1:C:34:ILE:HG13	1:C:276:LEU:HD13	2.00	0.44
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.53	0.43
1:A:69:GLY:HA3	1:A:333:ASN:O	2.17	0.43
1:C:413:GLU:OE1	8:C:942:HOH:O	2.21	0.43
1:A:120:LYS:HE2	3:A:502:MLI:O8	2.20	0.42
1:C:69:GLY:HA3	1:C:333:ASN:O	2.18	0.42
1:B:92:PRO:HB2	1:C:208[A]:ASP:OD2	2.20	0.42
1:C:349:ILE:CG2	1:C:355:ARG:HH21	2.32	0.42
1:A:378:PHE:CE2	1:A:382[A]:LEU:HD12	2.55	0.42
1:A:382[B]:LEU:CD2	1:A:457:LEU:HB3	2.45	0.42
1:B:410:LEU:HD21	1:B:429:ARG:HB2	2.02	0.42
1:C:160:PRO:HG3	1:C:258:PRO:HA	2.02	0.42
1:C:140:LEU:HA	1:C:143:LYS:HE3	2.02	0.42
1:C:410:LEU:HD13	1:C:430:ALA:HB2	2.02	0.41
1:B:80:ILE:HG22	1:B:82:PRO:HD3	2.01	0.41
1:C:407:THR:HB	1:C:409:GLU:OE1	2.21	0.41
1:B:44:LEU:C	1:B:44:LEU:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HD2	8:A:1112:HOH:O	2.19	0.41
1:B:310:GLU:OE2	1:C:220:LYS:NZ	2.48	0.41
4:B:504:EDO:H11	8:B:1206:HOH:O	2.21	0.41
1:B:139:GLU:O	1:B:143:LYS:HE3	2.21	0.41
1:B:2:LYS:NZ	8:B:885:HOH:O	2.55	0.40
1:C:82:PRO:HG2	1:C:87:GLN:HG2	2.03	0.40
1:A:160:PRO:HG3	1:A:258:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

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

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/476 (100%)	471 (99%)	5 (1%)	0	100	100
1	B	468/476 (98%)	461 (98%)	7 (2%)	0	100	100
1	C	466/476 (98%)	460 (99%)	6 (1%)	0	100	100
All	All	1410/1428 (99%)	1392 (99%)	18 (1%)	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	381/378 (101%)	379 (100%)	2 (0%)	88	77
1	B	373/378 (99%)	370 (99%)	3 (1%)	81	64
1	C	371/378 (98%)	368 (99%)	3 (1%)	81	64
All	All	1125/1134 (99%)	1117 (99%)	8 (1%)	84	68

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	PHE
1	A	428	PHE
1	B	259	PHE
1	B	428	PHE
1	B	459	SER
1	C	259	PHE
1	C	410	LEU
1	C	428	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	125	ASN
1	C	326	GLN

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](#)

12 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	D	1	2	12,12,12	0.82	0	17,17,17	0.90	1 (5%)
2	GLC	D	2	2	11,11,12	0.67	0	15,15,17	0.99	1 (6%)
2	GLC	D	3	2	11,11,12	1.06	0	15,15,17	1.20	1 (6%)
2	GLC	D	4	2	11,11,12	1.25	0	15,15,17	1.32	3 (20%)
2	GLC	E	1	2	12,12,12	0.94	0	17,17,17	0.82	1 (5%)
2	GLC	E	2	2	11,11,12	0.62	0	15,15,17	0.96	1 (6%)
2	GLC	E	3	2	11,11,12	0.79	0	15,15,17	1.38	4 (26%)
2	GLC	E	4	2	11,11,12	1.23	0	15,15,17	1.39	2 (13%)
2	GLC	F	1	2	12,12,12	1.00	1 (8%)	17,17,17	1.08	1 (5%)
2	GLC	F	2	2	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
2	GLC	F	3	2	11,11,12	1.02	0	15,15,17	1.85	4 (26%)
2	GLC	F	4	2	11,11,12	1.28	0	15,15,17	1.87	4 (26%)

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	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	1/2/22/22	0/1/1/1
2	GLC	F	2	2	-	1/2/19/22	0/1/1/1
2	GLC	F	3	2	-	0/2/19/22	0/1/1/1
2	GLC	F	4	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	GLC	O3-C3	-2.28	1.37	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	GLC	C1-O5-C5	4.15	117.82	112.19
2	F	4	GLC	C1-C2-C3	3.82	114.36	109.67
2	E	4	GLC	C1-C2-C3	3.63	114.13	109.67
2	F	4	GLC	C1-O5-C5	3.19	116.52	112.19
2	F	1	GLC	O5-C5-C4	3.07	115.26	109.69
2	F	3	GLC	O5-C5-C4	2.96	118.04	110.83
2	F	4	GLC	C6-C5-C4	-2.70	106.67	113.00
2	F	3	GLC	C2-C3-C4	2.67	115.51	110.89
2	F	4	GLC	O5-C5-C4	2.63	117.23	110.83
2	E	1	GLC	O5-C5-C4	2.43	114.11	109.69
2	F	2	GLC	C1-O5-C5	2.43	115.49	112.19
2	E	4	GLC	O2-C2-C1	2.43	114.12	109.15
2	D	4	GLC	C1-C2-C3	2.42	112.64	109.67
2	E	2	GLC	C1-O5-C5	2.42	115.47	112.19
2	F	2	GLC	O5-C5-C4	2.40	116.67	110.83
2	E	3	GLC	C1-O5-C5	2.31	115.32	112.19
2	D	2	GLC	O5-C1-C2	2.23	114.22	110.77
2	E	3	GLC	C2-C3-C4	2.23	114.75	110.89
2	D	1	GLC	O5-C5-C4	2.20	113.69	109.69
2	D	4	GLC	O2-C2-C1	2.18	113.61	109.15
2	E	3	GLC	C6-C5-C4	-2.12	108.04	113.00
2	D	4	GLC	C6-C5-C4	-2.08	108.13	113.00
2	F	3	GLC	O3-C3-C2	-2.05	106.07	109.99
2	D	3	GLC	C6-C5-C4	-2.05	108.21	113.00
2	E	3	GLC	O5-C5-C6	2.02	110.36	107.20

There are no chirality outliers.

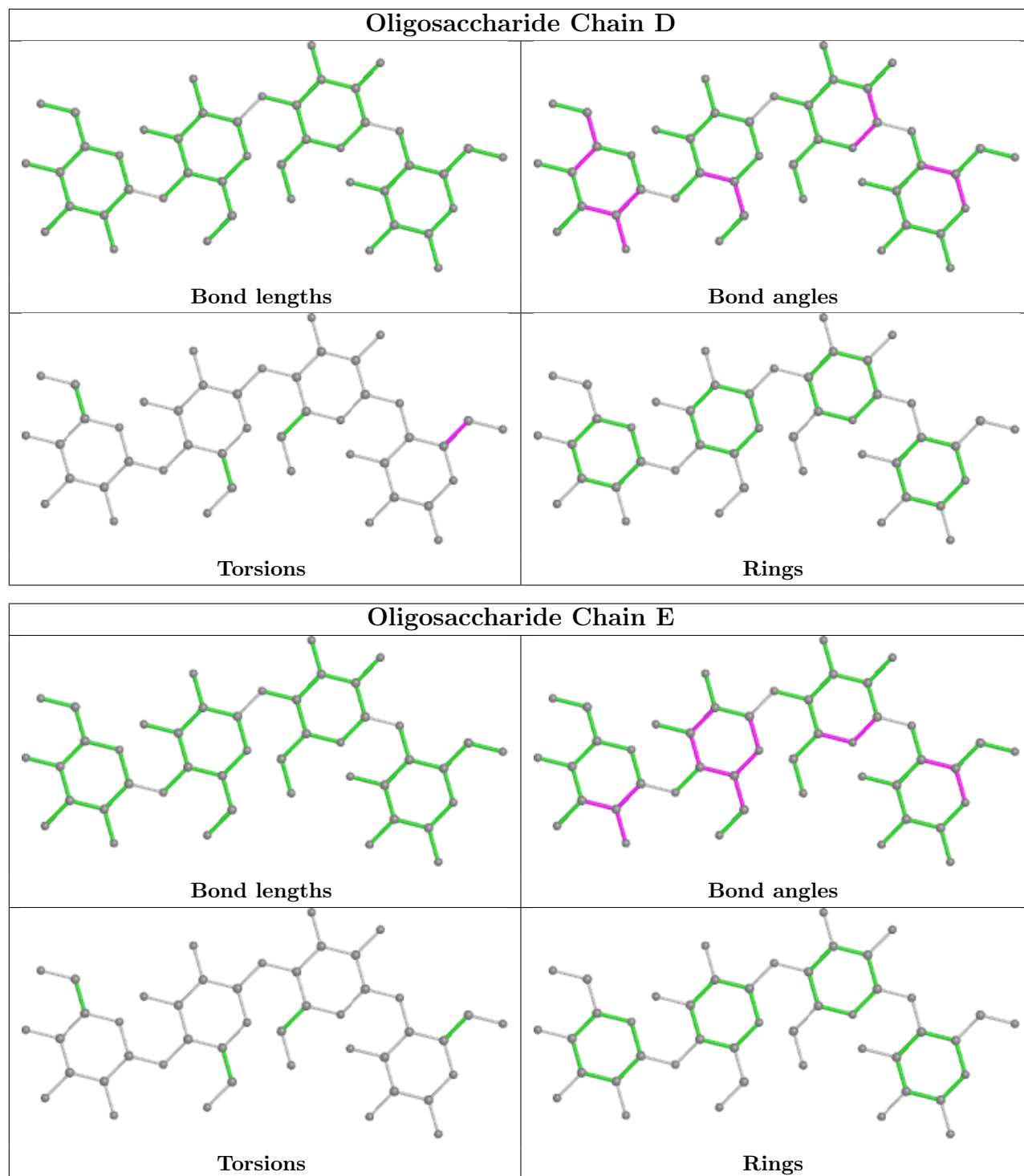
All (5) torsion outliers are listed below:

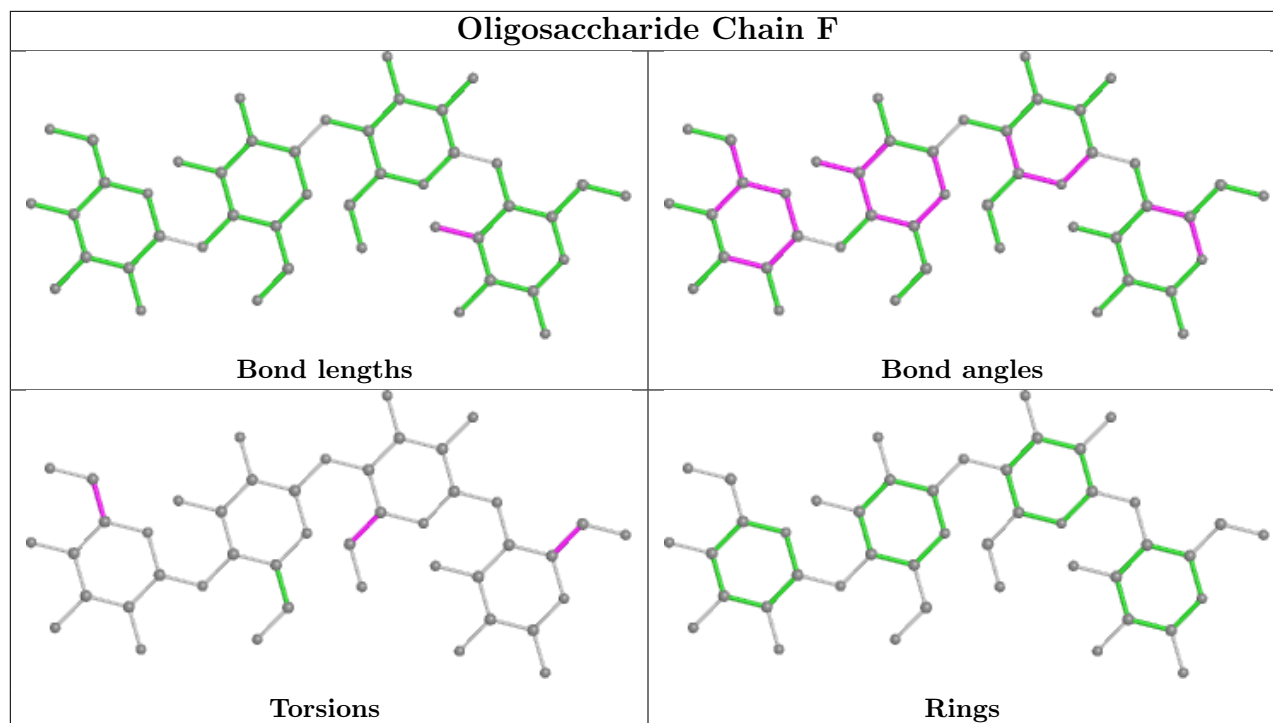
Mol	Chain	Res	Type	Atoms
2	F	4	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	F	4	GLC	O5-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6

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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
3	MLI	A	502	-	6,6,6	1.08	0	7,7,7	1.58	2 (28%)
4	EDO	C	503	-	3,3,3	0.49	0	2,2,2	0.15	0
5	ACT	A	504	-	3,3,3	0.55	0	3,3,3	1.56	1 (33%)
4	EDO	B	503	-	3,3,3	0.43	0	2,2,2	0.24	0
3	MLI	C	502	-	6,6,6	1.11	0	7,7,7	1.50	1 (14%)
7	PEG	C	504	-	6,6,6	0.60	0	5,5,5	0.75	0
4	EDO	B	505	-	3,3,3	0.50	0	2,2,2	0.25	0
5	ACT	C	505	-	3,3,3	0.67	0	3,3,3	1.01	0
5	ACT	B	506	-	3,3,3	0.73	0	3,3,3	1.14	0
3	MLI	B	502	-	6,6,6	1.25	0	7,7,7	1.31	0
4	EDO	B	504	-	3,3,3	0.60	0	2,2,2	0.13	0
4	EDO	A	503	-	3,3,3	0.48	0	2,2,2	0.42	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	MLI	A	502	-	-	0/4/4/4	-
4	EDO	C	503	-	-	0/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
3	MLI	C	502	-	-	0/4/4/4	-
7	PEG	C	504	-	-	2/4/4/4	-
4	EDO	B	505	-	-	0/1/1/1	-
3	MLI	B	502	-	-	0/4/4/4	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	MLI	O9-C3-C1	2.23	121.67	114.54
3	A	502	MLI	O7-C2-C1	2.05	121.07	114.54
3	A	502	MLI	O9-C3-C1	2.02	120.99	114.54
5	A	504	ACT	O-C-CH3	-2.00	114.53	122.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	504	PEG	O1-C1-C2-O2
7	C	504	PEG	C4-C3-O2-C2
4	B	504	EDO	O1-C1-C2-O2
4	A	503	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	MLI	1	0
5	A	504	ACT	1	0
5	C	505	ACT	1	0
5	B	506	ACT	1	0
4	B	504	EDO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	EDO	4	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	462/476 (97%)	-0.11	10 (2%) 62 66	9, 16, 31, 56	0
1	B	463/476 (97%)	-0.09	11 (2%) 59 63	11, 17, 31, 75	0
1	C	462/476 (97%)	0.02	17 (3%) 41 45	11, 19, 36, 65	0
All	All	1387/1428 (97%)	-0.06	38 (2%) 54 58	9, 17, 34, 75	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	462	SER	8.0
1	C	462	SER	5.2
1	B	463	GLU	4.9
1	B	174	ALA	4.9
1	C	172	TYR	4.4
1	C	174	ALA	4.2
1	B	172	TYR	4.1
1	B	1	MET	4.1
1	A	459	SER	3.8
1	C	1	MET	3.6
1	C	173	ALA	3.6
1	A	462	SER	3.5
1	C	404	ARG	3.5
1	C	175	GLY	3.4
1	C	461	HIS	3.3
1	A	460	ARG	3.2
1	C	355	ARG	3.1
1	C	460	ARG	3.1
1	A	174	ALA	3.0
1	A	175	GLY	2.9
1	C	142	ALA	2.9
1	A	142	ALA	2.8
1	B	142	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	404	ARG	2.8
1	B	460	ARG	2.7
1	C	144	GLY	2.6
1	B	144	GLY	2.5
1	C	402	SER	2.4
1	A	173	ALA	2.4
1	C	367	THR	2.3
1	B	459	SER	2.3
1	A	461	HIS	2.2
1	B	175	GLY	2.2
1	C	459	SER	2.1
1	B	176	LYS	2.1
1	A	314	LYS	2.0
1	C	379	VAL	2.0
1	C	143	LYS	2.0

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

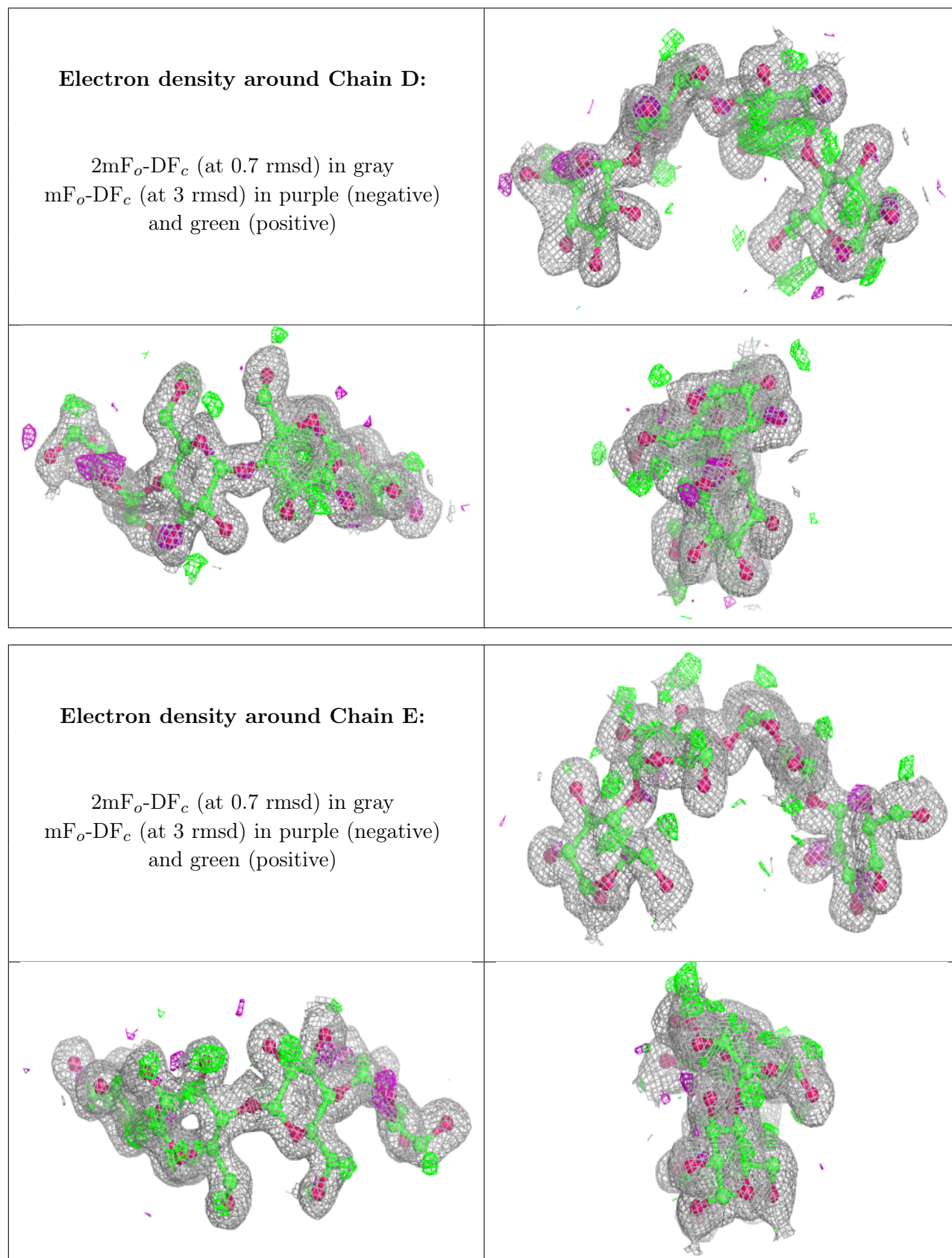
There are no non-standard protein/DNA/RNA residues in this entry.

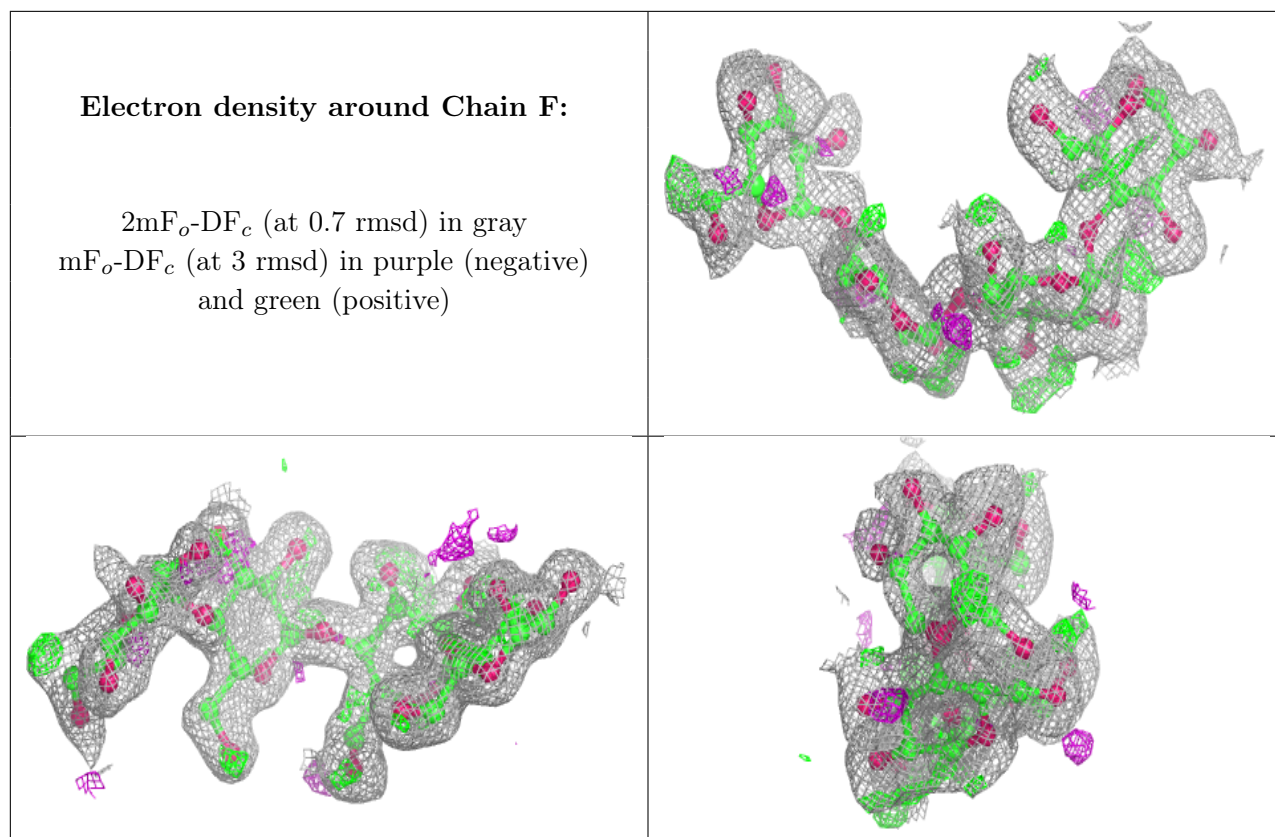
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	F	4	11/12	0.64	0.22	40,45,47,48	0
2	GLC	D	4	11/12	0.69	0.24	28,34,38,38	0
2	GLC	E	4	11/12	0.82	0.20	24,29,31,33	0
2	GLC	F	3	11/12	0.87	0.10	16,19,26,27	0
2	GLC	F	2	11/12	0.90	0.10	13,15,16,18	0
2	GLC	F	1	12/12	0.93	0.10	13,17,19,20	0
2	GLC	E	3	11/12	0.95	0.07	12,14,18,19	0
2	GLC	D	1	12/12	0.95	0.08	8,10,15,15	0
2	GLC	D	3	11/12	0.96	0.06	11,13,18,18	0
2	GLC	E	1	12/12	0.96	0.08	11,13,18,18	0
2	GLC	E	2	11/12	0.96	0.07	9,10,12,12	0
2	GLC	D	2	11/12	0.97	0.06	7,9,10,12	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(Å ²)	Q<0.9
4	EDO	B	503	4/4	0.79	0.13	28,28,35,36	0
4	EDO	A	503	4/4	0.81	0.23	26,29,31,42	0
4	EDO	C	503	4/4	0.81	0.17	38,42,46,48	0
7	PEG	C	504	7/7	0.82	0.11	34,41,49,52	0
4	EDO	B	504	4/4	0.88	0.17	25,29,31,34	0
6	NA	B	508	1/1	0.88	0.40	44,44,44,44	0
4	EDO	B	505	4/4	0.88	0.11	24,30,36,40	0
6	NA	C	506	1/1	0.91	0.10	25,25,25,25	0
3	MLI	B	502	7/7	0.91	0.17	18,24,32,38	0
5	ACT	C	505	4/4	0.92	0.11	16,17,20,23	0
5	ACT	A	504	4/4	0.92	0.11	11,16,16,21	0
3	MLI	C	502	7/7	0.94	0.13	19,25,31,36	0
5	ACT	B	506	4/4	0.94	0.11	8,15,15,18	0
3	MLI	A	502	7/7	0.95	0.18	18,23,25,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NA	B	507	1/1	0.96	0.10	20,20,20,20	0
6	NA	A	505	1/1	0.97	0.17	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.