



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:05 AM UTC

PDB ID : 4FWW / pdb_00004fww
Title : Crystal structure of the Sema-PSI extracellular domains of human RON receptor tyrosine kinase
Authors : Chao, K.L.; Herzberg, O.
Deposited on : 2012-07-02
Resolution : 1.85 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

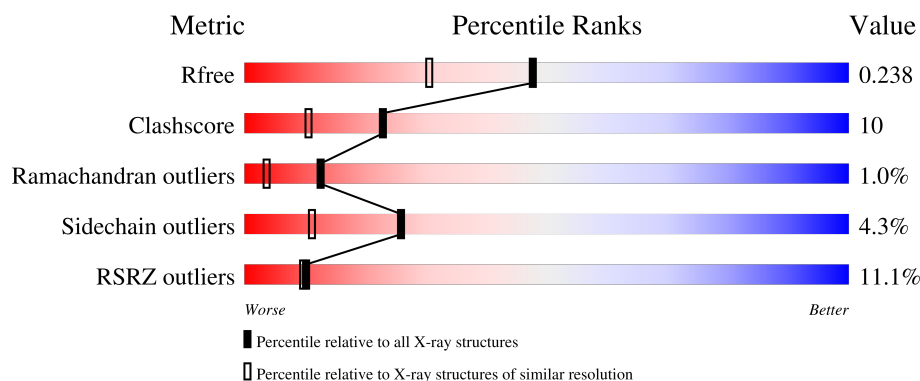
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	527	11% 80% 15% • •
2	B	4	25% 75%

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	ACT	A	607	-	-	X	-
4	ACT	A	611	-	-	X	-
6	EDO	A	616	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4330 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 Macrophage-stimulating protein receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	40	0	0
			3845	2430	672	716	27			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	LEU	ARG	conflict	UNP Q04912
A	307	VAL	ARG	conflict	UNP Q04912
A	308	PRO	ARG	conflict	UNP Q04912
A	311	SER	ALA	conflict	UNP Q04912
A	322	GLN	ARG	conflict	UNP Q04912

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



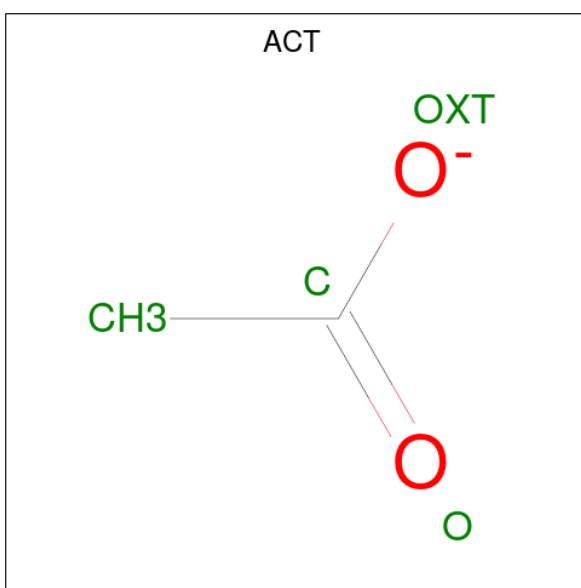
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



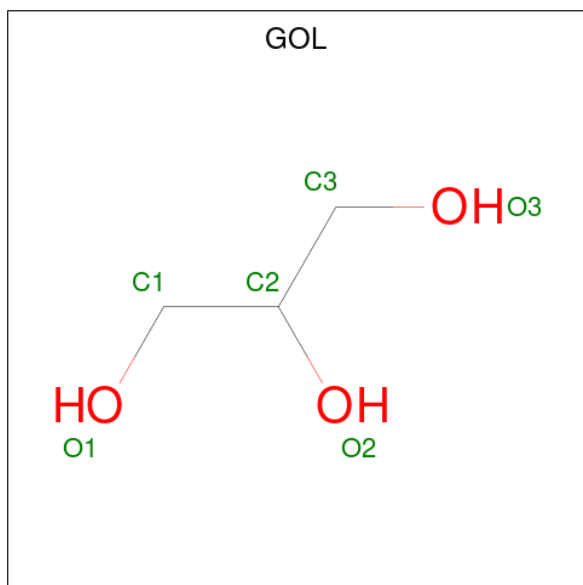
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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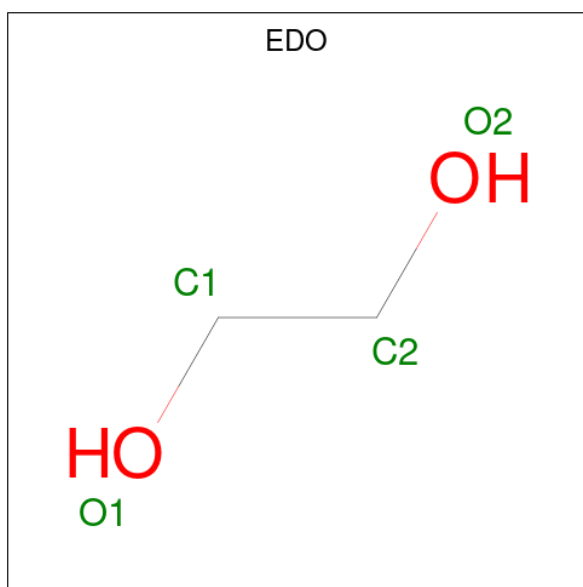
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



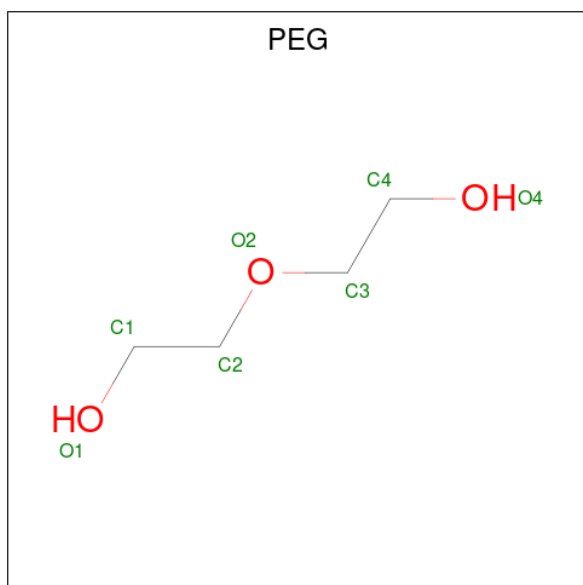
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

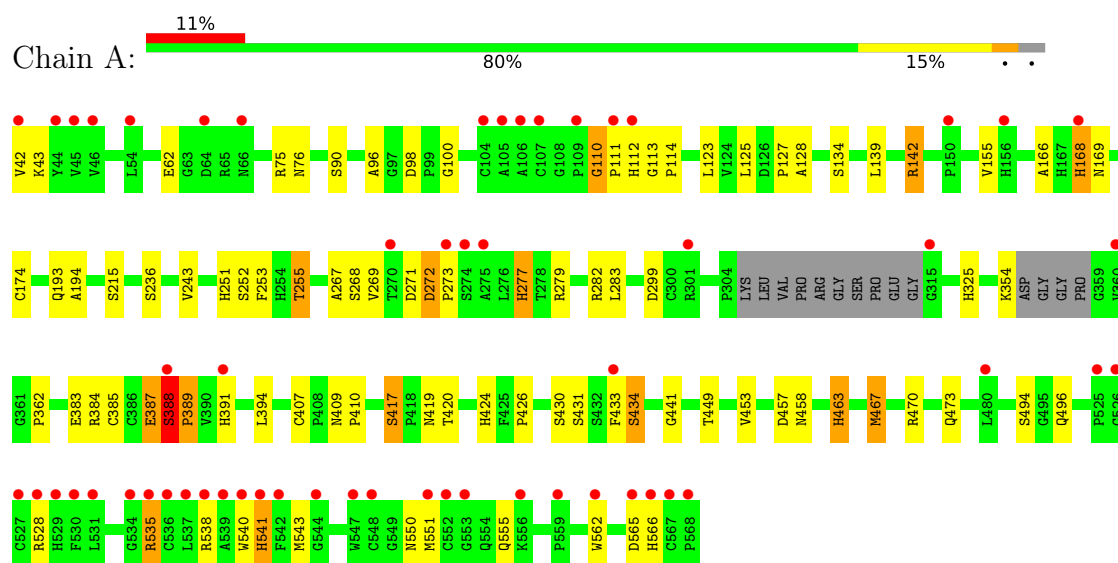
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	358	Total	O	0	0
			358	358		

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: Macrophage-stimulating protein receptor



- Molecule 2: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.40Å 73.30Å 87.90Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	19.32 – 1.85 19.32 – 1.85	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.32-1.85) 90.0 (19.32-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.191 , 0.232 0.208 , 0.238	Depositor DCC
R_{free} test set	2923 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4330	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% 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: ACT, BMA, NAG, PEG, GOL, SO4, EDO

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	1.01	4/3945 (0.1%)	0.99	10/5384 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	ARG	CB-CG	-17.14	1.01	1.52
1	A	538	ARG	CA-CB	-13.91	1.29	1.53
1	A	166	ALA	CA-CB	-7.15	1.42	1.53
1	A	463	HIS	CG-CD2	5.45	1.41	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	ARG	CB-CG-CD	11.77	138.37	111.30
1	A	538	ARG	CB-CA-C	9.02	129.17	110.31
1	A	535	ARG	CA-CB-CG	8.62	131.35	114.10
1	A	42	VAL	CA-CB-CG2	7.39	122.97	110.40
1	A	528	ARG	CG-CD-NE	-7.22	96.11	112.00
1	A	43	LYS	CB-CG-CD	6.39	125.99	111.30
1	A	391	HIS	CA-C-N	-6.10	114.33	120.31
1	A	391	HIS	C-N-CA	-6.10	114.33	120.31
1	A	538	ARG	CA-CB-CG	5.96	126.02	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	ARG	CB-CG-CD	5.27	123.42	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	GLU	Peptide
1	A	388	SER	Peptide

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	3845	0	3726	74	0
2	B	50	0	43	4	0
3	A	10	0	0	0	0
4	A	20	0	15	7	0
5	A	24	0	32	1	1
6	A	16	0	24	7	0
7	A	7	0	10	1	0
8	A	358	0	0	15	1
All	All	4330	0	3850	80	1

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 (80) 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:388:SER:HB3	1:A:389:PRO:CD	1.75	1.15
1:A:388:SER:HB3	1:A:389:PRO:HD2	1.21	1.12
1:A:139:LEU:HB3	1:A:142:ARG:HD3	1.32	1.11
6:A:616:EDO:H22	8:A:1178:HOH:O	1.74	0.88
1:A:388:SER:CB	1:A:389:PRO:CD	2.53	0.85
1:A:384:ARG:NH1	1:A:430:SER:OG	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:HIS:CE1	1:A:279:ARG:HE	1.93	0.85
1:A:127:PRO:HD2	8:A:1295:HOH:O	1.76	0.83
1:A:139:LEU:O	1:A:142:ARG:HD2	1.83	0.79
1:A:354:LYS:N	1:A:354:LYS:HD3	1.98	0.78
1:A:470:ARG:HH12	2:B:1:NAG:H61	1.47	0.78
1:A:277:HIS:HE1	1:A:279:ARG:HE	1.34	0.76
1:A:433:PHE:HD1	8:A:1245:HOH:O	1.68	0.76
1:A:123:LEU:H	4:A:611:ACT:H2	1.53	0.74
1:A:325:HIS:HD2	1:A:453:VAL:H	1.36	0.72
1:A:540:TRP:H	1:A:543:MET:HE3	1.55	0.72
4:A:607:ACT:CH3	8:A:1326:HOH:O	2.39	0.69
1:A:431:SER:HB2	8:A:1188:HOH:O	1.92	0.69
1:A:273:PRO:HB3	8:A:1297:HOH:O	1.92	0.68
1:A:325:HIS:CD2	1:A:453:VAL:H	2.11	0.66
1:A:215:SER:H	1:A:236:SER:HB3	1.60	0.66
1:A:215:SER:HB2	1:A:236:SER:HA	1.77	0.66
1:A:272:ASP:OD1	1:A:272:ASP:N	2.28	0.65
1:A:387:GLU:HG3	1:A:388:SER:HB2	1.76	0.65
1:A:362:PRO:HG3	1:A:441:GLY:HA2	1.78	0.65
1:A:388:SER:CB	1:A:389:PRO:HD2	2.13	0.63
1:A:112:HIS:HB3	8:A:1152:HOH:O	1.98	0.62
4:A:607:ACT:H1	8:A:1326:HOH:O	1.99	0.62
1:A:449:THR:HG21	1:A:467:MET:HE3	1.83	0.61
1:A:383:GLU:OE1	1:A:387:GLU:OE1	2.19	0.60
8:A:1298:HOH:O	2:B:1:NAG:H2	2.01	0.59
1:A:540:TRP:N	1:A:543:MET:HE3	2.20	0.57
1:A:252:SER:H	6:A:616:EDO:C1	2.18	0.56
1:A:388:SER:HA	8:A:1005:HOH:O	2.05	0.55
1:A:433:PHE:CD1	8:A:1245:HOH:O	2.50	0.55
1:A:426:PRO:HD3	7:A:620:PEG:H21	1.89	0.54
1:A:75:ARG:HG2	1:A:76:ASN:ND2	2.23	0.54
1:A:139:LEU:HB3	1:A:142:ARG:CD	2.23	0.53
1:A:252:SER:H	6:A:616:EDO:H12	1.73	0.53
1:A:251:HIS:HA	6:A:616:EDO:H12	1.91	0.52
1:A:139:LEU:O	1:A:142:ARG:CD	2.57	0.52
1:A:253:PHE:CD1	1:A:255:THR:HG22	2.45	0.52
4:A:611:ACT:H1	8:A:1124:HOH:O	2.09	0.51
1:A:194:ALA:HA	5:A:615:GOL:H31	1.92	0.51
1:A:299:ASP:OD2	1:A:434:SER:HB3	2.11	0.50
1:A:565:ASP:OD1	1:A:566:HIS:ND1	2.44	0.50
1:A:420:THR:HA	8:A:1019:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:SER:HB3	1:A:271:ASP:OD2	2.14	0.48
1:A:271:ASP:O	1:A:272:ASP:C	2.55	0.48
1:A:449:THR:CG2	1:A:467:MET:HE3	2.43	0.48
1:A:128:ALA:HB1	6:A:618:EDO:H21	1.96	0.47
1:A:269:VAL:HG23	8:A:1104:HOH:O	2.13	0.47
1:A:555:GLN:HA	1:A:562:TRP:CG	2.49	0.47
1:A:267:ALA:O	6:A:619:EDO:H22	2.16	0.46
1:A:385:CYS:O	1:A:407:CYS:HB3	2.15	0.46
1:A:354:LYS:HD3	1:A:354:LYS:H	1.76	0.46
1:A:169:ASN:OD1	1:A:174:CYS:SG	2.74	0.46
1:A:457:ASP:CG	1:A:458:ASN:H	2.18	0.46
1:A:470:ARG:NH1	2:B:1:NAG:H61	2.25	0.46
1:A:283:LEU:HD12	1:A:283:LEU:N	2.32	0.45
1:A:282:ARG:C	1:A:283:LEU:HD12	2.41	0.45
1:A:299:ASP:O	1:A:434:SER:HA	2.17	0.44
1:A:463:HIS:ND1	1:A:473:GLN:NE2	2.65	0.43
1:A:550:ASN:CG	1:A:550:ASN:O	2.61	0.43
1:A:215:SER:N	1:A:236:SER:HB3	2.31	0.42
1:A:252:SER:N	6:A:616:EDO:H12	2.34	0.42
1:A:494:SER:OG	1:A:496:GLN:HG3	2.19	0.42
2:B:3:BMA:H2	2:B:4:BMA:O2	2.20	0.42
1:A:98:ASP:OD1	1:A:100:GLY:N	2.38	0.42
1:A:409:ASN:HA	1:A:410:PRO:HD3	1.92	0.42
1:A:96:ALA:CB	1:A:139:LEU:HD13	2.49	0.41
1:A:113:GLY:HA2	1:A:114:PRO:C	2.44	0.41
1:A:424:HIS:HE1	4:A:607:ACT:H2	1.85	0.41
1:A:417:SER:OG	1:A:419:ASN:OD1	2.36	0.41
1:A:96:ALA:HB1	1:A:139:LEU:CD1	2.50	0.41
1:A:424:HIS:CE1	4:A:607:ACT:H2	2.55	0.41
1:A:134:SER:OG	4:A:610:ACT:H2	2.21	0.41
1:A:253:PHE:HD1	1:A:255:THR:HG22	1.85	0.40
1:A:541:HIS:HA	8:A:1230:HOH:O	2.21	0.40
1:A:110:GLY:HA3	1:A:111:PRO:HA	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:613:GOL:O1	8:A:1238:HOH:O[2_556]	2.00	0.20

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	507/527 (96%)	481 (95%)	21 (4%)	5 (1%)	12 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	388	SER
1	A	541	HIS
1	A	110	GLY
1	A	389	PRO

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	423/433 (98%)	405 (96%)	18 (4%)	26 11

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	90	SER
1	A	125	LEU
1	A	142	ARG
1	A	155	VAL
1	A	168	HIS

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Mol	Chain	Res	Type
1	A	193	GLN
1	A	243	VAL
1	A	255	THR
1	A	272	ASP
1	A	277	HIS
1	A	388	SER
1	A	394	LEU
1	A	417	SER
1	A	434	SER
1	A	467	MET
1	A	535	ARG
1	A	551	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	140	GLN
1	A	168	HIS
1	A	277	HIS
1	A	316	GLN
1	A	322	GLN
1	A	325	HIS
1	A	409	ASN
1	A	473	GLN
1	A	496	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](#)

4 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	B	1	2,1	14,14,15	0.86	1 (7%)	17,19,21	2.47	6 (35%)
2	NAG	B	2	2	14,14,15	0.48	0	17,19,21	1.77	2 (11%)
2	BMA	B	3	2	11,11,12	0.62	0	15,15,17	2.68	6 (40%)
2	BMA	B	4	2	11,11,12	0.91	0	15,15,17	1.80	3 (20%)

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	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	BMA	B	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	B	1	NAG	O5-C1	-2.39	1.39	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	5.86	120.04	112.19
2	B	3	BMA	O3-C3-C2	5.77	121.83	110.05
2	B	2	NAG	C2-N2-C7	5.69	130.53	122.90
2	B	1	NAG	O5-C1-C2	5.11	119.20	111.29
2	B	3	BMA	C1-C2-C3	-4.80	102.65	109.64
2	B	4	BMA	C1-O5-C5	-4.51	106.14	112.19
2	B	3	BMA	C3-C4-C5	4.11	117.69	110.23
2	B	3	BMA	C1-O5-C5	4.08	117.66	112.19
2	B	1	NAG	C6-C5-C4	-3.32	104.88	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	BMA	C2-C3-C4	2.47	115.20	110.86
2	B	1	NAG	C4-C3-C2	2.40	114.54	111.02
2	B	3	BMA	O5-C5-C4	2.39	116.63	110.83
2	B	1	NAG	O6-C6-C5	-2.27	103.61	111.33
2	B	2	NAG	O7-C7-C8	-2.26	118.04	122.05
2	B	4	BMA	C1-C2-C3	2.22	112.88	109.64
2	B	3	BMA	O2-C2-C3	2.05	114.39	110.15
2	B	1	NAG	C3-C4-C5	2.02	113.89	110.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

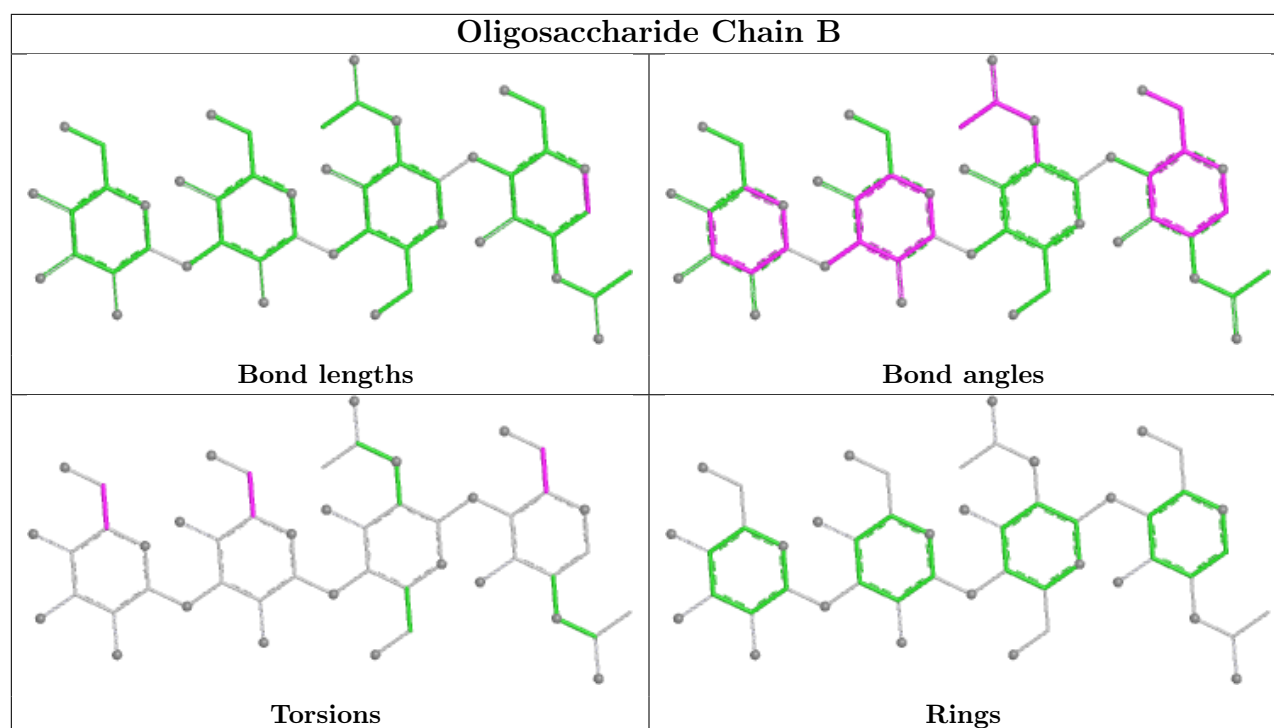
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	4	BMA	C4-C5-C6-O6
2	B	4	BMA	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	BMA	1	0
2	B	3	BMA	1	0
2	B	1	NAG	3	0

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](#)

16 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	$\# Z > 2$
4	ACT	A	609	-	3,3,3	0.72	0	3,3,3	1.09	0
4	ACT	A	611	-	3,3,3	0.72	0	3,3,3	1.00	0
7	PEG	A	620	-	6,6,6	0.54	0	5,5,5	0.37	0
4	ACT	A	608	-	3,3,3	0.75	0	3,3,3	1.01	0
6	EDO	A	617	-	3,3,3	0.47	0	2,2,2	0.41	0
3	SO4	A	606	-	4,4,4	0.36	0	6,6,6	0.55	0
5	GOL	A	613	-	5,5,5	0.59	0	5,5,5	0.44	0
5	GOL	A	614	-	5,5,5	0.28	0	5,5,5	1.08	1 (20%)
6	EDO	A	616	-	3,3,3	0.61	0	2,2,2	0.07	0
5	GOL	A	615	-	5,5,5	0.29	0	5,5,5	0.38	0
4	ACT	A	607	-	3,3,3	0.78	0	3,3,3	0.83	0
4	ACT	A	610	-	3,3,3	0.93	0	3,3,3	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	618	-	3,3,3	0.50	0	2,2,2	0.28	0
6	EDO	A	619	-	3,3,3	0.56	0	2,2,2	0.41	0
5	GOL	A	612	-	5,5,5	0.39	0	5,5,5	0.36	0
3	SO4	A	605	-	4,4,4	0.38	0	6,6,6	0.57	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
7	PEG	A	620	-	-	3/4/4/4	-
6	EDO	A	617	-	-	1/1/1/1	-
5	GOL	A	614	-	-	2/4/4/4	-
5	GOL	A	613	-	-	1/4/4/4	-
6	EDO	A	616	-	-	1/1/1/1	-
5	GOL	A	615	-	-	0/4/4/4	-
6	EDO	A	618	-	-	0/1/1/1	-
6	EDO	A	619	-	-	1/1/1/1	-
5	GOL	A	612	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	614	GOL	O3-C3-C2	-2.20	100.45	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	614	GOL	C1-C2-C3-O3
5	A	614	GOL	O2-C2-C3-O3
7	A	620	PEG	O1-C1-C2-O2
7	A	620	PEG	O2-C3-C4-O4
5	A	612	GOL	O1-C1-C2-C3
5	A	613	GOL	O1-C1-C2-C3
6	A	616	EDO	O1-C1-C2-O2
6	A	617	EDO	O1-C1-C2-O2
6	A	619	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	612	GOL	C1-C2-C3-O3
7	A	620	PEG	C4-C3-O2-C2

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	611	ACT	2	0
7	A	620	PEG	1	0
5	A	613	GOL	0	1
6	A	616	EDO	5	0
5	A	615	GOL	1	0
4	A	607	ACT	4	0
4	A	610	ACT	1	0
6	A	618	EDO	1	0
6	A	619	EDO	1	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 ⓘ

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	513/527 (97%)	0.62	57 (11%)	10 10	20, 48, 95, 126	9 (1%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	531	LEU	4.4
1	A	42	VAL	4.1
1	A	391	HIS	3.9
1	A	530	PHE	3.7
1	A	537	LEU	3.6
1	A	540	TRP	3.6
1	A	539	ALA	3.5
1	A	547	TRP	3.5
1	A	526	GLY	3.3
1	A	274	SER	3.3
1	A	275	ALA	3.3
1	A	541	HIS	3.2
1	A	556	LYS	3.2
1	A	44	TYR	3.1
1	A	168	HIS	3.1
1	A	565	ASP	3.0
1	A	552	CYS	3.0
1	A	480	LEU	2.9
1	A	46	VAL	2.9
1	A	542	PHE	2.9
1	A	388	SER	2.7
1	A	270	THR	2.7
1	A	105	ALA	2.7
1	A	553	GLY	2.7
1	A	528	ARG	2.7
1	A	562	TRP	2.7
1	A	544	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	107	CYS	2.7
1	A	54	LEU	2.6
1	A	551	MET	2.6
1	A	360	VAL	2.6
1	A	568	PRO	2.6
1	A	109	PRO	2.5
1	A	66	ASN	2.5
1	A	538	ARG	2.5
1	A	566	HIS	2.5
1	A	534	GLY	2.4
1	A	150	PRO	2.4
1	A	567	CYS	2.4
1	A	45	VAL	2.4
1	A	525	PRO	2.3
1	A	433	PHE	2.3
1	A	106	ALA	2.3
1	A	535	ARG	2.3
1	A	104	CYS	2.2
1	A	64	ASP	2.2
1	A	559	PRO	2.2
1	A	315	GLY	2.2
1	A	111	PRO	2.2
1	A	536	CYS	2.1
1	A	301	ARG	2.1
1	A	112	HIS	2.1
1	A	529	HIS	2.1
1	A	548	CYS	2.1
1	A	156	HIS	2.1
1	A	273	PRO	2.1
1	A	527	CYS	2.0

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

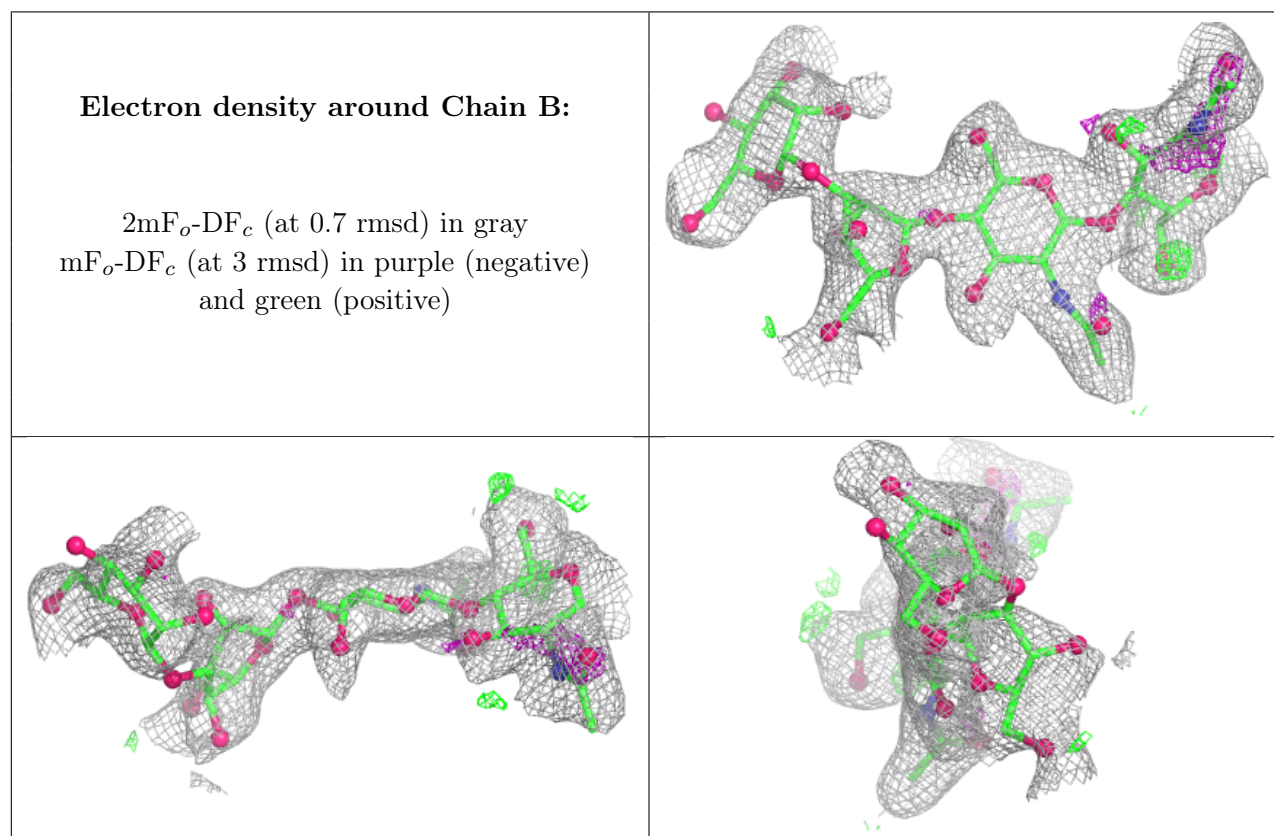
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	BMA	B	3	11/12	0.66	0.15	59,73,79,82	0
2	BMA	B	4	11/12	0.75	0.12	60,69,79,82	0
2	NAG	B	1	14/15	0.92	0.10	29,40,57,60	0
2	NAG	B	2	14/15	0.93	0.08	35,41,54,55	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 ⓘ

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	ACT	A	609	4/4	0.71	0.16	47,57,60,60	0
6	EDO	A	618	4/4	0.87	0.11	57,58,59,62	0
6	EDO	A	619	4/4	0.87	0.14	48,49,53,55	0
5	GOL	A	613	6/6	0.89	0.14	36,43,45,45	0
7	PEG	A	620	7/7	0.89	0.11	36,41,48,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	612	6/6	0.90	0.10	37,46,51,58	0
5	GOL	A	614	6/6	0.91	0.11	39,41,44,49	0
4	ACT	A	611	4/4	0.91	0.11	44,55,59,61	0
4	ACT	A	608	4/4	0.91	0.14	42,56,59,61	0
4	ACT	A	610	4/4	0.91	0.15	33,43,48,49	0
5	GOL	A	615	6/6	0.92	0.11	33,45,54,60	0
6	EDO	A	616	4/4	0.92	0.12	34,40,42,45	0
6	EDO	A	617	4/4	0.92	0.15	27,39,44,54	0
3	SO4	A	606	5/5	0.99	0.08	32,33,37,39	0
4	ACT	A	607	4/4	0.99	0.05	23,23,23,25	4
3	SO4	A	605	5/5	0.99	0.09	24,26,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.