Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2024 – 01:43 am BST

PDB ID	:	9FYO
Title	:	Lacto-N-biosidase from Trueperella pyogenes
Authors	:	Vuillemin, M.; Siebenhaar, S.; Zeuner, B.; Morth, J.P.
Deposited on	:	2024-07-03
Resolution	:	2.77 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 (1)) were used in the production of this report:

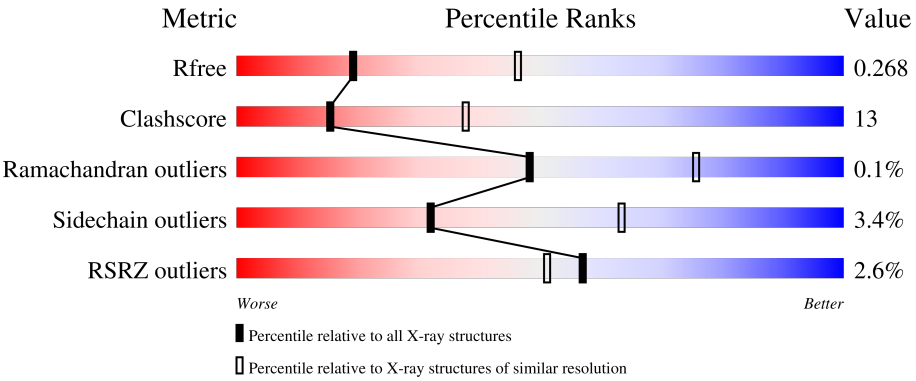
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

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	771	3% 72% 23%
2	C	2	50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11724 atoms, of which 5791 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 TrpyGH20.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	759	11651	3719	5770	999	1145	18	0	0	0

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	2	47	14	21	1	11	0	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
3	A	3	3	3	0	0

- Molecule 4 is water.

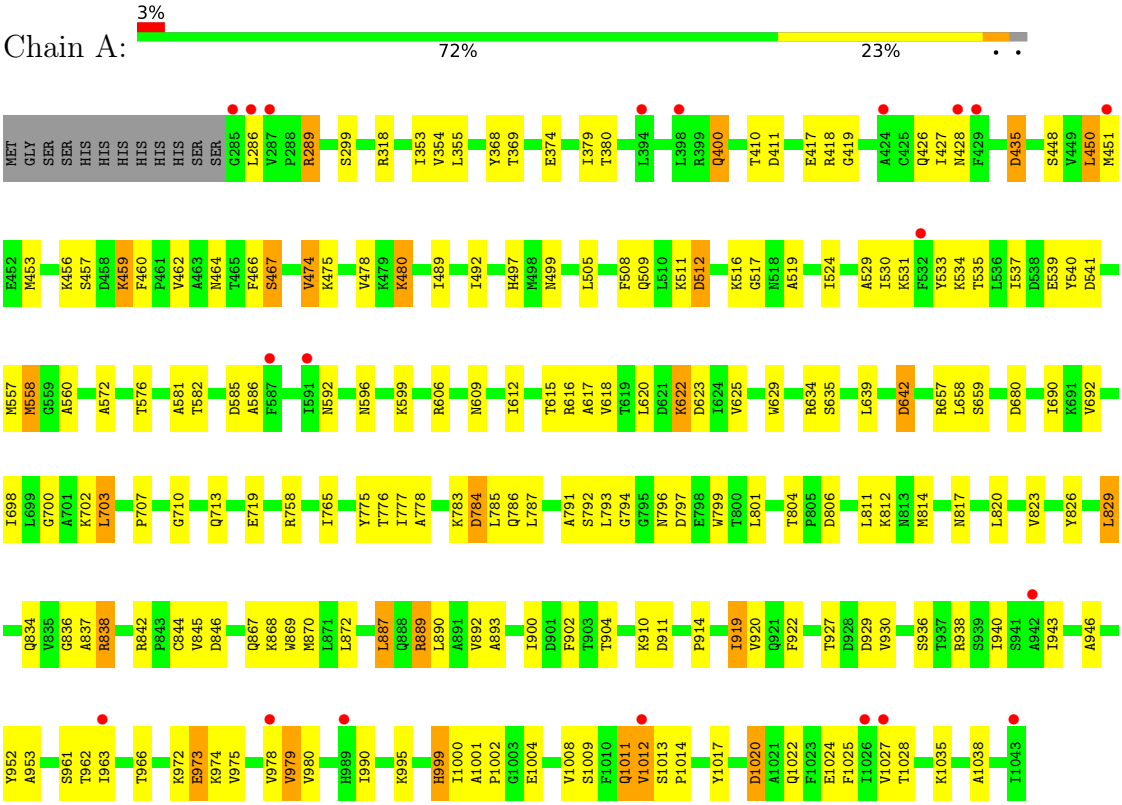
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	23	23	23	0	0

3 Residue-property plots (i)

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

• Molecule 1: TrpyGH20

Chain A:



• Molecule 2: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.76Å 93.69Å 94.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.30 – 2.77 65.30 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.5 (65.30-2.77) 98.5 (65.30-2.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.268 0.235 , 0.268	Depositor DCC
R_{free} test set	1097 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	77.9	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k 0.000 for -l,-k,-h 0.005 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11724	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NAG, NI, GAL

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	0.55	1/6012 (0.0%)	0.91	27/8165 (0.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	887	LEU	CG-CD1	6.85	1.77	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	887	LEU	CB-CG-CD2	14.58	135.79	111.00
1	A	435	ASP	CB-CG-OD1	-10.47	108.88	118.30
1	A	620	LEU	CB-CG-CD1	10.21	128.35	111.00
1	A	541	ASP	CB-CG-OD2	-9.19	110.03	118.30
1	A	1011	GLN	CA-CB-CG	8.36	131.80	113.40
1	A	658	LEU	CB-CG-CD1	7.82	124.29	111.00
1	A	620	LEU	CB-CG-CD2	-7.53	98.20	111.00
1	A	919	ILE	CG1-CB-CG2	-7.12	95.73	111.40
1	A	690	ILE	CG1-CB-CG2	-6.96	96.08	111.40
1	A	887	LEU	CB-CG-CD1	-6.76	99.50	111.00
1	A	887	LEU	CA-CB-CG	-6.75	99.78	115.30
1	A	480	LYS	CB-CG-CD	-6.56	94.55	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	541	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	829	LEU	CB-CG-CD1	6.10	121.38	111.00
1	A	450	LEU	CB-CG-CD2	-6.07	100.68	111.00
1	A	1012	VAL	CG1-CB-CG2	6.02	120.53	110.90
1	A	558	MET	CG-SD-CE	-5.88	90.78	100.20
1	A	639	LEU	CB-CG-CD2	-5.88	101.00	111.00
1	A	450	LEU	CB-CG-CD1	5.79	120.85	111.00
1	A	978	VAL	CG1-CB-CG2	-5.76	101.68	110.90
1	A	979	VAL	CG1-CB-CG2	-5.56	102.00	110.90
1	A	355	LEU	CB-CG-CD2	5.35	120.09	111.00
1	A	703	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	A	1011	GLN	CB-CA-C	-5.24	99.93	110.40
1	A	459	LYS	CB-CG-CD	-5.09	98.37	111.60
1	A	558	MET	CB-CG-SD	-5.06	97.22	112.40
1	A	541	ASP	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	ARG	Peptide
1	A	474	VAL	Mainchain
1	A	758	ARG	Sidechain

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	5881	5770	5770	156	0
2	C	26	21	24	1	0
3	A	3	0	0	0	0
4	A	23	0	0	8	0
All	All	5933	5791	5794	156	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 13.

All (156) 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:887:LEU:CG	1:A:887:LEU:CD1	1.77	1.63
1:A:887:LEU:CD1	1:A:887:LEU:CB	2.52	0.87
1:A:380:THR:O	4:A:1201:HOH:O	1.93	0.86
1:A:369:THR:O	4:A:1201:HOH:O	1.98	0.81
1:A:990:ILE:HG12	1:A:1012:VAL:HG12	1.66	0.76
1:A:775:TYR:CD1	1:A:801:LEU:HD23	2.20	0.76
1:A:497:HIS:H	1:A:558:MET:CE	2.01	0.74
1:A:995:LYS:HE2	1:A:1009:SER:O	1.87	0.73
1:A:785:LEU:HD11	1:A:919:ILE:HD12	1.68	0.73
1:A:887:LEU:CD1	1:A:887:LEU:CD2	2.67	0.72
1:A:796:ASN:O	1:A:796:ASN:OD1	2.08	0.71
1:A:980:VAL:HG21	1:A:1008:VAL:HG21	1.74	0.70
1:A:980:VAL:HG12	1:A:1027:VAL:HG12	1.75	0.68
1:A:557:MET:HG3	1:A:560:ALA:HB3	1.77	0.67
1:A:572:ALA:O	1:A:576:THR:HG23	1.95	0.67
1:A:927:THR:HG23	1:A:929:ASP:OD1	1.95	0.67
1:A:845:VAL:HG22	1:A:846:ASP:H	1.61	0.64
1:A:910:LYS:HD2	1:A:911:ASP:N	2.12	0.64
1:A:943:ILE:HG22	1:A:966:THR:CG2	2.29	0.63
1:A:474:VAL:O	1:A:478:VAL:HG23	2.00	0.61
1:A:974:LYS:HZ2	1:A:999:HIS:HB3	1.65	0.61
1:A:787:LEU:HD13	1:A:791:ALA:HB2	1.83	0.61
1:A:606:ARG:HG2	1:A:625:VAL:HG22	1.82	0.61
1:A:791:ALA:HB3	1:A:919:ILE:HG21	1.82	0.60
1:A:962:THR:HG1	1:A:1011:GLN:CD	2.04	0.60
1:A:622:LYS:O	1:A:622:LYS:HG3	2.01	0.60
1:A:836:GLY:O	1:A:838:ARG:HD2	2.01	0.59
1:A:354:VAL:HG23	1:A:380:THR:HG23	1.84	0.59
1:A:612:ILE:O	1:A:612:ILE:HD12	2.02	0.59
1:A:943:ILE:HG22	1:A:966:THR:HG22	1.85	0.58
1:A:823:VAL:HG11	1:A:842:ARG:HD3	1.86	0.58
1:A:820:LEU:HG	1:A:869:TRP:CZ2	2.38	0.58
1:A:1017:TYR:OH	1:A:1020:ASP:O	2.22	0.58
1:A:615:THR:HB	1:A:618:VAL:O	2.04	0.58
1:A:974:LYS:NZ	1:A:999:HIS:HB3	2.19	0.58
1:A:910:LYS:CD	1:A:911:ASP:N	2.67	0.57
1:A:369:THR:N	4:A:1201:HOH:O	2.18	0.57
1:A:606:ARG:HG2	1:A:625:VAL:CG2	2.34	0.57
1:A:902:PHE:CE2	1:A:914:PRO:HD3	2.40	0.56
1:A:457:SER:OG	1:A:464:ASN:OD1	2.21	0.56
1:A:900:ILE:HD11	1:A:904:THR:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ASP:OD1	1:A:617:ALA:N	2.34	0.56
1:A:995:LYS:HD3	1:A:1008:VAL:HB	1.87	0.56
1:A:451:MET:HG2	1:A:453:MET:HG2	1.88	0.56
1:A:592:ASN:O	1:A:596:ASN:ND2	2.39	0.56
1:A:900:ILE:HD11	1:A:904:THR:HG23	1.88	0.56
1:A:776:THR:HG23	1:A:936:SER:HA	1.88	0.55
1:A:765:ILE:HD11	1:A:872:LEU:CD1	2.37	0.55
1:A:999:HIS:C	1:A:1000:ILE:HD12	2.27	0.55
1:A:765:ILE:HD11	1:A:872:LEU:HD13	1.89	0.54
1:A:979:VAL:HB	1:A:1028:THR:HG22	1.89	0.54
1:A:533:TYR:CE1	1:A:537:ILE:HD11	2.42	0.54
1:A:353:ILE:HD13	1:A:379:ILE:HB	1.90	0.54
1:A:783:LYS:HB2	1:A:793:LEU:HG	1.90	0.53
1:A:834:GLN:HG2	1:A:837:ALA:HB2	1.90	0.53
1:A:615:THR:CB	1:A:618:VAL:O	2.57	0.53
1:A:616:ARG:HH11	1:A:616:ARG:HG2	1.74	0.53
1:A:973:GLU:N	1:A:1002:PRO:HG3	2.24	0.53
1:A:380:THR:N	4:A:1201:HOH:O	2.31	0.53
1:A:972:LYS:O	1:A:973:GLU:HG2	2.10	0.52
1:A:887:LEU:CD1	1:A:887:LEU:HB2	2.37	0.52
1:A:1000:ILE:HD12	1:A:1000:ILE:N	2.25	0.51
1:A:889:ARG:HH21	1:A:930:VAL:HG12	1.74	0.51
1:A:622:LYS:HD2	1:A:642:ASP:O	2.10	0.51
1:A:596:ASN:HA	1:A:599:LYS:HE3	1.94	0.50
1:A:535:THR:O	1:A:539:GLU:HG3	2.11	0.50
1:A:459:LYS:HD3	1:A:539:GLU:OE1	2.12	0.50
1:A:785:LEU:HD11	1:A:919:ILE:CD1	2.41	0.50
1:A:450:LEU:HD12	1:A:489:ILE:O	2.11	0.49
1:A:427:ILE:HG21	1:A:710:GLY:HA3	1.93	0.49
1:A:826:TYR:CD2	1:A:834:GLN:HB2	2.48	0.49
1:A:826:TYR:HD2	1:A:834:GLN:HB2	1.77	0.49
1:A:952:TYR:HD1	1:A:953:ALA:O	1.96	0.49
1:A:369:THR:CA	4:A:1201:HOH:O	2.58	0.49
1:A:943:ILE:CG2	1:A:966:THR:HG22	2.42	0.49
1:A:890:LEU:HD11	1:A:919:ILE:HD11	1.93	0.49
1:A:508:PHE:CD1	1:A:529:ALA:HB2	2.48	0.49
1:A:973:GLU:OE2	1:A:973:GLU:HA	2.13	0.49
1:A:1022:GLN:OE1	1:A:1038:ALA:O	2.29	0.48
1:A:940:ILE:HD11	1:A:975:VAL:HG11	1.94	0.48
1:A:492:ILE:HD11	1:A:540:TYR:CE1	2.49	0.48
1:A:512:ASP:OD2	1:A:516:LYS:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:MET:HG2	1:A:872:LEU:CD2	2.44	0.48
1:A:609:ASN:O	1:A:612:ILE:HG13	2.13	0.47
1:A:692:VAL:HB	1:A:698:ILE:HD11	1.96	0.47
1:A:797:ASP:N	1:A:938:ARG:HH22	2.13	0.47
1:A:845:VAL:HG22	1:A:846:ASP:N	2.26	0.47
1:A:910:LYS:HD2	1:A:911:ASP:O	2.15	0.47
1:A:462:VAL:HG23	1:A:505:LEU:HD21	1.97	0.47
1:A:474:VAL:O	1:A:475:LYS:C	2.53	0.46
1:A:459:LYS:CD	1:A:459:LYS:N	2.78	0.46
1:A:572:ALA:HB1	1:A:581:ALA:HB1	1.97	0.46
1:A:777:ILE:HD12	1:A:799:TRP:CG	2.49	0.46
1:A:804:THR:HG21	1:A:868:LYS:HD3	1.98	0.46
1:A:299:SER:OG	1:A:410:THR:O	2.34	0.46
1:A:775:TYR:CD1	1:A:801:LEU:CD2	2.97	0.46
1:A:979:VAL:HB	1:A:1028:THR:CG2	2.45	0.46
1:A:524:ILE:HD11	1:A:586:ALA:HB1	1.97	0.45
1:A:953:ALA:N	1:A:1014:PRO:HG2	2.32	0.45
1:A:417:GLU:O	1:A:700:GLY:HA3	2.17	0.45
1:A:786:GLN:HG2	1:A:794:GLY:HA3	1.98	0.45
1:A:806:ASP:OD2	1:A:868:LYS:NZ	2.49	0.45
1:A:466:PHE:CG	1:A:467:SER:HA	2.52	0.45
1:A:1001:ALA:HB3	1:A:1004:GLU:HG3	1.98	0.45
1:A:492:ILE:HD11	1:A:540:TYR:CZ	2.51	0.45
1:A:659:SER:O	1:A:659:SER:OG	2.32	0.45
1:A:1024:GLU:OE2	1:A:1035:LYS:CD	2.65	0.45
1:A:582:THR:HG23	1:A:585:ASP:H	1.81	0.44
1:A:286:LEU:HD21	1:A:400:GLN:HB2	1.99	0.44
1:A:531:LYS:O	1:A:535:THR:OG1	2.29	0.44
1:A:612:ILE:CD1	1:A:634:ARG:HB2	2.48	0.44
1:A:428:ASN:O	1:A:887:LEU:HD13	2.18	0.44
1:A:380:THR:CA	4:A:1201:HOH:O	2.65	0.44
1:A:911:ASP:C	1:A:911:ASP:OD2	2.56	0.43
1:A:943:ILE:HG22	1:A:966:THR:HG23	1.99	0.43
1:A:963:ILE:HG21	1:A:1025:PHE:CE1	2.54	0.43
1:A:368:TYR:CZ	1:A:411:ASP:HB3	2.53	0.43
1:A:419:GLY:HA2	1:A:448:SER:O	2.19	0.43
1:A:791:ALA:HB1	1:A:919:ILE:HD13	1.99	0.43
1:A:812:LYS:HD2	1:A:844:CYS:SG	2.58	0.43
1:A:289:ARG:N	1:A:289:ARG:CD	2.81	0.43
1:A:817:ASN:ND2	1:A:1022:GLN:HG2	2.33	0.43
1:A:426:GLN:HB2	1:A:829:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ARG:N	1:A:289:ARG:HD3	2.34	0.43
1:A:657:ARG:HD3	1:A:713:GLN:HB2	2.01	0.43
1:A:380:THR:HB	4:A:1201:HOH:O	2.19	0.42
1:A:893:ALA:CB	1:A:914:PRO:HB2	2.49	0.42
1:A:961:SER:O	1:A:1012:VAL:HG22	2.20	0.42
1:A:419:GLY:O	1:A:702:LYS:HA	2.20	0.42
1:A:599:LYS:HD3	1:A:623:ASP:OD2	2.19	0.42
1:A:511:LYS:HD3	1:A:517:GLY:CA	2.49	0.42
1:A:920:VAL:HG21	1:A:922:PHE:CZ	2.54	0.42
1:A:289:ARG:NE	1:A:289:ARG:H	2.18	0.42
1:A:972:LYS:HA	1:A:1002:PRO:HB3	2.02	0.42
1:A:892:VAL:O	1:A:892:VAL:CG2	2.67	0.41
1:A:973:GLU:H	1:A:1002:PRO:HG3	1.84	0.41
1:A:530:ILE:HG23	1:A:534:LYS:HE3	2.02	0.41
1:A:719:GLU:HG3	4:A:1205:HOH:O	2.19	0.41
1:A:435:ASP:OD1	1:A:480:LYS:HD3	2.21	0.41
1:A:612:ILE:O	1:A:612:ILE:CD1	2.68	0.41
1:A:680:ASP:OD1	1:A:680:ASP:N	2.54	0.41
1:A:870:MET:HG2	1:A:872:LEU:HD22	2.03	0.41
1:A:946:ALA:HB1	1:A:961:SER:OG	2.20	0.41
1:A:456:LYS:HG3	1:A:464:ASN:ND2	2.36	0.41
1:A:509:GLN:HG2	1:A:519:ALA:HA	2.03	0.41
1:A:943:ILE:CG2	1:A:966:THR:CG2	2.98	0.41
1:A:980:VAL:HG22	1:A:995:LYS:O	2.20	0.41
1:A:354:VAL:CG2	1:A:380:THR:HG23	2.49	0.41
1:A:629:TRP:CE2	2:C:1:NAG:H83	2.56	0.41
1:A:785:LEU:HD12	1:A:792:SER:O	2.20	0.41
1:A:927:THR:CG2	1:A:929:ASP:H	2.33	0.41
1:A:778:ALA:CB	1:A:784:ASP:HA	2.51	0.41
1:A:787:LEU:CD1	1:A:791:ALA:HB2	2.51	0.40
1:A:980:VAL:HG23	1:A:995:LYS:HB2	2.03	0.40
1:A:784:ASP:O	1:A:793:LEU:HD12	2.22	0.40
1:A:460:PHE:N	1:A:460:PHE:CD1	2.90	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	757/771 (98%)	723 (96%)	33 (4%)	1 (0%)	48 76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	707	PRO

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	626/637 (98%)	605 (97%)	21 (3%)	32 63

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	ARG
1	A	318	ARG
1	A	374	GLU
1	A	400	GLN
1	A	467	SER
1	A	499	ASN
1	A	512	ASP
1	A	622	LYS
1	A	635	SER
1	A	642	ASP

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Mol	Chain	Res	Type
1	A	703	LEU
1	A	784	ASP
1	A	811	LEU
1	A	814	MET
1	A	838	ARG
1	A	867	GLN
1	A	889	ARG
1	A	973	GLU
1	A	999	HIS
1	A	1013	SER
1	A	1020	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	779	GLN
1	A	796	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	C	1	2	15,15,15	0.54	0	21,21,21	0.75	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	C	2	2	11,11,12	1.26	1 (9%)	15,15,17	1.20	1 (6%)

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	C	1	2	-	3/6/26/26	0/1/1/1
2	GAL	C	2	2	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GAL	O5-C5	2.54	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GAL	C1-C2-C3	2.77	113.06	109.67
2	C	1	NAG	C1-O5-C5	2.51	118.40	113.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C1-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
2	C	2	GAL	O5-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

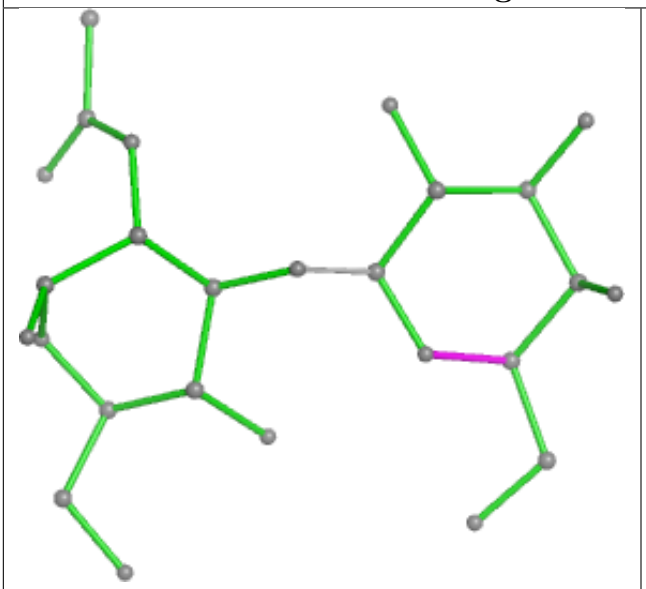
There are no ring outliers.

1 monomer is involved in 1 short contact:

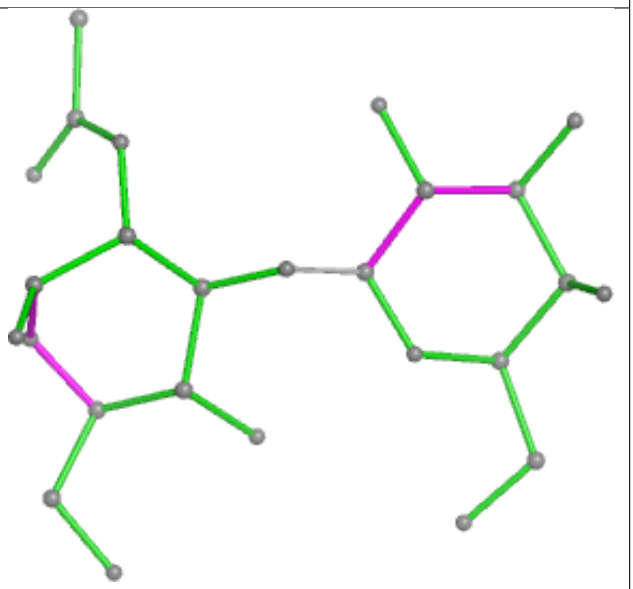
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

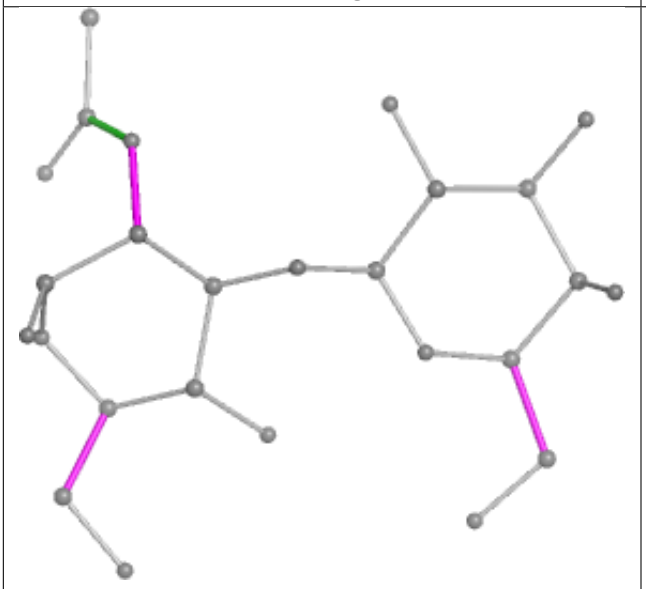
Oligosaccharide Chain C



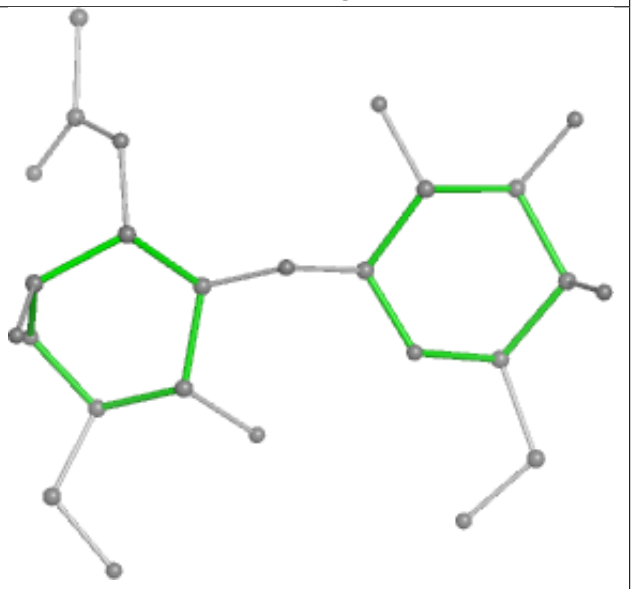
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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, 95^{th} 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	759/771 (98%)	0.04	20 (2%) 57 51	59, 94, 143, 169	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	GLY	4.4
1	A	963	ILE	3.7
1	A	287	VAL	3.1
1	A	591	ILE	2.8
1	A	398	LEU	2.8
1	A	532	PHE	2.8
1	A	1027	VAL	2.7
1	A	451	MET	2.7
1	A	1043	ILE	2.6
1	A	587	PHE	2.6
1	A	424	ALA	2.5
1	A	978	VAL	2.3
1	A	429	PHE	2.3
1	A	989	HIS	2.2
1	A	286	LEU	2.2
1	A	1026	ILE	2.1
1	A	942	ALA	2.1
1	A	1012	VAL	2.0
1	A	394	LEU	2.0
1	A	428	ASN	2.0

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 (i)

SUGAR-RSR INFOmissingINFO

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, 95^{th} 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	NI	A	1103	1/1	0.87	0.08	128,128,128,128	0
3	NI	A	1102	1/1	0.88	0.17	131,131,131,131	0
3	NI	A	1101	1/1	0.93	0.08	92,92,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.