



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 04:05 PM EDT

PDB ID : 6R1H
Title : Crystal structure of the LRR ectodomain of the receptor kinase SOBIR1 from Arabidopsis thaliana.
Authors : Hohmann, U.; Hothorn, M.
Deposited on : 2019-03-14
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

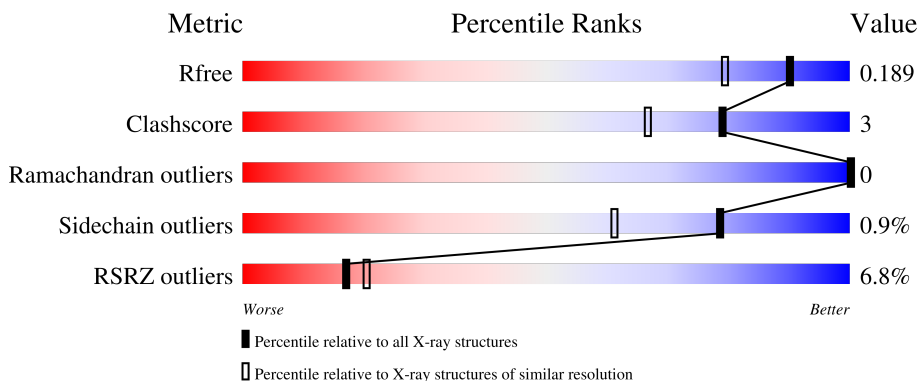
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	300	 5% 57% 39%
1	B	300	 3% 58% 40%
2	C	2	 100%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 6296 atoms, of which 3050 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 Leucine-rich repeat receptor-like serine/threonine/tyrosine-protein kinase SOBIR1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	184	2993	932	1512	271	274	4	0	9	0
1	B	181	2986	920	1518	272	272	4	0	9	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	LEU	-	expression tag	UNP Q9SKB2
A	272	GLU	-	expression tag	UNP Q9SKB2
A	273	LEU	-	expression tag	UNP Q9SKB2
A	274	GLU	-	expression tag	UNP Q9SKB2
A	275	ASN	-	expression tag	UNP Q9SKB2
A	276	LEU	-	expression tag	UNP Q9SKB2
A	277	TYR	-	expression tag	UNP Q9SKB2
A	278	PHE	-	expression tag	UNP Q9SKB2
A	279	GLN	-	expression tag	UNP Q9SKB2
A	280	GLY	-	expression tag	UNP Q9SKB2
A	281	ALA	-	expression tag	UNP Q9SKB2
A	282	TRP	-	expression tag	UNP Q9SKB2
A	283	SER	-	expression tag	UNP Q9SKB2
A	284	HIS	-	expression tag	UNP Q9SKB2
A	285	PRO	-	expression tag	UNP Q9SKB2
A	286	GLN	-	expression tag	UNP Q9SKB2
A	287	PHE	-	expression tag	UNP Q9SKB2
A	288	GLU	-	expression tag	UNP Q9SKB2
A	289	LYS	-	expression tag	UNP Q9SKB2
A	290	GLY	-	expression tag	UNP Q9SKB2
A	291	SER	-	expression tag	UNP Q9SKB2
A	292	HIS	-	expression tag	UNP Q9SKB2
A	293	HIS	-	expression tag	UNP Q9SKB2
A	294	HIS	-	expression tag	UNP Q9SKB2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	295	HIS	-	expression tag	UNP Q9SKB2
A	296	HIS	-	expression tag	UNP Q9SKB2
A	297	HIS	-	expression tag	UNP Q9SKB2
A	298	HIS	-	expression tag	UNP Q9SKB2
A	299	HIS	-	expression tag	UNP Q9SKB2
A	300	HIS	-	expression tag	UNP Q9SKB2
B	271	LEU	-	expression tag	UNP Q9SKB2
B	272	GLU	-	expression tag	UNP Q9SKB2
B	273	LEU	-	expression tag	UNP Q9SKB2
B	274	GLU	-	expression tag	UNP Q9SKB2
B	275	ASN	-	expression tag	UNP Q9SKB2
B	276	LEU	-	expression tag	UNP Q9SKB2
B	277	TYR	-	expression tag	UNP Q9SKB2
B	278	PHE	-	expression tag	UNP Q9SKB2
B	279	GLN	-	expression tag	UNP Q9SKB2
B	280	GLY	-	expression tag	UNP Q9SKB2
B	281	ALA	-	expression tag	UNP Q9SKB2
B	282	TRP	-	expression tag	UNP Q9SKB2
B	283	SER	-	expression tag	UNP Q9SKB2
B	284	HIS	-	expression tag	UNP Q9SKB2
B	285	PRO	-	expression tag	UNP Q9SKB2
B	286	GLN	-	expression tag	UNP Q9SKB2
B	287	PHE	-	expression tag	UNP Q9SKB2
B	288	GLU	-	expression tag	UNP Q9SKB2
B	289	LYS	-	expression tag	UNP Q9SKB2
B	290	GLY	-	expression tag	UNP Q9SKB2
B	291	SER	-	expression tag	UNP Q9SKB2
B	292	HIS	-	expression tag	UNP Q9SKB2
B	293	HIS	-	expression tag	UNP Q9SKB2
B	294	HIS	-	expression tag	UNP Q9SKB2
B	295	HIS	-	expression tag	UNP Q9SKB2
B	296	HIS	-	expression tag	UNP Q9SKB2
B	297	HIS	-	expression tag	UNP Q9SKB2
B	298	HIS	-	expression tag	UNP Q9SKB2
B	299	HIS	-	expression tag	UNP Q9SKB2
B	300	HIS	-	expression tag	UNP Q9SKB2

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

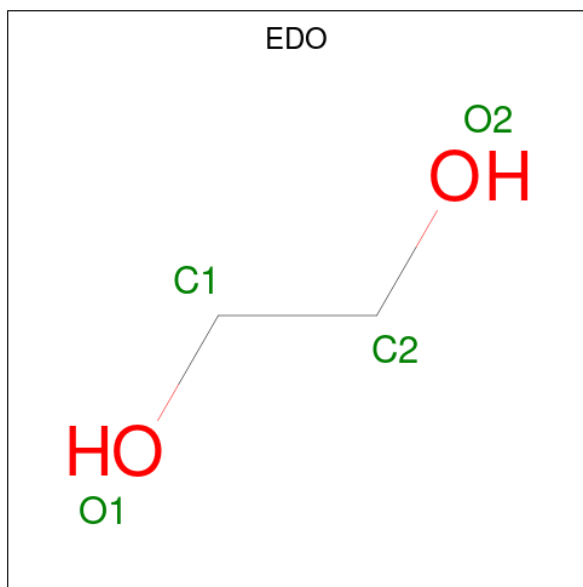


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	124	Total	O	0	0
			124	124		
6	B	130	Total	O	0	0
			130	130		

4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	82.25Å 82.25Å 109.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.50 – 1.55 43.50 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.50-1.55) 99.9 (43.50-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.55Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.172 , 0.188 0.172 , 0.189	Depositor DCC
R_{free} test set	3019 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtrriage
Anisotropy	0.453	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.051 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6296	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: EDO, GOL, NAG, CL

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	0.29	0/1542	0.51	0/2081
1	B	0.30	0/1518	0.50	0/2044
All	All	0.30	0/3060	0.50	0/4125

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1481	1512	1508	11	0
1	B	1468	1518	1508	7	0
2	C	28	0	25	0	0
3	A	1	0	0	1	0
4	B	8	12	12	0	0
5	B	6	8	8	0	0
6	A	124	0	0	2	0
6	B	130	0	0	3	0
All	All	3246	3050	3061	17	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 (17) 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:95:ARG:NH2	6:B:501:HOH:O	2.22	0.71
1:A:65:ASN:OD1	1:B:70:ARG:NH2	2.26	0.68
1:B:144:LYS:HD2	6:B:505:HOH:O	2.08	0.54
1:A:97:ARG:HD3	6:A:509:HOH:O	2.08	0.53
1:A:64:VAL:HG13	1:A:65:ASN:H	1.74	0.53
1:B:143[A]:ARG:NE	6:B:505:HOH:O	2.47	0.47
1:A:64:VAL:HG13	1:A:65:ASN:N	2.31	0.46
1:A:73:PHE:HB3	1:A:91:ARG:HB2	1.99	0.43
1:A:97:ARG:HH11	1:A:97:ARG:HG3	1.83	0.42
1:A:42:LEU:O	1:A:46:GLN:HG2	2.20	0.42
1:A:112:GLU:OE1	1:A:136[A]:GLN:NE2	2.48	0.42
1:A:186[B]:ASN:ND2	6:A:502:HOH:O	2.34	0.42
1:A:106:VAL:O	1:A:106:VAL:HG12	2.19	0.41
1:A:93:VAL:HG12	3:A:403:CL:CL	2.58	0.41
1:B:154:ASN:OD1	1:B:154:ASN:N	2.52	0.41
1:B:42:LEU:HD13	1:B:66:PRO:HG2	2.02	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	189/300 (63%)	180 (95%)	9 (5%)	0	100	100
1	B	186/300 (62%)	178 (96%)	8 (4%)	0	100	100
All	All	375/600 (62%)	358 (96%)	17 (4%)	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	175/270 (65%)	173 (99%)	2 (1%)	73	53
1	B	172/270 (64%)	171 (99%)	1 (1%)	86	73
All	All	347/540 (64%)	344 (99%)	3 (1%)	78	61

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	155	PHE
1	B	154	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.34	0	17,19,21	0.45	0
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.46	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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

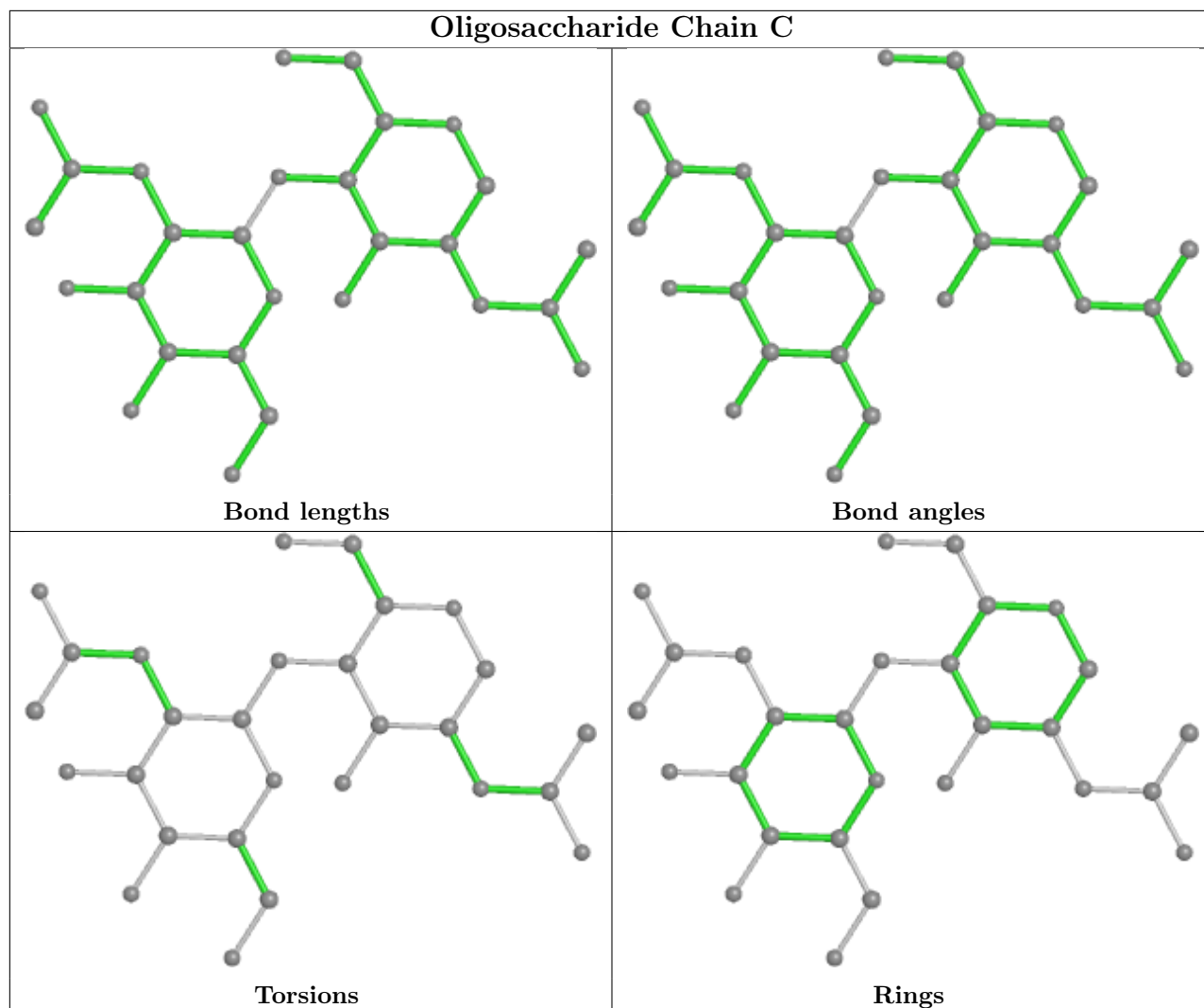
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
4	EDO	B	401	-	3,3,3	0.47	0	2,2,2	0.30	0
4	EDO	B	402	-	3,3,3	0.47	0	2,2,2	0.27	0
5	GOL	B	403	-	5,5,5	0.80	0	5,5,5	0.94	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
4	EDO	B	401	-	-	1/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
5	GOL	B	403	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	403	GOL	C1-C2-C3-O3
5	B	403	GOL	O2-C2-C3-O3
5	B	403	GOL	O1-C1-C2-C3
4	B	401	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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

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	184/300 (61%)	0.79	16 (8%) 10 11	22, 34, 90, 128	0
1	B	181/300 (60%)	0.55	9 (4%) 28 33	22, 35, 64, 95	0
All	All	365/600 (60%)	0.67	25 (6%) 17 20	22, 34, 73, 128	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	TRP	10.7
1	B	34	TRP	9.7
1	A	64	VAL	8.2
1	A	56	SER	6.3
1	A	55	ASN	5.6
1	A	224	PRO	5.3
1	A	223	ALA	4.9
1	A	82	THR	4.9
1	B	223	ALA	4.6
1	B	153	GLY	4.1
1	B	65	ASN	4.1
1	A	42	LEU	3.9
1	A	80	ALA	3.9
1	A	54	VAL	3.4
1	A	65	ASN	2.9
1	A	83	GLY	2.9
1	A	85	TYR	2.8
1	B	222	PRO	2.7
1	B	36	ASP	2.5
1	B	218	TYR	2.3
1	B	85	TYR	2.2
1	A	79	SER	2.2
1	A	203	VAL	2.2
1	A	152	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	35	LEU	2.1

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

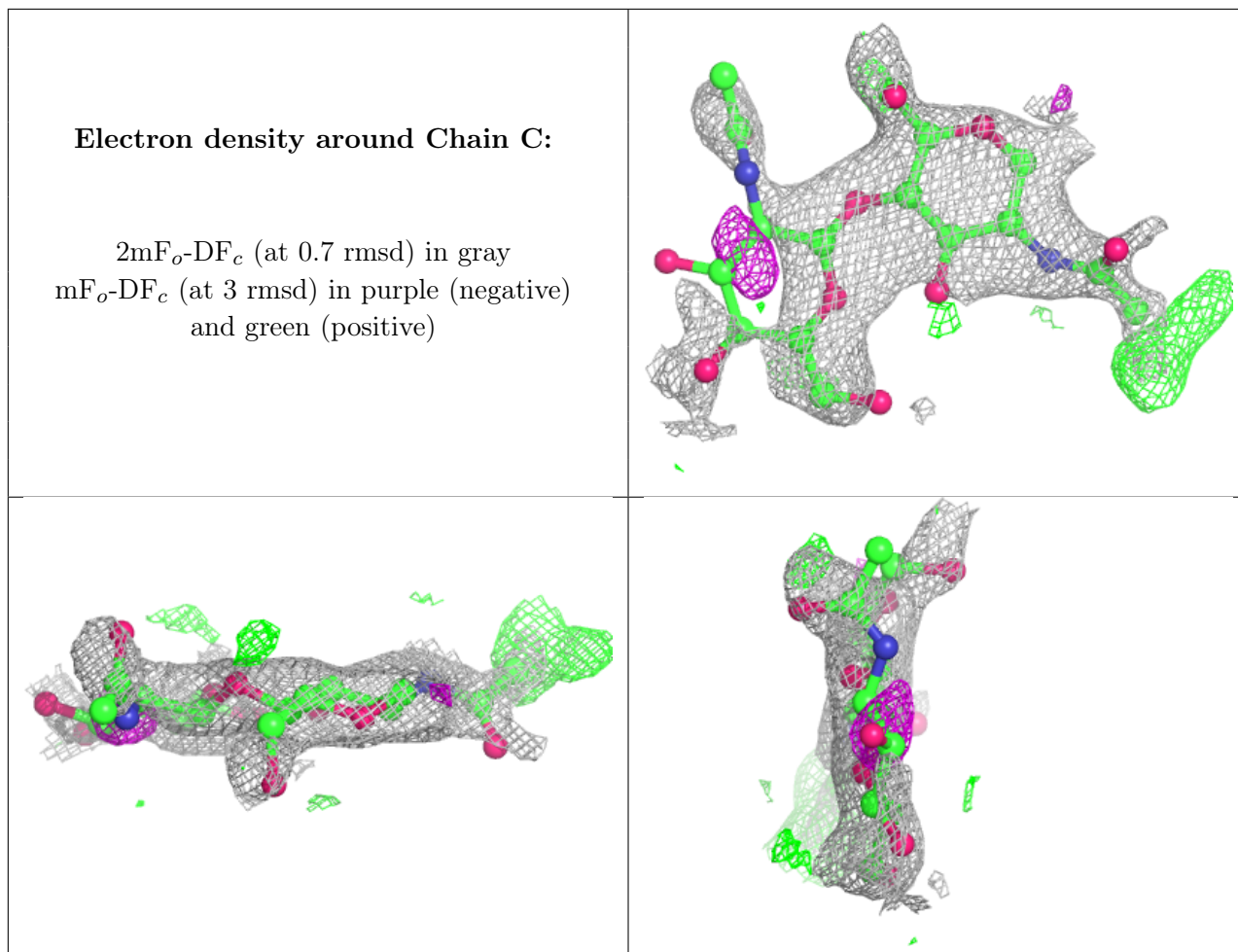
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NAG	C	2	14/15	0.58	0.31	88,93,97,98	0
2	NAG	C	1	14/15	0.75	0.21	67,77,81,86	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	401	4/4	0.60	0.33	63,75,82,83	0
5	GOL	B	403	6/6	0.68	0.29	62,74,88,89	0
4	EDO	B	402	4/4	0.73	0.28	77,93,94,94	0
3	CL	A	403	1/1	0.99	0.07	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.