



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:00 AM UTC

PDB ID : 1N7Q / pdb_00001n7q
Title : Streptococcus pneumoniae Hyaluronate Lyase W291A/W292A Double Mutant complex with hyaluronan hexasacchride
Authors : Nukui, M.; Taylor, K.B.; McPherson, D.T.; Shigenaga, M.; Jedrzejewski, M.J.
Deposited on : 2002-11-16
Resolution : 2.30 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

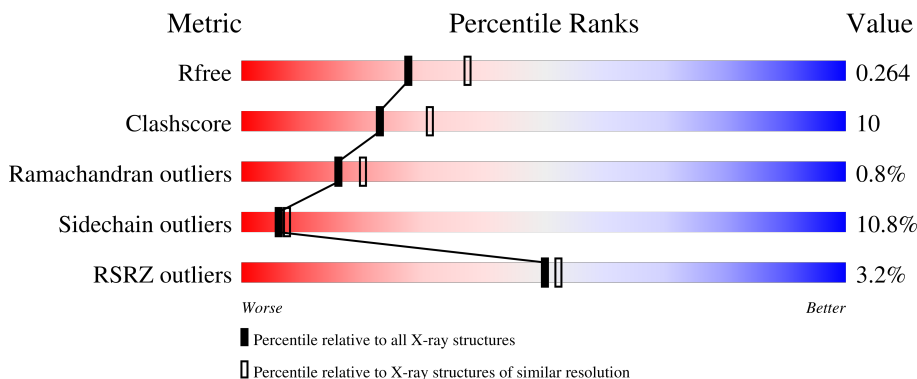
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

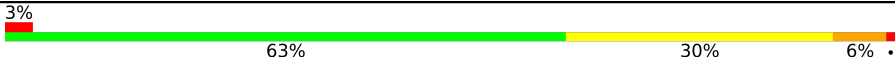
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	721	 3% 63% 30% 6%
2	B	6	 100%

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	5	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6325 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.

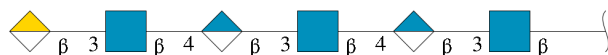
- Molecule 1 is a protein called HYALURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5766	3622	966	1156	22			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ALA	TRP	engineered mutation	GB 437705
A	292	ALA	TRP	engineered mutation	GB 437705
A	731	VAL	GLY	SEE REMARK 999	GB 437705

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			79	42	3	34			

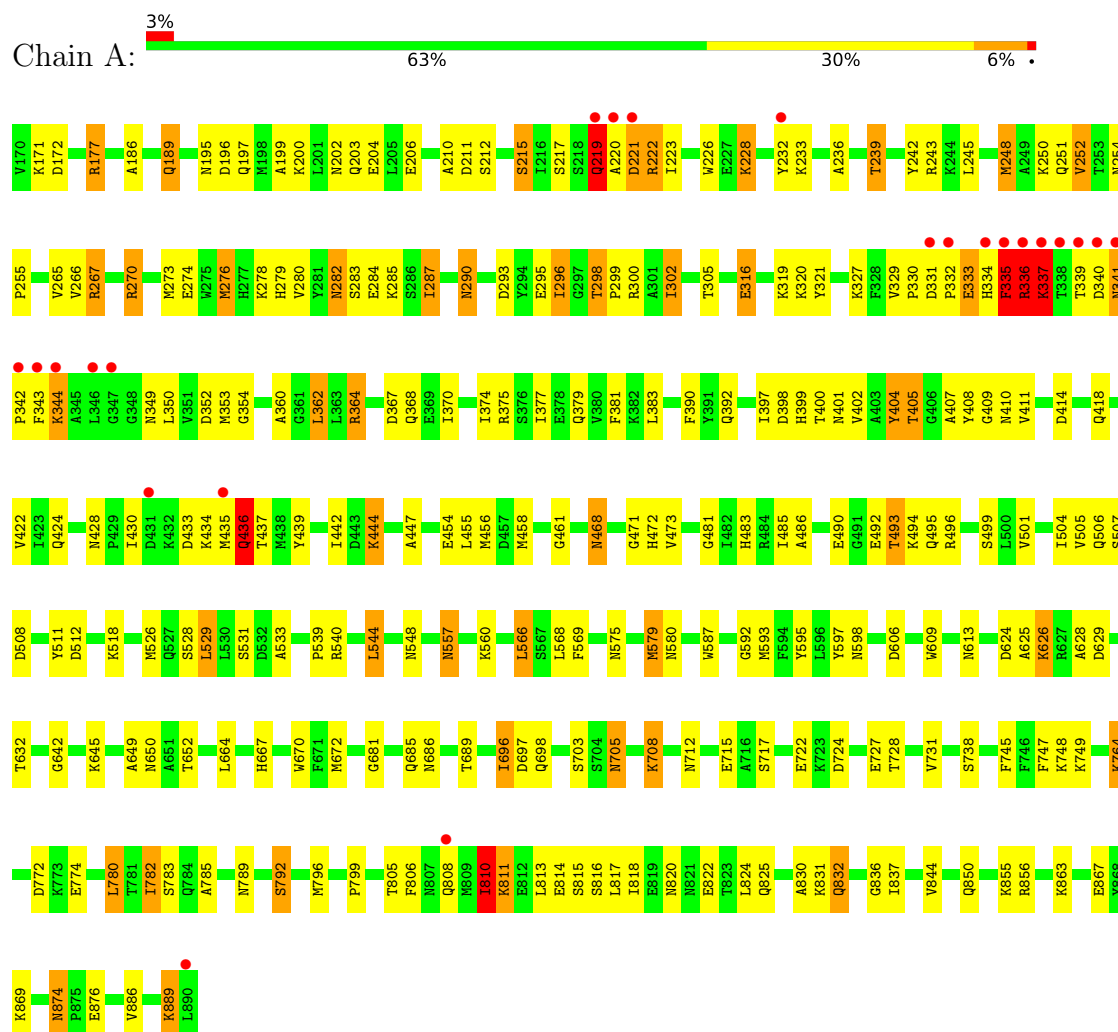
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	480	Total	O	0	0
			480	480		

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: HYALURONIDASE



• Molecule 2: beta-D-galactopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
BDP2
MAG3
BDP4
MAG5
GTR6

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.26Å 102.00Å 103.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 98.3 (20.00-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.249 0.208 , 0.264	Depositor DCC
R_{free} test set	820 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6325	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 3.91% 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: NAG, BDP, GTR

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	1.90	111/5881 (1.9%)	1.44	36/7941 (0.5%)

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	3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	MET	SD-CE	-24.24	1.19	1.79
1	A	579	MET	SD-CE	9.36	2.02	1.79
1	A	248	MET	SD-CE	9.13	2.02	1.79
1	A	447	ALA	CA-CB	-8.73	1.46	1.54
1	A	697	ASP	C-O	-8.53	1.12	1.23
1	A	727	GLU	CA-C	8.37	1.64	1.53
1	A	305	THR	C-O	-7.75	1.15	1.24
1	A	267	ARG	CB-CG	7.72	1.75	1.52
1	A	397	ILE	CA-CB	7.58	1.64	1.54
1	A	444	LYS	C-O	-7.48	1.15	1.24
1	A	844	VAL	CA-CB	7.45	1.62	1.53
1	A	511	TYR	CA-C	7.43	1.61	1.52
1	A	526	MET	C-O	-7.38	1.15	1.24
1	A	368	GLN	CG-CD	7.20	1.70	1.52
1	A	458	MET	SD-CE	6.96	1.97	1.79
1	A	280	VAL	CA-CB	6.93	1.62	1.55
1	A	512	ASP	C-O	-6.79	1.15	1.24
1	A	287	ILE	CA-CB	6.74	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	ARG	NE-CZ	6.70	1.40	1.33
1	A	267	ARG	CD-NE	6.69	1.55	1.46
1	A	223	ILE	C-O	-6.63	1.16	1.24
1	A	830	ALA	CA-CB	6.59	1.63	1.53
1	A	219	GLN	CA-C	6.53	1.61	1.52
1	A	267	ARG	CG-CD	6.53	1.72	1.52
1	A	609	TRP	C-O	6.49	1.31	1.24
1	A	808	GLN	CD-OE1	6.42	1.35	1.23
1	A	501	VAL	C-O	-6.37	1.17	1.24
1	A	473	VAL	C-O	6.37	1.31	1.24
1	A	499	SER	C-O	-6.35	1.16	1.24
1	A	341	ASN	CA-C	6.33	1.62	1.52
1	A	831	LYS	CA-C	6.32	1.61	1.52
1	A	200	LYS	CA-C	6.31	1.60	1.52
1	A	302	ILE	CA-CB	-6.29	1.47	1.54
1	A	436	GLN	N-CA	6.26	1.54	1.46
1	A	531	SER	C-O	-6.24	1.15	1.24
1	A	370	ILE	CA-C	6.22	1.60	1.52
1	A	236	ALA	CA-CB	6.21	1.64	1.53
1	A	342	PRO	CA-C	6.17	1.61	1.52
1	A	606	ASP	C-O	6.14	1.31	1.23
1	A	628	ALA	CA-C	6.07	1.60	1.52
1	A	265	VAL	CA-CB	6.05	1.61	1.54
1	A	418	GLN	C-O	-6.02	1.17	1.24
1	A	341	ASN	N-CA	5.99	1.52	1.46
1	A	290	ASN	CA-C	5.98	1.60	1.52
1	A	785	ALA	CA-CB	5.96	1.63	1.53
1	A	505	VAL	CA-CB	5.96	1.61	1.54
1	A	507	SER	C-O	-5.96	1.16	1.24
1	A	336	ARG	CA-C	5.95	1.60	1.52
1	A	352	ASP	CA-C	5.91	1.60	1.52
1	A	210	ALA	N-CA	5.89	1.53	1.46
1	A	442	ILE	C-O	-5.89	1.17	1.24
1	A	506	GLN	C-O	-5.89	1.16	1.24
1	A	876	GLU	C-O	-5.89	1.17	1.24
1	A	824	LEU	CA-C	5.87	1.59	1.52
1	A	362	LEU	CA-C	5.86	1.60	1.52
1	A	189	GLN	CG-CD	5.86	1.66	1.52
1	A	632	THR	CA-CB	5.80	1.63	1.53
1	A	544	LEU	N-CA	-5.80	1.39	1.46
1	A	649	ALA	CA-CB	5.74	1.62	1.54
1	A	270	ARG	CD-NE	-5.73	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	ILE	CA-CB	5.72	1.61	1.54
1	A	529	LEU	CA-C	5.69	1.60	1.52
1	A	818	ILE	C-O	-5.66	1.17	1.23
1	A	598	ASN	CG-ND2	5.60	1.45	1.33
1	A	652	THR	C-O	-5.59	1.17	1.23
1	A	705	ASN	CB-CG	5.57	1.66	1.52
1	A	811	LYS	CG-CD	5.52	1.69	1.52
1	A	645	LYS	C-O	-5.51	1.17	1.24
1	A	889	LYS	CG-CD	5.47	1.68	1.52
1	A	186	ALA	N-CA	5.43	1.53	1.46
1	A	172	ASP	C-O	-5.43	1.20	1.24
1	A	731	VAL	C-O	5.42	1.29	1.24
1	A	287	ILE	CA-C	5.41	1.58	1.52
1	A	405	THR	CA-C	5.38	1.59	1.52
1	A	204	GLU	CA-C	5.37	1.59	1.52
1	A	764	LYS	C-O	-5.36	1.17	1.24
1	A	255	PRO	CA-C	5.35	1.60	1.52
1	A	353	MET	SD-CE	5.34	1.92	1.79
1	A	468	ASN	CB-CG	5.31	1.65	1.52
1	A	344	LYS	CA-C	5.30	1.59	1.52
1	A	626	LYS	CG-CD	5.28	1.68	1.52
1	A	810	ILE	C-O	-5.28	1.17	1.24
1	A	796	MET	SD-CE	-5.26	1.66	1.79
1	A	816	SER	C-O	-5.25	1.17	1.24
1	A	782	ILE	C-O	5.23	1.29	1.24
1	A	747	PHE	C-O	-5.23	1.18	1.24
1	A	696	ILE	N-CA	5.22	1.53	1.46
1	A	728	THR	N-CA	5.20	1.52	1.46
1	A	242	TYR	CA-C	5.20	1.59	1.52
1	A	508	ASP	CA-CB	5.19	1.59	1.53
1	A	405	THR	C-O	5.18	1.30	1.24
1	A	505	VAL	CA-C	5.17	1.59	1.52
1	A	811	LYS	CD-CE	5.17	1.68	1.52
1	A	199	ALA	C-O	-5.14	1.17	1.24
1	A	533	ALA	CA-CB	5.13	1.61	1.53
1	A	856	ARG	C-O	-5.13	1.17	1.23
1	A	390	PHE	C-O	-5.10	1.17	1.23
1	A	504	ILE	CA-CB	5.10	1.60	1.54
1	A	210	ALA	C-O	-5.09	1.18	1.24
1	A	221	ASP	CA-C	5.08	1.59	1.52
1	A	539	PRO	C-O	-5.08	1.17	1.23
1	A	228	LYS	CG-CD	5.07	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	799	PRO	CA-C	5.06	1.58	1.52
1	A	367	ASP	C-O	-5.06	1.18	1.24
1	A	672	MET	C-O	-5.06	1.17	1.24
1	A	233	LYS	CA-C	5.05	1.59	1.52
1	A	806	PHE	CA-C	5.03	1.59	1.52
1	A	334	HIS	CA-C	5.03	1.58	1.52
1	A	629	ASP	C-O	5.03	1.30	1.24
1	A	468	ASN	CA-C	5.02	1.59	1.52
1	A	197	GLN	N-CA	5.01	1.52	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	886	VAL	N-CA-C	8.09	121.46	113.53
1	A	792	SER	CA-CB-OG	-7.52	96.06	111.10
1	A	642	GLY	N-CA-C	7.46	121.45	110.63
1	A	267	ARG	CA-CB-CG	7.14	128.38	114.10
1	A	270	ARG	NE-CZ-NH2	-7.06	112.84	119.20
1	A	832	GLN	N-CA-C	-6.80	105.14	113.50
1	A	195	ASN	CB-CA-C	6.61	121.35	110.78
1	A	867	GLU	N-CA-C	6.56	119.78	110.14
1	A	540	ARG	NE-CZ-NH1	-6.43	115.06	121.50
1	A	245	LEU	N-CA-C	6.06	117.96	111.36
1	A	493	THR	N-CA-CB	6.03	119.08	110.16
1	A	548	ASN	N-CA-C	5.96	118.54	111.33
1	A	333	GLU	N-CA-C	5.96	120.61	113.23
1	A	368	GLN	CB-CG-CD	5.80	122.47	112.60
1	A	401	ASN	N-CA-C	5.72	119.38	111.71
1	A	471	GLY	N-CA-C	5.71	119.80	112.83
1	A	566	LEU	CA-C-N	5.54	129.79	122.42
1	A	566	LEU	C-N-CA	5.54	129.79	122.42
1	A	341	ASN	N-CA-C	5.51	118.41	108.55
1	A	270	ARG	CG-CD-NE	-5.45	100.00	112.00
1	A	342	PRO	N-CA-C	5.45	123.70	112.47
1	A	266	VAL	CA-C-N	5.43	127.87	120.54
1	A	266	VAL	C-N-CA	5.43	127.87	120.54
1	A	337	LYS	N-CA-C	5.41	118.97	112.38
1	A	343	PHE	N-CA-C	5.39	117.46	109.69
1	A	724	ASP	CB-CA-C	5.39	118.42	109.53
1	A	609	TRP	N-CA-C	5.24	119.87	112.75
1	A	402	VAL	N-CA-C	5.20	115.45	108.17
1	A	335	PHE	N-CA-C	5.20	117.09	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ASP	N-CA-C	5.19	116.98	110.24
1	A	195	ASN	CA-C-N	5.14	127.48	120.54
1	A	195	ASN	C-N-CA	5.14	127.48	120.54
1	A	266	VAL	CA-C-O	-5.13	115.73	121.17
1	A	270	ARG	CD-NE-CZ	5.04	131.46	124.40
1	A	805	THR	N-CA-C	5.03	116.45	111.07
1	A	270	ARG	NE-CZ-NH1	5.01	126.51	121.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	GLN	Peptide
1	A	220	ALA	Peptide
1	A	270	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	A	5766	0	5585	119	1
2	B	79	0	51	27	0
3	A	480	0	0	5	0
All	All	6325	0	5636	119	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 (119) 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:267:ARG:CB	1:A:267:ARG:CG	1.75	1.62
1:A:579:MET:SD	1:A:579:MET:CE	2.03	1.47
1:A:248:MET:SD	1:A:248:MET:CE	2.02	1.45
1:A:276:MET:CE	1:A:276:MET:SD	1.18	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:CE1	2:B:3:NAG:H82	1.75	1.19
1:A:276:MET:SD	1:A:276:MET:HE2	1.76	1.16
1:A:276:MET:SD	1:A:276:MET:HE3	1.76	1.10
1:A:276:MET:SD	1:A:276:MET:HE1	1.76	1.07
1:A:276:MET:CE	1:A:276:MET:CG	2.40	1.00
1:A:613:ASN:H	1:A:698:GLN:HE22	1.13	0.95
1:A:580:ASN:ND2	2:B:2:BDP:O3	2.01	0.92
1:A:408:TYR:CE1	2:B:3:NAG:C8	2.56	0.88
1:A:483:HIS:NE2	1:A:529:LEU:HG	1.91	0.85
1:A:414:ASP:OD2	2:B:5:NAG:O6	2.05	0.74
1:A:217:SER:HB3	1:A:222:ARG:HD2	1.67	0.74
1:A:408:TYR:CD1	2:B:3:NAG:H82	2.23	0.74
1:A:874:ASN:C	1:A:874:ASN:HD22	1.96	0.73
1:A:316:GLU:H	1:A:316:GLU:CD	1.97	0.73
1:A:243:ARG:HH12	2:B:4:BDP:C6	2.03	0.70
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.56	0.70
1:A:243:ARG:HD3	2:B:5:NAG:H82	1.72	0.69
1:A:557:ASN:HD22	1:A:557:ASN:C	2.01	0.67
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.75	0.67
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.59	0.66
1:A:202:ASN:ND2	1:A:251:GLN:HE22	1.94	0.66
1:A:243:ARG:HD3	2:B:5:NAG:C8	2.26	0.65
1:A:243:ARG:NH2	2:B:5:NAG:H83	2.14	0.62
1:A:250:LYS:HZ1	2:B:6:GTR:C3	2.11	0.62
1:A:296:ILE:HD11	1:A:335:PHE:CZ	2.35	0.61
1:A:414:ASP:OD2	2:B:5:NAG:C6	2.48	0.61
1:A:483:HIS:NE2	1:A:529:LEU:CG	2.63	0.61
1:A:374:ILE:HG23	1:A:430:ILE:HD11	1.82	0.61
1:A:439:TYR:CZ	3:A:1268:HOH:O	2.51	0.61
1:A:243:ARG:HH22	2:B:4:BDP:C6	2.14	0.60
1:A:587:TRP:O	3:A:901:HOH:O	2.16	0.59
1:A:350:LEU:HD21	1:A:379:GLN:HG2	1.85	0.57
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.36	0.56
1:A:850:GLN:HE21	1:A:863:LYS:HE3	1.69	0.56
1:A:243:ARG:CZ	2:B:5:NAG:HN2	2.20	0.55
1:A:254:ASN:C	1:A:254:ASN:HD22	2.15	0.54
1:A:300:ARG:HH22	2:B:5:NAG:H4	1.73	0.54
1:A:336:ARG:HH12	2:B:1:NAG:H4	1.73	0.54
1:A:360:ALA:O	1:A:364:ARG:HG3	2.08	0.54
1:A:481:GLY:O	1:A:485:ILE:HG12	2.08	0.54
1:A:414:ASP:OD2	2:B:5:NAG:H61	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.57	0.53
1:A:874:ASN:C	1:A:874:ASN:ND2	2.66	0.53
1:A:336:ARG:HH22	2:B:1:NAG:H4	1.73	0.53
1:A:337:LYS:O	1:A:337:LYS:HD3	2.09	0.53
1:A:243:ARG:NH2	2:B:4:BDP:O6B	2.32	0.52
1:A:407:ALA:O	1:A:411:VAL:HG23	2.10	0.52
1:A:708:LYS:HE3	1:A:715:GLU:OE2	2.09	0.52
1:A:222:ARG:HH11	1:A:222:ARG:CG	2.23	0.51
1:A:316:GLU:CD	1:A:316:GLU:N	2.68	0.51
1:A:287:ILE:HD12	1:A:339:THR:CG2	2.40	0.51
1:A:349:ASN:ND2	3:A:910:HOH:O	2.44	0.51
1:A:557:ASN:ND2	1:A:560:LYS:H	2.09	0.49
1:A:296:ILE:CD1	1:A:335:PHE:CZ	2.95	0.49
1:A:569:PHE:CE2	1:A:575:ASN:HB3	2.47	0.49
1:A:250:LYS:NZ	2:B:6:GTR:C3	2.76	0.48
1:A:580:ASN:HD21	2:B:2:BDP:C3	2.21	0.48
1:A:211:ASP:O	1:A:215:SER:HB2	2.13	0.48
1:A:337:LYS:O	1:A:337:LYS:CD	2.62	0.48
1:A:557:ASN:C	1:A:557:ASN:ND2	2.71	0.48
1:A:408:TYR:CD1	2:B:3:NAG:C8	2.92	0.47
1:A:295:GLU:C	1:A:296:ILE:HD12	2.39	0.47
1:A:274:GLU:OE2	1:A:321:TYR:OH	2.25	0.47
1:A:273:MET:HE1	1:A:302:ILE:HG12	1.96	0.47
1:A:298:THR:HB	1:A:299:PRO:HD3	1.97	0.47
1:A:177:ARG:HG3	1:A:422:VAL:HG13	1.97	0.46
1:A:282:ASN:C	1:A:282:ASN:HD22	2.24	0.46
1:A:486:ALA:O	1:A:494:LYS:HG3	2.15	0.46
1:A:745:PHE:HB2	1:A:810:ILE:HG22	1.96	0.46
1:A:276:MET:CE	1:A:276:MET:HG2	2.42	0.46
1:A:566:LEU:HD11	1:A:670:TRP:CE2	2.51	0.46
1:A:283:SER:O	1:A:327:LYS:NZ	2.41	0.45
1:A:202:ASN:O	1:A:206:GLU:HG2	2.17	0.45
1:A:579:MET:CE	1:A:579:MET:CG	2.91	0.45
1:A:686:ASN:H	1:A:789:ASN:ND2	2.14	0.45
1:A:250:LYS:HZ3	2:B:6:GTR:C4	2.29	0.45
1:A:624:ASP:O	1:A:625:ALA:C	2.60	0.44
1:A:202:ASN:HD21	1:A:251:GLN:HE22	1.62	0.44
1:A:430:ILE:CG2	1:A:435:MET:CE	2.95	0.44
1:A:439:TYR:CE1	3:A:1268:HOH:O	2.69	0.44
1:A:667:HIS:O	1:A:681:GLY:HA2	2.17	0.44
1:A:764:LYS:HD2	1:A:772:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:CE1	2:B:2:BDP:C6	3.00	0.44
1:A:544:LEU:C	1:A:544:LEU:HD23	2.42	0.44
1:A:568:LEU:HD23	1:A:592:GLY:HA2	2.00	0.44
1:A:399:HIS:O	1:A:400:THR:HB	2.18	0.44
1:A:454:GLU:HB2	1:A:472:HIS:CE1	2.53	0.44
1:A:243:ARG:NH1	2:B:4:BDP:O6A	2.49	0.43
1:A:248:MET:O	1:A:252:VAL:HB	2.18	0.43
1:A:483:HIS:NE2	1:A:529:LEU:HB2	2.33	0.43
1:A:282:ASN:ND2	1:A:285:LYS:HG2	2.34	0.43
1:A:780:LEU:C	1:A:780:LEU:HD12	2.44	0.43
1:A:410:ASN:HD21	1:A:455:LEU:CD2	2.31	0.43
1:A:331:ASP:OD1	1:A:332:PRO:HD2	2.19	0.43
1:A:212:SER:HB3	1:A:226:TRP:CZ2	2.54	0.43
1:A:381:PHE:O	1:A:437:THR:HG21	2.19	0.43
1:A:569:PHE:CD2	1:A:575:ASN:HB3	2.53	0.42
1:A:836:GLY:C	1:A:837:ILE:HG13	2.45	0.42
1:A:250:LYS:NZ	2:B:6:GTR:C4	2.83	0.42
1:A:405:THR:O	1:A:409:GLY:HA3	2.20	0.42
1:A:295:GLU:OE2	1:A:336:ARG:HA	2.20	0.42
1:A:593:MET:HE2	1:A:595:TYR:CZ	2.54	0.42
1:A:239:THR:HG21	1:A:293:ASP:OD2	2.20	0.42
1:A:430:ILE:HG22	1:A:435:MET:CE	2.49	0.42
1:A:278:LYS:HG2	1:A:279:HIS:CD2	2.56	0.41
1:A:267:ARG:CB	1:A:267:ARG:CD	2.90	0.41
1:A:177:ARG:HB3	1:A:362:LEU:HD13	2.03	0.41
1:A:444:LYS:NZ	3:A:939:HOH:O	2.53	0.41
1:A:483:HIS:NE2	1:A:529:LEU:CB	2.83	0.41
1:A:664:LEU:HA	1:A:685:GLN:O	2.20	0.41
1:A:404:TYR:CE1	1:A:461:GLY:HA3	2.55	0.41
1:A:696:ILE:N	1:A:782:ILE:O	2.54	0.40
1:A:290:ASN:ND2	2:B:2:BDP:O3	2.55	0.40
1:A:456:MET:HG2	1:A:597:TYR:CE2	2.57	0.40
1:A:408:TYR:CZ	2:B:3:NAG:C8	3.04	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)
1:A:340:ASP:O	1:A:815:SER:OG[4_546]	2.19	0.01

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	719/721 (100%)	675 (94%)	38 (5%)	6 (1%)	16 20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	336	ARG
1	A	436	GLN
1	A	712	ASN
1	A	330	PRO
1	A	428	ASN

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	636/638 (100%)	567 (89%)	69 (11%)	6 7

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LYS
1	A	177	ARG
1	A	189	GLN
1	A	196	ASP
1	A	203	GLN

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Mol	Chain	Res	Type
1	A	215	SER
1	A	221	ASP
1	A	222	ARG
1	A	228	LYS
1	A	232	TYR
1	A	239	THR
1	A	252	VAL
1	A	282	ASN
1	A	284	GLU
1	A	296	ILE
1	A	298	THR
1	A	316	GLU
1	A	319	LYS
1	A	320	LYS
1	A	329	VAL
1	A	333	GLU
1	A	335	PHE
1	A	336	ARG
1	A	337	LYS
1	A	341	ASN
1	A	344	LYS
1	A	364	ARG
1	A	375	ARG
1	A	383	LEU
1	A	392	GLN
1	A	398	ASP
1	A	404	TYR
1	A	424	GLN
1	A	433	ASP
1	A	434	LYS
1	A	436	GLN
1	A	468	ASN
1	A	490	GLU
1	A	492	GLU
1	A	493	THR
1	A	495	GLN
1	A	496	ARG
1	A	518	LYS
1	A	528	SER
1	A	557	ASN
1	A	626	LYS
1	A	689	THR

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Mol	Chain	Res	Type
1	A	703	SER
1	A	705	ASN
1	A	708	LYS
1	A	717	SER
1	A	722	GLU
1	A	738	SER
1	A	748	LYS
1	A	749	LYS
1	A	774	GLU
1	A	780	LEU
1	A	783	SER
1	A	792	SER
1	A	810	ILE
1	A	811	LYS
1	A	813	LEU
1	A	814	GLU
1	A	817	LEU
1	A	822	GLU
1	A	855	LYS
1	A	869	LYS
1	A	874	ASN
1	A	889	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	251	GLN
1	A	254	ASN
1	A	277	HIS
1	A	282	ASN
1	A	341	ASN
1	A	349	ASN
1	A	436	GLN
1	A	498	GLN
1	A	557	ASN
1	A	578	HIS
1	A	580	ASN
1	A	583	ASN
1	A	662	GLN
1	A	685	GLN
1	A	698	GLN

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Mol	Chain	Res	Type
1	A	759	GLN
1	A	789	ASN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN
1	A	850	GLN
1	A	874	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 ⓘ

6 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	15,15,15	2.12	5 (33%)	21,21,21	1.16	2 (9%)
2	BDP	B	2	2	12,12,13	3.64	5 (41%)	14,17,19	1.74	4 (28%)
2	NAG	B	3	2	14,14,15	2.38	6 (42%)	17,19,21	1.10	2 (11%)
2	BDP	B	4	2	12,12,13	3.76	5 (41%)	14,17,19	2.12	4 (28%)
2	NAG	B	5	2	14,14,15	2.50	7 (50%)	17,19,21	1.23	2 (11%)
2	GTR	B	6	2	12,12,13	5.55	4 (33%)	14,17,19	4.29	7 (50%)

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	-	2/6/26/26	0/1/1/1
2	BDP	B	2	2	-	2/4/21/24	0/1/1/1
2	NAG	B	3	2	-	0/6/23/26	0/1/1/1
2	BDP	B	4	2	-	2/4/21/24	0/1/1/1
2	NAG	B	5	2	-	4/6/23/26	0/1/1/1
2	GTR	B	6	2	-	0/4/21/24	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	GTR	O4-C4	-14.64	1.06	1.43
2	B	6	GTR	C4-C5	-10.45	1.36	1.53
2	B	4	BDP	C5-C6	-8.29	1.35	1.53
2	B	2	BDP	C5-C6	-7.63	1.37	1.53
2	B	2	BDP	C4-C5	7.18	1.65	1.53
2	B	4	BDP	C4-C5	6.87	1.64	1.53
2	B	2	BDP	O5-C5	5.39	1.54	1.43
2	B	3	NAG	O5-C1	5.35	1.52	1.43
2	B	6	GTR	O5-C5	5.21	1.53	1.43
2	B	5	NAG	O5-C1	4.91	1.51	1.43
2	B	4	BDP	O5-C5	4.87	1.53	1.43
2	B	1	NAG	C2-N2	4.29	1.52	1.45
2	B	5	NAG	C2-N2	3.64	1.52	1.46
2	B	1	NAG	O5-C1	3.59	1.51	1.42
2	B	3	NAG	C1-C2	3.44	1.57	1.52
2	B	6	GTR	C5-C6	-3.32	1.46	1.53
2	B	5	NAG	C4-C5	3.20	1.59	1.53
2	B	3	NAG	O5-C5	3.20	1.49	1.43
2	B	5	NAG	O5-C5	3.14	1.49	1.43
2	B	1	NAG	C4-C5	3.08	1.59	1.53
2	B	5	NAG	C7-N2	3.02	1.44	1.34
2	B	4	BDP	C2-C3	2.99	1.57	1.52
2	B	5	NAG	C1-C2	2.96	1.56	1.52
2	B	1	NAG	C1-C2	2.94	1.56	1.52
2	B	3	NAG	C2-N2	2.88	1.51	1.46
2	B	3	NAG	C4-C5	2.75	1.58	1.53
2	B	2	BDP	C2-C3	2.16	1.55	1.52
2	B	2	BDP	O4-C4	2.16	1.48	1.43
2	B	5	NAG	C4-C3	2.09	1.57	1.52
2	B	4	BDP	O4-C4	2.08	1.48	1.43
2	B	1	NAG	O5-C5	2.07	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	NAG	C7-N2	2.04	1.40	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	GTR	C2-C3-C4	11.97	131.91	110.86
2	B	6	GTR	O4-C4-C3	7.33	127.65	110.38
2	B	4	BDP	O4-C4-C5	-4.26	100.03	109.76
2	B	6	GTR	O4-C4-C5	4.00	118.90	109.76
2	B	6	GTR	C1-C2-C3	-4.00	103.82	109.64
2	B	4	BDP	O4-C4-C3	3.71	119.12	110.38
2	B	2	BDP	O4-C4-C5	-3.32	102.17	109.76
2	B	4	BDP	C3-C4-C5	3.19	114.78	109.30
2	B	1	NAG	C8-C7-N2	-2.81	111.47	116.12
2	B	2	BDP	C3-C4-C5	2.80	114.12	109.30
2	B	6	GTR	O5-C1-C2	-2.79	104.14	110.79
2	B	5	NAG	O7-C7-N2	2.70	126.75	121.98
2	B	6	GTR	O6B-C6-O6A	2.67	130.14	124.08
2	B	4	BDP	O6B-C6-O6A	2.63	130.06	124.08
2	B	5	NAG	C8-C7-N2	-2.55	111.89	116.12
2	B	6	GTR	O3-C3-C2	-2.43	105.10	110.05
2	B	2	BDP	O6B-C6-O6A	2.43	129.58	124.08
2	B	3	NAG	C2-N2-C7	-2.35	119.74	122.90
2	B	1	NAG	O7-C7-N2	2.32	126.08	121.98
2	B	2	BDP	O4-C4-C3	2.27	115.72	110.38
2	B	3	NAG	C8-C7-N2	-2.26	112.37	116.12

There are no chirality outliers.

All (10) torsion outliers are listed below:

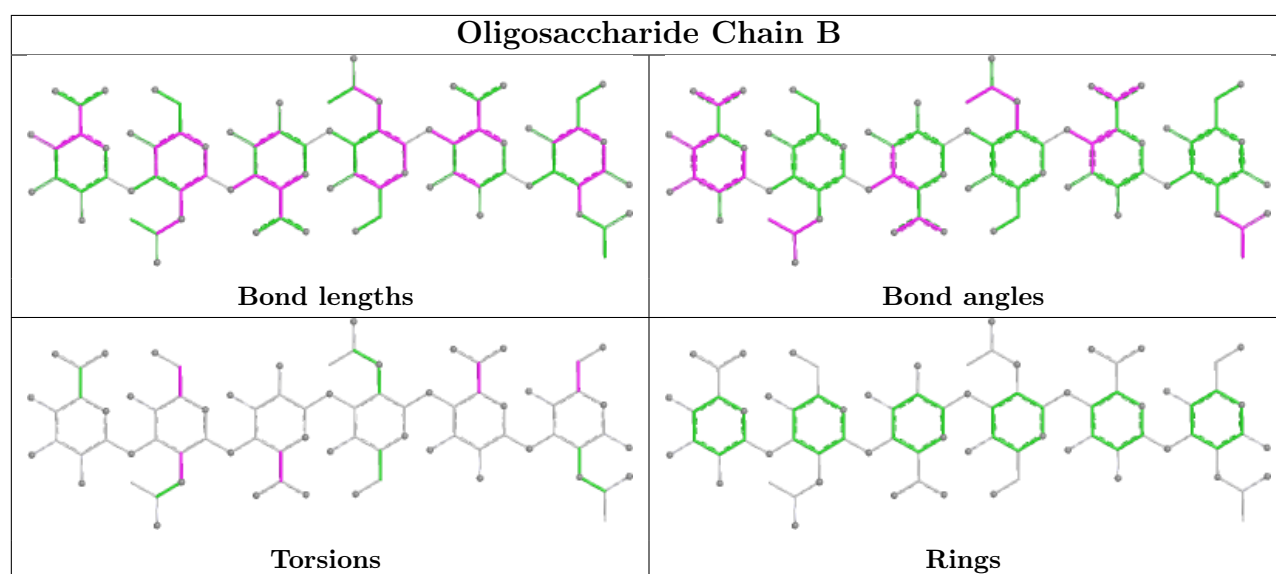
Mol	Chain	Res	Type	Atoms
2	B	2	BDP	C4-C5-C6-O6A
2	B	2	BDP	C4-C5-C6-O6B
2	B	5	NAG	C4-C5-C6-O6
2	B	5	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	5	NAG	C3-C2-N2-C7
2	B	1	NAG	C4-C5-C6-O6
2	B	5	NAG	C1-C2-N2-C7
2	B	4	BDP	O5-C5-C6-O6A
2	B	4	BDP	O5-C5-C6-O6B

There are no ring outliers.

6 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	BDP	4	0
2	B	2	BDP	4	0
2	B	3	NAG	5	0
2	B	5	NAG	8	0
2	B	6	GTR	4	0
2	B	1	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](#)

There are no ligands in this entry.

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	721/721 (100%)	0.03	23 (3%)	50 52	24, 36, 62, 129	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	HIS	4.6
1	A	338	THR	4.4
1	A	342	PRO	4.4
1	A	343	PHE	4.2
1	A	232	TYR	3.8
1	A	219	GLN	3.8
1	A	435	MET	3.7
1	A	347	GLY	3.4
1	A	335	PHE	3.3
1	A	341	ASN	3.0
1	A	340	ASP	2.9
1	A	890	LEU	2.9
1	A	344	LYS	2.8
1	A	336	ARG	2.8
1	A	332	PRO	2.8
1	A	346	LEU	2.8
1	A	221	ASP	2.7
1	A	808	GLN	2.7
1	A	337	LYS	2.7
1	A	339	THR	2.7
1	A	220	ALA	2.4
1	A	331	ASP	2.3
1	A	431	ASP	2.3

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

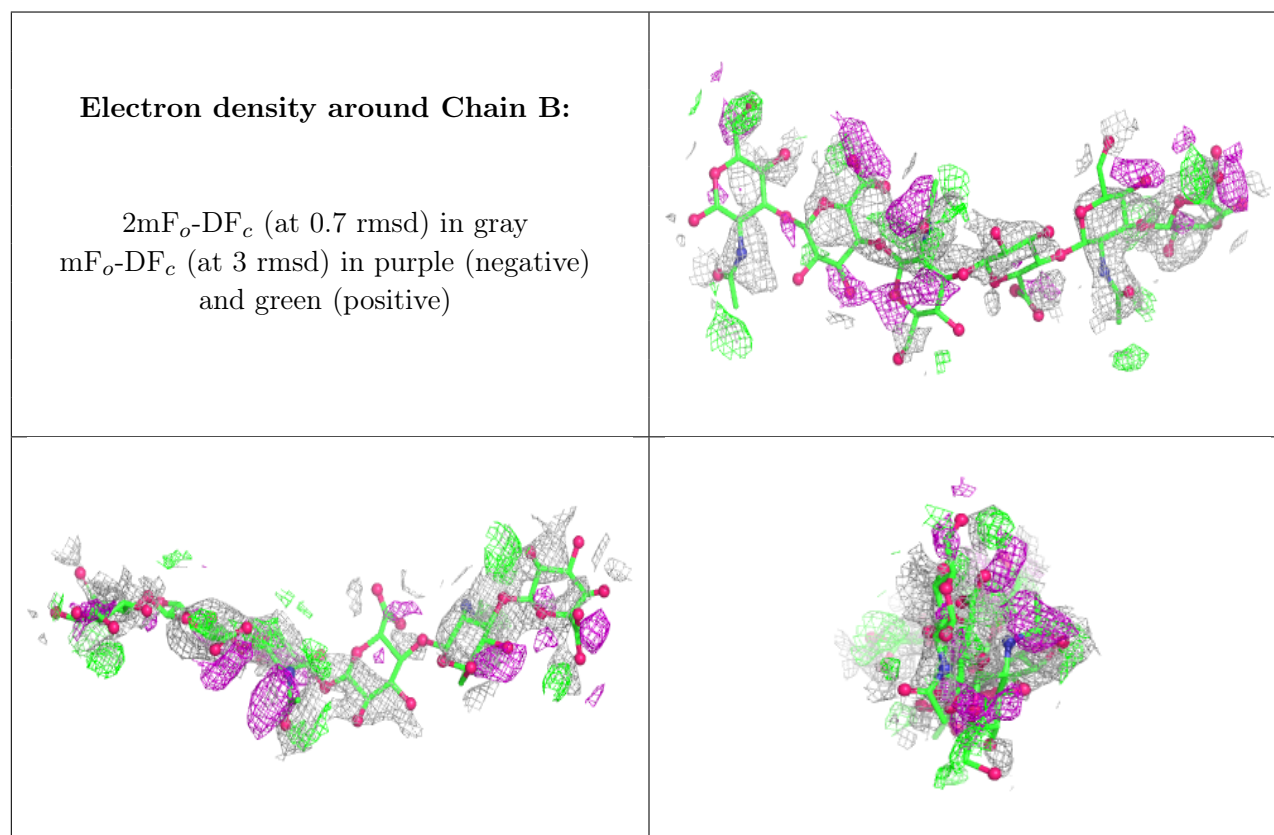
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NAG	B	3	14/15	0.35	0.34	96,105,107,109	0
2	NAG	B	1	15/15	0.46	0.24	115,118,119,119	0
2	NAG	B	5	14/15	0.49	0.26	115,117,118,119	0
2	BDP	B	2	12/13	0.50	0.28	103,108,112,113	0
2	BDP	B	4	12/13	0.59	0.22	110,111,113,115	0
2	GTR	B	6	12/13	0.64	0.27	115,119,120,120	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.