Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 10:30 PM EDT

PDB ID	:	3R4L
Title	:	Human very long half life Plasminogen Activator Inhibitor type-1
Authors	:	Yang, J.; Zheng, H.; Han, Q.; Skrzypczak-Jankun, E.; Jankun, J.
Deposited on	:	2011-03-17
Resolution	:	2.70 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 (i) 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 (i)) 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	:	2.35
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)	:	2.35
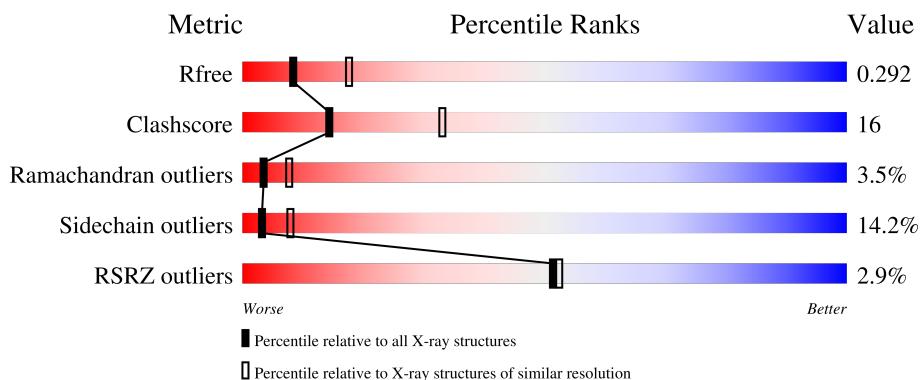
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
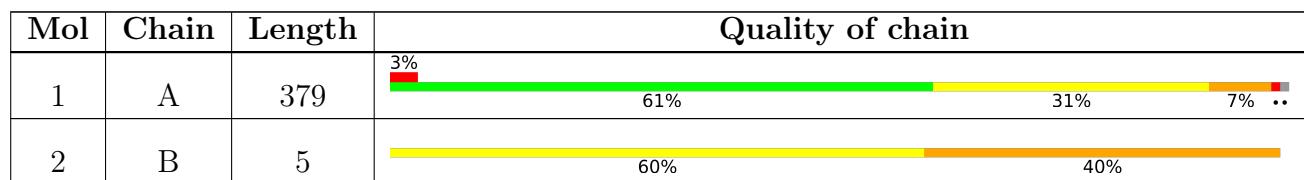
The reported resolution of this entry is 2.70 Å.

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	Percentile Ranks	Value
Rfree		0.292
Clashscore		16
Ramachandran outliers		3.5%
Sidechain outliers		14.2%
RSRZ outliers		2.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	379	3% 61% 31% 7% ••
2	B	5	60% 40%

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
2	NAG	B	1	X	-	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3086 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.
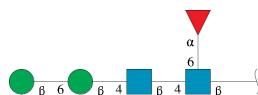
- Molecule 1 is a protein called Plasminogen activator inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2995	1918	511	548	18			

There are 2 discrepancies between the modelled and reference sequences:
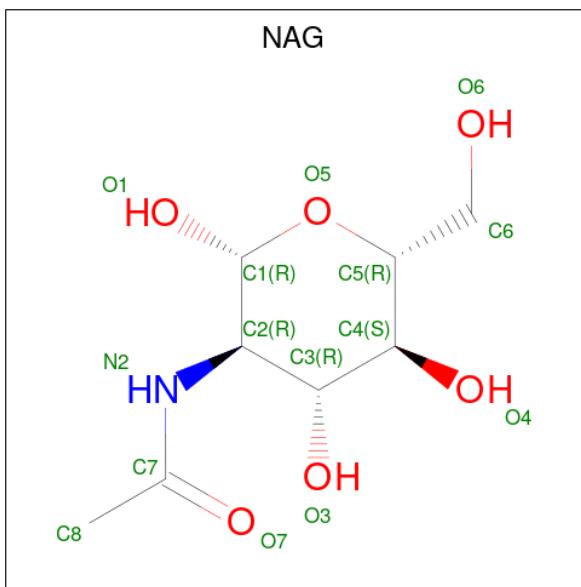
Chain	Residue	Modelled	Actual	Comment	Reference
A	197	CYS	GLN	engineered mutation	UNP P05121
A	355	CYS	GLY	engineered mutation	UNP P05121

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-aceta mido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
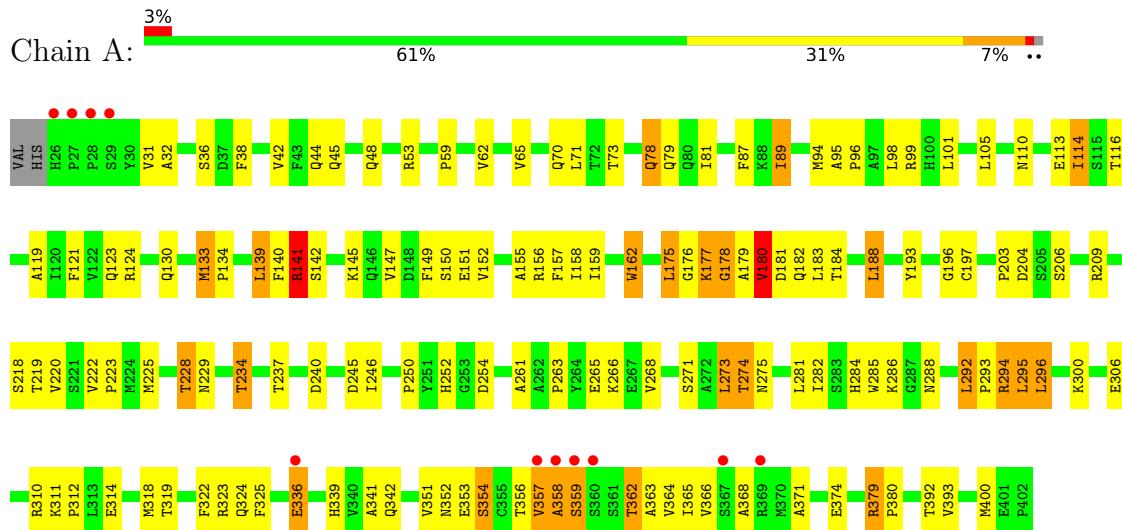
• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		

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: Plasminogen activator inhibitor 1

Chain A:

• Molecule 2: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	72.01Å 72.01Å 194.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.00 – 2.70 33.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.8 (33.00-2.70) 81.8 (33.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.12 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, R_{free}	0.209 , 0.282 0.210 , 0.292	Depositor DCC
R_{free} test set	709 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	60.1	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 37.0	EDS
L-test for twinning[2]	$< |L| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3086	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FUC, BMA, NAG

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	0.70	0/3068	0.84	1/4160 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	ARG	O-C-N	-5.53	113.86	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	GLU	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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2995	0	2983	94	0
2	B	60	0	52	1	0
3	A	14	0	13	2	0
4	A	17	0	0	1	0
All	All	3086	0	3048	95	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 16.

All (95) 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:123:GLN:HE22	1:A:149:PHE:H	1.03	0.94
1:A:155:ALA:O	1:A:158:ILE:HG22	1.68	0.93
1:A:123:GLN:NE2	1:A:149:PHE:H	1.72	0.87
1:A:123:GLN:HE22	1:A:149:PHE:N	1.79	0.78
1:A:133:MET:HB2	1:A:134:PRO:CD	2.18	0.74
1:A:156:ARG:CZ	1:A:177:LYS:HA	2.17	0.74
1:A:31:VAL:HG12	1:A:94:MET:HE1	1.70	0.73
1:A:197:CYS:HB2	1:A:252:HIS:HD2	1.53	0.73
1:A:70:GLN:NE2	1:A:89:ILE:H	1.87	0.73
1:A:292:LEU:HD23	1:A:293:PRO:HD2	1.73	0.70
1:A:265:GLU:HB2	1:A:268:VAL:HG23	1.73	0.69
1:A:156:ARG:HB3	1:A:175:LEU:HD12	1.76	0.67
1:A:300:LYS:HG3	1:A:352:ASN:HB3	1.79	0.65
2:B:3:BMA:H62	2:B:4:BMA:O2	1.95	0.65
1:A:70:GLN:HE22	1:A:89:ILE:H	1.41	0.65
1:A:179:ALA:O	1:A:180:VAL:HB	1.99	0.63
1:A:284:HIS:O	1:A:288:ASN:HB2	1.98	0.62
1:A:322:PHE:O	1:A:339:HIS:HD2	1.81	0.62
1:A:324:GLN:HG3	1:A:325:PHE:CD2	2.35	0.62
1:A:38:PHE:O	1:A:42:VAL:HG23	1.98	0.61
1:A:250:PRO:HG3	3:A:408:NAG:H81	1.82	0.61
1:A:31:VAL:HG12	1:A:94:MET:CE	2.30	0.61
1:A:203:PRO:HB2	1:A:206:SER:OG	2.01	0.61
1:A:362:THR:HG22	1:A:363:ALA:HA	1.83	0.61
1:A:188:LEU:N	1:A:188:LEU:HD23	2.16	0.60
1:A:133:MET:HA	1:A:133:MET:CE	2.32	0.58
1:A:133:MET:HA	1:A:133:MET:HE3	1.86	0.57
1:A:250:PRO:HG3	3:A:408:NAG:C8	2.35	0.57
1:A:263:PRO:HD3	1:A:273:LEU:HD13	1.87	0.57
1:A:101:LEU:O	1:A:105:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:O	1:A:314:GLU:HG3	2.05	0.56
1:A:263:PRO:HG2	1:A:379:ARG:NH2	2.20	0.56
1:A:113:GLU:HG2	1:A:196:GLY:HA2	1.86	0.55
1:A:265:GLU:HB2	1:A:268:VAL:CG2	2.35	0.55
1:A:133:MET:HB2	1:A:134:PRO:HD3	1.89	0.55
1:A:295:LEU:HD13	1:A:374:GLU:HG3	1.88	0.55
1:A:292:LEU:HD22	1:A:294:ARG:HH11	1.73	0.54
1:A:188:LEU:HD23	1:A:188:LEU:H	1.74	0.53
1:A:123:GLN:HE21	1:A:149:PHE:HD2	1.58	0.52
1:A:62:VAL:HA	1:A:65:VAL:HG12	1.92	0.52
1:A:184:THR:HG23	1:A:341:ALA:CB	2.41	0.51
1:A:133:MET:CB	1:A:134:PRO:CD	2.88	0.50
1:A:357:VAL:C	1:A:359:SER:H	2.15	0.50
1:A:36:SER:OG	1:A:392:THR:HA	2.12	0.50
1:A:324:GLN:OE1	1:A:324:GLN:HA	2.12	0.50
1:A:282:ILE:O	1:A:285:TRP:HB2	2.12	0.49
1:A:356:THR:O	1:A:358:ALA:N	2.45	0.49
1:A:145:LYS:HE3	1:A:162:TRP:CH2	2.48	0.49
1:A:114:ILE:HA	1:A:193:TYR:O	2.13	0.49
1:A:81:ILE:HG12	1:A:318:MET:HG2	1.95	0.49
1:A:245:ASP:O	1:A:261:ALA:HA	2.13	0.48
1:A:133:MET:HB2	1:A:134:PRO:HD2	1.95	0.48
1:A:300:LYS:NZ	1:A:353:GLU:OE1	2.43	0.47
1:A:42:VAL:O	1:A:45:GLN:HB2	2.14	0.47
1:A:157:PHE:CD1	1:A:157:PHE:C	2.87	0.47
1:A:176:GLY:O	1:A:178:GLY:N	2.48	0.47
1:A:322:PHE:O	1:A:339:HIS:CD2	2.66	0.47
1:A:95:ALA:HB3	1:A:96:PRO:HD3	1.97	0.47
1:A:324:GLN:O	1:A:325:PHE:HB2	2.16	0.46
1:A:158:ILE:CG2	1:A:159:ILE:N	2.79	0.46
1:A:181:ASP:O	1:A:183:LEU:N	2.48	0.46
1:A:274:THR:HG22	1:A:275:ASN:OD1	2.16	0.46
1:A:31:VAL:HG23	1:A:32:ALA:N	2.30	0.45
1:A:151:GLU:OE2	1:A:151:GLU:HA	2.16	0.45
1:A:222:VAL:HB	1:A:223:PRO:CD	2.47	0.45
1:A:354:SER:C	1:A:356:THR:H	2.20	0.44
1:A:158:ILE:HG23	1:A:159:ILE:N	2.31	0.44
1:A:252:HIS:C	1:A:254:ASP:H	2.19	0.44
1:A:265:GLU:O	1:A:266:LYS:C	2.54	0.44
1:A:162:TRP:CD1	1:A:162:TRP:C	2.91	0.44
1:A:357:VAL:O	1:A:359:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:C	1:A:141:ARG:O	2.56	0.44
1:A:319:THR:HB	1:A:323:ARG:NH1	2.33	0.43
1:A:119:ALA:HB1	1:A:121:PHE:CE1	2.53	0.43
1:A:311:LYS:HB2	1:A:312:PRO:HD3	2.00	0.43
1:A:366:VAL:HG12	1:A:366:VAL:O	2.18	0.43
1:A:139:LEU:N	1:A:139:LEU:HD23	2.33	0.43
1:A:271:SER:HA	1:A:274:THR:HB	2.01	0.42
1:A:44:GLN:O	1:A:45:GLN:C	2.58	0.42
1:A:156:ARG:NH1	1:A:177:LYS:HA	2.35	0.42
1:A:114:ILE:O	1:A:114:ILE:HG12	2.19	0.41
1:A:379:ARG:HD3	1:A:380:PRO:O	2.20	0.41
1:A:175:LEU:HD22	1:A:175:LEU:HA	1.83	0.41
1:A:228:THR:HG22	1:A:295:LEU:HD23	2.01	0.41
1:A:225:MET:SD	1:A:353:GLU:HG3	2.60	0.41
1:A:295:LEU:HD22	1:A:296:LEU:N	2.35	0.41
1:A:310:ARG:NH2	4:A:516:HOH:O	2.52	0.41
1:A:176:GLY:C	1:A:178:GLY:N	2.74	0.41
1:A:204:ASP:N	1:A:362:THR:HG23	2.35	0.41
1:A:234:THR:CG2	1:A:246:ILE:HD13	2.51	0.41
1:A:274:THR:HG22	1:A:275:ASN:N	2.35	0.41
1:A:59:PRO:HG2	1:A:393:VAL:CG1	2.51	0.41
1:A:73:THR:OG1	1:A:78:GLN:CG	2.68	0.40
1:A:87:PHE:HB2	1:A:94:MET:HE2	2.03	0.40
1:A:65:VAL:HG22	1:A:188:LEU:HD12	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	375/379 (99%)	326 (87%)	36 (10%)	13 (4%)	3	8

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	VAL
1	A	336	GLU
1	A	357	VAL
1	A	358	ALA
1	A	152	VAL
1	A	178	GLY
1	A	368	ALA
1	A	141	ARG
1	A	142	SER
1	A	177	LYS
1	A	218	SER
1	A	371	ALA
1	A	182	GLN

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	332/334 (99%)	285 (86%)	47 (14%)	3	8

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	53	ARG
1	A	71	LEU
1	A	78	GLN
1	A	79	GLN
1	A	89	ILE
1	A	98	LEU
1	A	99	ARG
1	A	110	ASN
1	A	114	ILE
1	A	116	THR
1	A	130	GLN

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Mol	Chain	Res	Type
1	A	133	MET
1	A	139	LEU
1	A	141	ARG
1	A	147	VAL
1	A	150	SER
1	A	162	TRP
1	A	175	LEU
1	A	180	VAL
1	A	188	LEU
1	A	209	ARG
1	A	219	THR
1	A	220	VAL
1	A	228	THR
1	A	229	ASN
1	A	234	THR
1	A	237	THR
1	A	240	ASP
1	A	273	LEU
1	A	274	THR
1	A	281	LEU
1	A	286	LYS
1	A	292	LEU
1	A	294	ARG
1	A	295	LEU
1	A	296	LEU
1	A	306	GLU
1	A	342	GLN
1	A	351	VAL
1	A	354	SER
1	A	359	SER
1	A	362	THR
1	A	364	VAL
1	A	365	ILE
1	A	379	ARG
1	A	400	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	70	GLN
1	A	82	GLN
1	A	123	GLN

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Mol	Chain	Res	Type
1	A	130	GLN
1	A	135	HIS
1	A	146	GLN
1	A	227	GLN
1	A	229	ASN
1	A	326	GLN
1	A	339	HIS

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 ⓘ

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	NAG	B	1	1,2	14,14,15	0.72	0	17,19,21	2.24	5 (29%)
2	NAG	B	2	2	14,14,15	0.53	0	17,19,21	2.15	3 (17%)
2	BMA	B	3	2	11,11,12	0.72	0	15,15,17	1.37	2 (13%)
2	BMA	B	4	2	11,11,12	0.94	1 (9%)	15,15,17	2.18	7 (46%)
2	FUC	B	5	2	10,10,11	0.70	0	14,14,16	1.23	1 (7%)

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	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	BMA	B	4	2	-	2/2/19/22	0/1/1/1
2	FUC	B	5	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	BMA	C1-C2	2.01	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	6.77	121.36	112.19
2	B	1	NAG	C1-O5-C5	5.99	120.31	112.19
2	B	4	BMA	C3-C4-C5	-4.12	102.90	110.24
2	B	4	BMA	O5-C5-C6	3.77	113.12	107.20
2	B	1	NAG	C2-N2-C7	-3.57	117.83	122.90
2	B	4	BMA	C1-O5-C5	2.67	115.81	112.19
2	B	3	BMA	C3-C4-C5	2.64	114.94	110.24
2	B	1	NAG	O3-C3-C2	-2.53	104.23	109.47
2	B	4	BMA	O4-C4-C5	2.48	115.47	109.30
2	B	4	BMA	O5-C1-C2	2.34	114.39	110.77
2	B	4	BMA	O2-C2-C1	2.32	113.91	109.15
2	B	3	BMA	C1-C2-C3	2.32	112.52	109.67
2	B	1	NAG	C1-C2-N2	-2.31	106.54	110.49
2	B	4	BMA	C1-C2-C3	2.29	112.48	109.67
2	B	2	NAG	C4-C3-C2	-2.17	107.83	111.02
2	B	1	NAG	C3-C4-C5	-2.15	106.41	110.24
2	B	5	FUC	O3-C3-C2	2.07	113.96	109.99
2	B	2	NAG	C1-C2-N2	2.01	113.92	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6

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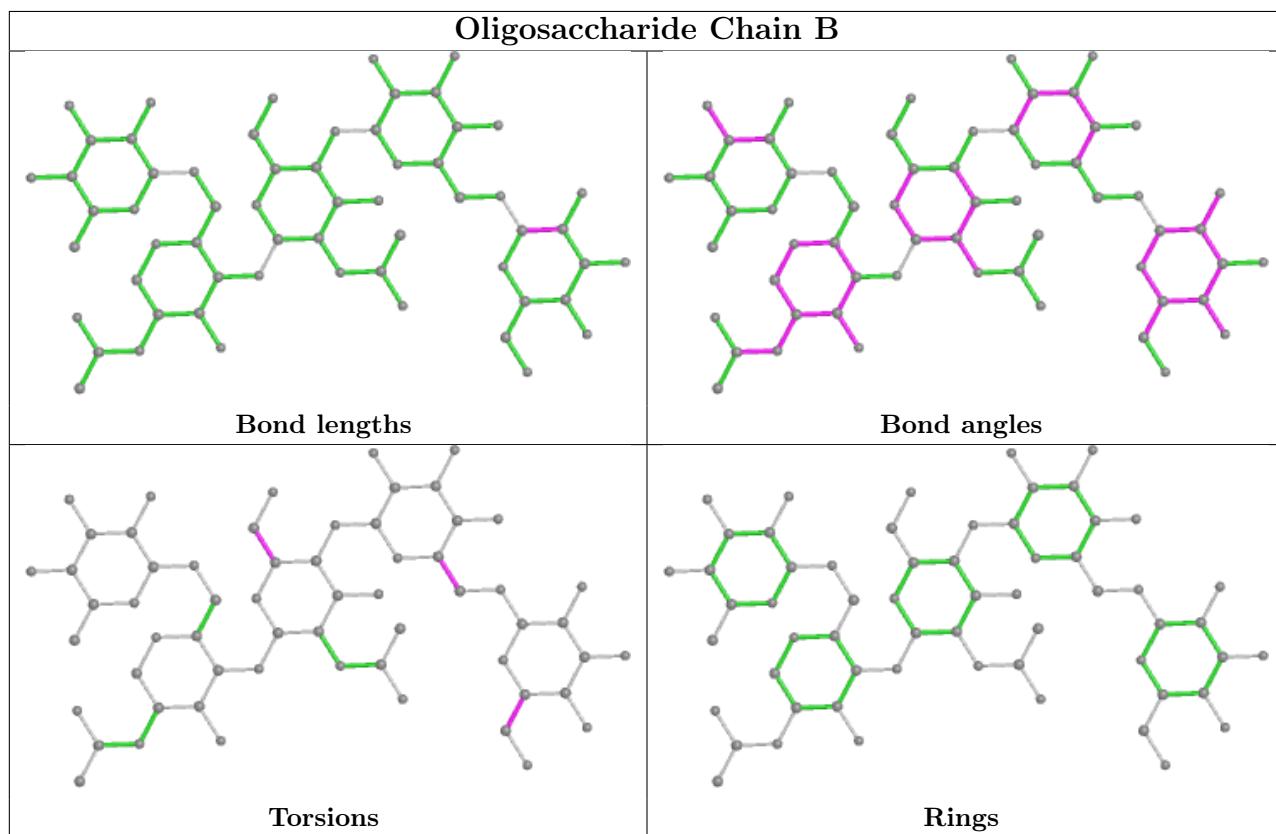
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	C4-C5-C6-O6
2	B	4	BMA	O5-C5-C6-O6
2	B	4	BMA	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

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

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

1 ligand is 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	A	408	1	14,14,15	0.49	0	17,19,21	3.03	8 (47%)

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	A	408	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	408	NAG	C1-O5-C5	7.21	121.96	112.19
3	A	408	NAG	C2-N2-C7	5.49	130.72	122.90
3	A	408	NAG	C8-C7-N2	4.45	123.63	116.10
3	A	408	NAG	O5-C5-C6	3.70	113.01	107.20
3	A	408	NAG	O7-C7-C8	-3.54	115.47	122.06
3	A	408	NAG	O5-C1-C2	2.80	115.71	111.29
3	A	408	NAG	O5-C5-C4	2.73	117.46	110.83
3	A	408	NAG	C3-C4-C5	2.27	114.28	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	408	NAG	C8-C7-N2-C2
3	A	408	NAG	O7-C7-N2-C2
3	A	408	NAG	C4-C5-C6-O6
3	A	408	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	408	NAG	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	377/379 (99%)	-0.48	11 (2%)	51	52	38, 64, 111, 155	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	HIS	4.0
1	A	357	VAL	3.8
1	A	359	SER	3.7
1	A	27	PRO	3.6
1	A	360	SER	3.5
1	A	336	GLU	3.0
1	A	367	SER	2.4
1	A	358	ALA	2.4
1	A	369	ARG	2.3
1	A	29	SER	2.2
1	A	28	PRO	2.1

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.
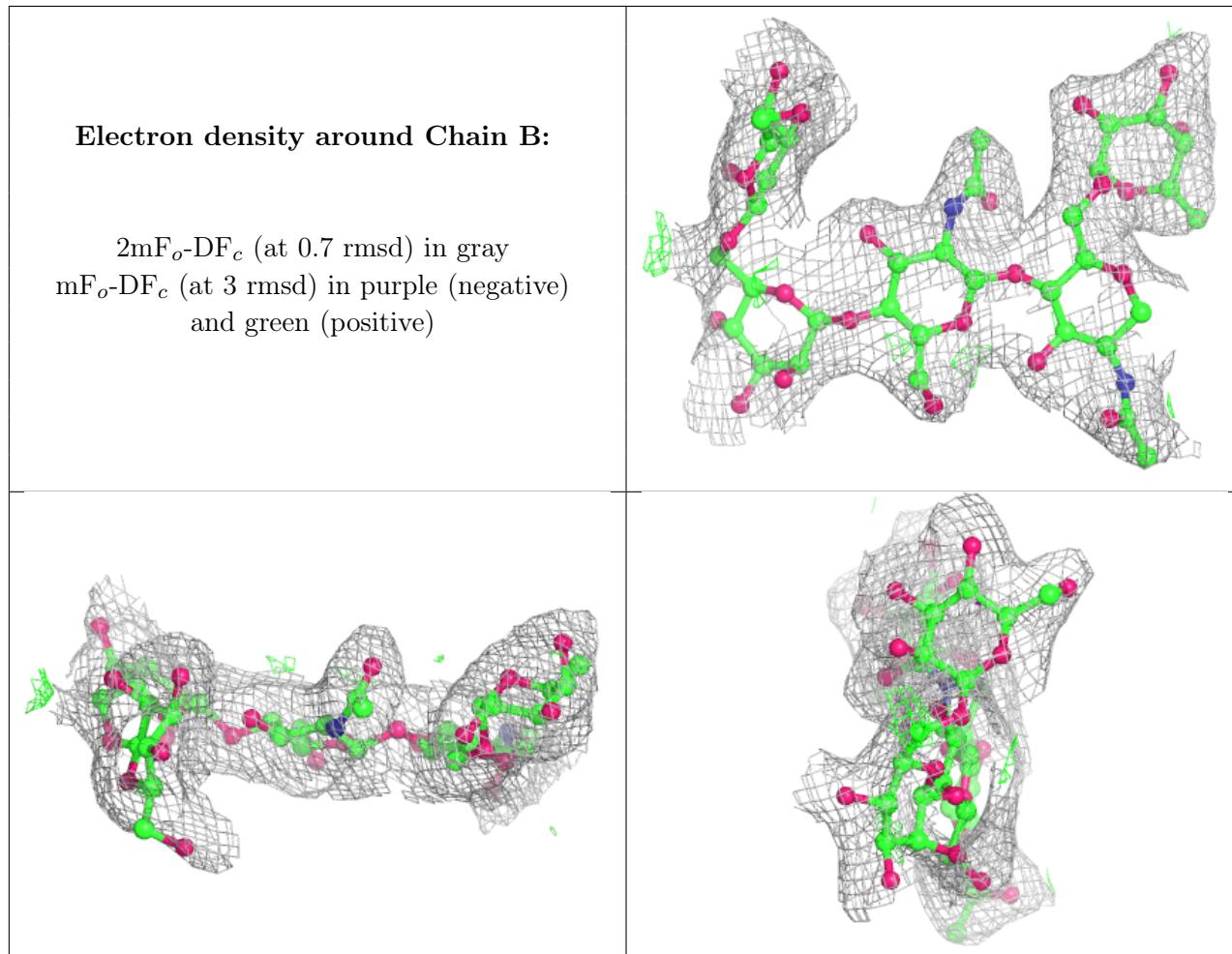
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	B	4	11/12	0.71	0.28	85,109,118,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	B	3	11/12	0.81	0.22	94,111,125,126	0
2	NAG	B	2	14/15	0.94	0.13	65,81,90,90	0
2	NAG	B	1	14/15	0.96	0.08	57,64,80,82	0
2	FUC	B	5	10/11	0.96	0.10	49,57,65,67	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.

Electron density around Chain B:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

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
3	NAG	A	408	14/15	0.91	0.14	65,88,106,122	0

6.5 Other polymers (i)

There are no such residues in this entry.