



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:35 AM BST

PDB ID : 2F1B  
Title : GOLGI ALPHA-MANNOSIDASE II COMPLEX WITH (2R,3R,4S,5R)-2-({[(1R)-2-hydroxy-1-phenylethyl]amino}methyl)-5-methylpyrrolidine-3,4-diol  
Authors : Kuntz, D.A.; Rose, D.R.  
Deposited on : 2005-11-14  
Resolution : 1.45 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
buster-report : 1.1.7 (2018)  
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) : 2.13.1

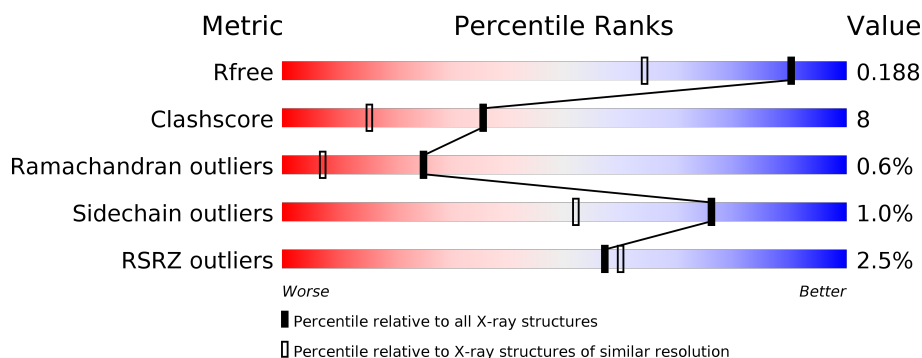
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1045	<div> <div>2%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	A	1801	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9491 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 alpha-mannosidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1014	Total	C	N	O	S	0	34	0
			8291	5266	1447	1535	43			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	expression tag	GB 517481
A	2	SER	-	expression tag	GB 517481
A	3	SER	-	expression tag	GB 517481
A	4	HIS	-	expression tag	GB 517481
A	5	HIS	-	expression tag	GB 517481
A	6	HIS	-	expression tag	GB 517481
A	7	HIS	-	expression tag	GB 517481
A	8	HIS	-	expression tag	GB 517481
A	9	HIS	-	expression tag	GB 517481
A	10	GLY	-	expression tag	GB 517481
A	11	GLU	-	expression tag	GB 517481
A	12	PHE	-	expression tag	GB 517481

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

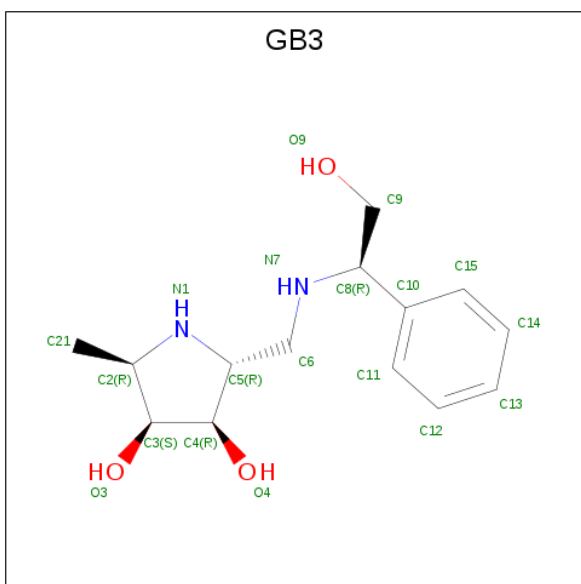


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (2R,3R,4S,5R)-2-({[(1R)-2-HYDROXY-1-PHENYLETHYL]AMINO}METHYL)-5-METHYLPYRROLIDINE-3,4-DIOL (three-letter code: GB3) (formula: C<sub>14</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	14	2	3		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		

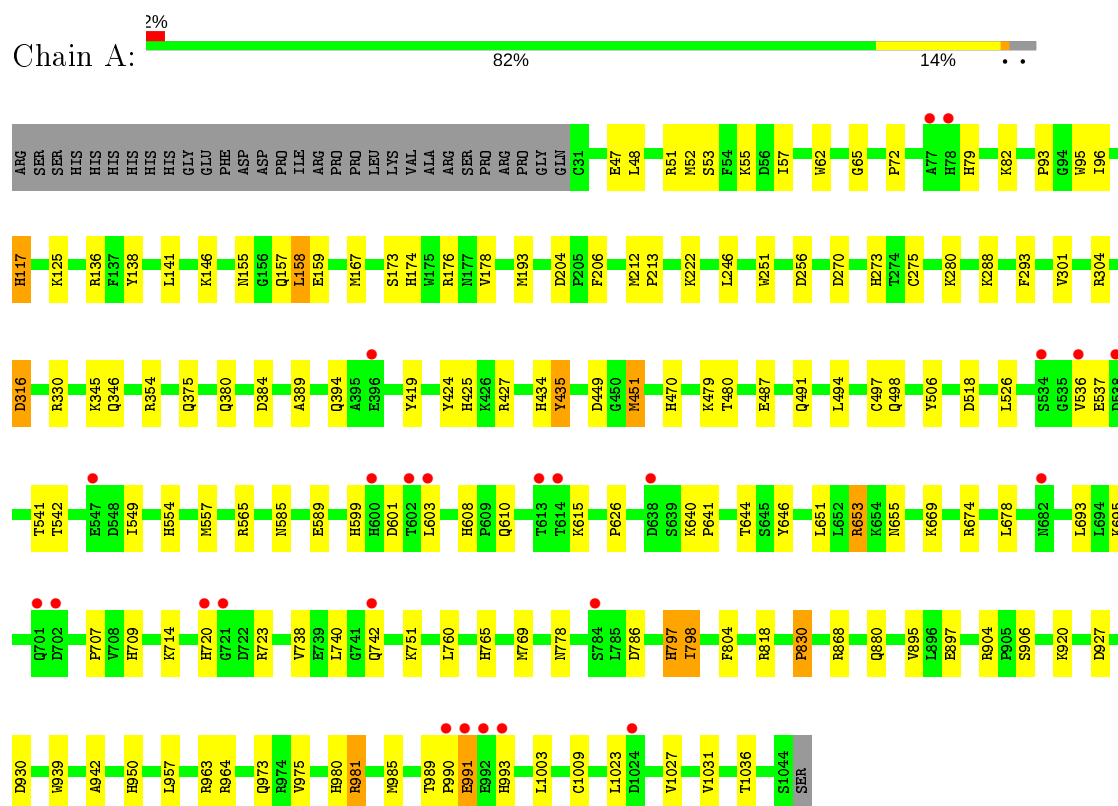
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1158	Total	O	0	0
			1158	1158		

### 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: alpha-mannosidase II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.43Å 110.58Å 139.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 1.45 29.56 – 1.45	Depositor EDS
% Data completeness (in resolution range)	91.0 (29.56-1.45) 91.2 (29.56-1.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 1.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.173 , 0.194 0.166 , 0.188	Depositor DCC
$R_{free}$ test set	4254 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, GB3, ZN, 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	1.06	5/8687 (0.1%)	0.93	14/11790 (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	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	830	PRO	N-CD	-18.27	1.22	1.47
1	A	72	PRO	N-CD	-18.11	1.22	1.47
1	A	497	CYS	CB-SG	-6.84	1.70	1.82
1	A	804	PHE	CE1-CZ	5.04	1.47	1.37
1	A	424	TYR	CD1-CE1	5.03	1.46	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	963	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	868	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	557	MET	CG-SD-CE	6.33	110.33	100.20
1	A	565	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	427	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	818	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	818	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	674	ARG	NE-CZ-NH2	-5.57	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	963	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	167	MET	N-CA-C	-5.14	97.12	111.00
1	A	518	ASP	N-CA-C	-5.09	97.26	111.00
1	A	330	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	1027	VAL	CG1-CB-CG2	-5.07	102.80	110.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117[B]	HIS	Mainchain
1	A	316[B]	ASP	Mainchain
1	A	435[B]	TYR	Mainchain
1	A	506	TYR	Sidechain
1	A	797[B]	HIS	Mainchain

## 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	8291	0	8060	131	0
2	A	14	0	13	1	0
3	A	1	0	0	0	0
4	A	19	0	20	0	0
5	A	8	0	14	3	0
6	A	1158	0	0	37	0
All	All	9491	0	8107	134	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 8.

All (134) 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:610:GLN:HG3	6:A:2865:HOH:O	1.37	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLN:HG2	6:A:2260:HOH:O	1.56	1.03
1:A:981:ARG:HH11	1:A:981:ARG:HB2	1.25	1.00
1:A:280:LYS:NZ	1:A:301:VAL:HG21	1.78	0.99
1:A:47:GLU:OE2	1:A:51:ARG:HD3	1.62	0.98
1:A:709[A]:HIS:HD2	6:A:1815:HOH:O	1.50	0.93
1:A:280:LYS:HZ3	1:A:301:VAL:HG21	1.33	0.92
1:A:498[B]:GLN:HG2	1:A:526:LEU:HD12	1.52	0.90
1:A:82:LYS:HD2	1:A:375:GLN:HE22	1.38	0.88
1:A:117[B]:HIS:HE1	1:A:354:ARG:HE	1.19	0.87
1:A:981:ARG:HH11	1:A:981:ARG:CB	1.88	0.87
1:A:709[A]:HIS:CD2	6:A:1815:HOH:O	2.24	0.86
1:A:48:LEU:O	1:A:52[B]:MET:HG3	1.77	0.83
1:A:599:HIS:CD2	6:A:2865:HOH:O	2.32	0.83
1:A:256:ASP:HB2	6:A:2303:HOH:O	1.77	0.83
1:A:695[A]:LYS:HG3	1:A:709[A]:HIS:CE1	2.16	0.81
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.65	0.80
1:A:136:ARG:HD3	6:A:1988:HOH:O	1.82	0.79
1:A:435[B]:TYR:CE1	6:A:2430:HOH:O	2.35	0.79
1:A:541:THR:HG23	6:A:2064:HOH:O	1.82	0.79
1:A:435[B]:TYR:CZ	6:A:2430:HOH:O	2.36	0.78
5:A:1801:MPD:H13	6:A:1923:HOH:O	1.83	0.77
1:A:155:ASN:HD21	1:A:157:GLN:HE21	1.31	0.76
1:A:280:LYS:NZ	1:A:301:VAL:CG2	2.50	0.75
1:A:981:ARG:CZ	6:A:2214:HOH:O	2.35	0.75
1:A:707:PRO:HG2	1:A:797[B]:HIS:CE1	2.21	0.74
5:A:1801:MPD:H11	6:A:2832:HOH:O	1.88	0.73
1:A:957:LEU:HD13	1:A:981:ARG:NH1	2.05	0.72
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.37	0.71
1:A:498[A]:GLN:HE21	1:A:526:LEU:H	1.38	0.71
1:A:723:ARG:HH11	1:A:723:ARG:HG2	1.57	0.69
1:A:742:GLN:HG3	6:A:2135:HOH:O	1.95	0.67
1:A:47:GLU:OE1	1:A:51:ARG:NH1	2.27	0.67
1:A:957:LEU:HD13	1:A:981:ARG:HH12	1.60	0.66
1:A:536:VAL:O	1:A:537[B]:GLU:HG2	1.96	0.66
1:A:280:LYS:HZ1	1:A:301:VAL:CG2	2.10	0.65
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.80	0.65
1:A:981:ARG:NH1	1:A:981:ARG:HB2	2.06	0.64
1:A:82:LYS:HD2	1:A:375:GLN:NE2	2.10	0.64
1:A:989:THR:HG22	1:A:991:GLU:HG3	1.78	0.64
1:A:981:ARG:HH11	1:A:981:ARG:CG	2.10	0.64
1:A:280:LYS:HZ1	1:A:301:VAL:HG21	1.60	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:NZ	6:A:2714:HOH:O	2.31	0.63
1:A:117[B]:HIS:CE1	1:A:354:ARG:HE	2.10	0.62
1:A:222[A]:LYS:HD3	6:A:2236:HOH:O	1.99	0.61
1:A:53[B]:SER:OG	1:A:55:LYS:HG2	1.99	0.61
1:A:693:LEU:HD13	6:A:2855:HOH:O	2.01	0.61
1:A:765:HIS:HE1	6:A:2880:HOH:O	1.85	0.59
1:A:981:ARG:NH2	6:A:2214:HOH:O	2.34	0.59
1:A:714:LYS:HE3	1:A:738:VAL:HG22	1.86	0.57
1:A:904:ARG:HG2	1:A:985:MET:SD	2.44	0.57
1:A:273:HIS:HE1	5:A:1801:MPD:O4	1.87	0.57
1:A:603:LEU:N	1:A:603:LEU:HD22	2.19	0.57
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.34	0.57
1:A:950:HIS:HE1	6:A:2324:HOH:O	1.88	0.57
1:A:494:LEU:O	1:A:498[B]:GLN:HG3	2.05	0.56
1:A:980:HIS:HE1	6:A:2221:HOH:O	1.88	0.55
1:A:48:LEU:O	1:A:52[A]:MET:HG3	2.06	0.55
1:A:695[A]:LYS:HG3	1:A:709[A]:HIS:HE1	1.70	0.55
1:A:589:GLU:OE2	1:A:751:LYS:HD3	2.07	0.55
1:A:626:PRO:O	1:A:950:HIS:HD2	1.90	0.54
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.43	0.53
1:A:293:PHE:HE1	1:A:346[B]:GLN:HE21	1.56	0.53
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.92	0.53
1:A:714:LYS:HD2	6:A:2848:HOH:O	2.07	0.53
1:A:541:THR:CG2	6:A:2064:HOH:O	2.49	0.53
1:A:435[B]:TYR:CE1	1:A:526:LEU:HD13	2.43	0.53
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.92	0.52
1:A:720:HIS:CD2	6:A:2943:HOH:O	2.63	0.51
1:A:678:LEU:HD13	1:A:769[A]:MET:HE3	1.93	0.51
1:A:480:THR:H	1:A:880:GLN:HE22	1.58	0.51
1:A:989:THR:CG2	1:A:991:GLU:HG3	2.42	0.50
1:A:786:ASP:CB	6:A:2939:HOH:O	2.60	0.50
1:A:678:LEU:HD12	1:A:769[A]:MET:HE1	1.93	0.49
1:A:425:HIS:HE1	1:A:487:GLU:OE1	1.95	0.49
2:A:1802:NAG:H81	6:A:1972:HOH:O	2.12	0.49
1:A:542:THR:OG1	1:A:615:LYS:HD2	2.13	0.49
1:A:786:ASP:HB3	6:A:2939:HOH:O	2.12	0.48
1:A:554:HIS:HE1	6:A:2096:HOH:O	1.95	0.48
1:A:304:ARG:NH1	6:A:2642:HOH:O	2.44	0.48
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.95	0.48
1:A:141:LEU:O	1:A:146[B]:LYS:NZ	2.46	0.48
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:HIS:HD2	6:A:2480:HOH:O	1.97	0.48
1:A:990:PRO:O	1:A:991:GLU:C	2.52	0.47
1:A:158[A]:LEU:HD23	1:A:159:GLU:N	2.29	0.47
1:A:906:SER:HB3	6:A:1894:HOH:O	2.13	0.47
1:A:389:ALA:HB1	1:A:394:GLN:CG	2.44	0.47
1:A:389:ALA:HB1	1:A:394:GLN:HG2	1.97	0.47
1:A:981:ARG:CZ	1:A:1031:VAL:O	2.63	0.47
1:A:173[B]:SER:OG	1:A:178:VAL:HG23	2.15	0.47
1:A:601:ASP:HB2	1:A:608:HIS:HE1	1.79	0.47
1:A:723:ARG:CG	1:A:723:ARG:HH11	2.25	0.47
1:A:990:PRO:O	1:A:991:GLU:O	2.32	0.47
1:A:601:ASP:HB2	1:A:608:HIS:CE1	2.50	0.46
1:A:920:LYS:HG3	6:A:2453:HOH:O	2.16	0.46
1:A:434:HIS:CE1	1:A:930:ASP:OD1	2.56	0.46
1:A:345:LYS:HD3	1:A:346[A]:GLN:NE2	2.31	0.46
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.46	0.46
1:A:419:TYR:CE2	1:A:830:PRO:HD3	2.51	0.46
1:A:345:LYS:HD3	1:A:346[A]:GLN:HE22	1.81	0.46
1:A:740:LEU:HD22	1:A:760:LEU:HD22	1.99	0.45
1:A:536:VAL:C	1:A:537[B]:GLU:HG2	2.36	0.45
1:A:380:GLN:CG	6:A:2260:HOH:O	2.33	0.44
1:A:641:PRO:HG2	1:A:644:THR:HB	2.00	0.44
1:A:270:ASP:OD1	1:A:273:HIS:HD2	2.01	0.44
1:A:138[A]:TYR:CE1	1:A:193[A]:MET:CE	3.01	0.43
1:A:251:TRP:CD1	1:A:251:TRP:C	2.91	0.43
1:A:981:ARG:NE	6:A:2214:HOH:O	2.47	0.43
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.54	0.43
1:A:57[B]:ILE:HG23	6:A:1916:HOH:O	2.18	0.43
1:A:449:ASP:OD2	1:A:451:MET:HB2	2.19	0.42
1:A:981:ARG:NH1	1:A:981:ARG:CG	2.74	0.42
1:A:212[A]:MET:HB2	1:A:213:PRO:CD	2.49	0.42
1:A:47:GLU:CD	1:A:51:ARG:HH11	2.20	0.42
1:A:419:TYR:CZ	1:A:830:PRO:HD3	2.55	0.42
1:A:48:LEU:HG	1:A:52[B]:MET:SD	2.60	0.42
1:A:138[A]:TYR:CE1	1:A:193[A]:MET:HE1	2.55	0.42
1:A:939:TRP:CD2	1:A:942:ALA:HB2	2.56	0.41
1:A:125:LYS:HE3	6:A:2274:HOH:O	2.20	0.41
1:A:640:LYS:HD2	1:A:646:TYR:CE1	2.56	0.41
1:A:1009:CYS:SG	1:A:1023:LEU:HD12	2.61	0.40
1:A:212[B]:MET:HB3	1:A:213:PRO:CD	2.51	0.40
1:A:79:HIS:HE1	6:A:2565:HOH:O	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:LYS:HB3	1:A:714:LYS:HE2	1.84	0.40
1:A:797[B]:HIS:O	1:A:798:ILE:C	2.58	0.40
1:A:96:ILE:HD12	1:A:479:LYS:HE2	2.04	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	1046/1045 (100%)	1012 (97%)	28 (3%)	6 (1%)	25	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	991	GLU
1	A	95	TRP
1	A	993	HIS
1	A	204	ASP
1	A	549	ILE
1	A	798	ILE

### 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	935/929 (101%)	925 (99%)	10 (1%)	73	48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158[A]	LEU
1	A	158[B]	LEU
1	A	206	PHE
1	A	275	CYS
1	A	451	MET
1	A	585	ASN
1	A	653	ARG
1	A	655	ASN
1	A	669	LYS
1	A	981	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	91	ASN
1	A	148	GLN
1	A	157	GLN
1	A	191	GLN
1	A	240	GLN
1	A	249	GLN
1	A	273	HIS
1	A	347	ASN
1	A	375	GLN
1	A	388	GLN
1	A	394	GLN
1	A	425	HIS
1	A	434	HIS
1	A	460	GLN
1	A	469	GLN
1	A	470	HIS
1	A	488	GLN
1	A	554	HIS
1	A	599	HIS
1	A	608	HIS
1	A	655	ASN
1	A	765	HIS

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Mol	Chain	Res	Type
1	A	812	GLN
1	A	880	GLN
1	A	885	ASN
1	A	901	ASN
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	986	GLN
1	A	993	HIS
1	A	1018	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 ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z  > 2$
2	NAG	A	1802	1	14,14,15	0.71	0	17,19,21	1.14	1 (5%)
5	MPD	A	1801	-	7,7,7	0.89	0	9,10,10	0.46	0
4	GB3	A	1803	3	20,20,20	1.54	4 (20%)	19,27,27	1.71	5 (26%)

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	A	1802	1	-	4/6/23/26	0/1/1/1
5	MPD	A	1801	-	1/1/2/2	2/5/5/5	-
4	GB3	A	1803	3	-	2/11/27/27	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1803	GB3	C11-C10	3.92	1.45	1.39
4	A	1803	GB3	C15-C10	3.47	1.44	1.39
4	A	1803	GB3	C14-C15	2.52	1.44	1.38
4	A	1803	GB3	C12-C11	2.07	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1803	GB3	C3-C4-C5	3.61	108.27	102.55
4	A	1803	GB3	O3-C3-C2	3.33	119.32	111.16
2	A	1802	NAG	C2-N2-C7	-3.14	118.43	122.90
4	A	1803	GB3	C9-C8-N7	2.71	115.89	108.81
4	A	1803	GB3	O4-C4-C5	-2.54	106.13	112.92
4	A	1803	GB3	C13-C12-C11	2.25	123.61	120.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1801	MPD	C4

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1802	NAG	C8-C7-N2-C2
2	A	1802	NAG	O7-C7-N2-C2
5	A	1801	MPD	C2-C3-C4-O4
4	A	1803	GB3	N1-C5-C6-N7
2	A	1802	NAG	O5-C5-C6-O6
2	A	1802	NAG	C4-C5-C6-O6
5	A	1801	MPD	C2-C3-C4-C5

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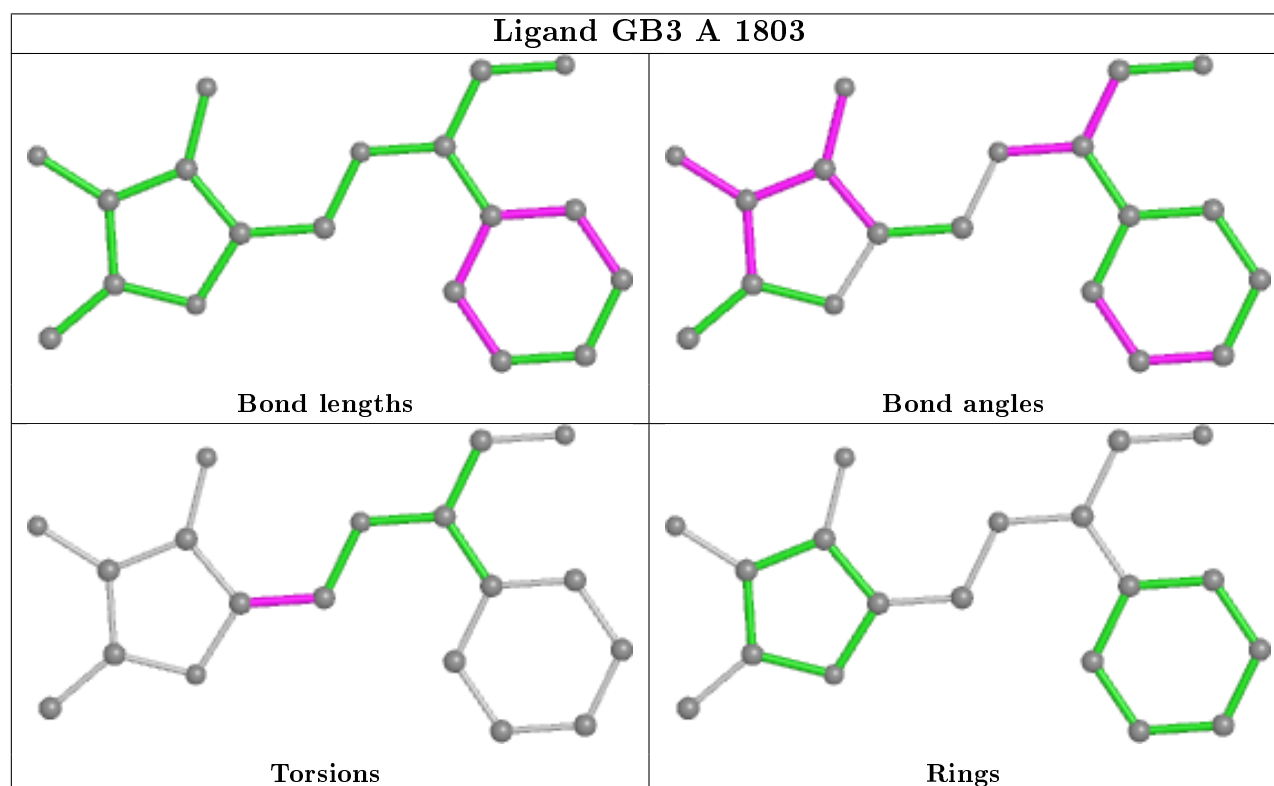
Mol	Chain	Res	Type	Atoms
4	A	1803	GB3	C4-C5-C6-N7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1802	NAG	1	0
5	A	1801	MPD	3	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	316[B]:ASP	C	317:LEU	N	1.62

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1014/1045 (97%)	-0.07	25 (2%) 57 60	7, 14, 28, 57	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	6.0
1	A	603	LEU	5.1
1	A	702	ASP	5.1
1	A	78	HIS	4.9
1	A	701	GLN	4.9
1	A	991	GLU	4.9
1	A	638	ASP	4.1
1	A	602	THR	4.0
1	A	992	GLU	3.9
1	A	600	HIS	3.9
1	A	990	PRO	3.8
1	A	720	HIS	3.3
1	A	1024	ASP	3.2
1	A	534	SER	3.1
1	A	682	ASN	3.1
1	A	538	ASP	2.9
1	A	547	GLU	2.7
1	A	721	GLY	2.4
1	A	742	GLN	2.3
1	A	613	THR	2.2
1	A	396	GLU	2.1
1	A	784	SER	2.1
1	A	77	ALA	2.1
1	A	536	VAL	2.1
1	A	614	THR	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](#)

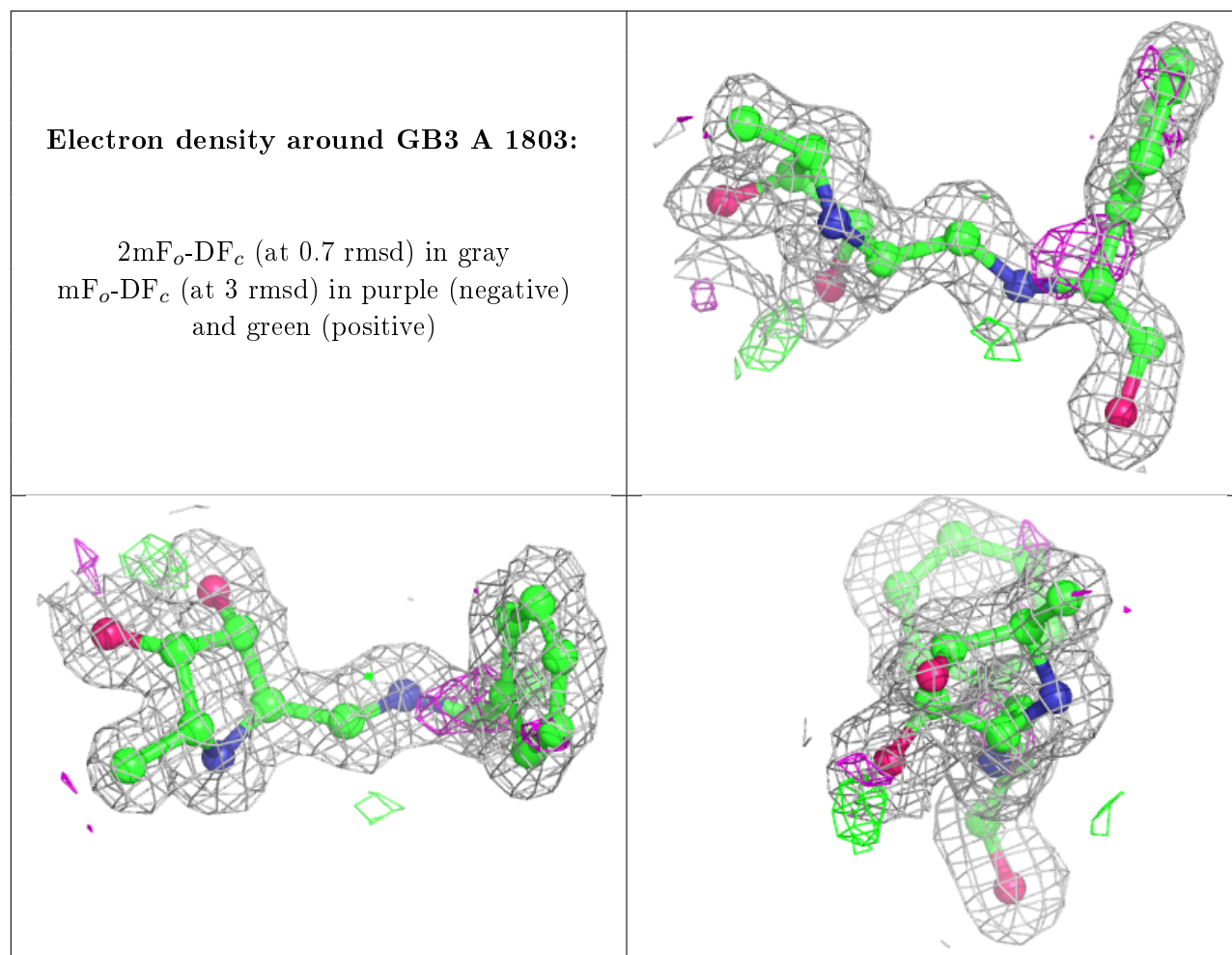
There are no monosaccharides in this entry.

## 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	1802	14/15	0.72	0.33	34,41,44,46	0
5	MPD	A	1801	8/8	0.91	0.12	18,21,22,23	0
4	GB3	A	1803	19/19	0.94	0.11	11,14,17,20	0
3	ZN	A	1804	1/1	1.00	0.04	9,9,9,9	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 ⓘ

There are no such residues in this entry.