



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:36 PM UTC

PDB ID : 3DDF / pdb_00003ddf
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

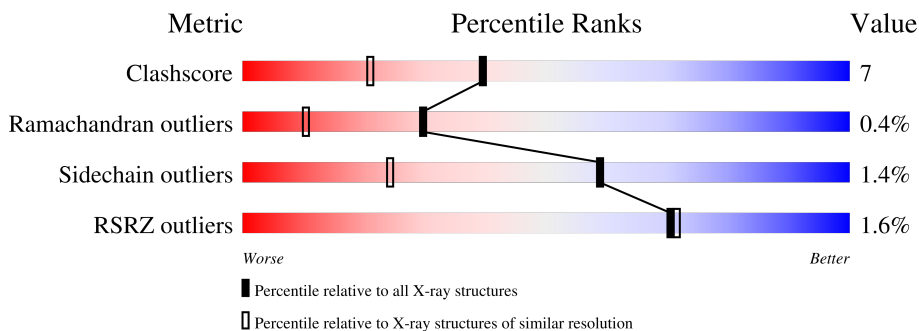
1 Overall quality at a glance

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	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1045	 2% 84% 11% . .

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
			Total	C	N	O	S			
1	A	1015	8468	5408	1471	1546	43	0	51	0

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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

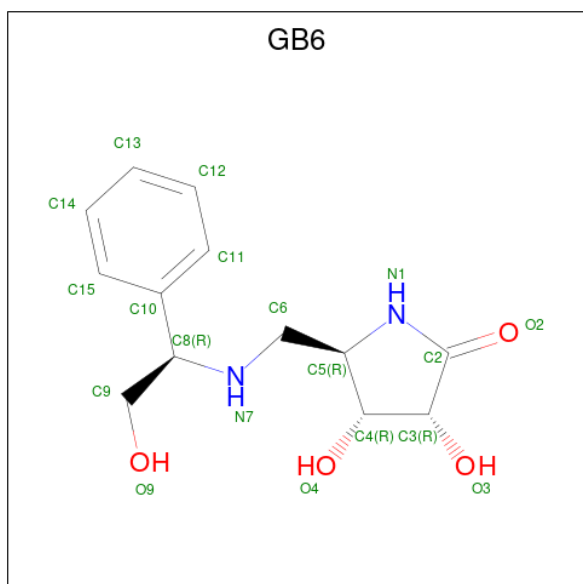


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

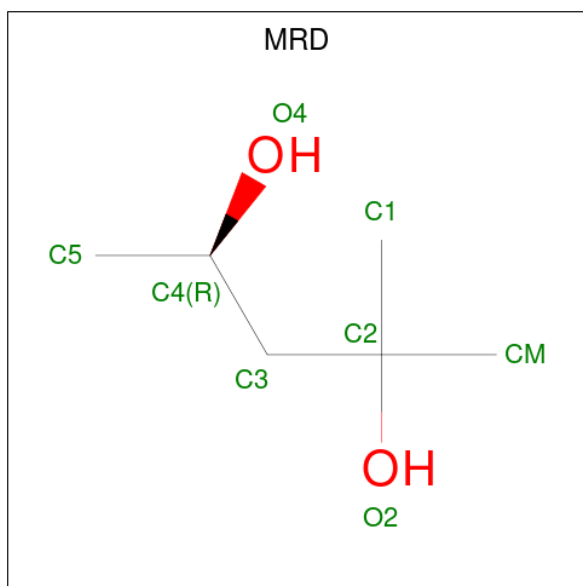
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

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



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

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

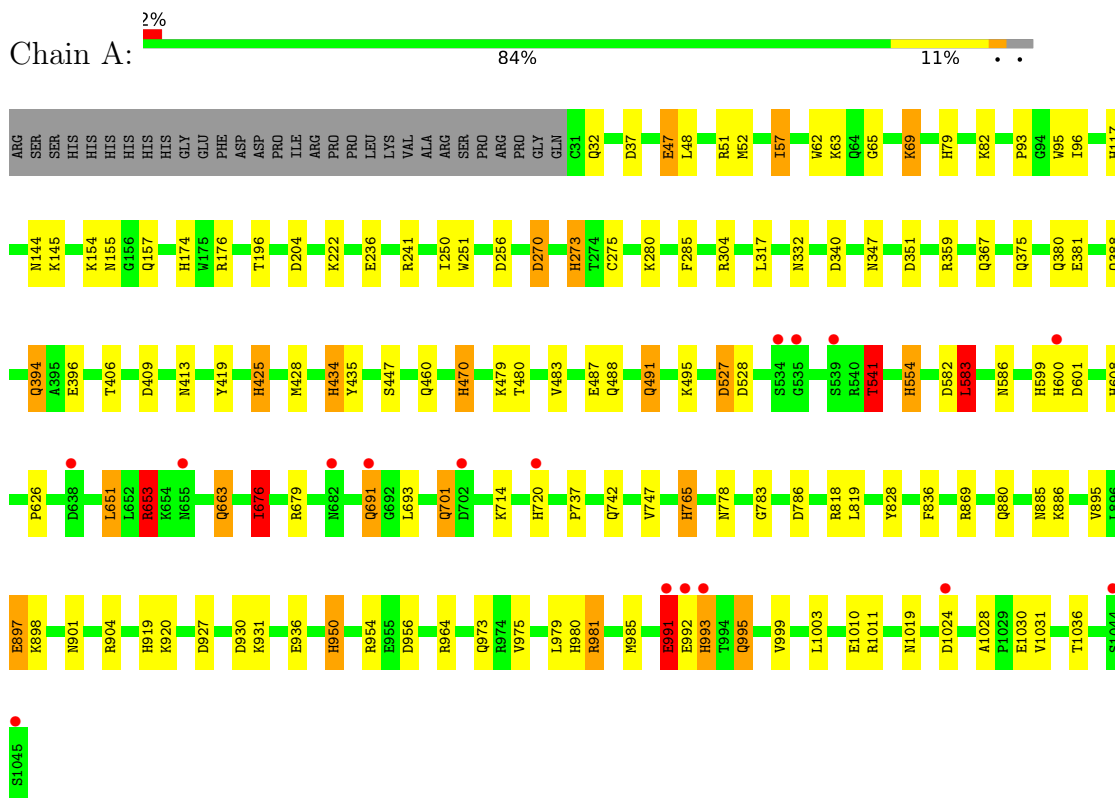
- Molecule 7 is water.

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, 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 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 20.00 – 1.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-1.20) 92.3 (20.00-1.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.60 (at 1.20Å)	Xtrriage
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	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, NAG, MPD, ZN, GB6

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	0.89	9/8836 (0.1%)	1.21	49/11990 (0.4%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	ASP	C-O	-7.03	1.14	1.23
1	A	819	LEU	C-O	-6.83	1.16	1.24
1	A	196	THR	C-O	-6.56	1.19	1.25
1	A	381	GLU	CD-OE1	-6.55	1.12	1.25
1	A	583	LEU	C-O	-5.83	1.14	1.23
1	A	317	LEU	C-O	-5.42	1.17	1.24
1	A	981[A]	ARG	CD-NE	-5.39	1.38	1.46
1	A	981[B]	ARG	CD-NE	-5.39	1.38	1.46
1	A	897	GLU	C-O	-5.36	1.17	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	HIS	CA-CB-CG	-8.71	105.09	113.80
1	A	993	HIS	CA-CB-CG	8.14	121.94	113.80
1	A	340	ASP	CA-CB-CG	7.60	120.20	112.60
1	A	995	GLN	OE1-CD-NE2	7.53	130.13	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	901	ASN	OD1-CG-ND2	7.42	130.02	122.60
1	A	783	GLY	CA-C-O	-7.35	111.81	121.51
1	A	37	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	1028	ALA	O-C-N	-6.91	115.64	121.23
1	A	586	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	270	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	836	PHE	CA-CB-CG	6.76	120.56	113.80
1	A	765	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	A	347	ASN	OD1-CG-ND2	6.43	129.03	122.60
1	A	367	GLN	OE1-CD-NE2	6.37	128.97	122.60
1	A	600	HIS	N-CA-CB	6.31	119.75	110.35
1	A	273	HIS	CB-CG-CD2	-6.30	123.01	131.20
1	A	1024	ASP	CA-C-O	6.21	128.02	121.19
1	A	413	ASN	CA-CB-CG	6.21	118.81	112.60
1	A	663	GLN	OE1-CD-NE2	6.17	128.77	122.60
1	A	409	ASP	CA-CB-CG	6.16	118.75	112.60
1	A	273	HIS	CB-CG-ND1	6.09	131.83	122.70
1	A	950	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	A	1028	ALA	CA-C-O	6.04	123.22	119.29
1	A	1030	GLU	CA-C-O	6.04	128.88	121.99
1	A	425	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	A	676	ILE	CA-CB-CG2	5.95	120.61	110.50
1	A	144	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	554	HIS	CB-CG-ND1	5.92	131.57	122.70
1	A	470	HIS	CB-CG-CD2	-5.89	123.55	131.20
1	A	950	HIS	CB-CG-ND1	5.88	131.53	122.70
1	A	1028	ALA	CA-C-N	-5.88	113.91	119.85
1	A	1028	ALA	C-N-CA	-5.88	113.91	119.85
1	A	765	HIS	CB-CG-ND1	5.81	131.42	122.70
1	A	818[A]	ARG	CA-C-O	-5.67	114.46	120.92
1	A	818[B]	ARG	CA-C-O	-5.67	114.46	120.92
1	A	541	THR	N-CA-CB	5.62	119.33	110.23
1	A	47	GLU	CB-CG-CD	5.49	121.93	112.60
1	A	460	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	A	434	HIS	CB-CG-CD2	-5.41	124.16	131.20
1	A	653	ARG	CG-CD-NE	5.34	123.74	112.00
1	A	991	GLU	O-C-N	-5.28	115.56	122.59
1	A	992	GLU	CA-C-N	5.28	131.63	121.54
1	A	992	GLU	C-N-CA	5.28	131.63	121.54
1	A	527	ASP	O-C-N	-5.25	117.13	123.27
1	A	394	GLN	OE1-CD-NE2	5.24	127.84	122.60
1	A	285	PHE	CA-CB-CG	-5.22	108.58	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	A	347	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	491[A]	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	A	491[B]	GLN	OE1-CD-NE2	-5.15	117.45	122.60

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 [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	8468	0	8386	105	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	113	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 7.

All (113) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:651:LEU:CD1	1:A:653:ARG:HG2	2.33	0.58
1:A:1019:ASN:HB3	7:A:6201:HOH:O	2.02	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:47:GLU:CD	1:A:51:ARG:HD3	2.32	0.55
1:A:63:LYS:HE2	7:A:7720:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:428:MET:HE1	1:A:491[B]:GLN:HG2	1.90	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: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
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:435[B]:TYR:OH	1:A:528:ASP:OD2	2.29	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
1:A:954[B]:ARG:HD2	1:A:956:ASP:OD1	2.16	0.46
6:A:5002:MPD:O4	6:A:5002:MPD:HM1	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:434:HIS:CE1	1:A:930:ASP:OD1	2.58	0.45
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.98	0.45
1:A:82[A]:LYS:CE	7:A:6241:HOH:O	2.64	0.45
6:A:5002:MPD:H11	7:A:6992:HOH:O	2.17	0.45
1:A:32:GLN:NE2	7:A:6870:HOH:O	2.49	0.45
1:A:96[A]:ILE:HG23	1:A:479:LYS:HE2	1.99	0.45
1:A:886:LYS:NZ	7:A:6602:HOH:O	2.49	0.45
1:A:304[A]:ARG:NH2	7:A:6304:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304[B]:ARG:HH11	1:A:304[B]:ARG:HD2	1.65	0.44
1:A:251:TRP:C	1:A:251:TRP:CD1	2.94	0.44
1:A:491[B]:GLN:NE2	7:A:6951:HOH:O	2.48	0.44
2:A:2001:NAG:H83	2:A:2001:NAG:H2	1.52	0.44
1:A:653:ARG:NH1	7:A:7416:HOH:O	2.49	0.44
1:A:48:LEU:HG	1:A:52[A]:MET:SD	2.58	0.43
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: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:679:ARG:HH22	1:A:701[B]:GLN:CD	2.28	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
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:434:HIS:CD2	1:A:927:ASP:HA	2.56	0.40
1:A:919:HIS:HE1	7:A:7131:HOH:O	2.03	0.40
1:A:954[B]:ARG:HH11	1:A:954[B]:ARG:HD3	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%)	30 10

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%)	937 (98%)	16 (2%)	53 18

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	69	LYS
1	A	275	CYS
1	A	396	GLU
1	A	447[A]	SER
1	A	447[B]	SER
1	A	541	THR
1	A	651	LEU
1	A	653	ARG
1	A	676	ILE
1	A	691	GLN
1	A	701[A]	GLN
1	A	701[B]	GLN
1	A	720[A]	HIS
1	A	720[B]	HIS
1	A	898	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	121	ASN
1	A	148	GLN
1	A	157	GLN
1	A	191	GLN
1	A	240	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
1	A	554	HIS
1	A	608	HIS
1	A	610	GLN
1	A	655	ASN
1	A	691	GLN
1	A	698	GLN
1	A	765	HIS
1	A	812	GLN
1	A	880	GLN
1	A	885	ASN
1	A	919	HIS
1	A	923	GLN
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	993	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

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
5	MRD	A	5001	-	7,7,7	0.72	0	9,10,10	1.35	1 (11%)
2	NAG	A	2001	1	14,14,15	0.81	0	17,19,21	2.72	8 (47%)
4	GB6	A	4001	3	20,20,20	2.15	5 (25%)	25,27,27	1.57	5 (20%)
6	MPD	A	5002	-	7,7,7	0.71	0	9,10,10	0.77	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
5	MRD	A	5001	-	-	2/5/5/5	-
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
6	MPD	A	5002	-	-	0/5/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4001	GB6	C15-C10	6.77	1.49	1.39
4	A	4001	GB6	C8-N7	3.76	1.52	1.47
4	A	4001	GB6	C9-C8	3.07	1.57	1.53
4	A	4001	GB6	O3-C3	2.19	1.46	1.42
4	A	4001	GB6	C10-C8	2.15	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NAG	C2-N2-C7	-8.38	111.66	122.90
4	A	4001	GB6	C14-C15-C10	-3.63	116.30	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NAG	C3-C4-C5	3.51	116.59	110.23
4	A	4001	GB6	O9-C9-C8	-3.41	103.86	111.51
2	A	2001	NAG	C1-O5-C5	2.94	116.13	112.19
2	A	2001	NAG	O5-C1-C2	-2.67	107.16	111.29
4	A	4001	GB6	C9-C8-C10	-2.63	104.85	111.08
4	A	4001	GB6	O2-C2-C3	-2.61	123.59	126.23
4	A	4001	GB6	O3-C3-C2	-2.47	106.56	111.80
2	A	2001	NAG	C1-C2-N2	2.27	114.00	110.43
5	A	5001	MRD	CM-C2-C1	-2.26	105.56	110.63
2	A	2001	NAG	O3-C3-C2	-2.20	104.83	109.40
2	A	2001	NAG	C8-C7-N2	-2.10	112.63	116.12
2	A	2001	NAG	O5-C5-C4	2.10	115.93	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

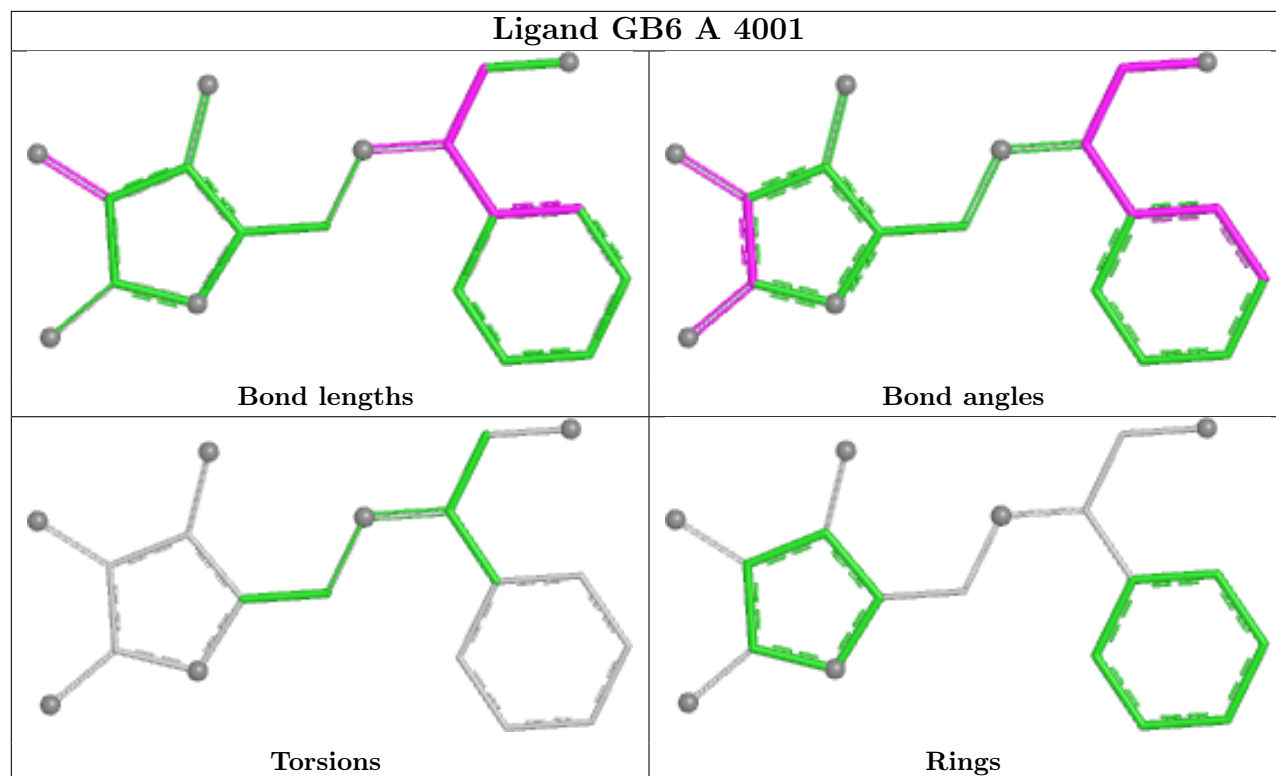
Mol	Chain	Res	Type	Atoms
2	A	2001	NAG	C8-C7-N2-C2
2	A	2001	NAG	O7-C7-N2-C2
5	A	5001	MRD	C2-C3-C4-O4
5	A	5001	MRD	C2-C3-C4-C5

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5001	MRD	3	0
2	A	2001	NAG	5	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%)	-0.33	16 (1%) 70 71	4, 12, 29, 73	51 (5%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1045	SER	4.8
1	A	993	HIS	4.1
1	A	691	GLN	3.5
1	A	992	GLU	3.1
1	A	991	GLU	2.9
1	A	702	ASP	2.7
1	A	682	ASN	2.5
1	A	720[A]	HIS	2.4
1	A	534	SER	2.3
1	A	655	ASN	2.3
1	A	1044	SER	2.3
1	A	600	HIS	2.2
1	A	638	ASP	2.2
1	A	535	GLY	2.2
1	A	1024	ASP	2.1
1	A	539	SER	2.1

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

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

6.3 Carbohydrates [i](#)

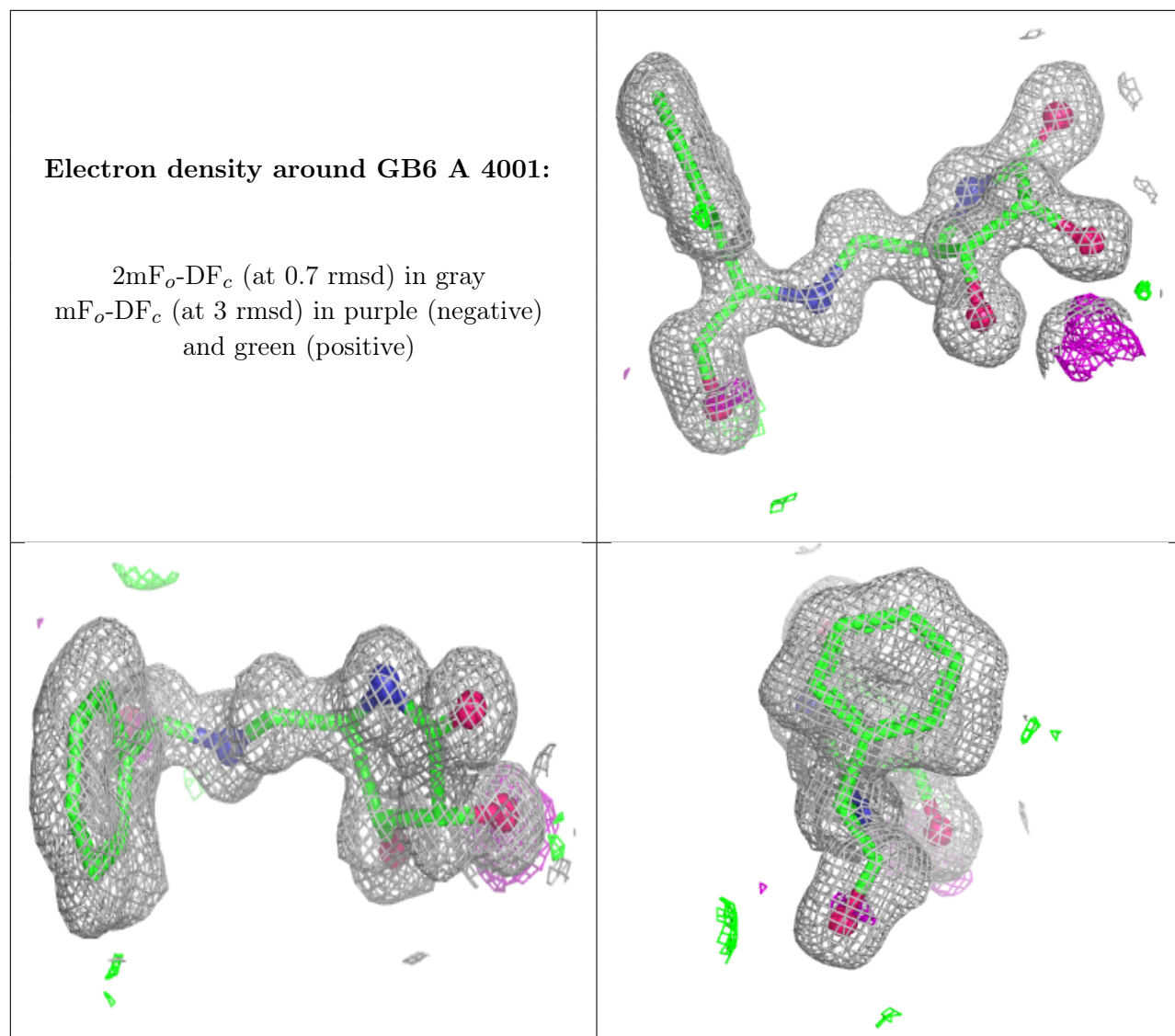
There are no oligosaccharides in this entry.

6.4 Ligands

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	0.79	0.14	25,31,42,47	0
2	NAG	A	2001	14/15	0.87	0.12	26,46,66,71	0
5	MRD	A	5001	8/8	0.96	0.07	11,13,18,22	0
4	GB6	A	4001	19/19	0.99	0.04	7,9,18,19	0
3	ZN	A	3001	1/1	1.00	0.02	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.