



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:18 AM UTC

PDB ID : 7PKI / pdb_00007pki
Title : Crystal structure of human ACE2 bound to the spike receptor-binding domain from a cave bat sarbecovirus closely related to SARS-CoV-2.
Authors : Baquero, E.; Rey, F.A.
Deposited on : 2021-08-25
Resolution : 2.94 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

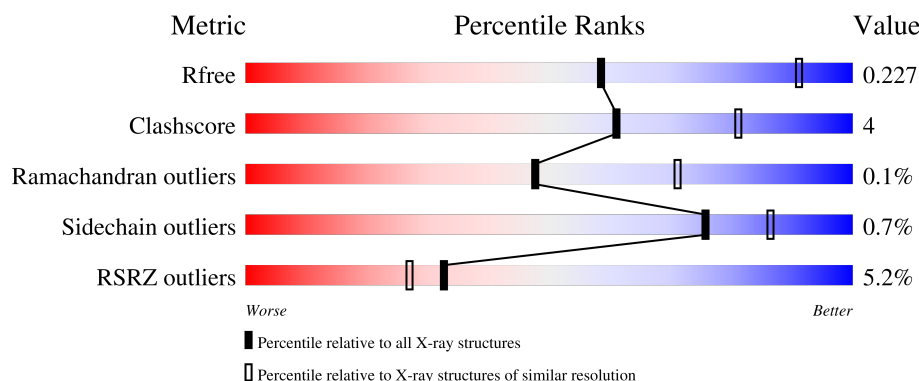
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

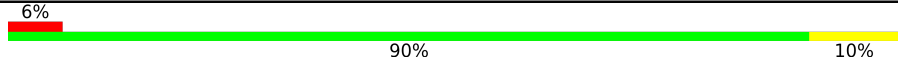
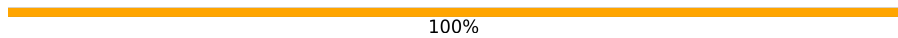
The reported resolution of this entry is 2.94 Å.

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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	596	
2	E	197	
3	B	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PEG	A	710	-	X	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6610 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			

- Molecule 2 is a protein called BANAL 236 coronavirus spike receptor-binding domain.

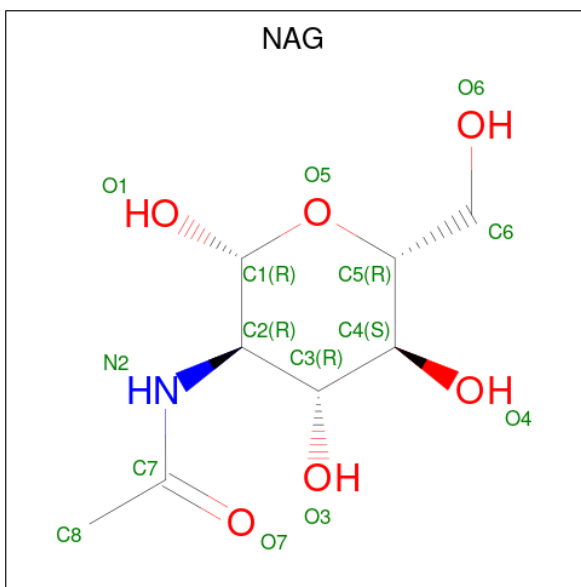
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	197	Total	C	N	O	S	0	0	0
			1556	999	257	292	8			

- Molecule 3 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
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



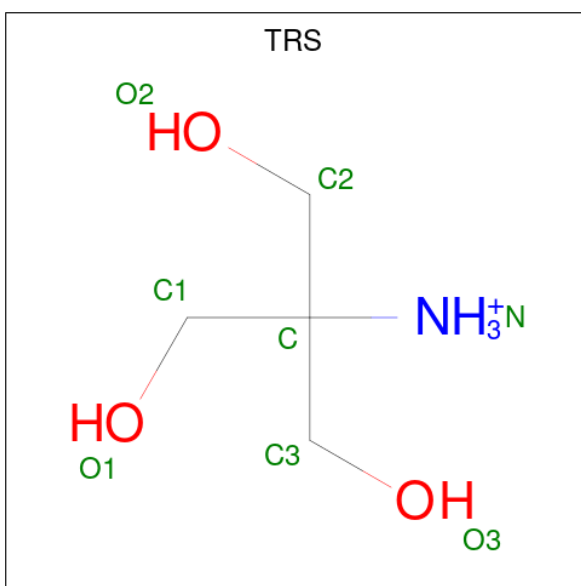
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



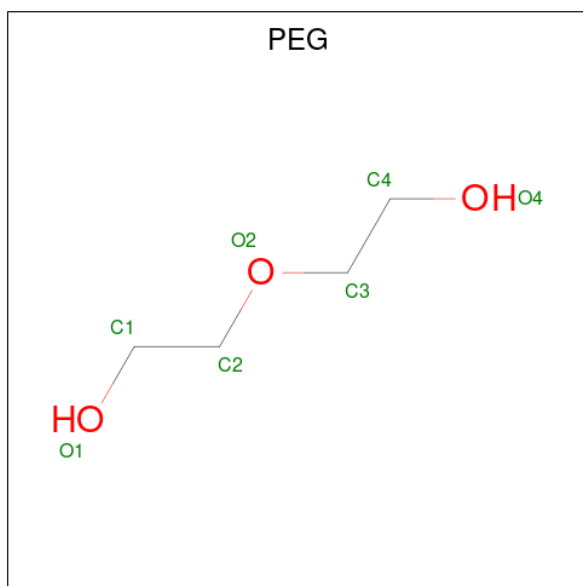
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		

- 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		
7	A	1	Total	C	O	0	0
			7	4	3		
7	E	1	Total	C	O	0	0
			7	4	3		
7	E	1	Total	C	O	0	0
			7	4	3		
7	E	1	Total	C	O	0	0
			7	4	3		

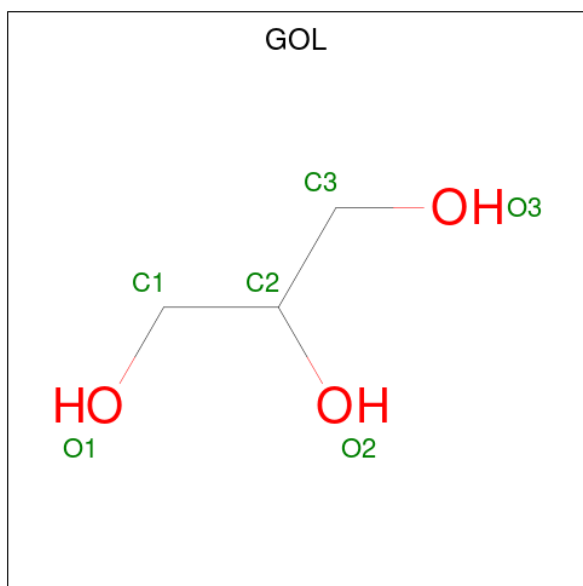
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	2	Total	Cl	0	0
			2	2		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	O	0	0
			6	3	3		

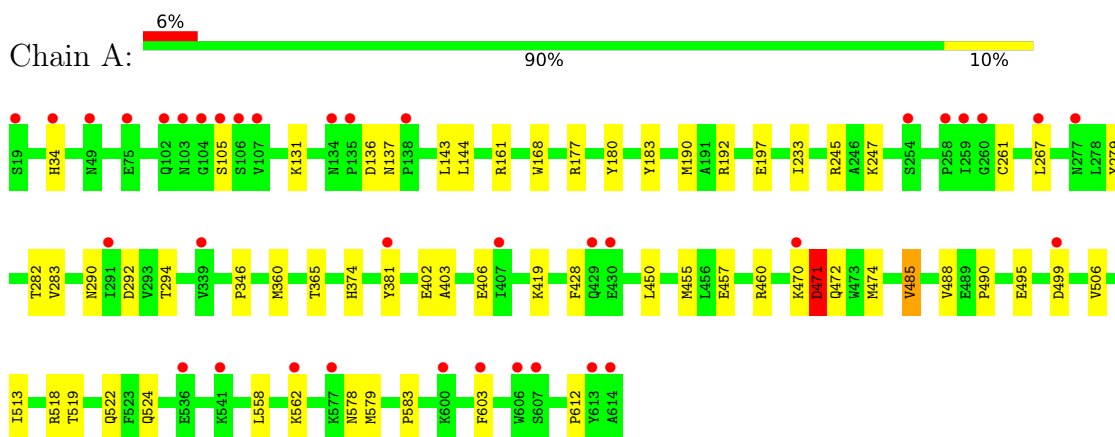
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	5	Total	O	0	0
			5	5		
11	E	3	Total	O	0	0
			3	3		

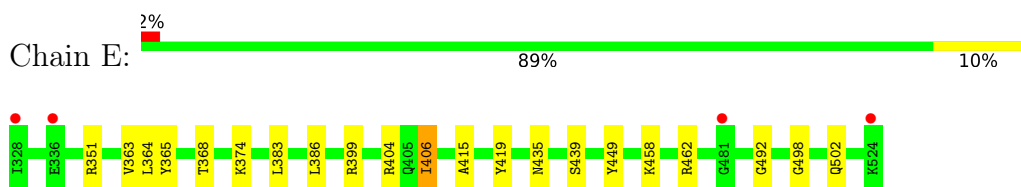
3 Residue-property plots [i](#)

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.

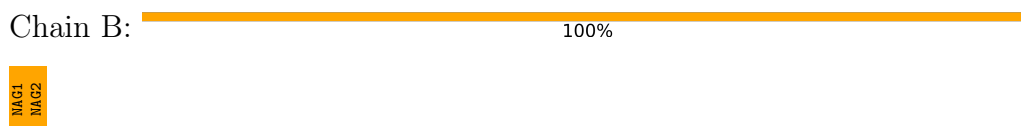
- Molecule 1: Processed angiotensin-converting enzyme 2



- Molecule 2: BANAL 236 coronavirus spike receptor-binding domain



- Molecule 3: 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	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	341.54Å 341.54Å 68.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.30 – 2.94 49.30 – 2.94	Depositor EDS
% Data completeness (in resolution range)	87.0 (49.30-2.94) 86.9 (49.30-2.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.214 , 0.227 0.215 , 0.227	Depositor DCC
R_{free} test set	2170 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6610	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL, CL, NAG, SO4, TRS, PEG

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	0.14	0/4999	0.32	2/6792 (0.0%)
2	E	0.24	0/1600	0.34	0/2179
All	All	0.17	0/6599	0.33	2/8971 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	ASP	CA-C-N	-6.93	110.64	122.56
1	A	471	ASP	C-N-CA	-6.93	110.64	122.56

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	4862	0	4634	38	0
2	E	1556	0	1479	15	0
3	B	28	0	25	2	0
4	A	56	0	52	0	0
4	E	28	0	26	3	0
5	A	15	0	0	0	0
5	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	0	12	0	0
7	A	14	0	20	0	0
7	E	21	0	30	2	0
8	A	1	0	0	0	0
9	E	2	0	0	1	0
10	E	6	0	8	2	0
11	A	5	0	0	0	0
11	E	3	0	0	1	0
All	All	6610	0	6286	54	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 4.

All (54) 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)
2:E:374:LYS:NZ	9:E:1705:CL:CL	2.58	0.72
2:E:492:GLY:H	7:E:1706:PEG:H42	1.58	0.68
1:A:470:LYS:HD3	1:A:470:LYS:N	2.10	0.66
3:B:1:NAG:H61	3:B:2:NAG:HN2	1.59	0.66
2:E:368:THR:HG22	4:E:1702:NAG:H62	1.79	0.65
1:A:406:GLU:HG3	1:A:518:ARG:HH21	1.61	0.64
1:A:161:ARG:NH2	1:A:267:LEU:O	2.32	0.63
3:B:2:NAG:O7	3:B:2:NAG:O3	2.18	0.62
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.85	0.59
1:A:34:HIS:ND1	2:E:449:TYR:OH	2.39	0.56
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.88	0.55
1:A:470:LYS:HD3	1:A:470:LYS:H	1.71	0.54
1:A:419:LYS:HD2	1:A:428:PHE:HB3	1.91	0.53
1:A:455:MET:HE2	1:A:485:VAL:HG21	1.90	0.53
1:A:192:ARG:NH2	1:A:197:GLU:O	2.42	0.53
1:A:261:CYS:HB2	1:A:488:VAL:HB	1.92	0.52
1:A:578:ASN:OD1	1:A:579:MET:N	2.41	0.52
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.91	0.51
2:E:435:ASN:O	2:E:439:SER:OG	2.26	0.51
1:A:136:ASP:OD1	1:A:137:ASN:N	2.43	0.51
1:A:245:ARG:NH1	1:A:603:PHE:O	2.45	0.50
2:E:383:LEU:HA	2:E:386:LEU:HB2	1.94	0.50
1:A:474:MET:HE1	1:A:499:ASP:HB2	1.95	0.48
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.96	0.47
1:A:177:ARG:NH1	1:A:470:LYS:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.95	0.47
1:A:403:ALA:HA	1:A:518:ARG:HG3	1.97	0.47
1:A:374:HIS:NE2	1:A:402:GLU:OE2	2.48	0.47
1:A:279:TYR:O	1:A:283:VAL:HG23	2.15	0.46
1:A:290:ASN:HD21	1:A:292:ASP:HB3	1.81	0.46
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.99	0.45
2:E:462:ARG:NH1	10:E:1709:GOL:O2	2.47	0.45
1:A:460:ARG:NH2	1:A:506:VAL:HA	2.32	0.45
1:A:471:ASP:O	1:A:495:GLU:CD	2.60	0.45
1:A:455:MET:HE3	1:A:455:MET:HB3	1.80	0.45
1:A:177:ARG:NH2	1:A:495:GLU:O	2.50	0.45
2:E:399:ARG:HD2	7:E:1706:PEG:H32	1.99	0.45
1:A:346:PRO:HB3	1:A:360:MET:HE2	1.98	0.44
1:A:381:TYR:HE1	1:A:558:LEU:HA	1.81	0.44
2:E:498:GLY:O	2:E:502:GLN:HG3	2.17	0.44
2:E:415:ALA:HA	2:E:419:TYR:O	2.18	0.44
2:E:404:ARG:NH2	11:E:1801:HOH:O	2.51	0.44
1:A:381:TYR:CD1	1:A:558:LEU:HD22	2.52	0.43
1:A:105:SER:HB2	1:A:190:MET:HE3	2.01	0.43
1:A:519:THR:O	1:A:522:GLN:HG2	2.19	0.43
1:A:247:LYS:HB2	1:A:282:THR:HG22	2.01	0.42
2:E:364:LEU:O	4:E:1701:NAG:N2	2.48	0.42
2:E:363:VAL:O	4:E:1701:NAG:O3	2.30	0.42
1:A:294:THR:HG23	1:A:365:THR:HA	2.00	0.41
1:A:144:LEU:HB2	1:A:168:TRP:CH2	2.54	0.41
1:A:562:LYS:HB2	1:A:562:LYS:HE3	1.76	0.41
2:E:351:ARG:HD2	10:E:1709:GOL:H2	2.03	0.41
2:E:406:ILE:HG22	2:E:406:ILE:O	2.21	0.40
1:A:105:SER:CB	1:A:190:MET:HE3	2.52	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	594/596 (100%)	584 (98%)	10 (2%)	0	100	100
2	E	195/197 (99%)	191 (98%)	3 (2%)	1 (0%)	24	49
All	All	789/793 (100%)	775 (98%)	13 (2%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	406	ILE

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	526/526 (100%)	523 (99%)	3 (1%)	78	89
2	E	171/171 (100%)	169 (99%)	2 (1%)	63	78
All	All	697/697 (100%)	692 (99%)	5 (1%)	76	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	ASP
1	A	472	GLN
1	A	485	VAL
2	E	365	TYR
2	E	458	LYS

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	64	ASN
1	A	96	GLN
1	A	154	ASN
1	A	345	HIS
1	A	380	GLN

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Mol	Chain	Res	Type
1	A	552	GLN
2	E	446	ASN
2	E	477	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 ⓘ

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
3	NAG	B	1	3,1	14,14,15	0.90	1 (7%)	17,19,21	2.18	4 (23%)
3	NAG	B	2	3	14,14,15	0.81	1 (7%)	17,19,21	1.38	4 (23%)

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	NAG	B	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	B	2	3	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	NAG	O5-C1	3.16	1.49	1.43
3	B	2	NAG	O5-C1	2.59	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C1-O5-C5	6.06	120.31	112.19
3	B	1	NAG	C1-C2-N2	3.52	115.98	110.43
3	B	1	NAG	C4-C3-C2	-3.37	106.08	111.02
3	B	2	NAG	C1-O5-C5	2.91	116.09	112.19
3	B	1	NAG	C2-N2-C7	2.90	126.78	122.90
3	B	2	NAG	C1-C2-N2	2.37	114.17	110.43
3	B	2	NAG	C4-C3-C2	-2.30	107.65	111.02
3	B	2	NAG	O3-C3-C2	2.15	113.88	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

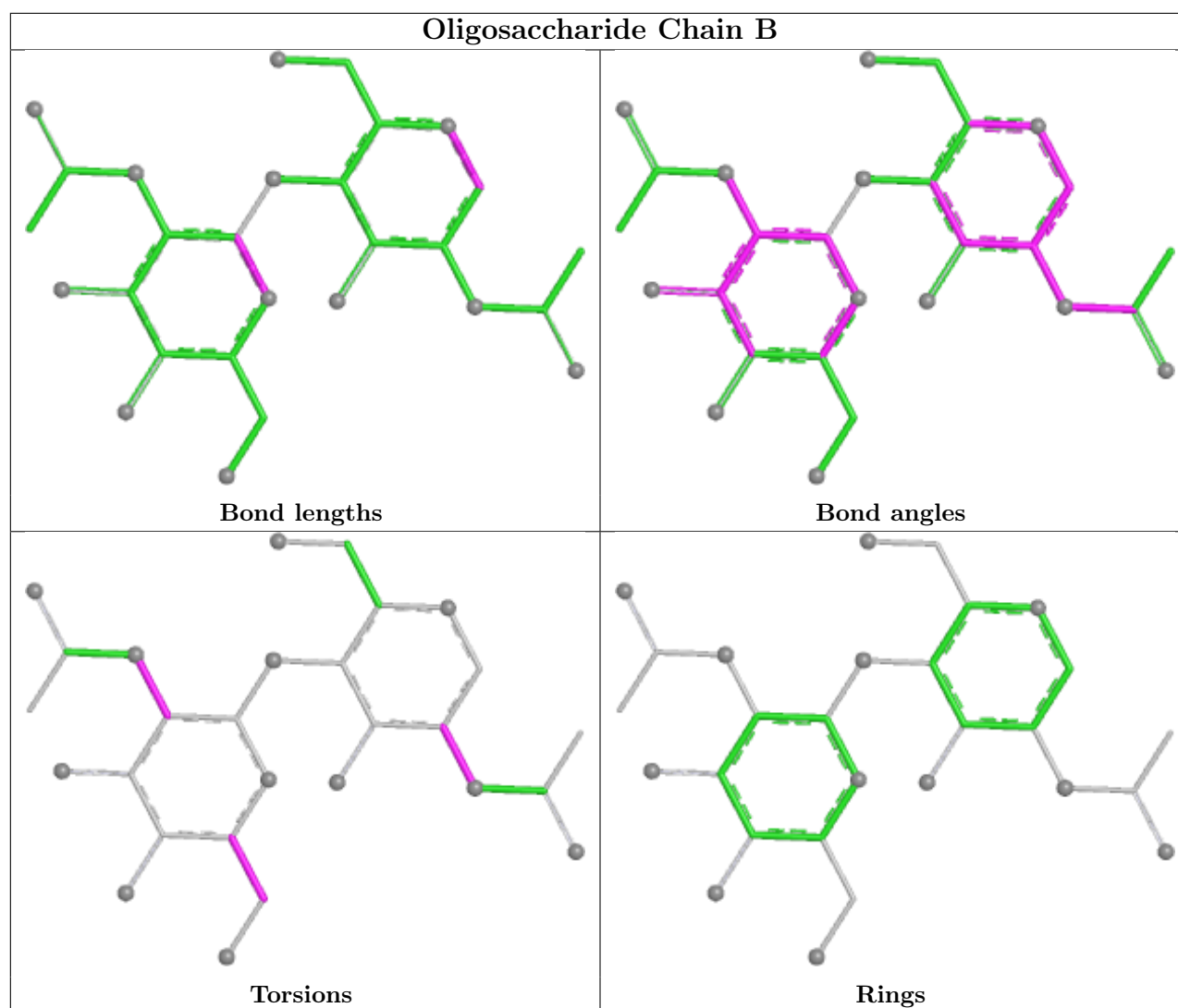
Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C1-C2-N2-C7
3	B	2	NAG	O5-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	B	2	NAG	C1-C2-N2-C7
3	B	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	NAG	1	0
3	B	2	NAG	2	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](#)

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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	NAG	E	1702	2	14,14,15	0.70	1 (7%)	17,19,21	2.17	6 (35%)
7	PEG	A	709	-	6,6,6	0.50	0	5,5,5	0.26	0
5	SO4	E	1703	-	4,4,4	0.23	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PEG	A	710	-	6,6,6	2.16	3 (50%)	5,5,5	5.35	5 (100%)
7	PEG	E	1708	-	6,6,6	0.50	0	5,5,5	0.26	0
4	NAG	A	704	1	14,14,15	0.33	0	17,19,21	0.39	0
4	NAG	E	1701	2	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	A	701	1	14,14,15	0.25	0	17,19,21	0.47	0
6	TRS	A	708	-	7,7,7	0.33	0	9,9,9	0.33	0
7	PEG	E	1707	-	6,6,6	0.50	0	5,5,5	0.24	0
5	SO4	A	707	-	4,4,4	0.24	0	6,6,6	0.08	0
4	NAG	A	702	1	14,14,15	0.29	0	17,19,21	0.39	0
7	PEG	E	1706	-	6,6,6	0.50	0	5,5,5	0.20	0
4	NAG	A	703	1	14,14,15	0.32	0	17,19,21	0.45	0
5	SO4	A	706	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	A	705	-	4,4,4	0.23	0	6,6,6	0.12	0
10	GOL	E	1709	-	5,5,5	0.42	0	5,5,5	0.25	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	NAG	E	1702	2	-	0/6/23/26	0/1/1/1
7	PEG	E	1708	-	-	1/4/4/4	-
7	PEG	A	710	-	-	4/4/4/4	-
4	NAG	A	704	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1701	2	-	2/6/23/26	0/1/1/1
4	NAG	A	701	1	-	0/6/23/26	0/1/1/1
6	TRS	A	708	-	-	0/9/9/9	-
7	PEG	E	1707	-	-	2/4/4/4	-
4	NAG	A	702	1	-	1/6/23/26	0/1/1/1
7	PEG	E	1706	-	-	3/4/4/4	-
4	NAG	A	703	1	-	2/6/23/26	0/1/1/1
7	PEG	A	709	-	-	0/4/4/4	-
10	GOL	E	1709	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	710	PEG	O1-C1	3.56	1.60	1.42
7	A	710	PEG	O2-C3	2.91	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	710	PEG	O4-C4	2.17	1.53	1.42
4	E	1702	NAG	C8-C7	2.00	1.54	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	710	PEG	O2-C3-C4	7.38	142.63	110.11
7	A	710	PEG	O2-C2-C1	7.28	142.17	110.11
4	E	1702	NAG	C1-O5-C5	6.53	120.94	112.19
7	A	710	PEG	O1-C1-C2	3.85	134.49	111.82
7	A	710	PEG	C3-O2-C2	3.60	129.02	113.26
7	A	710	PEG	O4-C4-C3	2.85	128.61	111.82
4	E	1702	NAG	C1-C2-N2	2.42	114.24	110.43
4	E	1702	NAG	C3-C4-C5	2.32	114.44	110.23
4	E	1702	NAG	O5-C5-C6	-2.16	103.46	107.66
4	E	1702	NAG	C2-N2-C7	2.03	125.62	122.90
4	E	1702	NAG	O5-C5-C4	2.02	115.74	110.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	E	1709	GOL	O1-C1-C2-C3
4	A	703	NAG	O5-C5-C6-O6
4	A	704	NAG	O5-C5-C6-O6
4	A	703	NAG	C4-C5-C6-O6
4	E	1701	NAG	O5-C5-C6-O6
4	A	704	NAG	C4-C5-C6-O6
7	A	710	PEG	O2-C3-C4-O4
7	E	1706	PEG	O2-C3-C4-O4
7	E	1707	PEG	O1-C1-C2-O2
10	E	1709	GOL	O1-C1-C2-O2
4	E	1701	NAG	C4-C5-C6-O6
7	E	1706	PEG	C1-C2-O2-C3
7	E	1708	PEG	C1-C2-O2-C3
7	E	1707	PEG	C1-C2-O2-C3
7	A	710	PEG	C4-C3-O2-C2
7	E	1706	PEG	C4-C3-O2-C2
7	A	710	PEG	O1-C1-C2-O2
7	A	710	PEG	C1-C2-O2-C3
4	A	702	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1702	NAG	1	0
4	E	1701	NAG	2	0
7	E	1706	PEG	2	0
10	E	1709	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	596/596 (100%)	0.47	37 (6%) 26 22	41, 66, 92, 156	0
2	E	197/197 (100%)	0.06	4 (2%) 65 56	34, 50, 76, 110	0
All	All	793/793 (100%)	0.37	41 (5%) 33 27	34, 62, 90, 156	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	328	ILE	6.6
2	E	481	GLY	5.6
1	A	105	SER	5.1
1	A	339	VAL	4.9
1	A	614	ALA	4.8
1	A	102	GLN	4.6
1	A	138	PRO	3.9
1	A	103	ASN	3.7
1	A	430	GLU	3.7
1	A	135	PRO	3.6
1	A	104	GLY	3.2
1	A	381	TYR	3.1
1	A	260	GLY	3.1
1	A	106	SER	2.9
1	A	107	VAL	2.9
1	A	34	HIS	2.8
1	A	49	ASN	2.6
1	A	536	GLU	2.4
2	E	336	GLU	2.4
1	A	499	ASP	2.4
1	A	291	ILE	2.4
1	A	134	ASN	2.3
1	A	603	PHE	2.3
1	A	259	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	607	SER	2.3
1	A	577	LYS	2.3
1	A	254	SER	2.3
1	A	429	GLN	2.2
1	A	541	LYS	2.2
1	A	470	LYS	2.2
1	A	19	SER	2.2
1	A	407	ILE	2.1
1	A	75	GLU	2.1
1	A	277	ASN	2.1
1	A	600	LYS	2.1
1	A	267	LEU	2.1
1	A	613	TYR	2.1
1	A	606	TRP	2.0
1	A	562	LYS	2.0
1	A	258	PRO	2.0
2	E	524	LYS	2.0

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

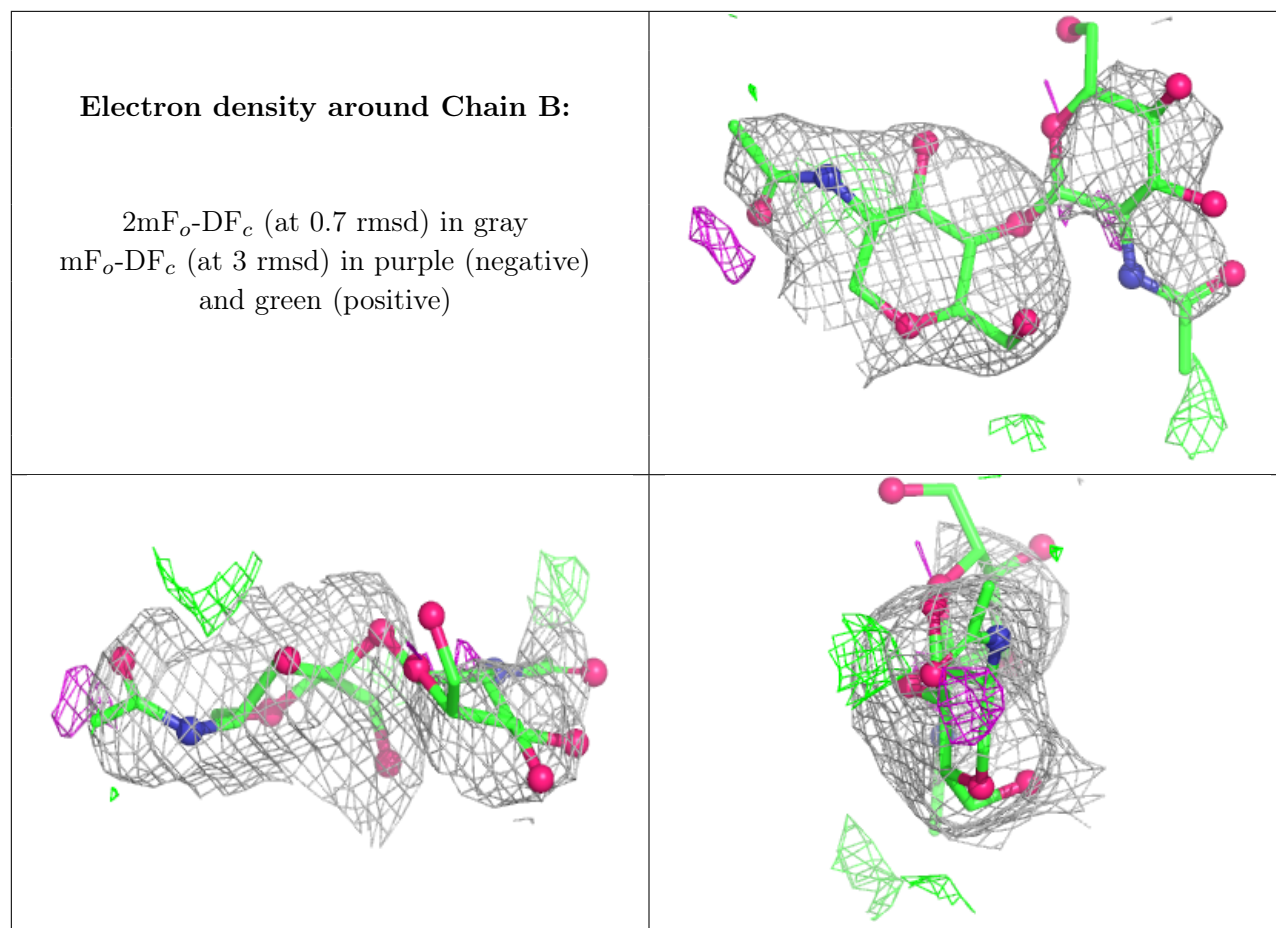
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	NAG	B	1	14/15	-	-	56,73,87,106	0
3	NAG	B	2	14/15	-	-	90,124,142,144	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	NAG	A	703	14/15	0.26	0.29	90,130,152,153	0
4	NAG	E	1702	14/15	0.37	0.22	106,129,144,148	0
4	NAG	A	702	14/15	0.70	0.18	90,108,125,136	0
4	NAG	A	704	14/15	0.72	0.23	73,98,113,113	0
5	SO4	E	1703	5/5	0.72	0.39	98,108,123,176	0
5	SO4	A	705	5/5	0.73	0.21	101,102,110,118	0
7	PEG	E	1706	7/7	0.74	0.38	67,75,78,81	0
7	PEG	A	710	7/7	0.78	0.39	103,123,133,136	0
10	GOL	E	1709	6/6	0.79	0.21	71,82,90,92	0
6	TRS	A	708	8/8	0.80	0.17	67,93,114,115	0
5	SO4	A	706	5/5	0.81	0.32	96,97,108,143	0
7	PEG	E	1708	7/7	0.82	0.23	66,74,80,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CL	E	1704	1/1	0.82	0.20	78,78,78,78	0
7	PEG	A	709	7/7	0.82	0.20	67,78,97,98	0
4	NAG	E	1701	14/15	0.86	0.12	63,81,91,105	0
5	SO4	A	707	5/5	0.87	0.32	86,91,116,128	0
7	PEG	E	1707	7/7	0.90	0.18	60,78,82,86	0
4	NAG	A	701	14/15	0.92	0.09	51,64,72,73	0
9	CL	E	1705	1/1	0.94	0.19	73,73,73,73	0
8	ZN	A	711	1/1	0.98	0.09	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.