



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 11:50 AM EST

PDB ID : 3L4Y
Title : Crystal complex of N-terminal Human Maltase-Glucoamylase with NR4-8II
Authors : Sim, L.; Rose, D.R.
Deposited on : 2009-12-21
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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

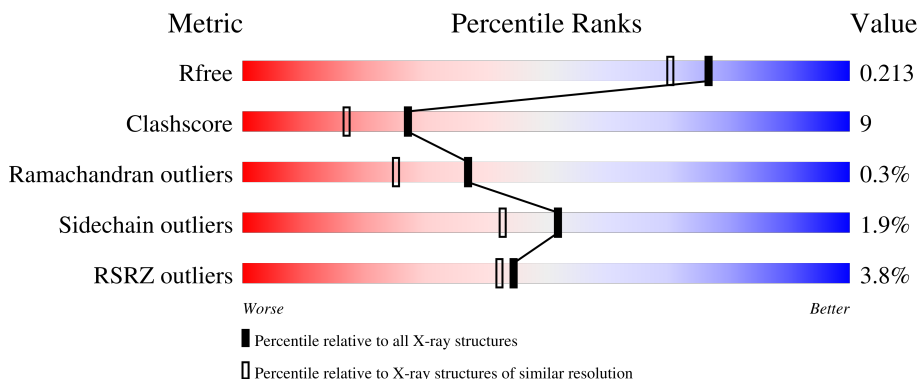
1 Overall quality at a glance

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	A	875	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
2	B	2	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7888 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 Maltase-glucoamylase, intestinal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	863	Total	C	N	O	S	0	9	0
			6970	4445	1181	1317	27			

There are 8 discrepancies between the modelled and reference sequences:

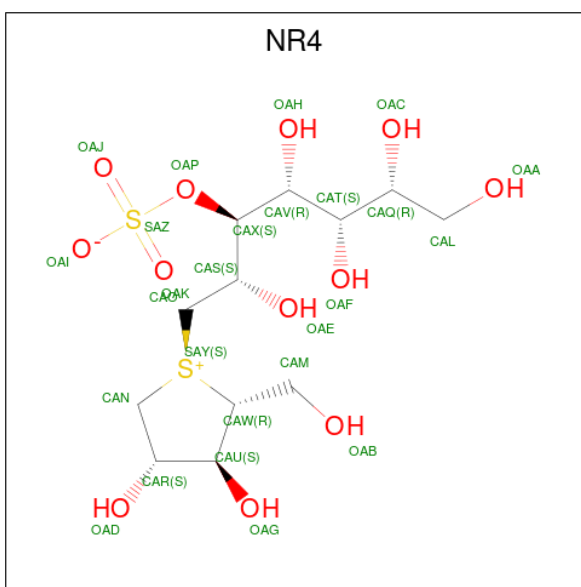
Chain	Residue	Modelled	Actual	Comment	Reference
A	772	ASP	ASN	variant	UNP O43451
A	869	ALA	-	expression tag	UNP O43451
A	870	HIS	-	expression tag	UNP O43451
A	871	HIS	-	expression tag	UNP O43451
A	872	HIS	-	expression tag	UNP O43451
A	873	HIS	-	expression tag	UNP O43451
A	874	HIS	-	expression tag	UNP O43451
A	875	HIS	-	expression tag	UNP O43451

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



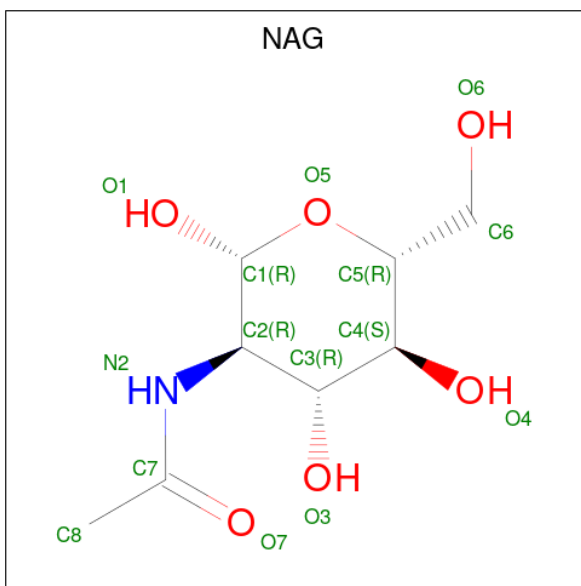
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is (1S,2R,3S,4R)-1-[(1S)-2-[(2R,3S,4S)-3,4-dihydroxy-2-(hydroxymethyl)tetrahydrothiophenium-1-yl]-1-hydroxyethyl]-2,3,4,5-tetrahydroxypentyl sulfate (three-letter code: NR4) (formula: C₁₂H₂₄O₁₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			26	12	12	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

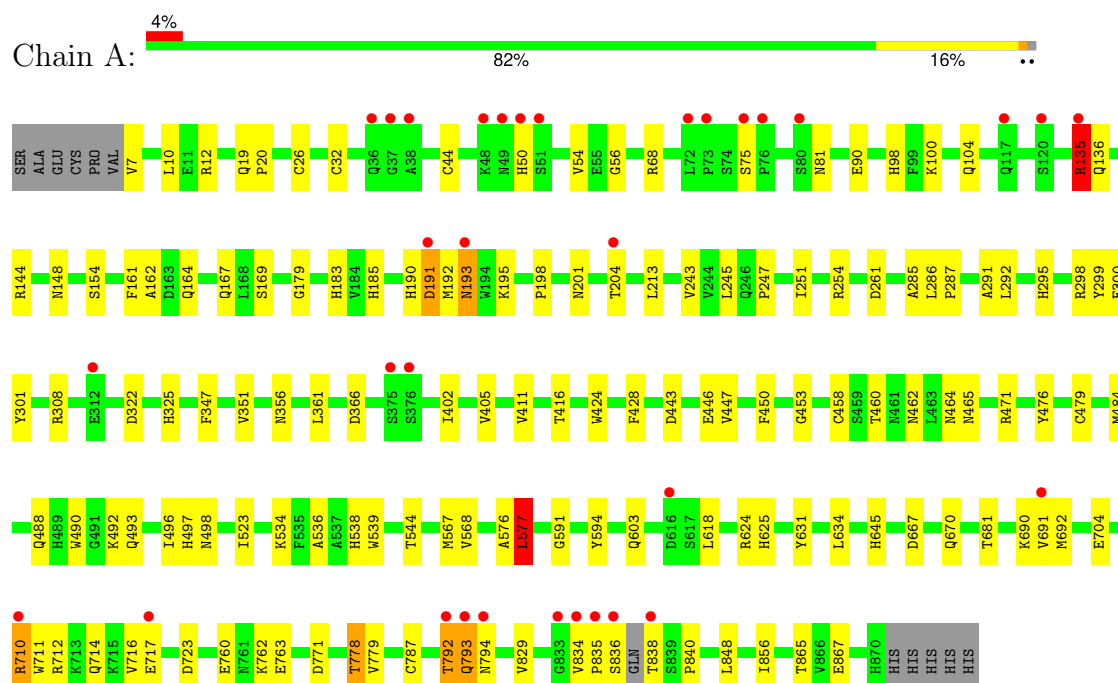
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	801	Total	O	0	0
			801	801		

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: Maltase-glucoamylase, intestinal



- 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 21	Depositor
Cell constants a, b, c, α , β , γ	87.13Å 109.36Å 109.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 1.80 19.91 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.91-1.80) 97.2 (19.91-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.174 , 0.214 0.173 , 0.213	Depositor DCC
R_{free} test set	4714 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7888	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: NR4, NAG, GOL, SO4

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	0.80	1/7187 (0.0%)	0.81	7/9801 (0.1%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	787	CYS	CB-SG	-5.00	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	A	624	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	A	135	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	144	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	12	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	624	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	191	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	HIS	Peptide
1	A	792	THR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6970	0	6649	125	1
2	B	28	0	25	0	0
3	A	26	0	24	1	0
4	A	28	0	26	0	1
5	A	30	0	40	8	0
6	A	5	0	0	0	0
7	A	801	0	0	20	1
All	All	7888	0	6764	125	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 9.

All (125) 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:479[A]:CYS:SG	7:A:4843:HOH:O	1.96	1.21
1:A:98:HIS:HE1	1:A:261:ASP:OD1	1.50	0.95
1:A:793:GLN:HA	7:A:4827:HOH:O	1.68	0.93
1:A:712:ARG:H	1:A:714:GLN:HE21	1.17	0.92
1:A:771:ASP:OD2	1:A:778:THR:HG21	1.71	0.91
1:A:191:ASP:OD1	7:A:4879:HOH:O	1.95	0.84
1:A:56:GLY:O	1:A:135:ARG:NH2	2.11	0.82
1:A:492:LYS:HE3	7:A:4798:HOH:O	1.80	0.80
1:A:829:VAL:O	1:A:836:SER:HB3	1.84	0.77
1:A:68[A]:ARG:HG2	1:A:104:GLN:NE2	2.02	0.75
1:A:493:GLN:NE2	1:A:497:HIS:HD2	1.87	0.73
1:A:493:GLN:HE21	1:A:497:HIS:HD2	1.38	0.72
1:A:670:GLN:NE2	7:A:4418:HOH:O	2.23	0.70
1:A:471:ARG:HD2	7:A:4610:HOH:O	1.91	0.70
1:A:245:LEU:HD23	1:A:251[B]:ILE:HG12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLU:HG3	1:A:603:GLN:HE21	1.56	0.69
1:A:98:HIS:CE1	1:A:261:ASP:OD1	2.39	0.69
1:A:135:ARG:HB2	1:A:136:GLN:HE21	1.58	0.68
1:A:471:ARG:CD	7:A:4610:HOH:O	2.42	0.67
1:A:201:ASN:O	1:A:497:HIS:HE1	1.77	0.67
1:A:794:ASN:N	7:A:4831:HOH:O	2.28	0.66
1:A:100:LYS:HD2	7:A:4255:HOH:O	1.95	0.66
1:A:690:LYS:HB3	1:A:717:GLU:OE2	1.95	0.66
1:A:68[A]:ARG:HG2	1:A:104:GLN:HE22	1.60	0.65
1:A:245:LEU:CD2	1:A:251[B]:ILE:HG12	2.26	0.65
1:A:446:GLU:N	1:A:447:VAL:HA	2.13	0.63
1:A:183:HIS:HE1	1:A:198:PRO:O	1.81	0.63
1:A:691:VAL:HG23	7:A:4273:HOH:O	1.99	0.63
1:A:836:SER:C	1:A:838:THR:N	2.53	0.62
1:A:179:GLY:O	1:A:190:HIS:HE1	1.82	0.62
1:A:493:GLN:NE2	1:A:497:HIS:CD2	2.68	0.61
1:A:26:CYS:HG	1:A:44:CYS:HG	1.48	0.61
1:A:68[A]:ARG:HE	1:A:104:GLN:HE22	1.48	0.61
1:A:464:ASN:ND2	1:A:484:MET:H	1.98	0.61
1:A:544:THR:CG2	1:A:577:LEU:HD22	2.32	0.60
1:A:135:ARG:HB2	1:A:136:GLN:NE2	2.17	0.59
1:A:54:VAL:HB	1:A:135:ARG:HB3	1.85	0.59
1:A:295:HIS:HD2	1:A:325:HIS:NE2	2.02	0.58
1:A:183:HIS:HD2	1:A:185:HIS:NE2	2.02	0.57
1:A:488:GLN:HB2	1:A:496:ILE:HD11	1.85	0.57
1:A:191:ASP:OD1	1:A:192:MET:N	2.37	0.57
1:A:692:MET:SD	1:A:717:GLU:OE1	2.62	0.57
1:A:443:ASP:OD2	3:A:1001:NR4:HANA	2.04	0.56
1:A:591:GLY:HA2	1:A:594:TYR:CD2	2.41	0.56
1:A:576:ALA:O	1:A:577:LEU:HB2	2.04	0.56
1:A:840:PRO:HB3	1:A:856:ILE:CG2	2.36	0.56
1:A:191:ASP:OD2	1:A:193:ASN:HB2	2.06	0.55
1:A:625:HIS:HE1	1:A:704:GLU:OE2	1.90	0.55
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.88	0.55
1:A:300:GLU:HG3	1:A:603:GLN:NE2	2.21	0.55
1:A:201:ASN:H	1:A:498:ASN:ND2	2.05	0.55
1:A:645:HIS:CE1	5:A:3005:GOL:H32	2.42	0.54
1:A:135:ARG:HE	1:A:136:GLN:HE21	1.56	0.54
1:A:190:HIS:HD2	7:A:4033:HOH:O	1.91	0.54
1:A:243:VAL:HG11	1:A:251[A]:ILE:HD11	1.90	0.54
1:A:424:TRP:CE2	1:A:428:PHE:HE2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:H	1:A:498:ASN:HD21	1.56	0.53
1:A:464:ASN:HD21	1:A:484:MET:H	1.56	0.53
1:A:54:VAL:HB	1:A:135:ARG:CB	2.39	0.53
1:A:90:GLU:OE1	1:A:98:HIS:HD2	1.90	0.53
1:A:760:GLU:OE2	7:A:4782:HOH:O	2.19	0.53
1:A:681:THR:HG22	1:A:691:VAL:HG11	1.91	0.53
1:A:68[A]:ARG:HE	1:A:104:GLN:NE2	2.06	0.52
1:A:836:SER:OG	1:A:838:THR:HG22	2.10	0.52
1:A:711:TRP:CG	1:A:716:VAL:HG11	2.45	0.51
1:A:81:ASN:HA	1:A:162:ALA:HA	1.92	0.51
1:A:291:ALA:O	1:A:295:HIS:HE1	1.94	0.51
1:A:450:PHE:CZ	5:A:3002:GOL:H32	2.46	0.51
1:A:645:HIS:NE2	5:A:3005:GOL:H32	2.27	0.50
1:A:68[A]:ARG:NE	1:A:104:GLN:HE22	2.08	0.50
1:A:692:MET:CE	1:A:717:GLU:OE1	2.59	0.50
1:A:191:ASP:OD2	1:A:193:ASN:CB	2.60	0.49
1:A:840:PRO:HB3	1:A:856:ILE:HG23	1.93	0.49
1:A:19:GLN:HB2	1:A:20:PRO:CD	2.42	0.49
1:A:450:PHE:CE1	5:A:3002:GOL:H32	2.47	0.49
1:A:183:HIS:CD2	1:A:185:HIS:NE2	2.80	0.49
1:A:523:ILE:H	5:A:3001:GOL:C1	2.26	0.48
1:A:191:ASP:OD1	1:A:191:ASP:N	2.46	0.48
1:A:164:GLN:HE22	1:A:462:ASN:HB2	1.79	0.48
1:A:631:TYR:HA	1:A:634:LEU:HG	1.96	0.47
1:A:308:ARG:NH2	7:A:4878:HOH:O	2.09	0.47
1:A:32:CYS:SG	7:A:4452:HOH:O	2.30	0.47
1:A:164:GLN:NE2	1:A:462:ASN:HD22	2.12	0.47
1:A:201:ASN:O	1:A:497:HIS:CE1	2.64	0.47
1:A:148:ASN:ND2	7:A:4364:HOH:O	2.47	0.47
1:A:476:TYR:HB2	1:A:479[A]:CYS:SG	2.55	0.47
1:A:618:LEU:HD11	1:A:723:ASP:HB3	1.96	0.46
1:A:834:VAL:HG12	1:A:835:PRO:O	2.16	0.46
1:A:865:THR:HG22	1:A:867:GLU:HG3	1.97	0.46
1:A:366:ASP:HB3	7:A:4121:HOH:O	2.16	0.46
1:A:135:ARG:NE	1:A:136:GLN:HE21	2.14	0.45
1:A:771:ASP:OD2	1:A:778:THR:CG2	2.55	0.45
1:A:285:ALA:HB3	5:A:3001:GOL:H31	1.98	0.45
1:A:351:VAL:HG22	1:A:361:LEU:HD22	1.99	0.44
1:A:793:GLN:HG2	7:A:4242:HOH:O	2.15	0.44
1:A:135:ARG:HE	1:A:136:GLN:NE2	2.15	0.44
1:A:534:LYS:NZ	7:A:4652:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:VAL:HB	5:A:3005:GOL:H12	1.99	0.44
1:A:762:LYS:HA	1:A:762:LYS:HD3	1.79	0.44
1:A:763:GLU:HG2	1:A:792:THR:HA	2.00	0.44
1:A:292:LEU:HD23	1:A:567:MET:CE	2.48	0.43
1:A:836:SER:O	1:A:838:THR:N	2.51	0.43
1:A:710:ARG:HD2	1:A:710:ARG:HA	1.61	0.43
1:A:167:GLN:NE2	1:A:254:ARG:HE	2.17	0.43
1:A:416:THR:HB	1:A:490:TRP:CG	2.53	0.43
1:A:538:HIS:O	1:A:568:VAL:HA	2.18	0.43
1:A:10:LEU:HD22	1:A:247:PRO:HG2	2.00	0.43
1:A:204:THR:HG23	1:A:213:LEU:HD23	2.01	0.43
1:A:298:ARG:HG2	1:A:301:TYR:CZ	2.54	0.43
1:A:26:CYS:CB	1:A:44:CYS:HG	2.31	0.42
1:A:243:VAL:CG1	1:A:251[A]:ILE:HD11	2.48	0.42
1:A:836:SER:HG	1:A:838:THR:N	2.18	0.42
1:A:286:LEU:HD12	1:A:287:PRO:HD2	2.02	0.42
1:A:7:VAL:HG23	7:A:4270:HOH:O	2.19	0.42
1:A:536:ALA:HA	5:A:3001:GOL:H11	2.02	0.42
1:A:471:ARG:HD3	7:A:4610:HOH:O	2.12	0.41
1:A:298:ARG:HG2	1:A:301:TYR:CE1	2.55	0.41
1:A:300:GLU:HG3	1:A:603:GLN:HG3	2.03	0.41
1:A:493:GLN:HE21	1:A:497:HIS:CD2	2.27	0.41
1:A:838:THR:O	1:A:838:THR:HG23	2.21	0.41
1:A:464:ASN:HD21	1:A:484:MET:N	2.18	0.41
1:A:453:GLY:HA3	1:A:458:CYS:SG	2.61	0.40
1:A:460:THR:HA	1:A:465:ASN:ND2	2.37	0.40
1:A:154:SER:HA	1:A:169:SER:O	2.21	0.40
1:A:402:ILE:HD13	1:A:411:VAL:HG12	2.02	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:A:20:PRO:O	1:A:356[B]:ASN:ND2[3_544]	2.17	0.03
4:A:2003:NAG:O4	7:A:4367:HOH:O[2_555]	2.17	0.03

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	868/875 (99%)	824 (95%)	41 (5%)	3 (0%)	37 25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	793	GLN
1	A	577	LEU
1	A	405	VAL

5.3.2 Protein sidechains [i](#)

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	765/767 (100%)	751 (98%)	14 (2%)	54 45

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	A	135	ARG
1	A	161	PHE
1	A	193	ASN
1	A	195	LYS
1	A	299	TYR
1	A	322	ASP
1	A	347	PHE

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Mol	Chain	Res	Type
1	A	539	TRP
1	A	577	LEU
1	A	667	ASP
1	A	710	ARG
1	A	778	THR
1	A	848	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	62	ASN
1	A	84	ASN
1	A	98	HIS
1	A	104	GLN
1	A	107	ASN
1	A	136	GLN
1	A	148	ASN
1	A	164	GLN
1	A	167	GLN
1	A	183	HIS
1	A	190	HIS
1	A	193	ASN
1	A	239	ASN
1	A	295	HIS
1	A	464	ASN
1	A	465	ASN
1	A	493	GLN
1	A	497	HIS
1	A	498	ASN
1	A	603	GLN
1	A	625	HIS
1	A	628	ASN
1	A	669	HIS
1	A	714	GLN
1	A	781	ASN
1	A	799	ASN
1	A	802	GLN
1	A	832	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	2,1	14,14,15	0.62	0	17,19,21	1.31	2 (11%)
2	NAG	B	2	2	14,14,15	0.57	0	17,19,21	1.46	1 (5%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	4.32	117.98	112.19
2	B	1	NAG	O5-C1-C2	-3.03	106.61	111.29
2	B	1	NAG	C1-O5-C5	2.58	115.65	112.19

There are no chirality outliers.

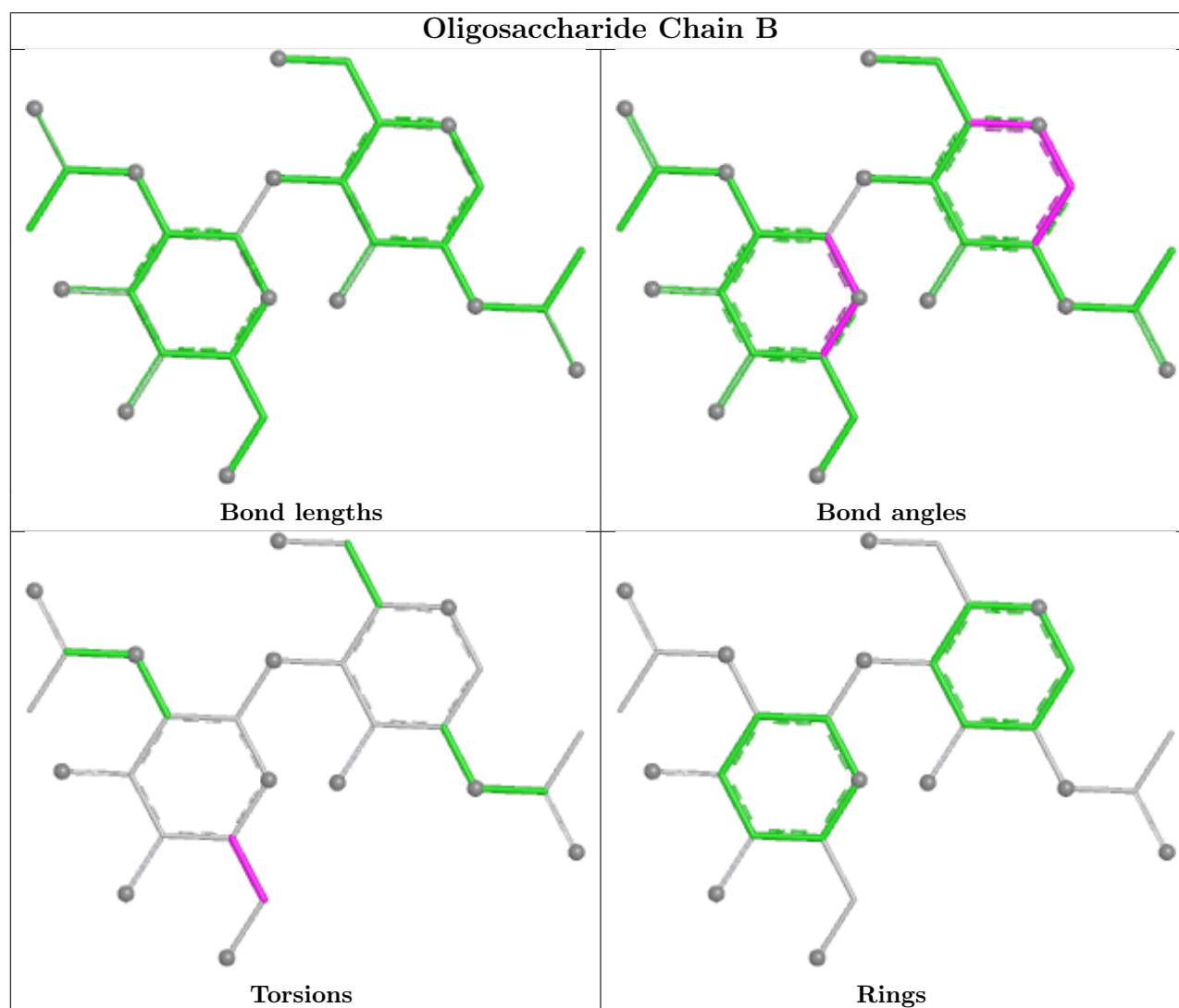
All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

9 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$
4	NAG	A	2004	1	14,14,15	0.45	0	17,19,21	2.77	3 (17%)
3	NR4	A	1001	-	21,26,26	1.17	2 (9%)	25,38,38	1.74	8 (32%)
5	GOL	A	3004	-	5,5,5	0.47	0	5,5,5	0.78	0
5	GOL	A	3005	-	5,5,5	0.81	0	5,5,5	0.91	0
5	GOL	A	3002	-	5,5,5	0.89	0	5,5,5	0.68	0
5	GOL	A	3001	-	5,5,5	0.61	0	5,5,5	1.35	0
4	NAG	A	2003	1	14,14,15	0.62	0	17,19,21	1.73	4 (23%)
5	GOL	A	3003	-	5,5,5	0.27	0	5,5,5	0.89	0
6	SO4	A	5001	-	4,4,4	0.26	0	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2004	1	-	2/6/23/26	0/1/1/1
3	NR4	A	1001	-	-	6/28/45/45	0/1/1/1
5	GOL	A	3004	-	-	3/4/4/4	-
5	GOL	A	3005	-	-	2/4/4/4	-
5	GOL	A	3002	-	-	2/4/4/4	-
5	GOL	A	3001	-	-	4/4/4/4	-
4	NAG	A	2003	1	-	3/6/23/26	0/1/1/1
5	GOL	A	3003	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NR4	OAP-SAZ	-2.79	1.48	1.57
3	A	1001	NR4	CAN-SAY	2.64	1.88	1.82

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2004	NAG	C1-O5-C5	9.92	125.48	112.19
3	A	1001	NR4	CAS-CAX-CAV	-4.34	104.22	113.60
4	A	2003	NAG	C1-O5-C5	4.32	117.98	112.19
4	A	2004	NAG	C6-C5-C4	-3.69	103.96	113.02
4	A	2003	NAG	O5-C1-C2	-2.77	107.01	111.29
4	A	2003	NAG	C2-N2-C7	2.73	126.56	122.90
3	A	1001	NR4	OAD-CAR-CAN	2.68	114.89	109.66
3	A	1001	NR4	OAH-CAV-CAT	2.60	115.53	109.46
3	A	1001	NR4	CAN-CAR-CAU	-2.55	104.21	106.43
4	A	2003	NAG	C1-C2-N2	-2.41	106.63	110.43
3	A	1001	NR4	CAR-CAU-CAW	-2.41	103.49	106.84
3	A	1001	NR4	CAQ-CAT-CAV	-2.35	108.87	112.48
3	A	1001	NR4	OAI-SAZ-OAP	2.35	111.77	106.37
4	A	2004	NAG	O3-C3-C4	-2.18	105.23	110.38
3	A	1001	NR4	OAC-CAQ-CAL	2.16	113.93	109.03

There are no chirality outliers.

All (23) torsion outliers are listed below:

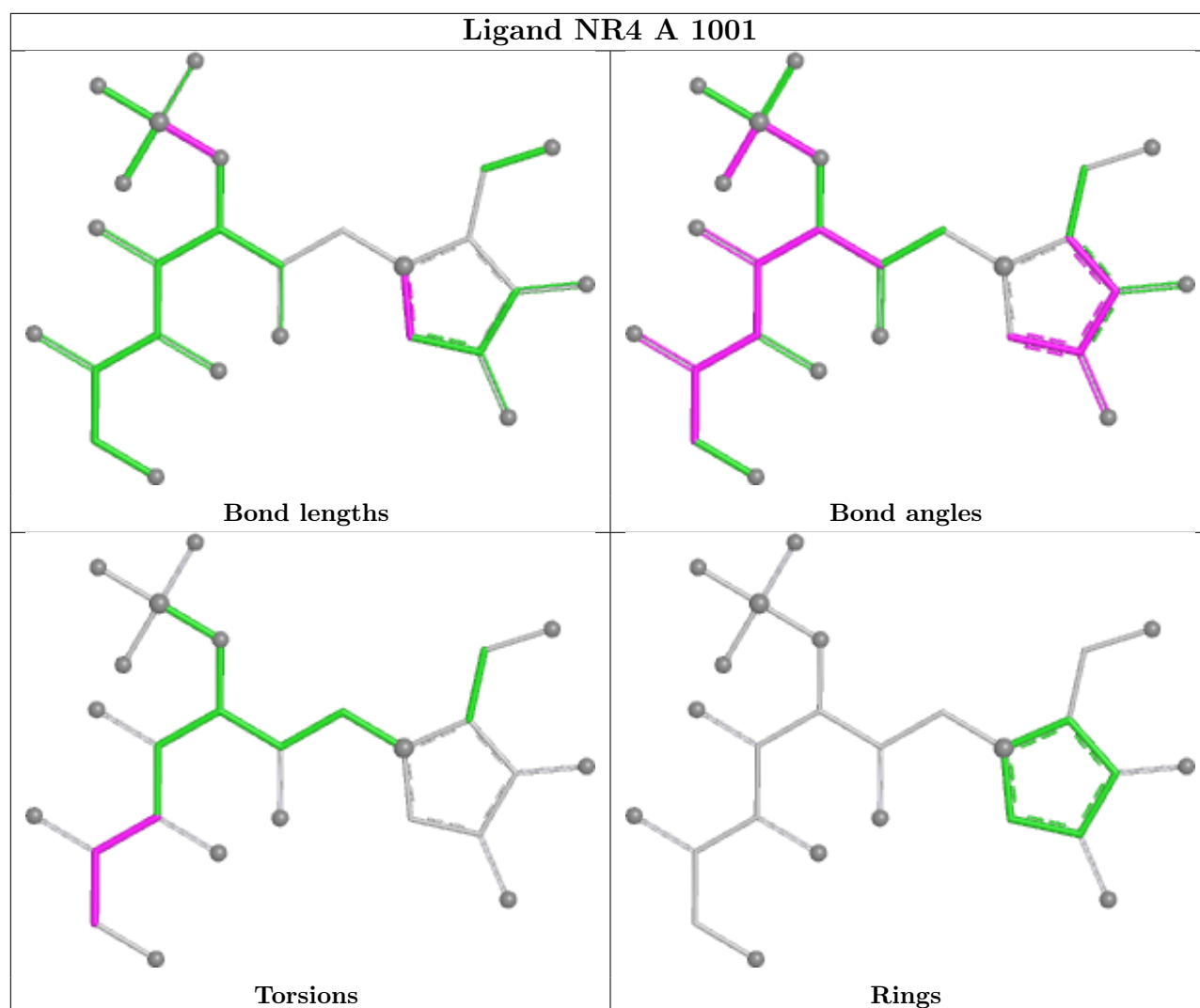
Mol	Chain	Res	Type	Atoms
3	A	1001	NR4	OAA-CAL-CAQ-OAC
4	A	2003	NAG	C8-C7-N2-C2
4	A	2003	NAG	O7-C7-N2-C2
5	A	3001	GOL	O1-C1-C2-C3
5	A	3001	GOL	C1-C2-C3-O3
5	A	3002	GOL	O1-C1-C2-C3
3	A	1001	NR4	OAA-CAL-CAQ-CAT
4	A	2004	NAG	C4-C5-C6-O6
4	A	2004	NAG	O5-C5-C6-O6
5	A	3002	GOL	O1-C1-C2-O2
3	A	1001	NR4	CAL-CAQ-CAT-OAF
3	A	1001	NR4	CAL-CAQ-CAT-CAV
5	A	3004	GOL	O1-C1-C2-C3
5	A	3005	GOL	C1-C2-C3-O3
5	A	3001	GOL	O1-C1-C2-O2
5	A	3001	GOL	O2-C2-C3-O3
5	A	3004	GOL	O1-C1-C2-O2
3	A	1001	NR4	OAC-CAQ-CAT-OAF
5	A	3004	GOL	O2-C2-C3-O3
5	A	3005	GOL	O2-C2-C3-O3
3	A	1001	NR4	OAC-CAQ-CAT-CAV
4	A	2003	NAG	C4-C5-C6-O6
5	A	3003	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	NR4	1	0
5	A	3005	GOL	3	0
5	A	3002	GOL	2	0
5	A	3001	GOL	3	0
4	A	2003	NAG	0	1

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	863/875 (98%)	-0.20	33 (3%) 44 42	8, 21, 35, 57	9 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	SER	5.0
1	A	836	SER	4.6
1	A	50	HIS	4.3
1	A	37	GLY	3.9
1	A	75	SER	3.8
1	A	135	ARG	3.7
1	A	835	PRO	3.7
1	A	838	THR	3.5
1	A	793	GLN	3.2
1	A	72	LEU	3.1
1	A	49	ASN	3.0
1	A	204	THR	3.0
1	A	375	SER	2.9
1	A	833	GLY	2.9
1	A	616	ASP	2.7
1	A	36	GLN	2.7
1	A	38	ALA	2.7
1	A	191	ASP	2.6
1	A	312	GLU	2.5
1	A	792	THR	2.4
1	A	691	VAL	2.4
1	A	834	VAL	2.4
1	A	193	ASN	2.4
1	A	80	SER	2.3
1	A	120	SER	2.3
1	A	73	PRO	2.3
1	A	710	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	717	GLU	2.2
1	A	117	GLN	2.2
1	A	794	ASN	2.2
1	A	376	SER	2.1
1	A	48	LYS	2.1
1	A	76	PRO	2.1

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

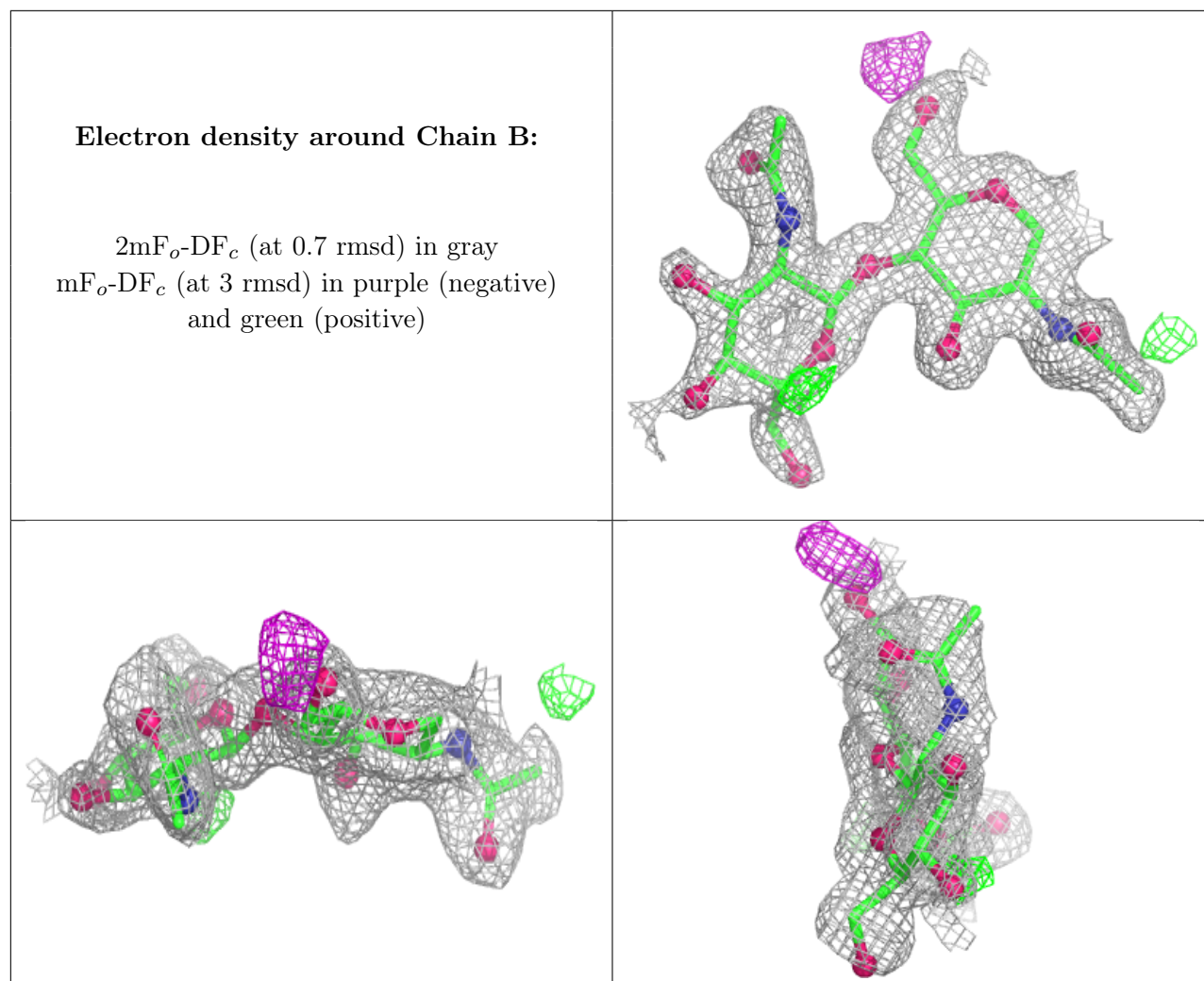
There are no non-standard protein/DNA/RNA residues in this entry.

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	0.80	0.12	38,42,49,50	0
2	NAG	B	1	14/15	0.92	0.08	24,28,33,34	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.

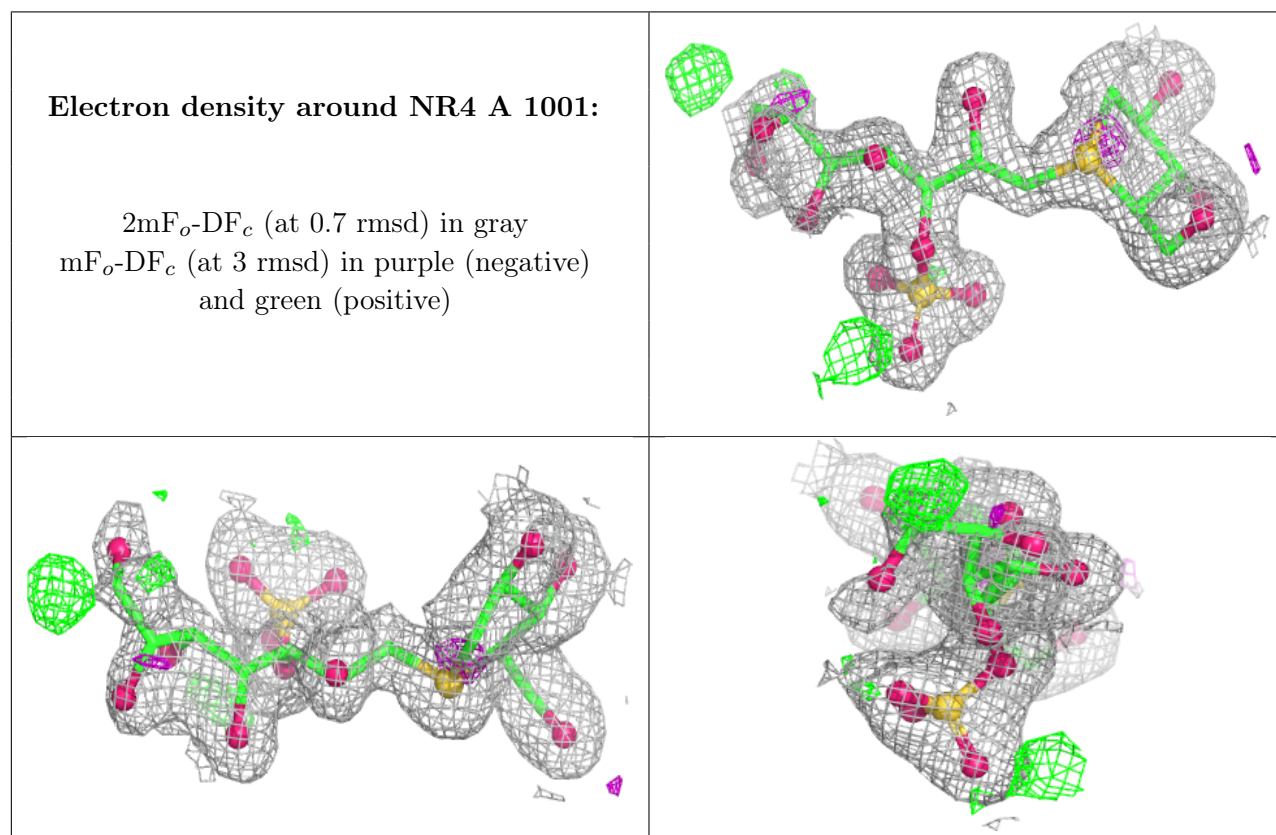


6.4 Ligands [i](#)

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	NAG	A	2003	14/15	0.75	0.15	30,34,44,47	0
4	NAG	A	2004	14/15	0.79	0.11	39,44,48,49	0
5	GOL	A	3002	6/6	0.83	0.14	49,53,55,55	0
5	GOL	A	3005	6/6	0.83	0.15	42,43,44,46	0
5	GOL	A	3003	6/6	0.85	0.14	34,40,44,49	0
5	GOL	A	3001	6/6	0.87	0.12	29,35,36,38	0
5	GOL	A	3004	6/6	0.90	0.09	32,33,35,37	0
3	NR4	A	1001	26/26	0.96	0.09	20,25,43,48	0
6	SO4	A	5001	5/5	0.96	0.08	37,38,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.