Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 08:11 AM EDT

PDB ID	:	2RHP
Title	:	The Thrombospondin-1 Polymorphism Asn700Ser Associated with Cornoary Artery Disease Causes Local and Long-Ranging Changes in Protein Structure
Authors	:	Carlson, C.B.; Keck, J.L.; Mosher, D.F.
Deposited on	:	2007-10-09
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

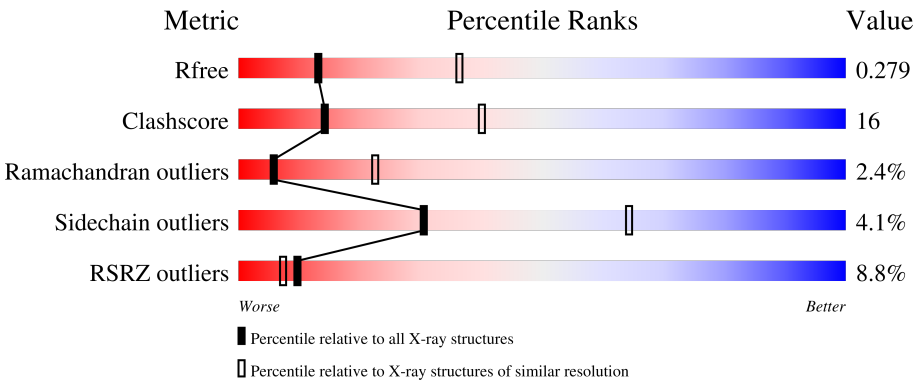
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	622	9%, 72%, 25%, •
2	B	2	50%, 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5007 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 Thrombospondin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	622	4850	2954	837	1018	41	0	0	0

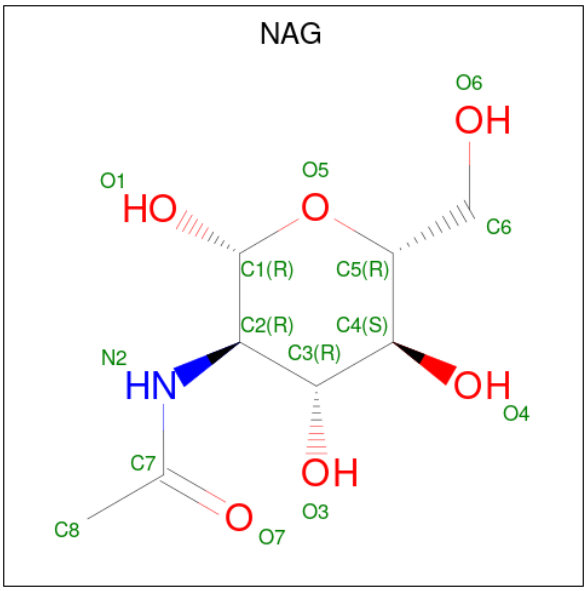
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	702	SER	ASN	engineered mutation	UNP P35442

- 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	28	16	2	10	0	0	0

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



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	30	30	30	0	0

- Molecule 5 is water.

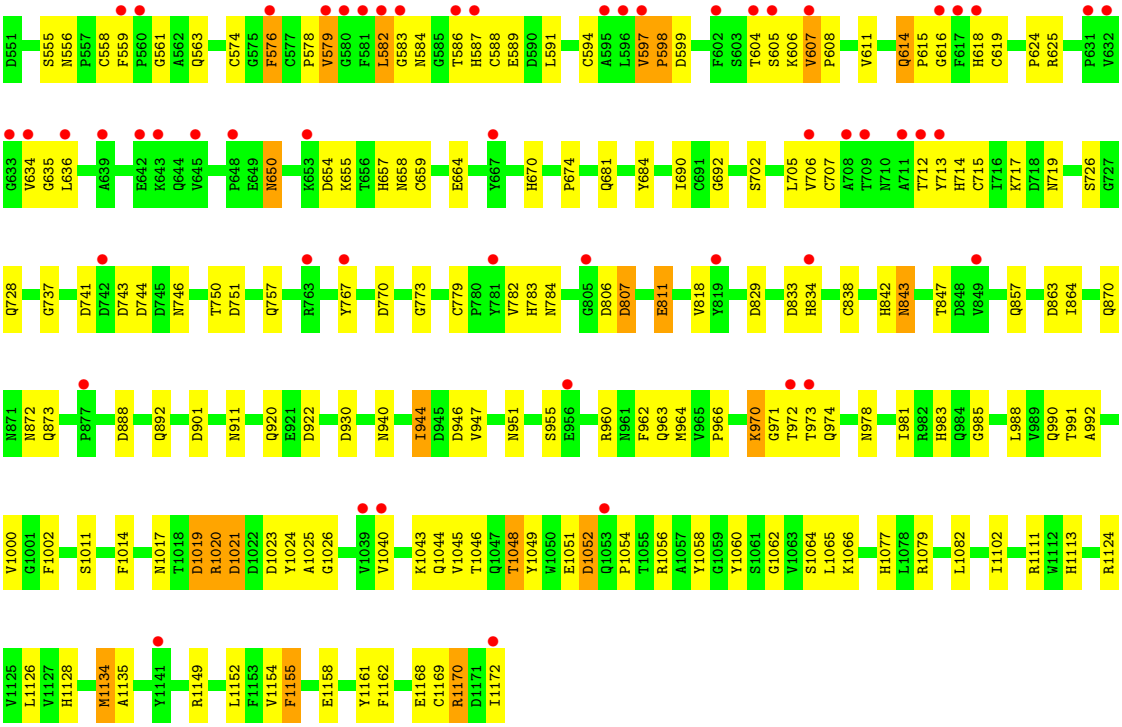
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	71	71	71	0	0

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: Thrombospondin-2

Chain A: 9% 72% 25%



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.89Å 122.65Å 155.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-2.90) 98.2 (29.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	0.61 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.227 , 0.277 0.227 , 0.279	Depositor DCC
R_{free} test set	1019 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5007	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.35	0/4973	0.52	0/6778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4850	0	4259	144	0
2	B	28	0	25	0	0
3	A	28	0	26	0	0
4	A	30	0	0	0	0
5	A	71	0	0	2	0
All	All	5007	0	4310	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (144) 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:614:GLN:HB2	1:A:615:PRO:HD3	1.31	1.10
1:A:597:VAL:HB	1:A:598:PRO:CD	1.87	1.04
1:A:597:VAL:HB	1:A:598:PRO:HD3	1.06	1.04
1:A:597:VAL:CB	1:A:598:PRO:HD3	1.90	1.01
1:A:1169:CYS:HB3	1:A:1172:ILE:HB	1.41	0.99
1:A:1019:ASP:OD1	1:A:1020:ARG:NH1	2.03	0.91
1:A:978:ASN:H	1:A:990:GLN:HE21	1.07	0.90
1:A:582:LEU:HD12	1:A:589:GLU:HB2	1.55	0.89
1:A:972:THR:HG22	1:A:973:THR:H	1.37	0.89
1:A:818:VAL:HG11	1:A:834:HIS:CD2	2.07	0.88
1:A:843:ASN:HB3	1:A:857:GLN:HG3	1.54	0.86
1:A:972:THR:HG22	1:A:973:THR:N	1.92	0.85
1:A:981:ILE:HD12	1:A:988:LEU:HD22	1.60	0.81
1:A:743:ASP:OD2	1:A:746:ASN:HA	1.81	0.80
1:A:705:LEU:C	1:A:707:CYS:H	1.85	0.79
1:A:981:ILE:CD1	1:A:988:LEU:HD22	2.15	0.77
1:A:1134:MET:HE2	1:A:1135:ALA:HB2	1.65	0.77
1:A:972:THR:CG2	1:A:973:THR:H	1.99	0.76
1:A:607:VAL:H	1:A:608:PRO:CD	1.99	0.75
1:A:614:GLN:HB2	1:A:615:PRO:CD	2.13	0.75
1:A:1124:ARG:NH2	1:A:1126:LEU:HD21	2.02	0.74
1:A:978:ASN:H	1:A:990:GLN:NE2	1.85	0.73
1:A:1014:PHE:HE2	1:A:1025:ALA:HB3	1.53	0.71
1:A:1172:ILE:HG22	1:A:1172:ILE:O	1.92	0.70
1:A:607:VAL:H	1:A:608:PRO:HD2	1.56	0.69
1:A:922:ASP:HA	1:A:930:ASP:OD1	1.93	0.67
1:A:962:PHE:CE2	1:A:981:ILE:HD11	2.29	0.67
1:A:847:THR:HG23	5:A:1198:HOH:O	1.95	0.66
1:A:972:THR:CG2	1:A:973:THR:N	2.58	0.66
1:A:606:LYS:HB3	1:A:608:PRO:HD2	1.79	0.65
1:A:674:PRO:HD2	1:A:944:ILE:HG23	1.78	0.65
1:A:1024:TYR:HB2	1:A:1155:PHE:HB3	1.79	0.65
1:A:1052:ASP:OD1	1:A:1052:ASP:N	2.28	0.64
1:A:657:HIS:HD2	1:A:659:CYS:H	1.44	0.64
1:A:741:ASP:HB3	1:A:744:ASP:OD1	1.99	0.63
1:A:582:LEU:N	1:A:589:GLU:O	2.31	0.63
1:A:962:PHE:HE2	1:A:981:ILE:HD11	1.63	0.62
1:A:563:GLN:H	1:A:576:PHE:HB2	1.64	0.62
1:A:1043:LYS:HE3	1:A:1045:VAL:O	2.00	0.62
1:A:1169:CYS:CB	1:A:1172:ILE:HB	2.24	0.62
1:A:963:GLN:OE1	1:A:1149:ARG:NH2	2.31	0.62
1:A:990:GLN:HE22	1:A:992:ALA:H	1.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:VAL:HG11	1:A:834:HIS:HD2	1.66	0.61
1:A:857:GLN:HG2	5:A:1230:HOH:O	2.00	0.60
1:A:1054:PRO:HG3	1:A:1077:HIS:HA	1.83	0.60
1:A:1168:GLU:OE1	1:A:1170:ARG:NH1	2.35	0.59
1:A:1011:SER:HB3	1:A:1113:HIS:HD2	1.67	0.58
1:A:719:ASN:H	1:A:728:GLN:HE22	1.49	0.58
1:A:591:LEU:HD21	1:A:636:LEU:HD13	1.84	0.58
1:A:1014:PHE:CE2	1:A:1025:ALA:HB3	2.37	0.58
1:A:584:ASN:HB3	1:A:587:HIS:O	2.03	0.57
1:A:963:GLN:HB3	1:A:1000:VAL:HG22	1.87	0.57
1:A:705:LEU:C	1:A:707:CYS:N	2.52	0.56
1:A:578:PRO:O	1:A:579:VAL:C	2.45	0.55
1:A:705:LEU:O	1:A:707:CYS:N	2.39	0.55
1:A:978:ASN:N	1:A:990:GLN:HE21	1.91	0.55
1:A:1044:GLN:HG2	1:A:1045:VAL:HG23	1.88	0.55
1:A:1024:TYR:CE2	1:A:1043:LYS:HB2	2.42	0.54
1:A:561:GLY:HA3	1:A:578:PRO:HG3	1.89	0.54
1:A:972:THR:C	1:A:974:GLN:H	2.08	0.54
1:A:947:VAL:HG22	1:A:955:SER:C	2.28	0.53
1:A:806:ASP:O	1:A:807:ASP:HB2	2.09	0.53
1:A:829:ASP:HB3	1:A:842:HIS:CD2	2.44	0.53
1:A:991:THR:O	1:A:1158:GLU:HB2	2.09	0.53
1:A:990:GLN:NE2	1:A:992:ALA:H	2.07	0.52
1:A:1152:LEU:HD22	1:A:1162:PHE:CD2	2.45	0.52
1:A:650:ASN:C	1:A:650:ASN:HD22	2.13	0.52
1:A:864:ILE:O	1:A:864:ILE:HG12	2.09	0.52
1:A:1048:THR:HB	1:A:1058:TYR:HD2	1.75	0.51
1:A:1062:GLY:HA2	1:A:1102:ILE:O	2.10	0.51
1:A:1011:SER:HB3	1:A:1113:HIS:CD2	2.44	0.51
1:A:951:ASN:HB2	1:A:1172:ILE:HG21	1.92	0.51
1:A:624:PRO:O	1:A:625:ARG:HB2	2.10	0.51
1:A:726:SER:O	1:A:983:HIS:CE1	2.64	0.51
1:A:888:ASP:HB3	1:A:901:ASP:HA	1.92	0.50
1:A:664:GLU:HG2	1:A:681:GLN:HG2	1.92	0.50
1:A:654:ASP:O	1:A:655:LYS:HG2	2.11	0.50
1:A:702:SER:O	1:A:717:LYS:HG3	2.12	0.50
1:A:843:ASN:CB	1:A:857:GLN:HG3	2.35	0.50
1:A:743:ASP:OD2	1:A:746:ASN:CA	2.54	0.50
1:A:737:GLY:O	1:A:741:ASP:HB2	2.12	0.49
1:A:964:MET:O	1:A:966:PRO:HD3	2.13	0.48
1:A:604:THR:HG22	1:A:604:THR:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:GLU:CG	1:A:681:GLN:HG2	2.43	0.48
1:A:1002:PHE:HA	1:A:1149:ARG:HH11	1.76	0.48
1:A:690:ILE:CG2	1:A:707:CYS:HB2	2.43	0.48
1:A:657:HIS:CD2	1:A:659:CYS:H	2.29	0.48
1:A:690:ILE:HG21	1:A:707:CYS:HB2	1.95	0.48
1:A:558:CYS:O	1:A:559:PHE:C	2.52	0.47
1:A:604:THR:O	1:A:605:SER:CB	2.62	0.47
1:A:611:VAL:HG23	1:A:618:HIS:HB3	1.96	0.47
1:A:990:GLN:HG3	1:A:1154:VAL:HG11	1.97	0.47
1:A:1048:THR:HB	1:A:1058:TYR:CD2	2.49	0.47
1:A:684:TYR:HA	1:A:692:GLY:O	2.14	0.47
1:A:946:ASP:OD1	1:A:955:SER:HA	2.15	0.47
1:A:751:ASP:O	1:A:757:GLN:NE2	2.48	0.46
1:A:574:CYS:SG	1:A:586:THR:HG22	2.55	0.46
1:A:951:ASN:HB2	1:A:1172:ILE:CG2	2.45	0.46
1:A:614:GLN:CB	1:A:615:PRO:HD3	2.20	0.46
1:A:616:GLY:HA3	1:A:634:VAL:HA	1.98	0.46
1:A:838:CYS:HB2	1:A:843:ASN:HD21	1.80	0.46
1:A:1052:ASP:HB3	1:A:1056:ARG:NH1	2.30	0.46
1:A:604:THR:O	1:A:605:SER:HB3	2.16	0.46
1:A:930:ASP:OD1	1:A:930:ASP:N	2.50	0.45
1:A:811:GLU:H	1:A:811:GLU:HG2	1.58	0.45
1:A:1172:ILE:O	1:A:1172:ILE:CG2	2.63	0.45
1:A:1152:LEU:HD22	1:A:1162:PHE:CG	2.52	0.45
1:A:1023:ASP:OD1	1:A:1043:LYS:NZ	2.50	0.45
1:A:597:VAL:CG1	1:A:598:PRO:HD3	2.45	0.44
1:A:818:VAL:CG1	1:A:834:HIS:CD2	2.92	0.44
1:A:579:VAL:HG12	1:A:635:GLY:HA2	1.97	0.44
1:A:625:ARG:HB3	1:A:670:HIS:CE1	2.53	0.44
1:A:779:CYS:HB2	1:A:784:ASN:ND2	2.33	0.44
1:A:960:ARG:HG3	1:A:985:GLY:HA3	1.99	0.44
1:A:598:PRO:HB2	1:A:599:ASP:H	1.55	0.43
1:A:1111:ARG:HB3	1:A:1128:HIS:HB2	2.01	0.43
1:A:1026:GLY:HA3	1:A:1040:VAL:O	2.18	0.43
1:A:1049:TYR:OH	1:A:1079:ARG:HD2	2.18	0.43
1:A:1066:LYS:NZ	1:A:1082:LEU:O	2.49	0.43
1:A:1046:THR:HG23	1:A:1060:TYR:HA	2.01	0.43
1:A:944:ILE:H	1:A:944:ILE:HG13	1.52	0.43
1:A:960:ARG:HG3	1:A:985:GLY:CA	2.49	0.43
1:A:972:THR:C	1:A:974:GLN:N	2.72	0.42
1:A:654:ASP:C	1:A:655:LYS:HG2	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASN:HD22	1:A:658:ASN:HA	1.66	0.42
1:A:872:ASN:OD1	1:A:873:GLN:HG3	2.19	0.42
1:A:555:SER:O	1:A:556:ASN:C	2.58	0.42
1:A:707:CYS:HB3	1:A:715:CYS:HB3	1.92	0.42
1:A:1134:MET:HG3	1:A:1135:ALA:N	2.35	0.42
1:A:1170:ARG:HD2	1:A:1170:ARG:HA	1.71	0.42
1:A:981:ILE:HD12	1:A:988:LEU:CD2	2.42	0.42
1:A:782:VAL:HG12	1:A:783:HIS:N	2.36	0.41
1:A:863:ASP:HB2	1:A:870:GLN:HA	2.03	0.41
1:A:597:VAL:CB	1:A:598:PRO:CD	2.65	0.41
1:A:770:ASP:HB3	1:A:783:HIS:CD2	2.55	0.41
1:A:842:HIS:O	1:A:843:ASN:HB3	2.20	0.41
1:A:1017:ASN:HB3	1:A:1161:TYR:CE2	2.55	0.41
1:A:911:ASN:OD1	1:A:920:GLN:OE1	2.39	0.41
1:A:559:PHE:HB2	1:A:586:THR:O	2.21	0.41
1:A:713:TYR:O	1:A:715:CYS:N	2.54	0.41
1:A:607:VAL:N	1:A:608:PRO:CD	2.69	0.40
1:A:611:VAL:HG22	1:A:618:HIS:O	2.22	0.40
1:A:970:LYS:HB2	1:A:971:GLY:H	1.69	0.40
1:A:1040:VAL:HA	1:A:1064:SER:O	2.22	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	620/622 (100%)	536 (86%)	69 (11%)	15 (2%)	6 22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	767	TYR
1	A	579	VAL
1	A	594	CYS
1	A	598	PRO
1	A	706	VAL
1	A	714	HIS
1	A	773	GLY
1	A	607	VAL
1	A	582	LEU
1	A	970	LYS
1	A	576	PHE
1	A	1021	ASP
1	A	583	GLY
1	A	843	ASN

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	541/541 (100%)	519 (96%)	22 (4%)	30 64

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	CYS
1	A	614	GLN
1	A	619	CYS
1	A	650	ASN
1	A	712	THR
1	A	750	THR
1	A	807	ASP
1	A	811	GLU
1	A	833	ASP
1	A	892	GLN
1	A	940	ASN
1	A	944	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1019	ASP
1	A	1020	ARG
1	A	1021	ASP
1	A	1048	THR
1	A	1051	GLU
1	A	1052	ASP
1	A	1065	LEU
1	A	1134	MET
1	A	1155	PHE
1	A	1170	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	587	HIS
1	A	650	ASN
1	A	657	HIS
1	A	658	ASN
1	A	728	GLN
1	A	783	HIS
1	A	834	HIS
1	A	842	HIS
1	A	990	GLN
1	A	1091	GLN

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	B	1	1,2	14,14,15	0.66	0	17,19,21	1.08	1 (5%)
2	NAG	B	2	2	14,14,15	0.61	0	17,19,21	0.67	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
2	NAG	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C4-C3-C2	2.47	114.64	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

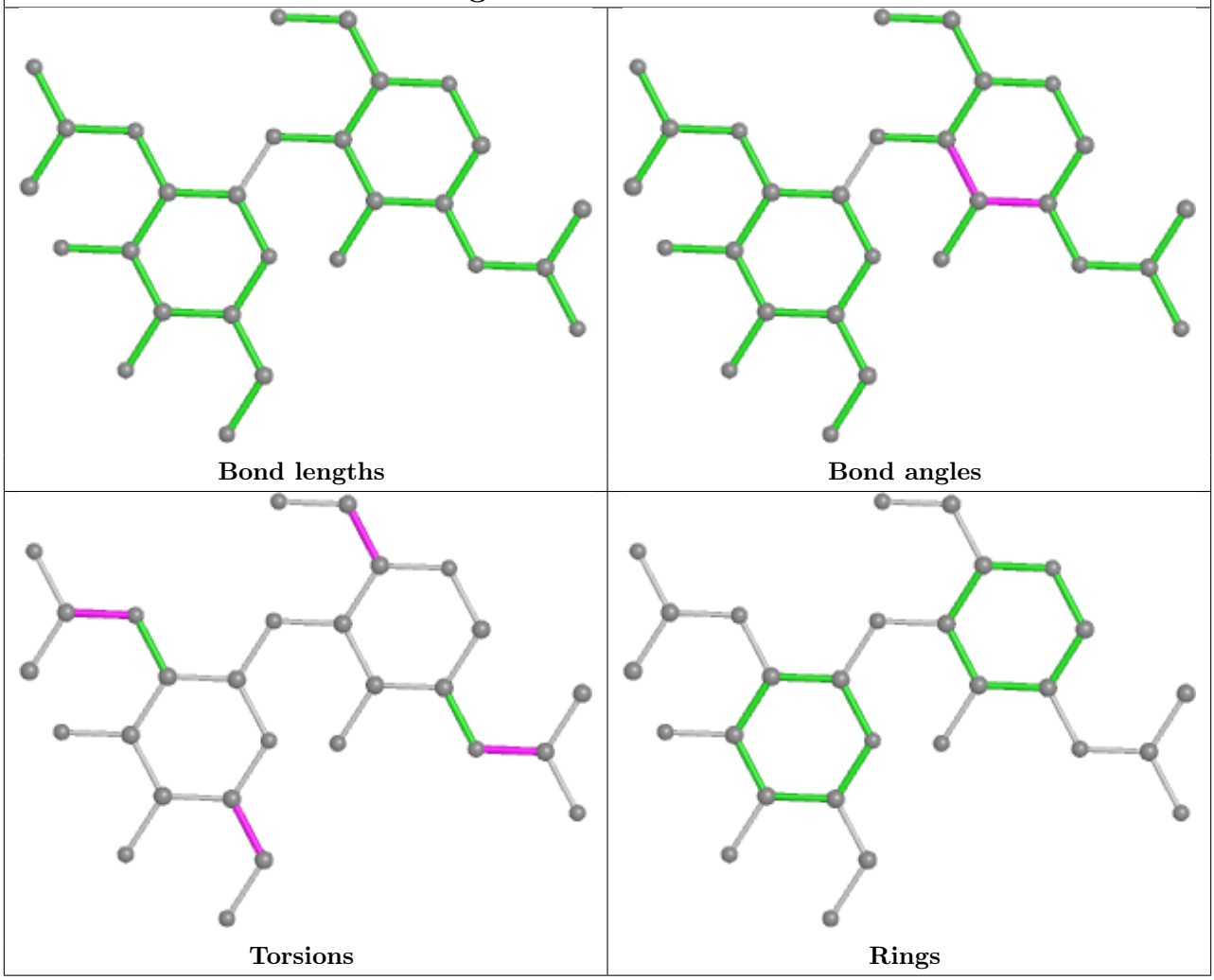
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

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.

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 30 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	6	1	14,14,15	0.49	0	17,19,21	1.21	1 (5%)
3	NAG	A	1	1	14,14,15	0.52	0	17,19,21	1.43	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
3	NAG	A	6	1	-	5/6/23/26	0/1/1/1
3	NAG	A	1	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	NAG	C1-O5-C5	4.39	118.14	112.19
3	A	6	NAG	C1-O5-C5	3.35	116.73	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NAG	C8-C7-N2-C2
3	A	1	NAG	O7-C7-N2-C2
3	A	6	NAG	C3-C2-N2-C7
3	A	6	NAG	C8-C7-N2-C2
3	A	6	NAG	O7-C7-N2-C2
3	A	6	NAG	O5-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
3	A	6	NAG	C4-C5-C6-O6

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	622/622 (100%)	0.74	55 (8%)	10	7	11, 34, 80, 86	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	834	HIS	7.0
1	A	596	LEU	6.6
1	A	709	THR	5.6
1	A	576	PHE	5.5
1	A	634	VAL	4.9
1	A	633	GLY	4.8
1	A	632	VAL	4.8
1	A	605	SER	4.3
1	A	617	PHE	4.2
1	A	805	GLY	4.0
1	A	973	THR	3.9
1	A	645	VAL	3.9
1	A	618	HIS	3.9
1	A	819	TYR	3.7
1	A	560	PRO	3.4
1	A	631	PRO	3.3
1	A	597	VAL	3.2
1	A	712	THR	3.2
1	A	604	THR	3.1
1	A	781	TYR	3.0
1	A	643	LYS	2.9
1	A	706	VAL	2.9
1	A	616	GLY	2.8
1	A	972	THR	2.8
1	A	642	GLU	2.8
1	A	1039	VAL	2.7
1	A	639	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	582	LEU	2.6
1	A	583	GLY	2.6
1	A	607	VAL	2.6
1	A	595	ALA	2.6
1	A	559	PHE	2.6
1	A	767	TYR	2.5
1	A	580	GLY	2.5
1	A	708	ALA	2.4
1	A	586	THR	2.4
1	A	587	HIS	2.4
1	A	1141	TYR	2.4
1	A	1053	GLN	2.3
1	A	579	VAL	2.3
1	A	648	PRO	2.2
1	A	877	PRO	2.2
1	A	581	PHE	2.2
1	A	1040	VAL	2.2
1	A	602	PHE	2.1
1	A	742	ASP	2.1
1	A	1172	ILE	2.1
1	A	713	TYR	2.1
1	A	711	ALA	2.1
1	A	849	VAL	2.1
1	A	636	LEU	2.0
1	A	763	ARG	2.0
1	A	653	LYS	2.0
1	A	956	GLU	2.0
1	A	667	TYR	2.0

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)

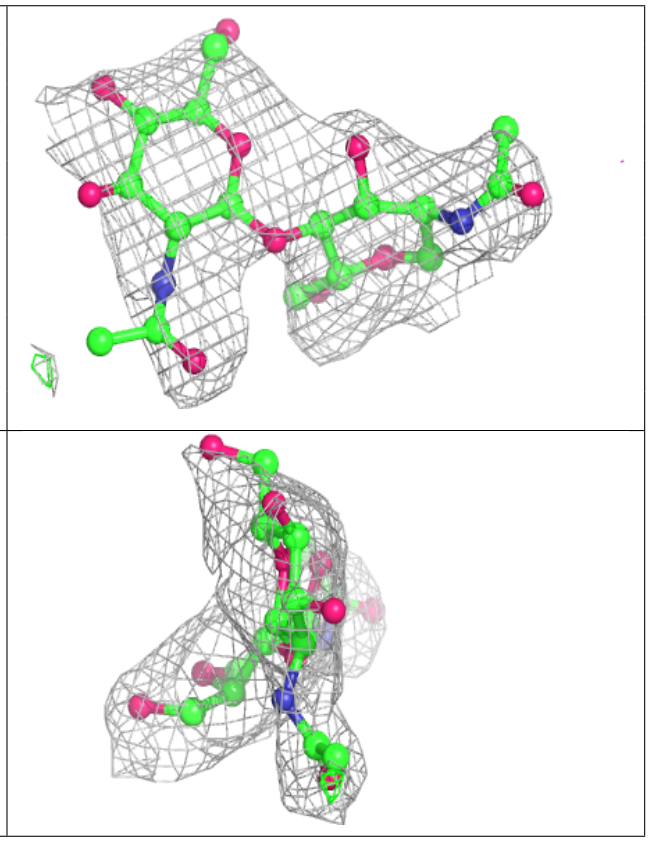
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.74	0.39	52,53,54,54	0
2	NAG	B	1	14/15	0.86	0.27	44,46,48,50	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	21	1/1	0.08	0.15	57,57,57,57	0
3	NAG	A	1	14/15	0.62	0.34	64,64,65,65	0
4	CA	A	25	1/1	0.77	0.12	35,35,35,35	0
4	CA	A	24	1/1	0.81	0.13	45,45,45,45	0
4	CA	A	26	1/1	0.81	0.10	34,34,34,34	0
4	CA	A	30	1/1	0.83	0.08	75,75,75,75	0
4	CA	A	29	1/1	0.85	0.13	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	22	1/1	0.85	0.10	67,67,67,67	0
4	CA	A	1175	1/1	0.86	0.08	31,31,31,31	0
4	CA	A	20	1/1	0.86	0.07	61,61,61,61	0
3	NAG	A	6	14/15	0.86	0.31	63,63,65,65	0
4	CA	A	10	1/1	0.88	0.10	25,25,25,25	0
4	CA	A	28	1/1	0.88	0.10	21,21,21,21	0
4	CA	A	1174	1/1	0.89	0.11	31,31,31,31	0
4	CA	A	1173	1/1	0.89	0.07	18,18,18,18	0
4	CA	A	17	1/1	0.90	0.06	30,30,30,30	0
4	CA	A	8	1/1	0.90	0.11	36,36,36,36	0
4	CA	A	1176	1/1	0.90	0.07	37,37,37,37	0
4	CA	A	12	1/1	0.90	0.07	31,31,31,31	0
4	CA	A	16	1/1	0.90	0.07	43,43,43,43	0
4	CA	A	11	1/1	0.91	0.08	24,24,24,24	0
4	CA	A	23	1/1	0.91	0.06	54,54,54,54	0
4	CA	A	13	1/1	0.92	0.08	15,15,15,15	0
4	CA	A	18	1/1	0.92	0.13	45,45,45,45	0
4	CA	A	14	1/1	0.92	0.12	24,24,24,24	0
4	CA	A	3	1/1	0.92	0.10	32,32,32,32	0
4	CA	A	15	1/1	0.94	0.15	30,30,30,30	0
4	CA	A	2	1/1	0.94	0.10	32,32,32,32	0
4	CA	A	7	1/1	0.95	0.05	32,32,32,32	0
4	CA	A	27	1/1	0.97	0.13	31,31,31,31	0
4	CA	A	19	1/1	0.97	0.05	34,34,34,34	0
4	CA	A	9	1/1	0.98	0.07	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.