



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 16, 2019 – 11:37 PM EDT

PDB ID : 3DDF
Title : GOLGI MANNOSIDASE II complex with (3R,4R,5R)-3,4-Dihydroxy-5-({[(1R)-2-hydroxy-1 phenylethyl]amino}methyl) pyrrolidin-2-one
Authors : Kuntz, D.A.; Rose, D.R.; Hoffman, D.
Deposited on : 2008-06-05
Resolution : 1.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

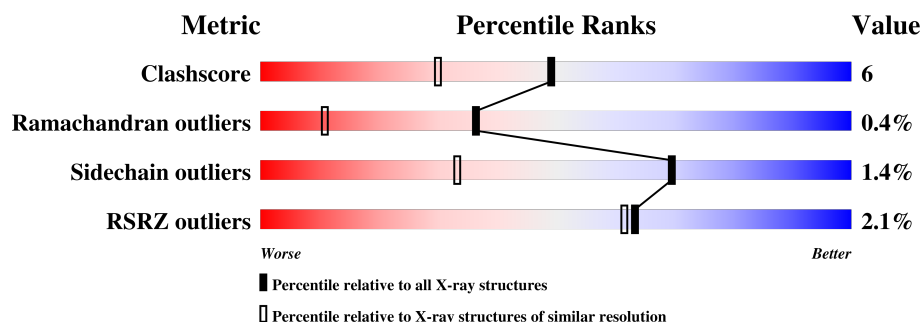
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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))
Clashscore	122126	1064 (1.22-1.18)
Ramachandran outliers	120053	1024 (1.22-1.18)
Sidechain outliers	120020	1023 (1.22-1.18)
RSRZ outliers	108989	1278 (1.24-1.16)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10110 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1015	Total	C	N	O	S	0	51	0
			8468	5408	1471	1546	43			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	EXPRESSION TAG	UNP Q24451
A	2	SER	-	EXPRESSION TAG	UNP Q24451
A	3	SER	-	EXPRESSION TAG	UNP Q24451
A	4	HIS	-	EXPRESSION TAG	UNP Q24451
A	5	HIS	-	EXPRESSION TAG	UNP Q24451
A	6	HIS	-	EXPRESSION TAG	UNP Q24451
A	7	HIS	-	EXPRESSION TAG	UNP Q24451
A	8	HIS	-	EXPRESSION TAG	UNP Q24451
A	9	HIS	-	EXPRESSION TAG	UNP Q24451
A	10	GLY	-	EXPRESSION TAG	UNP Q24451
A	11	GLU	-	EXPRESSION TAG	UNP Q24451
A	12	PHE	-	EXPRESSION TAG	UNP Q24451
A	907	LYS	GLU	VARIANT	UNP Q24451

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

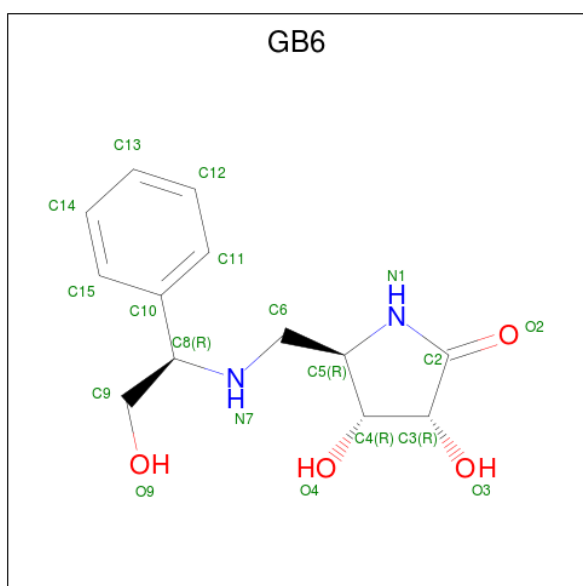


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

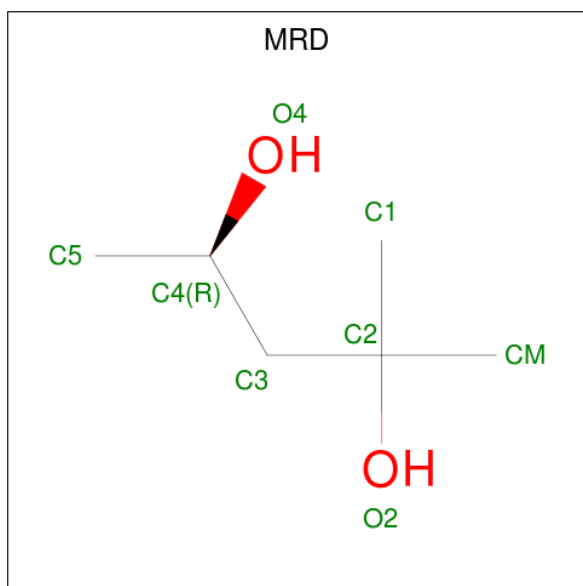
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (3R,4R,5R)-3,4-dihydroxy-5-({[(1R)-2-hydroxy-1-phenylethyl]amino}methyl)pyrrolidin-2-one (three-letter code: GB6) (formula: C₁₃H₁₈N₂O₄).



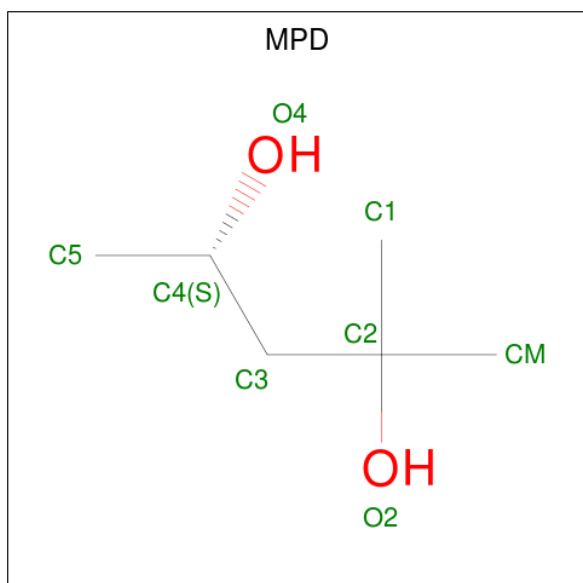
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	13	2	4		

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



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

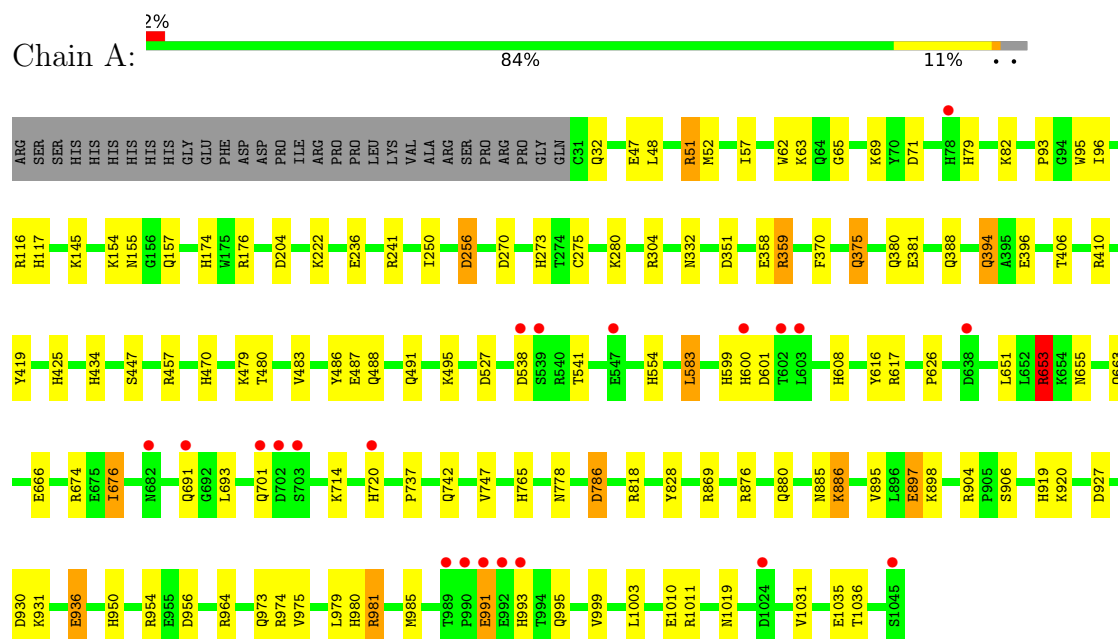
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1584	Total	O	0	8
			1592	1592		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.92Å 109.99Å 138.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.20 19.87 – 1.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-1.20) 92.3 (19.87-1.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.60 (at 1.20Å)	Xtriage
Refinement program	SHELXL-97, CNS, SHELX	Depositor
R, R_{free}	0.115 , 0.151 0.119 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	9.4	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10110	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: ZN, GB6, MPD, NAG, MRD

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	0.76	8/8836 (0.1%)	1.16	36/11990 (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	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	GLU	CD-OE1	-11.58	1.12	1.25
1	A	897	GLU	CD-OE2	-8.38	1.16	1.25
1	A	1035[A]	GLU	CD-OE1	-7.01	1.18	1.25
1	A	1035[B]	GLU	CD-OE1	-7.01	1.18	1.25
1	A	981[A]	ARG	CD-NE	-5.76	1.36	1.46
1	A	981[B]	ARG	CD-NE	-5.76	1.36	1.46
1	A	1035[A]	GLU	CB-CG	5.66	1.62	1.52
1	A	1035[B]	GLU	CB-CG	5.66	1.62	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	981[A]	ARG	NE-CZ-NH2	-22.78	108.91	120.30
1	A	981[B]	ARG	NE-CZ-NH2	-22.78	108.91	120.30
1	A	981[A]	ARG	NE-CZ-NH1	19.53	130.06	120.30
1	A	981[B]	ARG	NE-CZ-NH1	19.53	130.06	120.30
1	A	51	ARG	NE-CZ-NH2	-10.03	115.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	1035[A]	GLU	OE1-CD-OE2	-7.20	114.66	123.30
1	A	1035[B]	GLU	OE1-CD-OE2	-7.20	114.66	123.30
1	A	786	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	974	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	974	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	71	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	457	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	653	ARG	CG-CD-NE	5.69	123.74	111.80
1	A	116	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	936	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	A	359	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	359	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	616	TYR	CB-CG-CD1	-5.53	117.69	121.00
1	A	538	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	981[A]	ARG	CD-NE-CZ	5.32	131.05	123.60
1	A	981[B]	ARG	CD-NE-CZ	5.32	131.05	123.60
1	A	617	ARG	CD-NE-CZ	5.31	131.03	123.60
1	A	410	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	886	LYS	CD-CE-NZ	5.25	123.77	111.70
1	A	370	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	A	486	TYR	CB-CG-CD2	5.14	124.09	121.00
1	A	674	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	358	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	A	936	GLU	CG-CD-OE1	5.09	128.48	118.30
1	A	600	HIS	N-CA-CB	5.08	119.75	110.60
1	A	256	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	876	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	818[A]	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	818[B]	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	599	HIS	CA-CB-CG	-5.00	105.09	113.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	583	LEU	Peptide

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	8468	0	8386	101	0
2	A	14	0	13	5	0
3	A	1	0	0	0	0
4	A	19	0	16	0	0
5	A	8	0	14	3	0
6	A	8	0	14	3	0
7	A	1592	0	0	62	0
All	All	10110	0	8443	109	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 6.

All (109) 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:406[B]:THR:HG22	1:A:419:TYR:OH	1.73	0.88
1:A:47:GLU:OE2	1:A:51:ARG:HD3	1.78	0.83
1:A:406[B]:THR:HG21	1:A:828:TYR:O	1.79	0.83
1:A:155[A]:ASN:HD21	1:A:157:GLN:HE21	1.29	0.81
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.29	0.81
1:A:57:ILE:HG12	7:A:7555:HOH:O	1.83	0.78
5:A:5001:MRD:H1C1	7:A:6352:HOH:O	1.83	0.77
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.68	0.76
1:A:491[B]:GLN:HG3	7:A:6952:HOH:O	1.87	0.75
1:A:991:GLU:HG2	7:A:6842:HOH:O	1.88	0.74
1:A:222[B]:LYS:HD3	7:A:6210:HOH:O	1.88	0.72
2:A:2001:NAG:H81	7:A:6175:HOH:O	1.90	0.72
2:A:2001:NAG:H61	7:A:6712:HOH:O	1.91	0.71
1:A:280[B]:LYS:HE3	7:A:6059:HOH:O	1.92	0.69
1:A:1011:ARG:HD2	7:A:6860:HOH:O	1.92	0.69
1:A:69:LYS:HE3	7:A:7561:HOH:O	1.93	0.69
1:A:250:ILE:HD11	7:A:7600:HOH:O	1.93	0.68
1:A:1010:GLU:HG2	7:A:6201:HOH:O	1.93	0.67
1:A:693:LEU:HD13	7:A:6557:HOH:O	1.93	0.66
6:A:5002:MPD:HM2	7:A:7003:HOH:O	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:GLU:HG2	7:A:7081:HOH:O	1.97	0.64
5:A:5001:MRD:H1C3	7:A:6353:HOH:O	1.97	0.64
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.80	0.63
1:A:273:HIS:HE1	5:A:5001:MRD:O4	1.84	0.60
1:A:980:HIS:HE1	7:A:7135:HOH:O	1.84	0.59
1:A:154:LYS:NZ	2:A:2001:NAG:H83	2.17	0.59
1:A:47:GLU:OE2	1:A:51:ARG:CD	2.51	0.59
1:A:742[A]:GLN:HG3	7:A:7412:HOH:O	2.02	0.59
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.86	0.59
1:A:950:HIS:HE1	7:A:6821:HOH:O	1.86	0.59
1:A:1019:ASN:HB3	7:A:6201:HOH:O	2.02	0.58
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.33	0.58
1:A:541:THR:HG21	7:A:6940:HOH:O	2.03	0.58
1:A:663:GLN:HG3	7:A:7323:HOH:O	2.03	0.58
1:A:904:ARG:HG2	1:A:985:MET:SD	2.44	0.57
1:A:332:ASN:H	1:A:394:GLN:HE22	1.52	0.57
1:A:995:GLN:HG3	7:A:6835:HOH:O	2.05	0.57
1:A:626:PRO:O	1:A:950:HIS:HD2	1.87	0.57
1:A:32:GLN:HG3	7:A:6869:HOH:O	2.05	0.56
1:A:676:ILE:HD12	1:A:747:VAL:HG21	1.87	0.56
1:A:51:ARG:HG3	7:A:6476:HOH:O	2.04	0.56
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.35	0.56
1:A:154:LYS:HZ1	2:A:2001:NAG:H83	1.69	0.56
1:A:765:HIS:HE1	7:A:7581:HOH:O	1.88	0.56
1:A:691:GLN:NE2	7:A:7378:HOH:O	2.38	0.56
1:A:63:LYS:HE2	7:A:7720:HOH:O	2.05	0.55
1:A:388:GLN:NE2	7:A:6224:HOH:O	2.31	0.55
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.42	0.54
1:A:601:ASP:OD2	1:A:608:HIS:HE1	1.91	0.54
1:A:270:ASP:OD1	1:A:273:HIS:HD2	1.90	0.54
1:A:954[B]:ARG:NH2	7:A:6847:HOH:O	2.23	0.53
1:A:480:THR:H	1:A:880:GLN:HE22	1.57	0.52
1:A:79:HIS:HE1	7:A:6024:HOH:O	1.91	0.52
1:A:676:ILE:HD13	7:A:7409:HOH:O	2.10	0.52
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.93	0.52
1:A:96[B]:ILE:HD12	7:A:6651:HOH:O	2.11	0.51
1:A:583:LEU:HA	7:A:7259:HOH:O	2.11	0.51
1:A:47:GLU:CD	1:A:51:ARG:HD3	2.32	0.51
1:A:495:LYS:HE2	7:A:7005:HOH:O	2.10	0.50
1:A:256:ASP:HB2	7:A:6870:HOH:O	2.10	0.50
1:A:380:GLN:HG2	7:A:6720:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:HIS:HE1	1:A:487:GLU:OE1	1.94	0.50
1:A:583:LEU:HD12	7:A:7259:HOH:O	2.12	0.49
1:A:608:HIS:HD2	7:A:7431:HOH:O	1.95	0.49
1:A:82[A]:LYS:HE3	7:A:6241:HOH:O	2.13	0.49
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.47	0.48
1:A:554:HIS:HD2	7:A:6931:HOH:O	1.97	0.48
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.62	0.47
1:A:954[B]:ARG:NE	7:A:6847:HOH:O	2.47	0.47
1:A:527:ASP:O	1:A:931:LYS:HE3	2.15	0.46
1:A:737:PRO:HG3	7:A:6553:HOH:O	2.15	0.46
1:A:979[A]:LEU:HD21	1:A:999:VAL:HG11	1.97	0.46
1:A:82[B]:LYS:HE3	1:A:375[B]:GLN:NE2	2.30	0.46
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.50	0.46
6:A:5002:MPD:HM1	6:A:5002:MPD:O4	2.16	0.46
1:A:954[B]:ARG:HD2	1:A:956:ASP:OD1	2.16	0.46
1:A:981[A]:ARG:HD2	1:A:1031:VAL:O	2.16	0.46
1:A:241:ARG:HD3	7:A:6019:HOH:O	2.17	0.45
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.98	0.45
1:A:434:HIS:CE1	1:A:930:ASP:OD1	2.58	0.45
6:A:5002:MPD:H11	7:A:6992:HOH:O	2.17	0.45
1:A:82[A]:LYS:CE	7:A:6241:HOH:O	2.64	0.45
1:A:32:GLN:NE2	7:A:6870:HOH:O	2.49	0.45
1:A:886:LYS:NZ	7:A:6602:HOH:O	2.49	0.45
1:A:96[A]:ILE:HG23	1:A:479:LYS:HE2	1.99	0.45
1:A:304[B]:ARG:HD2	1:A:304[B]:ARG:HH11	1.65	0.44
1:A:304[A]:ARG:NH2	7:A:6304:HOH:O	2.49	0.44
1:A:491[B]:GLN:NE2	7:A:6951:HOH:O	2.48	0.44
2:A:2001:NAG:H2	2:A:2001:NAG:H83	1.52	0.44
1:A:653:ARG:NH1	7:A:7416:HOH:O	2.49	0.44
1:A:145:LYS:HE3	7:A:7524:HOH:O	2.18	0.43
1:A:483:VAL:HG11	7:A:6592:HOH:O	2.18	0.43
1:A:48:LEU:HG	1:A:52[A]:MET:SD	2.58	0.43
1:A:117[B]:HIS:HE1	1:A:351:ASP:OD1	2.02	0.43
1:A:964:ARG:HH11	1:A:973:GLN:NE2	2.08	0.43
1:A:82[A]:LYS:HG3	7:A:6241:HOH:O	2.18	0.43
1:A:359:ARG:HD3	7:A:6137:HOH:O	2.18	0.42
1:A:885:ASN:ND2	1:A:885:ASN:H	2.18	0.42
1:A:541:THR:HG23	7:A:6944:HOH:O	2.18	0.42
1:A:786:ASP:CB	7:A:7468:HOH:O	2.68	0.42
1:A:714:LYS:HD2	7:A:7452:HOH:O	2.19	0.41
1:A:979[B]:LEU:HD23	1:A:1031:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:GLN:NE2	7:A:7185:HOH:O	2.53	0.41
1:A:48:LEU:HD11	1:A:236:GLU:HG2	2.02	0.41
1:A:541:THR:HG23	7:A:6943:HOH:O	2.22	0.40
1:A:920:LYS:HG3	7:A:7219:HOH:O	2.21	0.40
1:A:919:HIS:HE1	7:A:7131:HOH:O	2.03	0.40
1:A:434:HIS:CD2	1:A:927:ASP:HA	2.56	0.40
1:A:954[B]:ARG:HD3	1:A:954[B]:ARG:HH11	1.66	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	1064/1045 (102%)	1034 (97%)	26 (2%)	4 (0%)	36 11

All (4) Ramachandran outliers are listed below:

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

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	953/929 (103%)	935 (98%)	18 (2%)	60 20

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	CYS
1	A	375[A]	GLN
1	A	375[B]	GLN
1	A	394	GLN
1	A	396	GLU
1	A	447[A]	SER
1	A	447[B]	SER
1	A	653	ARG
1	A	655	ASN
1	A	666[A]	GLU
1	A	666[B]	GLU
1	A	676	ILE
1	A	701[A]	GLN
1	A	701[B]	GLN
1	A	720[A]	HIS
1	A	720[B]	HIS
1	A	898	LYS
1	A	906	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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	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

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Mol	Chain	Res	Type
1	A	554	HIS
1	A	608	HIS
1	A	655	ASN
1	A	698	GLN
1	A	765	HIS
1	A	880	GLN
1	A	885	ASN
1	A	919	HIS
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	993	HIS
1	A	1018	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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	2001	1	14,14,15	0.80	0	17,19,21	2.60	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GB6	A	4001	3	20,20,20	2.03	4 (20%)	19,27,27	1.55	4 (21%)
5	MRD	A	5001	-	7,7,7	0.67	0	9,10,10	1.32	1 (11%)
6	MPD	A	5002	-	7,7,7	0.67	0	9,10,10	0.78	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	A	2001	1	-	2/6/23/26	0/1/1/1
4	GB6	A	4001	3	-	0/11/27/27	0/2/2/2
5	MRD	A	5001	-	-	2/5/5/5	-
6	MPD	A	5002	-	-	0/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4001	GB6	C15-C10	6.65	1.49	1.39
4	A	4001	GB6	C8-N7	3.01	1.52	1.47
4	A	4001	GB6	C9-C8	2.75	1.57	1.52
4	A	4001	GB6	O3-C3	2.09	1.46	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NAG	C2-N2-C7	-7.86	111.66	122.92
2	A	2001	NAG	C3-C4-C5	3.54	116.59	110.23
4	A	4001	GB6	C14-C15-C10	-3.50	116.30	120.64
4	A	4001	GB6	O9-C9-C8	-3.42	103.86	111.50
2	A	2001	NAG	C1-O5-C5	2.89	116.13	112.20
2	A	2001	NAG	O5-C1-C2	-2.67	107.16	111.36
4	A	4001	GB6	O3-C3-C2	-2.53	106.56	111.91
5	A	5001	MRD	CM-C2-C1	-2.38	105.56	110.57
4	A	4001	GB6	C9-C8-C10	-2.31	104.85	110.74
2	A	2001	NAG	O3-C3-C2	-2.16	104.83	109.38
2	A	2001	NAG	O5-C5-C4	2.10	115.93	110.83
2	A	2001	NAG	C1-C2-N2	2.06	114.00	110.49
2	A	2001	NAG	C8-C7-N2	-2.01	112.63	116.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

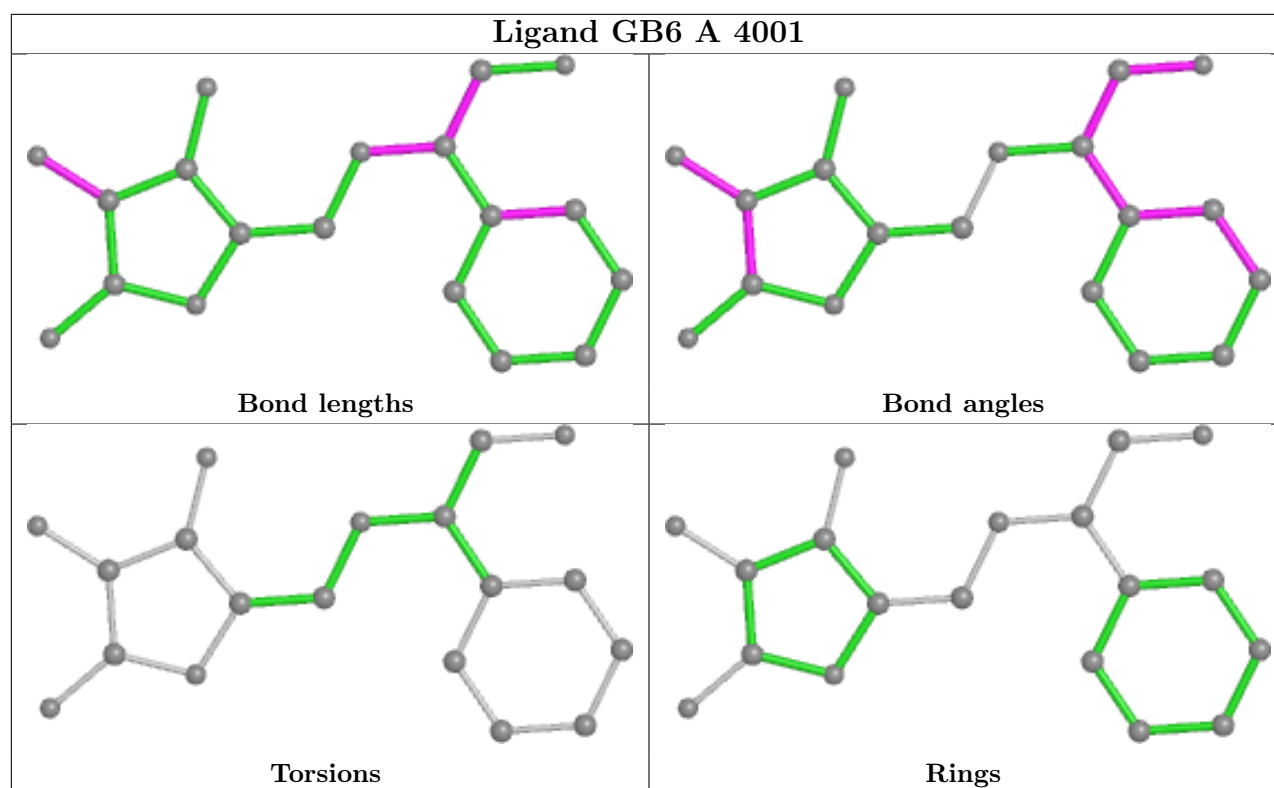
Mol	Chain	Res	Type	Atoms
2	A	2001	NAG	C8-C7-N2-C2
2	A	2001	NAG	O7-C7-N2-C2
5	A	5001	MRD	C2-C3-C4-O4
5	A	5001	MRD	C2-C3-C4-C5

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	NAG	5	0
5	A	5001	MRD	3	0
6	A	5002	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](#)

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	1015/1045 (97%)	-0.35	21 (2%) 63 61	6, 12, 29, 73	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	702	ASP	7.5
1	A	993	HIS	5.8
1	A	991	GLU	5.7
1	A	1045	SER	5.2
1	A	701[A]	GLN	4.8
1	A	992	GLU	4.7
1	A	78	HIS	4.2
1	A	638	ASP	4.0
1	A	720[A]	HIS	3.6
1	A	1024	ASP	3.5
1	A	990	PRO	3.4
1	A	602	THR	3.1
1	A	539	SER	2.9
1	A	682	ASN	2.7
1	A	691	GLN	2.4
1	A	600	HIS	2.3
1	A	989	THR	2.3
1	A	703	SER	2.2
1	A	538	ASP	2.2
1	A	603	LEU	2.0
1	A	547	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

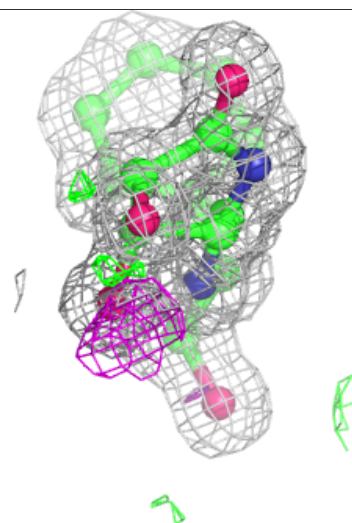
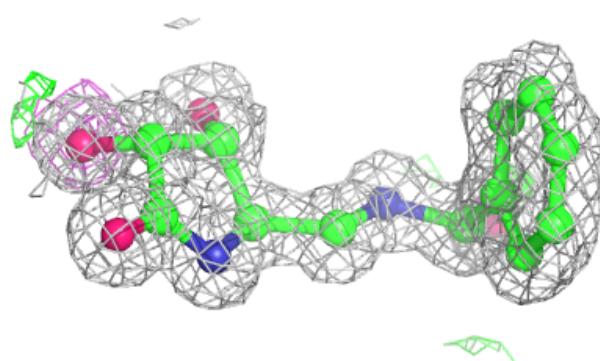
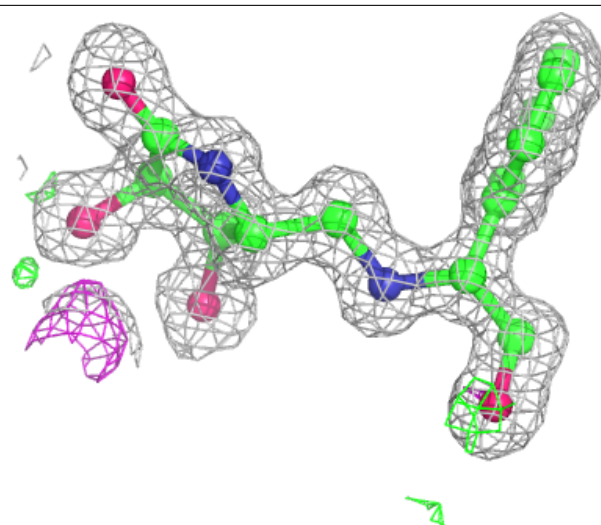
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MPD	A	5002	8/8	0.65	0.22	25,31,42,47	0
2	NAG	A	2001	14/15	0.87	0.27	26,46,66,71	0
5	MRD	A	5001	8/8	0.93	0.09	11,13,18,22	0
4	GB6	A	4001	19/19	0.98	0.06	7,9,18,19	0
3	ZN	A	3001	1/1	1.00	0.03	8,8,8,8	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.

Electron density around GB6 A 4001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.