



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:51 PM UTC

PDB ID : 1C7S / pdb_00001c7s
Title : BETA-N-ACETYLHEXOSAMINIDASE MUTANT D539A COMPLEXED
WITH DI-N-ACETYL-BETA-D-GLUCOSAMINE (CHITOBIASE)
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Deposited on : 2000-03-14
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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

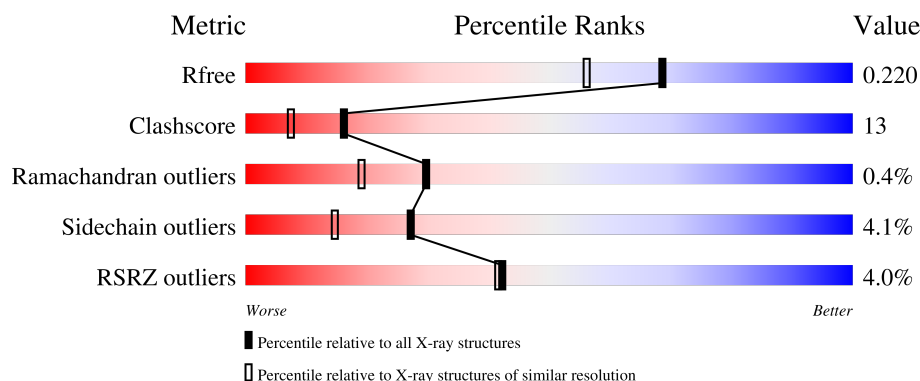
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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	A	858	4% 77% 18% ..
2	B	2	50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7656 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 BETA-N-ACETYLHEXOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	858	6786	4296	1190	1278	22	0	5	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	484	GLN	PRO	conflict	UNP Q54468
A	539	ALA	ASP	engineered mutation	UNP Q54468
A	828	GLY	ALA	conflict	UNP Q54468

- Molecule 2 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
			Total	C	N	O			
2	B	2	29	16	2	11	0	0	0

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



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

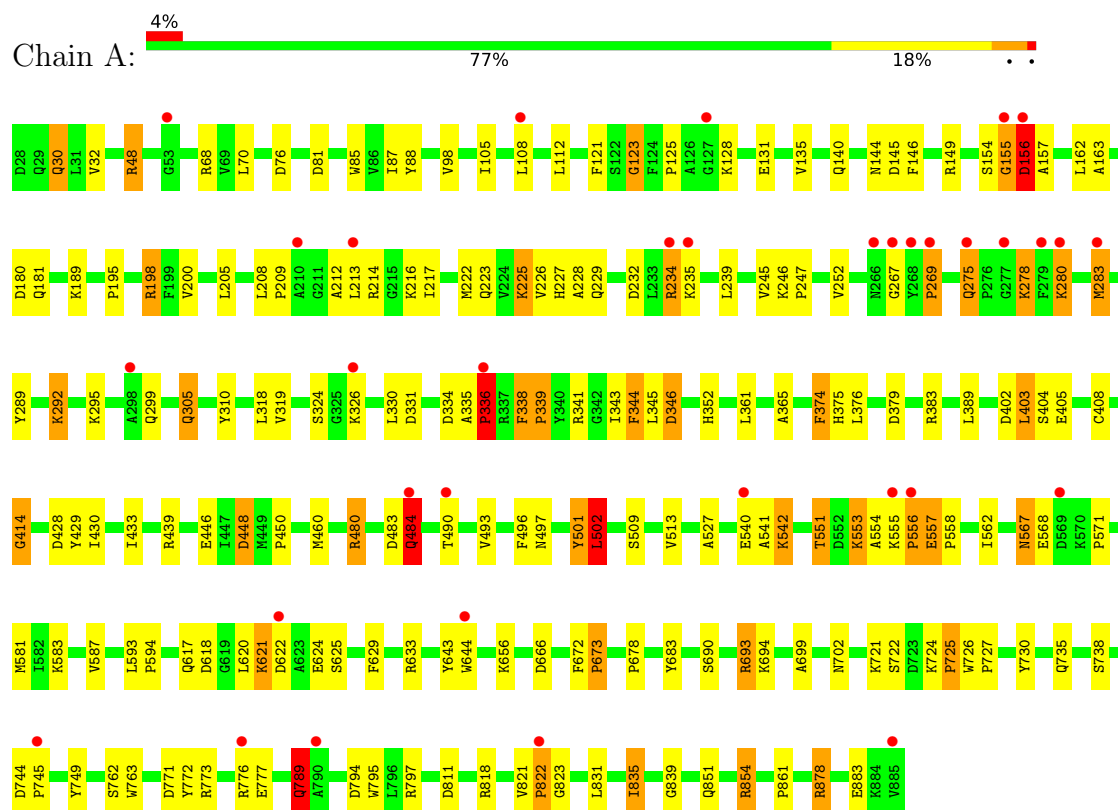
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	821	Total	O	0	0
			821	821		

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: BETA-N-ACETYLHEXOSAMINIDASE



• Molecule 2: 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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.79Å 99.96Å 86.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 15.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	86.9 (15.00-1.80) 86.7 (15.00-1.80)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.47 (at 1.80Å)	Xtriage
Refinement program	REFMAC / ARP	Depositor
R, R_{free}	0.171 , 0.224 0.178 , 0.220	Depositor DCC
R_{free} test set	8803 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7656	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: SO4, 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	0.88	3/6979 (0.0%)	1.56	93/9444 (1.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292[A]	LYS	CB-CG	-6.38	1.33	1.52
1	A	292[B]	LYS	CB-CG	-6.38	1.33	1.52
1	A	336	PRO	CA-C	-5.33	1.45	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280[A]	LYS	CG-CD-CE	16.13	148.40	111.30
1	A	280[B]	LYS	CG-CD-CE	16.13	148.40	111.30
1	A	305	GLN	OE1-CD-NE2	-10.79	111.81	122.60
1	A	229	GLN	OE1-CD-NE2	-10.60	112.00	122.60
1	A	223	GLN	OE1-CD-NE2	-10.44	112.17	122.60
1	A	338	PHE	CA-CB-CG	9.75	123.55	113.80
1	A	851	GLN	OE1-CD-NE2	-9.53	113.07	122.60
1	A	484	GLN	OE1-CD-NE2	-9.39	113.20	122.60
1	A	346	ASP	CA-CB-CG	9.27	121.87	112.60
1	A	181	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	A	794	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	48	ARG	CD-NE-CZ	7.92	135.49	124.40
1	A	556	PRO	CA-N-CD	-7.90	100.94	112.00
1	A	228	ALA	CA-C-N	-7.72	109.33	122.92
1	A	228	ALA	C-N-CA	-7.72	109.33	122.92
1	A	352	HIS	CA-CB-CG	-7.63	106.17	113.80
1	A	693	ARG	CD-NE-CZ	7.34	134.68	124.40
1	A	379	ASP	CA-C-O	-7.30	111.57	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	GLU	CB-CA-C	7.05	118.42	108.76
1	A	854	ARG	CD-NE-CZ	7.02	134.23	124.40
1	A	223	GLN	CG-CD-NE2	6.96	126.83	116.40
1	A	229	GLN	CG-CD-NE2	6.92	126.77	116.40
1	A	30	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	A	555	LYS	O-C-N	6.83	127.11	121.44
1	A	484	GLN	O-C-N	6.82	130.20	122.22
1	A	738	SER	N-CA-C	6.76	121.20	112.41
1	A	484	GLN	CG-CD-NE2	6.73	126.50	116.40
1	A	76	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	144	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	305	GLN	CG-CD-NE2	6.61	126.31	116.40
1	A	146	PHE	CA-CB-CG	-6.56	107.24	113.80
1	A	851	GLN	CG-CD-NE2	6.55	126.22	116.40
1	A	379	ASP	CA-C-N	-6.48	112.29	122.65
1	A	379	ASP	C-N-CA	-6.48	112.29	122.65
1	A	181	GLN	CG-CD-NE2	6.45	126.07	116.40
1	A	699	ALA	CA-C-N	6.35	125.97	119.56
1	A	699	ALA	C-N-CA	6.35	125.97	119.56
1	A	339	PRO	N-CA-CB	6.34	109.59	103.51
1	A	839	GLY	N-CA-C	-6.24	106.91	113.58
1	A	789	GLN	CB-CG-CD	6.17	123.09	112.60
1	A	480	ARG	CD-NE-CZ	6.10	132.94	124.40
1	A	617	GLN	N-CA-C	6.05	118.66	111.33
1	A	403	LEU	CA-C-N	-6.04	113.13	122.49
1	A	403	LEU	C-N-CA	-6.04	113.13	122.49
1	A	338	PHE	CA-C-N	6.01	125.63	119.56
1	A	338	PHE	C-N-CA	6.01	125.63	119.56
1	A	483	ASP	CA-C-N	5.91	128.79	120.28
1	A	483	ASP	C-N-CA	5.91	128.79	120.28
1	A	823	GLY	N-CA-C	-5.87	100.25	110.71
1	A	335	ALA	O-C-N	5.82	126.37	121.83
1	A	310	TYR	CA-C-O	5.74	126.57	119.97
1	A	345	LEU	CA-C-O	5.69	127.14	120.20
1	A	811	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	702	ASN	OD1-CG-ND2	5.55	128.15	122.60
1	A	878	ARG	NE-CZ-NH2	-5.54	114.22	119.20
1	A	554	ALA	O-C-N	5.52	127.97	122.12
1	A	557	GLU	N-CA-C	-5.51	102.00	110.32
1	A	414	GLY	O-C-N	5.47	127.55	122.57
1	A	379	ASP	O-C-N	5.43	128.95	122.27
1	A	725	PRO	N-CA-CB	5.43	108.38	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	878	ARG	CD-NE-CZ	5.37	131.92	124.40
1	A	162	LEU	N-CA-C	-5.37	101.42	109.15
1	A	383	ARG	CA-C-N	-5.36	115.54	122.99
1	A	383	ARG	C-N-CA	-5.36	115.54	122.99
1	A	556	PRO	N-CA-C	5.35	118.88	110.80
1	A	163	ALA	N-CA-C	5.34	117.79	111.33
1	A	555	LYS	CA-C-N	5.33	125.50	119.90
1	A	555	LYS	C-N-CA	5.33	125.50	119.90
1	A	389	LEU	CA-C-N	5.30	125.11	119.28
1	A	389	LEU	C-N-CA	5.30	125.11	119.28
1	A	344	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	343	ILE	N-CA-CB	5.27	118.98	111.82
1	A	123	GLY	N-CA-C	5.21	118.12	112.29
1	A	239	LEU	N-CA-C	5.20	117.09	108.20
1	A	821	VAL	O-C-N	5.19	127.01	121.10
1	A	376	LEU	N-CA-C	5.18	119.45	113.18
1	A	269	PRO	N-CA-C	5.16	119.30	111.15
1	A	678	PRO	N-CA-CB	5.16	108.34	103.19
1	A	428	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	361	LEU	CA-C-O	-5.14	115.11	120.55
1	A	198	ARG	CD-NE-CZ	5.13	131.58	124.40
1	A	336	PRO	CA-N-CD	-5.11	104.85	112.00
1	A	568	GLU	CA-C-N	-5.11	113.72	123.32
1	A	568	GLU	C-N-CA	-5.11	113.72	123.32
1	A	319	VAL	CA-C-N	5.11	125.08	120.03
1	A	319	VAL	C-N-CA	5.11	125.08	120.03
1	A	374	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	496	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	502	LEU	CA-C-O	-5.02	115.54	121.16
1	A	209	PRO	N-CA-CB	5.01	107.71	103.35
1	A	448	ASP	N-CA-C	5.01	117.69	110.28
1	A	673	PRO	N-CA-CB	5.00	107.98	103.33

There are no chirality outliers.

There are no planarity outliers.

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	6786	0	6603	176	0
2	B	29	0	27	1	0
3	A	20	0	0	1	0
4	A	821	0	0	27	1
All	All	7656	0	6630	176	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 13.

All (176) 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:540:GLU:CB	1:A:542[B]:LYS:HE3	1.26	1.60
1:A:540:GLU:HB2	1:A:542[B]:LYS:CE	1.21	1.56
1:A:267:GLY:O	1:A:269:PRO:HD3	1.51	1.07
1:A:773:ARG:HD2	1:A:776:ARG:CZ	1.85	1.06
1:A:214:ARG:O	1:A:216:LYS:HE2	1.58	1.04
1:A:484:GLN:HE21	1:A:484:GLN:HA	1.25	1.00
1:A:540:GLU:CA	1:A:542[B]:LYS:HE3	1.95	0.96
1:A:567:ASN:H	1:A:567:ASN:HD22	1.14	0.90
1:A:540:GLU:HB2	1:A:542[B]:LYS:NZ	1.87	0.89
1:A:234[B]:ARG:HG2	1:A:324:SER:O	1.72	0.88
1:A:542[B]:LYS:HG2	4:A:2454:HOH:O	1.71	0.88
1:A:789:GLN:HG2	4:A:2426:HOH:O	1.74	0.87
1:A:245:VAL:HG12	1:A:247:PRO:HD2	1.56	0.87
1:A:878:ARG:HD3	4:A:2310:HOH:O	1.75	0.86
1:A:542[B]:LYS:HD3	4:A:2424:HOH:O	1.77	0.84
1:A:336:PRO:HD3	1:A:763:TRP:CH2	2.13	0.83
1:A:336:PRO:HD3	1:A:763:TRP:CZ2	2.15	0.82
1:A:540:GLU:HB2	1:A:542[B]:LYS:HE2	1.60	0.81
1:A:540:GLU:CG	1:A:542[B]:LYS:HE3	2.12	0.80
1:A:108:LEU:HD12	1:A:112:LEU:CD2	2.13	0.78
1:A:776:ARG:HD2	4:A:2312:HOH:O	1.83	0.78
1:A:98:VAL:HG22	1:A:105:ILE:HD12	1.66	0.77
1:A:773:ARG:HD2	1:A:776:ARG:NE	1.99	0.77
1:A:581:MET:HE3	1:A:587:VAL:CG2	2.14	0.77
1:A:88:TYR:CE2	1:A:108:LEU:HD11	2.21	0.76
1:A:267:GLY:O	1:A:269:PRO:CD	2.32	0.76
1:A:540:GLU:CA	1:A:542[B]:LYS:CE	2.60	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASN:H	1:A:567:ASN:ND2	1.82	0.76
1:A:205:LEU:HD21	1:A:693:ARG:HH12	1.52	0.75
1:A:773:ARG:CD	1:A:776:ARG:CZ	2.64	0.74
1:A:540:GLU:CB	1:A:542[B]:LYS:CE	2.08	0.74
1:A:88:TYR:HE2	1:A:108:LEU:HD11	1.52	0.73
1:A:581:MET:HE3	1:A:587:VAL:HG21	1.72	0.71
1:A:773:ARG:CD	1:A:776:ARG:NH2	2.54	0.71
1:A:497:ASN:HB3	3:A:2001:SO4:O3	1.91	0.70
1:A:484:GLN:HA	1:A:484:GLN:NE2	2.00	0.70
1:A:227:HIS:NE2	1:A:331:ASP:OD1	2.24	0.68
1:A:85:TRP:CZ3	1:A:87:ILE:HD12	2.28	0.68
1:A:773:ARG:NH1	1:A:776:ARG:NH1	2.41	0.68
1:A:214:ARG:O	1:A:216:LYS:CE	2.40	0.67
1:A:429:TYR:CE2	1:A:433:ILE:HD11	2.31	0.66
1:A:621:LYS:HG2	1:A:622:ASP:N	2.10	0.66
1:A:156:ASP:N	4:A:2718:HOH:O	2.28	0.66
1:A:275:GLN:HG3	1:A:278:LYS:HG3	1.76	0.66
1:A:567:ASN:HD22	1:A:567:ASN:N	1.79	0.66
1:A:745:PRO:HD3	4:A:2164:HOH:O	1.96	0.66
1:A:446:GLU:OE2	1:A:448:ASP:OD1	2.14	0.65
1:A:108:LEU:HD12	1:A:112:LEU:CG	2.27	0.64
1:A:48:ARG:NH2	1:A:180:ASP:OD2	2.29	0.64
1:A:108:LEU:HD12	1:A:112:LEU:HG	1.78	0.64
1:A:245:VAL:HG12	1:A:247:PRO:CD	2.28	0.64
1:A:208:LEU:HB2	1:A:213:LEU:HD21	1.80	0.63
1:A:234[B]:ARG:CG	1:A:324:SER:O	2.45	0.63
1:A:212:ALA:C	1:A:213:LEU:HD22	2.23	0.63
1:A:673:PRO:HD3	1:A:683:TYR:O	1.99	0.62
1:A:336:PRO:HG3	1:A:763:TRP:CZ3	2.34	0.61
1:A:625:SER:HB3	1:A:656:LYS:HE3	1.82	0.61
1:A:581:MET:HE3	1:A:587:VAL:HG23	1.82	0.60
1:A:154:SER:O	1:A:155:GLY:C	2.45	0.60
1:A:252:VAL:HA	4:A:2520:HOH:O	2.01	0.60
1:A:773:ARG:HD2	1:A:776:ARG:NH2	2.16	0.60
1:A:344:PHE:HB3	1:A:735:GLN:HA	1.83	0.59
1:A:625:SER:CB	1:A:656:LYS:HE3	2.33	0.59
1:A:540:GLU:C	1:A:542[B]:LYS:HE3	2.27	0.59
1:A:225:LYS:CD	1:A:225:LYS:C	2.75	0.59
1:A:121:PHE:CZ	1:A:123:GLY:HA2	2.38	0.58
1:A:540:GLU:HG3	4:A:2497:HOH:O	2.03	0.58
1:A:540:GLU:HB2	1:A:542[B]:LYS:HE3	0.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASP:C	1:A:404:SER:H	2.11	0.57
1:A:854:ARG:CZ	4:A:2587:HOH:O	2.52	0.57
1:A:289:TYR:CE1	1:A:334:ASP:HB3	2.40	0.56
1:A:624:GLU:O	1:A:656:LYS:CE	2.53	0.56
1:A:195:PRO:HD3	1:A:198:ARG:HH12	1.70	0.56
1:A:450:PRO:HD2	4:A:2358:HOH:O	2.04	0.56
1:A:643:TYR:HE1	1:A:644:TRP:CE2	2.23	0.56
1:A:195:PRO:HD3	1:A:883:GLU:OE1	2.06	0.56
1:A:225:LYS:C	1:A:225:LYS:HD3	2.31	0.55
1:A:98:VAL:CG2	1:A:105:ILE:HD12	2.35	0.55
1:A:213:LEU:HD22	1:A:213:LEU:N	2.22	0.55
1:A:567:ASN:ND2	1:A:567:ASN:N	2.43	0.54
1:A:540:GLU:C	1:A:542[B]:LYS:CE	2.80	0.54
1:A:200:VAL:HG22	4:A:2575:HOH:O	2.08	0.53
1:A:346:ASP:HA	1:A:375:HIS:HB3	1.90	0.53
1:A:502:LEU:C	1:A:502:LEU:HD23	2.34	0.53
1:A:620:LEU:CD2	1:A:629:PHE:CZ	2.92	0.53
1:A:624:GLU:O	1:A:656:LYS:HE2	2.09	0.52
1:A:724:LYS:HB3	1:A:725:PRO:HD2	1.91	0.52
1:A:402:ASP:C	1:A:404:SER:N	2.66	0.52
1:A:225:LYS:HD3	1:A:226:VAL:N	2.25	0.52
1:A:365:ALA:HB2	1:A:439:ARG:HB3	1.92	0.51
1:A:721:LYS:HB2	1:A:777:GLU:HA	1.93	0.51
1:A:620:LEU:HD22	1:A:629:PHE:CZ	2.45	0.51
1:A:509:SER:O	1:A:513:VAL:HG23	2.10	0.51
1:A:797:ARG:HD2	4:A:2678:HOH:O	2.10	0.51
1:A:108:LEU:HD12	1:A:112:LEU:HD23	1.90	0.50
1:A:542[B]:LYS:CD	4:A:2424:HOH:O	2.50	0.50
1:A:721:LYS:HB3	1:A:777:GLU:HG3	1.92	0.50
1:A:854:ARG:NH2	4:A:2587:HOH:O	2.44	0.50
1:A:245:VAL:HG23	1:A:305:GLN:HE22	1.77	0.49
1:A:493:VAL:HG11	2:B:1:NAG:H5	1.93	0.49
1:A:551:THR:HG22	1:A:562:ILE:HA	1.95	0.49
1:A:149:ARG:HG3	1:A:414:GLY:O	2.12	0.49
1:A:222:MET:SD	1:A:283:MET:SD	3.10	0.49
1:A:32:VAL:HG23	1:A:154:SER:HB3	1.94	0.49
1:A:540:GLU:C	1:A:542[B]:LYS:CD	2.85	0.49
1:A:690:SER:HA	1:A:694:LYS:HD3	1.95	0.48
1:A:776:ARG:NE	4:A:2703:HOH:O	2.42	0.48
1:A:330:LEU:HD12	1:A:330:LEU:C	2.39	0.48
1:A:633:ARG:NH2	1:A:730:TYR:OH	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:MET:CE	1:A:587:VAL:HG21	2.43	0.47
1:A:232:ASP:OD1	1:A:234[B]:ARG:HG3	2.15	0.47
1:A:480:ARG:NH2	1:A:484:GLN:OE1	2.43	0.47
1:A:693:ARG:NH1	1:A:795:TRP:CD1	2.83	0.47
1:A:205:LEU:HD21	1:A:693:ARG:NH1	2.24	0.47
1:A:540:GLU:CB	1:A:542[B]:LYS:HE2	2.29	0.47
1:A:693:ARG:HG2	4:A:2388:HOH:O	2.15	0.47
1:A:541:ALA:C	1:A:542[B]:LYS:HD2	2.40	0.47
1:A:292[B]:LYS:HE2	1:A:292[B]:LYS:HB2	1.30	0.46
1:A:289:TYR:CZ	1:A:334:ASP:HB3	2.51	0.46
1:A:540:GLU:CA	1:A:542[B]:LYS:HE2	2.46	0.46
1:A:776:ARG:NH2	4:A:2703:HOH:O	2.43	0.46
1:A:123:GLY:O	1:A:125:PRO:HD3	2.15	0.45
1:A:156:ASP:O	1:A:157:ALA:C	2.56	0.45
1:A:341:ARG:HG2	1:A:762:SER:OG	2.17	0.45
1:A:540:GLU:O	1:A:540:GLU:HG2	2.17	0.45
1:A:672:PHE:HA	1:A:683:TYR:O	2.16	0.45
1:A:405:GLU:HA	1:A:408:CYS:O	2.17	0.45
1:A:280[B]:LYS:HG3	4:A:2781:HOH:O	2.17	0.45
1:A:722:SER:HB3	1:A:772:TYR:OH	2.17	0.45
1:A:773:ARG:NE	1:A:776:ARG:NH2	2.64	0.44
1:A:797:ARG:CD	4:A:2678:HOH:O	2.64	0.44
1:A:822:PRO:HA	1:A:835:ILE:HD12	1.99	0.44
1:A:217:ILE:HG13	1:A:318:LEU:HD21	1.99	0.44
1:A:480:ARG:HH12	1:A:484:GLN:CD	2.26	0.43
1:A:30:GLN:HG2	4:A:2823:HOH:O	2.19	0.43
1:A:656:LYS:HD2	1:A:656:LYS:HA	1.77	0.43
1:A:189:LYS:HE2	4:A:2414:HOH:O	2.19	0.43
1:A:480:ARG:NH1	1:A:484:GLN:HG2	2.33	0.43
1:A:593:LEU:N	1:A:594:PRO:CD	2.81	0.43
1:A:283:MET:HE3	1:A:283:MET:HB3	1.80	0.43
1:A:744:ASP:HB2	1:A:745:PRO:CD	2.48	0.42
1:A:493:VAL:HG23	4:A:2357:HOH:O	2.18	0.42
1:A:643:TYR:HE1	1:A:644:TRP:CZ2	2.37	0.42
1:A:88:TYR:CD2	1:A:108:LEU:HD11	2.51	0.42
1:A:336:PRO:HB2	4:A:2295:HOH:O	2.19	0.42
1:A:618:ASP:HB2	4:A:2221:HOH:O	2.18	0.42
1:A:749:TYR:CE2	1:A:818:ARG:HG3	2.55	0.42
1:A:154:SER:O	1:A:155:GLY:O	2.37	0.42
1:A:553:LYS:HB2	1:A:553:LYS:NZ	2.34	0.42
1:A:726:TRP:HA	1:A:727:PRO:HD2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HG2	1:A:135:VAL:HG22	2.01	0.42
1:A:338:PHE:O	1:A:341:ARG:NH1	2.47	0.42
1:A:540:GLU:HB2	1:A:542[B]:LYS:HZ1	1.77	0.41
1:A:620:LEU:HD23	1:A:629:PHE:CZ	2.55	0.41
1:A:339:PRO:HD2	1:A:730:TYR:O	2.21	0.41
1:A:557:GLU:HA	1:A:558:PRO:HD3	1.88	0.41
1:A:70:LEU:HD11	1:A:131:GLU:HB3	2.02	0.41
1:A:246:LYS:HB3	1:A:247:PRO:HD3	2.03	0.41
1:A:155:GLY:O	1:A:157:ALA:N	2.51	0.41
1:A:157:ALA:N	4:A:2431:HOH:O	2.53	0.41
1:A:480:ARG:NH1	1:A:484:GLN:OE1	2.51	0.41
1:A:501:TYR:CD1	1:A:501:TYR:N	2.89	0.41
1:A:797:ARG:HH11	1:A:797:ARG:HD3	1.72	0.41
1:A:81:ASP:HB2	4:A:2825:HOH:O	2.20	0.40
1:A:205:LEU:CD2	1:A:693:ARG:HH12	2.29	0.40
1:A:213:LEU:C	1:A:216:LYS:HG2	2.47	0.40
1:A:540:GLU:C	1:A:542[B]:LYS:HD3	2.46	0.40
1:A:831:LEU:HB3	1:A:861:PRO:HG2	2.02	0.40
1:A:460:MET:HA	1:A:460:MET:HE2	2.04	0.40
1:A:430:ILE:HG23	1:A:527:ALA:HB2	2.04	0.40
1:A:744:ASP:CB	1:A:745:PRO:CD	2.99	0.40
1:A:140:GLN:HA	1:A:145:ASP:OD2	2.21	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)
4:A:2247:HOH:O	4:A:2812:HOH:O[3_556]	0.16	2.04

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	860/858 (100%)	835 (97%)	22 (3%)	3 (0%)	36 25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	GLY
1	A	156	ASP
1	A	403	LEU

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	710/705 (101%)	679 (96%)	31 (4%)	25 13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LYS
1	A	156	ASP
1	A	225	LYS
1	A	234[A]	ARG
1	A	234[B]	ARG
1	A	235	LYS
1	A	275	GLN
1	A	278	LYS
1	A	283	MET
1	A	295	LYS
1	A	299	GLN
1	A	326	LYS
1	A	336	PRO
1	A	374	PHE
1	A	484	GLN
1	A	490	THR
1	A	501	TYR
1	A	502	LEU

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Mol	Chain	Res	Type
1	A	542[A]	LYS
1	A	542[B]	LYS
1	A	551	THR
1	A	553	LYS
1	A	556	PRO
1	A	567	ASN
1	A	571	PRO
1	A	583	LYS
1	A	621	LYS
1	A	666	ASP
1	A	789	GLN
1	A	822	PRO
1	A	835	ILE

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	275	GLN
1	A	427	GLN
1	A	510	GLN
1	A	567	ASN
1	A	716	ASN
1	A	717	HIS
1	A	789	GLN
1	A	853	GLN

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
2	NAG	B	1	2	15,15,15	1.22	2 (13%)	21,21,21	1.35	2 (9%)
2	NAG	B	2	2	14,14,15	1.31	2 (14%)	17,19,21	1.44	2 (11%)

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	-	0/6/26/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O7-C7	-3.32	1.15	1.23
2	B	1	NAG	O7-C7	-2.96	1.16	1.23
2	B	2	NAG	C2-N2	2.88	1.51	1.46
2	B	1	NAG	C2-N2	2.03	1.49	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	4.04	117.60	112.19
2	B	1	NAG	O1-C1-C2	3.92	117.35	109.22
2	B	1	NAG	O5-C1-C2	-3.02	106.48	109.52
2	B	2	NAG	C2-N2-C7	-2.81	119.14	122.90

There are no chirality outliers.

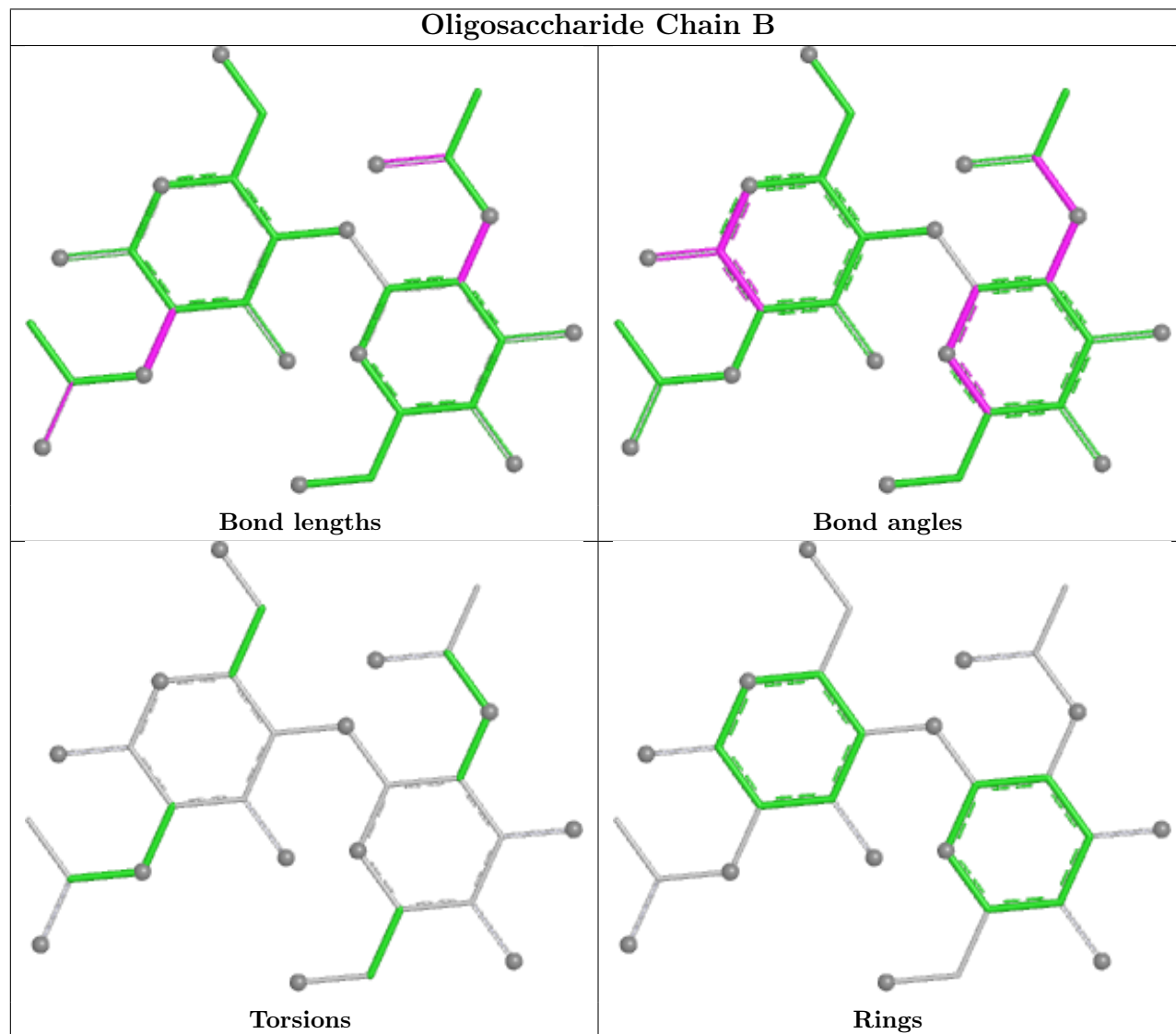
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	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.



5.6 Ligand geometry [i](#)

4 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	SO4	A	2001	-	4,4,4	0.75	0	6,6,6	0.40	0
3	SO4	A	2004	-	4,4,4	0.69	0	6,6,6	0.08	0
3	SO4	A	2002	-	4,4,4	0.72	0	6,6,6	0.27	0
3	SO4	A	2003	-	4,4,4	0.67	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	858/858 (100%)	0.02	34 (3%)	42 41	9, 19, 37, 55	5 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	PRO	4.4
1	A	156	ASP	4.4
1	A	155	GLY	4.1
1	A	267	GLY	4.0
1	A	277	GLY	3.9
1	A	484	GLN	3.7
1	A	540	GLU	3.7
1	A	555	LYS	3.6
1	A	569	ASP	3.2
1	A	266	ASN	3.1
1	A	283	MET	3.0
1	A	269	PRO	3.0
1	A	556	PRO	3.0
1	A	108	LEU	2.9
1	A	53	GLY	2.9
1	A	234[A]	ARG	2.8
1	A	326	LYS	2.8
1	A	622	ASP	2.7
1	A	275	GLN	2.7
1	A	885[A]	VAL	2.7
1	A	822	PRO	2.6
1	A	127	GLY	2.5
1	A	490	THR	2.5
1	A	213	LEU	2.4
1	A	644	TRP	2.4
1	A	268	TYR	2.3
1	A	745	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	279	PHE	2.2
1	A	776	ARG	2.2
1	A	280[A]	LYS	2.1
1	A	790	ALA	2.1
1	A	235	LYS	2.1
1	A	210	ALA	2.1
1	A	298	ALA	2.1

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

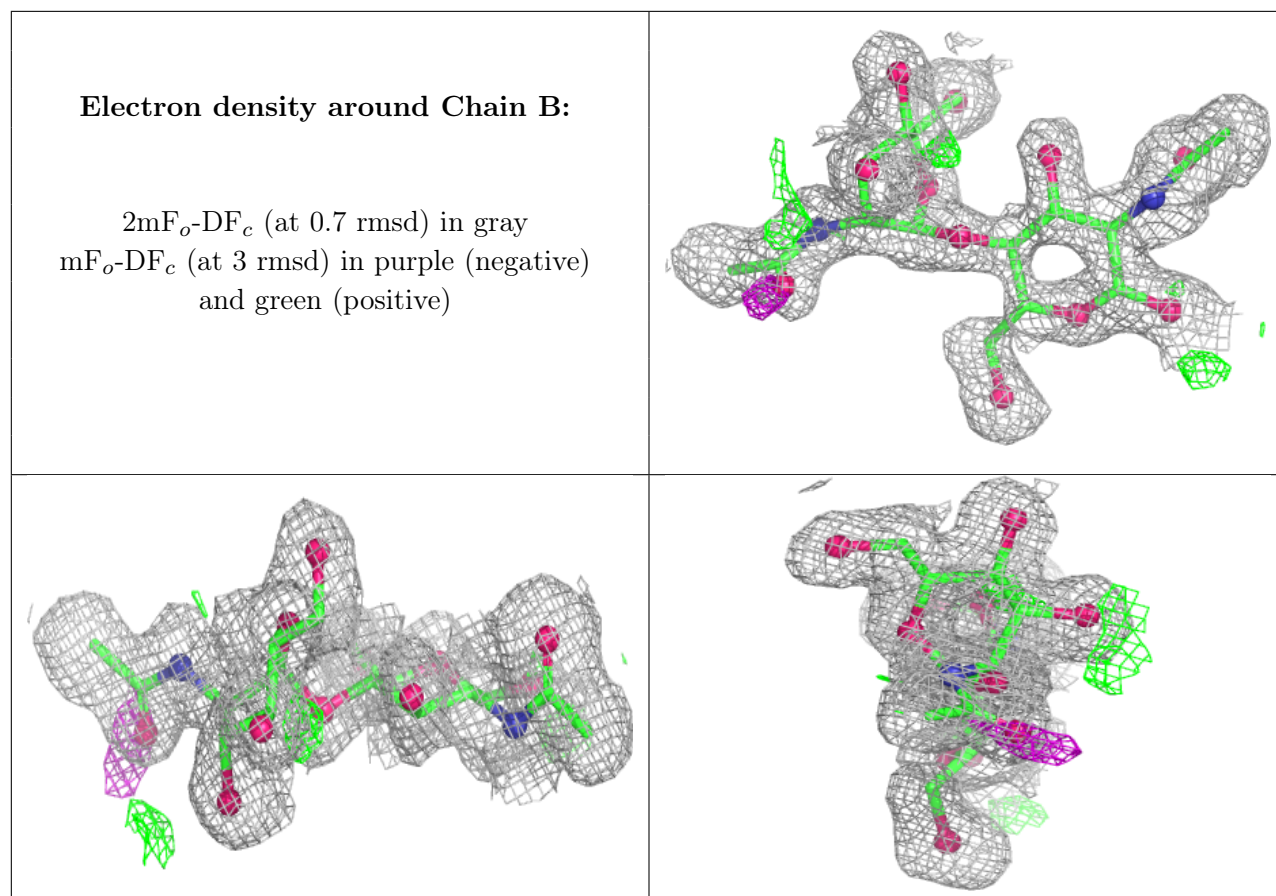
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.94	0.08	11,14,19,24	0
2	NAG	B	1	15/15	0.97	0.06	12,14,19,28	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($\text{\AA}^2$)	Q<0.9
3	SO4	A	2004	5/5	0.78	0.27	78,78,79,79	0
3	SO4	A	2003	5/5	0.85	0.17	72,72,73,73	0
3	SO4	A	2002	5/5	0.94	0.10	36,37,39,40	0
3	SO4	A	2001	5/5	0.96	0.09	17,17,18,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.