



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 01:44 am BST

PDB ID : 9QRM / pdb_00009qrm
Title : X-ray structure of Kp32gp38 in complex with K21 pyr5
Authors : Napolitano, V.; Squeglia, F.; Privitera, M.; Berisio, R.
Deposited on : 2025-04-03
Resolution : 1.80 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

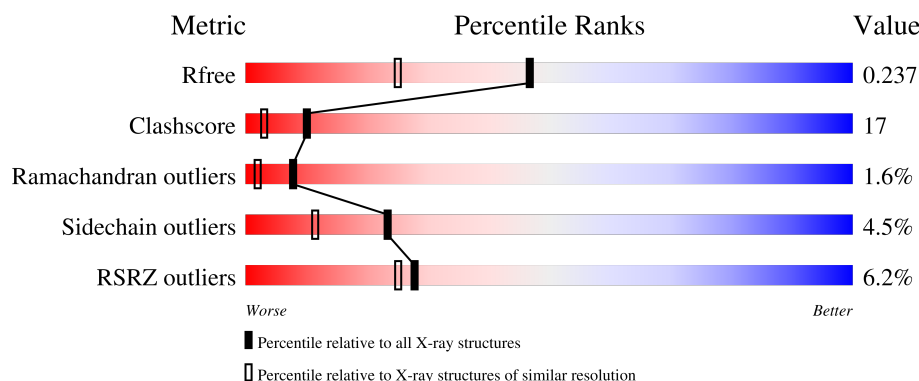
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	B	584	
2	A	5	

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	PEG	B	603	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4929 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 Depolymerase 2, capsule K21-specific.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	563	Total	C	N	O	S	0	18	0
			4340	2718	766	837	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	577	LYS	-	expression tag	UNP D1L2X1
B	578	GLY	-	expression tag	UNP D1L2X1
B	579	HIS	-	expression tag	UNP D1L2X1
B	580	HIS	-	expression tag	UNP D1L2X1
B	581	HIS	-	expression tag	UNP D1L2X1
B	582	HIS	-	expression tag	UNP D1L2X1
B	583	HIS	-	expression tag	UNP D1L2X1
B	584	HIS	-	expression tag	UNP D1L2X1

- Molecule 2 is an oligosaccharide called (2 {S},4 {a} {S},6 {R},7 {S},8 {R},8 {a} {R})-2-methyl-6,7,8-tris(oxidanyl)-4,4 {a},6,7,8,8 {a}-hexahydropyrano[3,2-d][1,3]dioxine-2-carboxylic acid-(4-4)-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	A	5	Total	C	O	0	0	0
			61	33	28			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

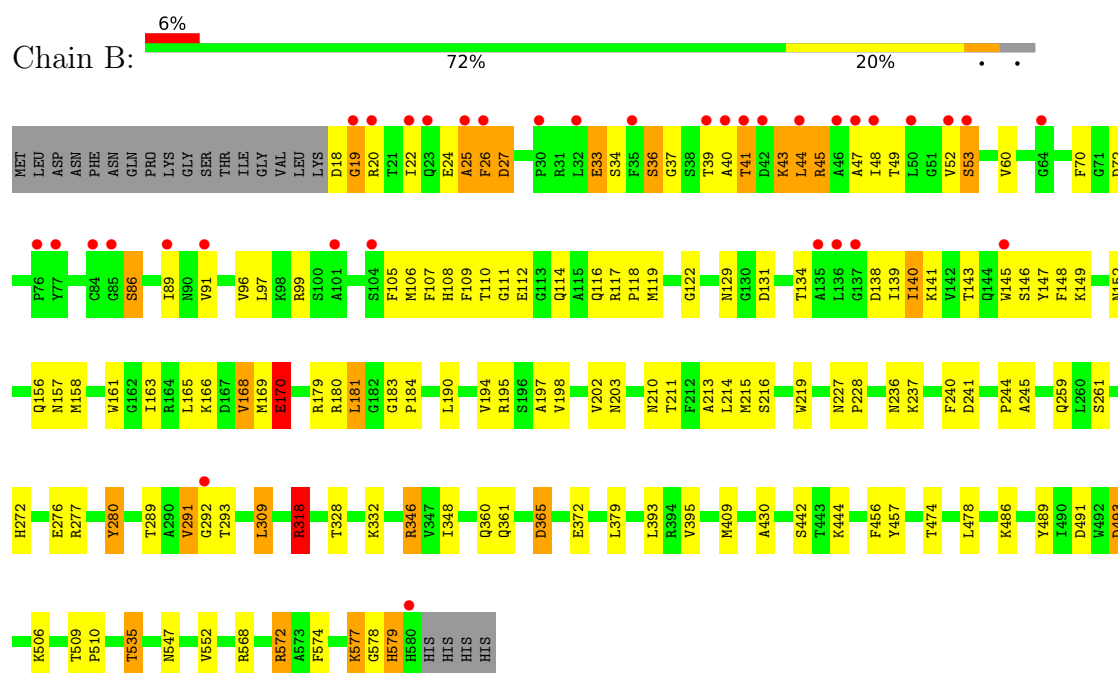
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	509	Total 509	O 509	0	0

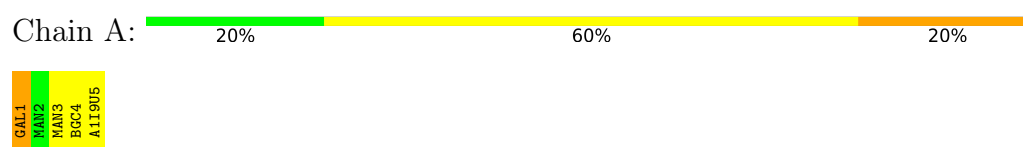
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Depolymerase 2, capsule K21-specific



- Molecule 2: (2 {S},4 {a} {S},6 {R},7 {S},8 {R},8 {a} {R})-2-methyl-6,7,8-tris(oxidanyl)-4,4 {a} {6,7,8,8 {a}-hexahydropyrano[3,2-d][1,3]dioxine-2-carboxylic acid-(4-4)-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.49Å 70.49Å 205.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.94 – 1.80 14.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (14.94-1.80) 95.3 (14.94-1.80)	Depositor EDS
R_{merge}	0.82	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.188 , 0.235 0.188 , 0.237	Depositor DCC
R_{free} test set	2751 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4929	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: A1I9U, GAL, BGC, GOL, MAN, 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	B	0.65	4/4416 (0.1%)	1.18	12/5998 (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	B	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	SER	CB-OG	11.70	1.65	1.42
1	B	37	GLY	C-O	9.09	1.36	1.23
1	B	34	SER	CB-OG	8.54	1.59	1.42
1	B	37	GLY	C-N	5.01	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	GLU	CB-CG-CD	7.03	124.55	112.60
1	B	109	PHE	CA-CB-CG	6.96	120.76	113.80
1	B	280	TYR	N-CA-CB	6.45	119.27	110.57
1	B	293	THR	CA-CB-OG1	-6.38	100.03	109.60
1	B	493	ASP	CA-CB-CG	5.99	118.59	112.60
1	B	276	GLU	CB-CG-CD	5.63	122.16	112.60
1	B	457	TYR	CB-CA-C	-5.43	100.36	109.48
1	B	365	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	474	THR	CA-CB-OG1	-5.35	101.57	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	PHE	CA-CB-CG	-5.24	108.56	113.80
1	B	116	GLN	N-CA-CB	-5.21	102.38	110.57
1	B	577	LYS	CB-CA-C	5.07	120.50	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	318[A]	ARG	Sidechain
1	B	346[A]	ARG	Sidechain
1	B	43	LYS	Peptide
1	B	572[A]	ARG	Sidechain

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	B	4340	0	4262	147	1
2	A	61	0	37	1	1
3	B	12	0	16	1	0
4	B	7	0	10	5	0
5	B	509	0	0	25	1
All	All	4929	0	4325	149	2

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 17.

All (149) 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:53:SER:OG	1:B:53:SER:CB	1.65	1.42
1:B:578:GLY:HA2	5:B:1044:HOH:O	1.20	1.28
1:B:346[B]:ARG:HH11	1:B:346[B]:ARG:CG	1.56	1.12
1:B:41:THR:O	1:B:44:LEU:HB2	1.46	1.12
1:B:346[B]:ARG:CG	1:B:346[B]:ARG:NH1	2.11	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346[B]:ARG:HH11	1:B:346[B]:ARG:HG3	0.89	1.02
1:B:535[B]:THR:HG21	5:B:747:HOH:O	1.58	1.02
1:B:346[B]:ARG:NH1	1:B:346[B]:ARG:HG3	1.70	0.99
1:B:318[B]:ARG:NH2	1:B:318[B]:ARG:HB2	1.78	0.98
1:B:165:LEU:HG	1:B:168:VAL:HG11	1.48	0.96
1:B:318[B]:ARG:HB2	1:B:318[B]:ARG:HH21	1.32	0.92
1:B:119:MET:HE3	1:B:147:TYR:CE2	2.05	0.92
1:B:509[B]:THR:HG22	1:B:552:VAL:H	1.35	0.91
1:B:346[B]:ARG:NH1	1:B:346[B]:ARG:HG2	1.84	0.91
1:B:119:MET:HE3	1:B:147:TYR:HE2	1.41	0.86
1:B:535[B]:THR:HG22	5:B:823:HOH:O	1.73	0.86
1:B:45:ARG:O	1:B:49:THR:N	2.08	0.83
1:B:97:LEU:HB2	1:B:106:MET:HE1	1.60	0.83
1:B:180[B]:ARG:HH22	1:B:245:ALA:H	1.28	0.78
1:B:163:ILE:HG22	1:B:165:LEU:HD13	1.68	0.76
1:B:97:LEU:CB	1:B:106:MET:HE1	2.16	0.75
1:B:442[A]:SER:HB2	5:B:704:HOH:O	1.87	0.74
1:B:346[B]:ARG:NE	5:B:703:HOH:O	2.06	0.74
1:B:535[B]:THR:CG2	5:B:747:HOH:O	2.22	0.74
1:B:509[B]:THR:CG2	1:B:552:VAL:H	2.01	0.74
1:B:372:GLU:OE2	5:B:702:HOH:O	2.06	0.73
1:B:568:ARG:HG3	4:B:603:PEG:H21	1.71	0.72
1:B:106:MET:HE2	1:B:107:PHE:CE2	2.24	0.72
1:B:45:ARG:HA	1:B:48:ILE:HB	1.72	0.70
1:B:163:ILE:HG22	1:B:165:LEU:CD1	2.22	0.70
1:B:430:ALA:HB3	5:B:783:HOH:O	1.91	0.69
1:B:291:VAL:HG22	1:B:292:GLY:N	2.09	0.67
1:B:509[B]:THR:OG1	1:B:510:PRO:HD2	1.96	0.66
1:B:117:ARG:HH12	1:B:145:TRP:C	2.03	0.66
1:B:110:THR:HG22	1:B:112:GLU:H	1.61	0.65
1:B:41:THR:OG1	1:B:70:PHE:HA	1.97	0.64
1:B:169[B]:MET:SD	1:B:203:ASN:ND2	2.69	0.64
1:B:318[A]:ARG:HB2	1:B:318[A]:ARG:HH11	1.63	0.63
1:B:572[A]:ARG:HH11	1:B:572[A]:ARG:HG3	1.64	0.63
1:B:535[B]:THR:CG2	5:B:823:HOH:O	2.38	0.62
1:B:213:ALA:O	1:B:215:MET:HG3	2.00	0.62
1:B:117:ARG:HH11	1:B:117:ARG:HG2	1.63	0.61
1:B:577:LYS:HE2	5:B:826:HOH:O	2.00	0.61
1:B:41:THR:O	1:B:44:LEU:CB	2.36	0.61
1:B:25:ALA:O	1:B:27:ASP:N	2.33	0.61
1:B:194:VAL:CG1	1:B:197:ALA:O	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:SER:HA	1:B:292:GLY:H	1.65	0.60
1:B:194:VAL:HG11	1:B:198:VAL:HA	1.82	0.60
1:B:259:GLN:HE21	1:B:289[B]:THR:CG2	2.15	0.59
1:B:33:GLU:OE1	1:B:43:LYS:HD2	2.02	0.59
1:B:139:ILE:HG22	1:B:140:ILE:HD13	1.85	0.58
1:B:108:HIS:HE1	1:B:143:THR:OG1	1.87	0.58
1:B:372:GLU:CD	5:B:702:HOH:O	2.44	0.58
1:B:25:ALA:O	1:B:26:PHE:C	2.47	0.57
1:B:259:GLN:HG2	1:B:289[B]:THR:HG23	1.86	0.57
1:B:291:VAL:CG2	1:B:292:GLY:N	2.67	0.57
1:B:53:SER:CB	1:B:53:SER:HG	2.09	0.56
1:B:41:THR:C	1:B:44:LEU:HB2	2.29	0.56
1:B:332[A]:LYS:HD3	5:B:717:HOH:O	2.06	0.56
1:B:509[B]:THR:HG23	1:B:510:PRO:O	2.04	0.56
3:B:601:GOL:H32	5:B:1030:HOH:O	2.06	0.55
1:B:348:ILE:HD11	1:B:360:GLN:HG3	1.89	0.55
1:B:41:THR:O	1:B:44:LEU:CD1	2.56	0.54
1:B:97:LEU:HB3	1:B:106:MET:CE	2.38	0.54
1:B:161:TRP:CE3	1:B:190:LEU:HB2	2.43	0.54
1:B:210:ASN:HB2	1:B:236:ASN:OD1	2.09	0.53
1:B:156:GLN:HA	1:B:181:LEU:HD13	1.91	0.52
1:B:99:ARG:O	1:B:131:ASP:HB3	2.09	0.52
1:B:328:THR:HB	5:B:1049:HOH:O	2.10	0.52
1:B:45:ARG:O	1:B:49:THR:CB	2.58	0.52
1:B:379:LEU:HD13	1:B:395:VAL:HG22	1.92	0.52
1:B:219:TRP:NE1	1:B:280:TYR:OH	2.42	0.51
1:B:110:THR:HG23	1:B:143:THR:HB	1.92	0.51
1:B:259:GLN:HE21	1:B:289[B]:THR:HG21	1.76	0.51
1:B:119:MET:HA	1:B:146:SER:O	2.10	0.51
1:B:568:ARG:HG3	4:B:603:PEG:C2	2.41	0.51
1:B:18:ASP:HA	1:B:25:ALA:H	1.76	0.50
1:B:194:VAL:HG13	1:B:197:ALA:O	2.10	0.50
1:B:107:PHE:CD2	1:B:140:ILE:HD11	2.47	0.50
1:B:105:PHE:HA	1:B:138:ASP:O	2.12	0.49
1:B:18:ASP:CB	1:B:24:GLU:HA	2.42	0.49
1:B:18:ASP:O	1:B:19:GLY:C	2.55	0.49
1:B:169[B]:MET:O	1:B:170:GLU:HB2	2.13	0.49
1:B:509[B]:THR:OG1	1:B:510:PRO:CD	2.59	0.49
1:B:72:ASP:HA	1:B:105:PHE:CE1	2.48	0.49
1:B:509[B]:THR:HG22	1:B:552:VAL:N	2.16	0.49
1:B:572[A]:ARG:HH11	1:B:572[A]:ARG:CG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:CB	1:B:106:MET:CE	2.87	0.48
1:B:169[B]:MET:HE1	2:A:1:GAL:H2	1.95	0.48
4:B:603:PEG:H21	4:B:603:PEG:H42	1.58	0.48
1:B:41:THR:O	1:B:44:LEU:HD13	2.14	0.48
1:B:365:ASP:HB3	5:B:1078:HOH:O	2.13	0.48
1:B:36:SER:OG	1:B:43:LYS:HB3	2.13	0.48
1:B:156:GLN:HA	1:B:179:ARG:O	2.14	0.47
1:B:579:HIS:HB3	5:B:1032:HOH:O	2.14	0.47
1:B:40:ALA:O	1:B:41:THR:CB	2.62	0.47
1:B:45:ARG:O	1:B:49:THR:HB	2.14	0.47
1:B:506:LYS:HE2	5:B:743:HOH:O	2.14	0.47
1:B:332[A]:LYS:HD3	5:B:1116:HOH:O	2.15	0.46
1:B:211:THR:HG23	1:B:237:LYS:HD2	1.97	0.46
1:B:131:ASP:N	1:B:131:ASP:OD1	2.48	0.46
1:B:47:ALA:O	1:B:52:VAL:HG12	2.16	0.46
1:B:442[A]:SER:HB3	1:B:456:PHE:HD2	1.81	0.46
1:B:579:HIS:CD2	1:B:579:HIS:C	2.94	0.46
1:B:183:GLY:HA2	1:B:216:SER:HB3	1.98	0.45
1:B:145:TRP:CD1	1:B:148:PHE:HB2	2.51	0.45
1:B:111:GLY:HA3	1:B:118:PRO:CD	2.46	0.45
1:B:346[B]:ARG:HD2	1:B:361:GLN:HB2	1.99	0.45
1:B:227:ASN:N	1:B:228:PRO:HD3	2.32	0.45
1:B:240:PHE:HB2	1:B:272:HIS:O	2.17	0.45
1:B:44:LEU:HD23	1:B:45:ARG:CD	2.47	0.45
1:B:86:SER:HA	1:B:152:ASN:ND2	2.31	0.45
1:B:165:LEU:CG	1:B:168:VAL:HG11	2.32	0.45
1:B:444[A]:LYS:NZ	5:B:701:HOH:O	2.49	0.44
1:B:506:LYS:CE	5:B:743:HOH:O	2.66	0.44
1:B:547:ASN:ND2	5:B:732:HOH:O	2.49	0.44
1:B:240:PHE:CD2	1:B:277:ARG:HD3	2.53	0.44
1:B:309:LEU:C	1:B:309:LEU:HD23	2.43	0.44
1:B:111:GLY:HA2	1:B:114:GLN:HE21	1.83	0.44
1:B:195:ARG:HH11	1:B:195:ARG:HD2	1.62	0.44
1:B:119:MET:HE3	1:B:147:TYR:CD2	2.51	0.43
1:B:18:ASP:O	1:B:20:ARG:N	2.51	0.43
1:B:122:GLY:HA3	1:B:149:LYS:O	2.18	0.43
1:B:147:TYR:CD1	1:B:170:GLU:HB3	2.53	0.43
1:B:486:LYS:NZ	5:B:741:HOH:O	2.51	0.43
1:B:332[A]:LYS:CD	5:B:1116:HOH:O	2.65	0.43
1:B:45:ARG:HG2	1:B:49:THR:OG1	2.17	0.43
1:B:346[B]:ARG:CZ	5:B:703:HOH:O	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLN:HE21	1:B:289[B]:THR:HG23	1.82	0.43
1:B:143:THR:HA	1:B:166:LYS:O	2.18	0.42
1:B:393:LEU:O	1:B:478:LEU:HA	2.19	0.42
1:B:106:MET:HE2	1:B:107:PHE:HE2	1.77	0.42
1:B:180[B]:ARG:NH1	1:B:244:PRO:HA	2.35	0.42
1:B:108:HIS:CE1	1:B:141:LYS:HE2	2.54	0.42
1:B:168:VAL:O	1:B:202:VAL:HA	2.20	0.42
1:B:219:TRP:N	1:B:219:TRP:CD1	2.88	0.42
1:B:491:ASP:OD1	1:B:572[A]:ARG:NH1	2.52	0.42
1:B:493:ASP:OD1	4:B:603:PEG:H22	2.19	0.42
1:B:409[B]:MET:HE3	1:B:409[B]:MET:HB2	1.97	0.41
1:B:489:TYR:CD1	1:B:489:TYR:C	2.99	0.41
1:B:96:VAL:O	1:B:97:LEU:HD23	2.21	0.41
1:B:117:ARG:HG2	1:B:117:ARG:NH1	2.31	0.41
1:B:129:ASN:HA	1:B:156:GLN:O	2.20	0.41
1:B:430:ALA:CB	5:B:783:HOH:O	2.60	0.41
1:B:572[A]:ARG:HG3	1:B:572[A]:ARG:NH1	2.33	0.40
1:B:493:ASP:CG	4:B:603:PEG:H22	2.46	0.40
1:B:163:ILE:CG2	1:B:165:LEU:CD1	2.97	0.40
1:B:194:VAL:HG11	1:B:197:ALA:O	2.20	0.40
1:B:261:SER:HA	1:B:292:GLY:N	2.32	0.40

All (2) 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)
1:B:241:ASP:OD1	2:A:1:GAL:O4[2_445]	1.98	0.22
5:B:1003:HOH:O	5:B:1155:HOH:O[3_545]	2.06	0.14

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	B	580/584 (99%)	530 (91%)	41 (7%)	9 (2%)	8 2

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	22	ILE
1	B	26	PHE
1	B	36	SER
1	B	19	GLY
1	B	41	THR
1	B	157	ASN
1	B	25	ALA
1	B	44	LEU
1	B	184	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	B	459/473 (97%)	437 (95%)	22 (5%)	21 10

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	ASP
1	B	33	GLU
1	B	39	THR
1	B	45	ARG
1	B	60	VAL
1	B	86	SER
1	B	89	ILE
1	B	91	VAL
1	B	134	THR
1	B	140	ILE
1	B	158	MET
1	B	168	VAL

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Mol	Chain	Res	Type
1	B	170	GLU
1	B	181	LEU
1	B	214	LEU
1	B	291	VAL
1	B	309	LEU
1	B	318[A]	ARG
1	B	318[B]	ARG
1	B	535[A]	THR
1	B	535[B]	THR
1	B	579	HIS

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

Mol	Chain	Res	Type
1	B	63	ASN
1	B	108	HIS
1	B	114	GLN
1	B	259	GLN
1	B	355	ASN
1	B	360	GLN
1	B	547	ASN
1	B	579	HIS

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](#)

5 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	GAL	A	1	2	12,12,12	0.77	0	17,17,17	1.18	2 (11%)
2	MAN	A	2	2	11,11,12	0.80	0	15,15,17	1.07	0
2	MAN	A	3	2	11,11,12	0.64	0	15,15,17	1.35	2 (13%)
2	BGC	A	4	2	10,10,12	0.31	0	11,13,17	1.02	1 (9%)
2	A1I9U	A	5	2	17,18,18	0.58	0	25,28,28	1.44	1 (4%)

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	GAL	A	1	2	-	1/2/22/22	0/1/1/1
2	MAN	A	2	2	-	2/2/19/22	0/1/1/1
2	MAN	A	3	2	-	0/2/19/22	0/1/1/1
2	BGC	A	4	2	-	0/2/15/22	0/1/1/1
2	A1I9U	A	5	2	-	3/5/37/37	1/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	A1I9U	O2-C5-C6	5.73	115.27	109.27
2	A	3	MAN	O3-C3-C2	3.45	116.60	109.99
2	A	3	MAN	C1-O5-C5	2.41	115.46	112.19
2	A	4	BGC	O5-C5-C4	-2.22	107.06	110.65
2	A	1	GAL	O3-C3-C2	2.22	115.48	110.35
2	A	1	GAL	O2-C2-C3	-2.01	105.70	110.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5	A1I9U	C1-C2-C9-O7
2	A	5	A1I9U	O2-C2-C9-O8
2	A	1	GAL	O5-C5-C6-O6
2	A	5	A1I9U	O2-C2-C9-O7

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Mol	Chain	Res	Type	Atoms
2	A	2	MAN	C4-C5-C6-O6
2	A	2	MAN	O5-C5-C6-O6

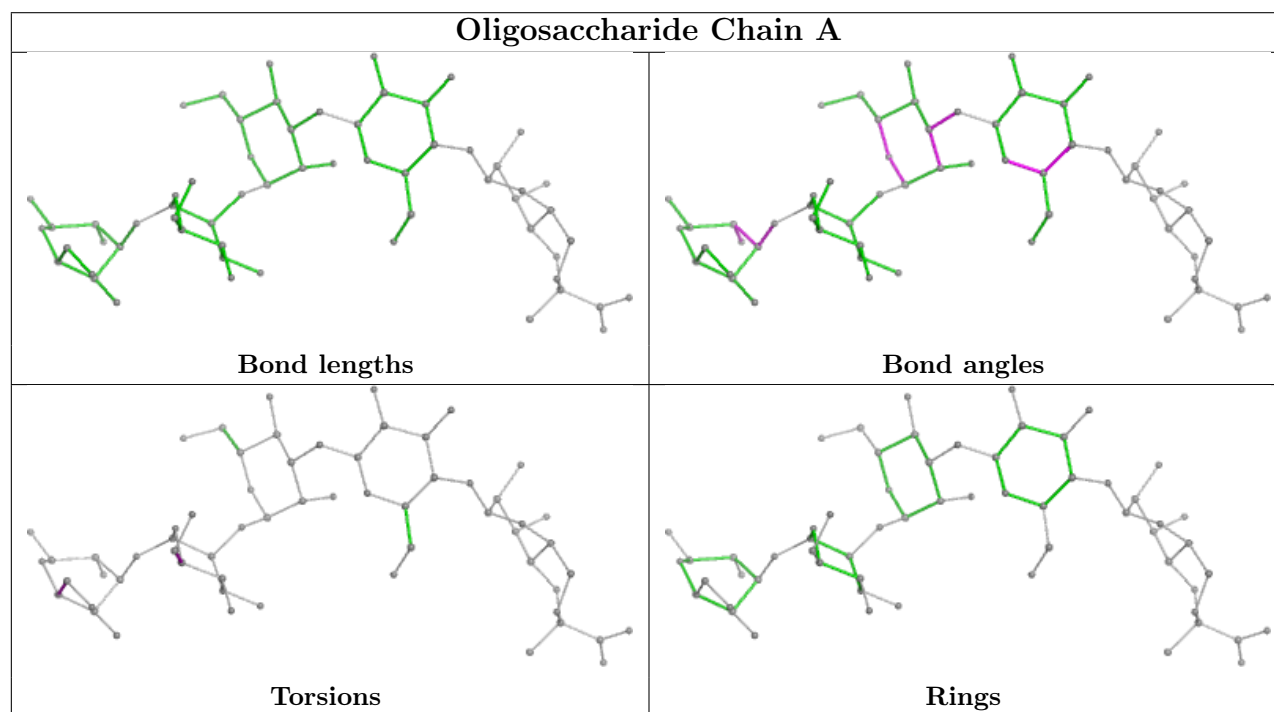
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5	A1I9U	C2-C3-C4-C5-O1-O2

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	GAL	1	1

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](#)

3 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	$\# Z > 2$
3	GOL	B	604	-	5,5,5	0.16	0	5,5,5	0.55	0
3	GOL	B	601	-	5,5,5	0.13	0	5,5,5	0.44	0
4	PEG	B	603	-	6,6,6	0.23	0	5,5,5	0.36	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	GOL	B	604	-	-	4/4/4/4	-
3	GOL	B	601	-	-	4/4/4/4	-
4	PEG	B	603	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	GOL	O1-C1-C2-C3
3	B	601	GOL	C1-C2-C3-O3
3	B	601	GOL	O2-C2-C3-O3
3	B	604	GOL	O1-C1-C2-C3
4	B	603	PEG	O1-C1-C2-O2
3	B	601	GOL	O1-C1-C2-O2
3	B	604	GOL	O1-C1-C2-O2
4	B	603	PEG	C4-C3-O2-C2
3	B	604	GOL	O2-C2-C3-O3
3	B	604	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	PEG	5	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	B	563/584 (96%)	0.04	35 (6%) 28 25	5, 37, 94, 116	18 (3%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	PHE	3.8
1	B	19	GLY	3.8
1	B	46	ALA	3.7
1	B	84	CYS	3.4
1	B	85	GLY	3.3
1	B	39	THR	3.2
1	B	136	LEU	3.2
1	B	40	ALA	3.0
1	B	35	PHE	2.9
1	B	137	GLY	2.9
1	B	42	ASP	2.9
1	B	20	ARG	2.8
1	B	104	SER	2.7
1	B	91	VAL	2.6
1	B	44	LEU	2.6
1	B	22	ILE	2.5
1	B	50	LEU	2.4
1	B	30	PRO	2.4
1	B	47	ALA	2.4
1	B	32	LEU	2.3
1	B	25	ALA	2.3
1	B	48	ILE	2.3
1	B	145	TRP	2.3
1	B	292	GLY	2.2
1	B	76	PRO	2.2
1	B	23	GLN	2.2
1	B	580	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	101	ALA	2.2
1	B	77	TYR	2.2
1	B	135	ALA	2.1
1	B	89	ILE	2.1
1	B	41	THR	2.1
1	B	64	GLY	2.1
1	B	52	VAL	2.0
1	B	53	SER	2.0

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

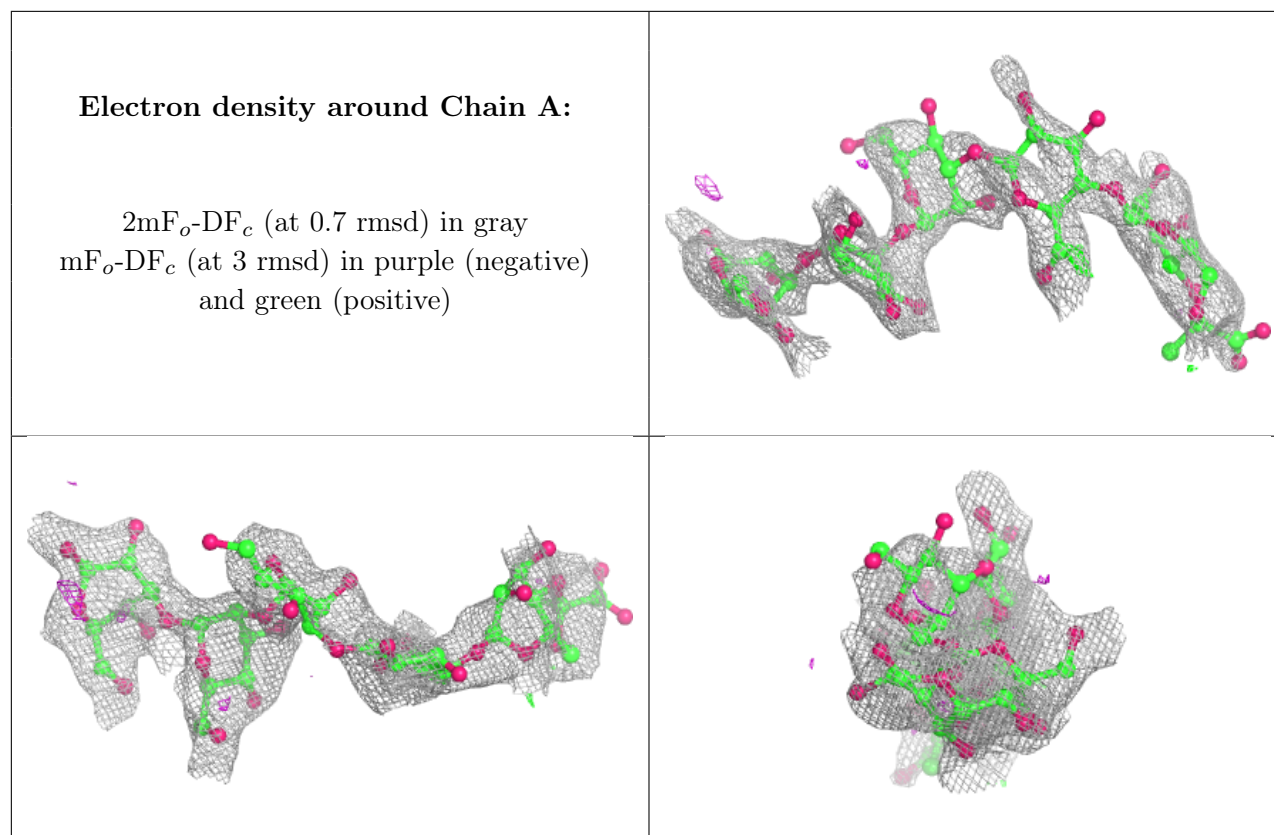
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
2	GAL	A	1	12/12	-	-	66,69,71,72	0
2	MAN	A	2	11/12	-	-	63,66,69,71	0
2	MAN	A	3	11/12	-	-	71,75,80,83	0
2	BGC	A	4	10/12	-	-	72,74,78,82	0
2	A1I9U	A	5	17/17	-	-	90,108,114,117	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(\AA^2)	Q<0.9
4	PEG	B	603	7/7	0.72	0.14	38,39,44,46	0
3	GOL	B	601	6/6	0.76	0.13	54,60,61,61	0
3	GOL	B	604	6/6	0.79	0.10	49,53,55,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.