



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:20 AM BST

PDB ID : 2FYV  
Title : Golgi alpha-mannosidase II complex with an amino-salacinol carboxylate analog  
Authors : Kuntz, D.A.; Hamlet, T.; Rose, D.R.  
Deposited on : 2006-02-08  
Resolution : 1.90 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](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

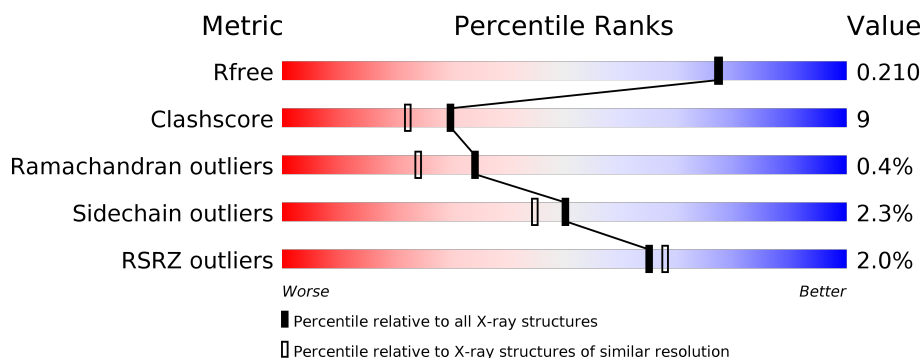
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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>80%</div> <div>16%</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	W72	A	2000	X	-	-	-
6	MPD	A	2001	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9313 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 putative golgi alpha-mannosidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1014	Total	C	N	O	S	0	10	0
			8216	5222	1438	1516	40			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	cloning artifact	GB 517481
A	2	SER	-	cloning artifact	GB 517481
A	3	SER	-	cloning artifact	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	-	cloning artifact	GB 517481
A	11	GLU	-	cloning artifact	GB 517481
A	12	PHE	-	cloning artifact	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 PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

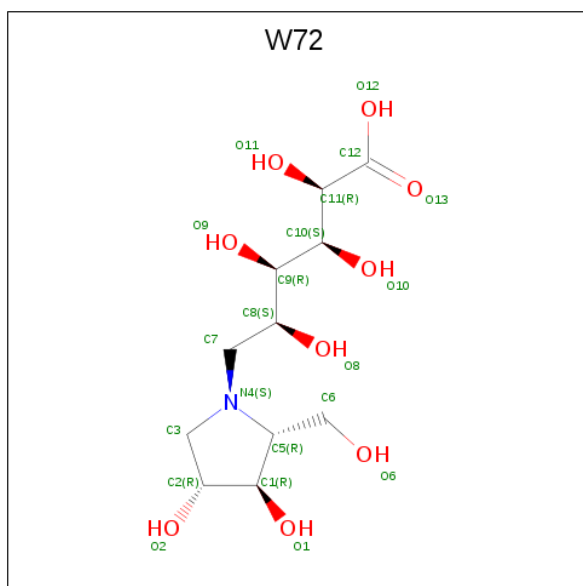


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

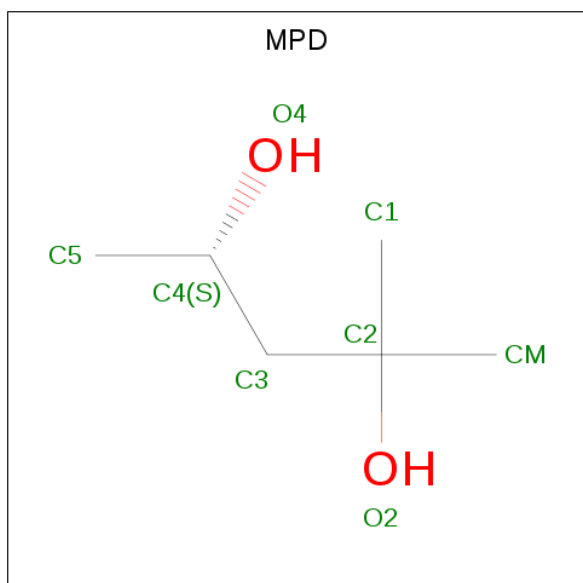
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 6-DEOXY-6-[(2R,3R,4R)-3,4-DIHYDROXY-2-(HYDROXYMETHYL)PYRRROLIDIN-1-YL]-L-GULONIC ACID (three-letter code: W72) (formula:  $C_{11}H_{21}NO_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	11	1	9		

- 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	1048	Total	O	0	0
			1048	1048		

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.

- Chain A:
- 
- 20% 80% 16%
- ARG SER SER HIS HIS HIS HIS GLY GIJ PHE ASP ASP PRO ARG ARG PRO LEU LYS VAL ALA ARG SER ARG ARG GLY GLN C31 N40 S53 F54 K55 D56 I57 D58 W62 G65 W66 K69 L73 K74 Y75 H76 H78 H79 K82 P93 G94 W95
- T96 Q97 T98 E101 R116 K125 S132 H139 D140 L141 K145 K146 I152 M155 G156 Q157 L158 M167 H174 W175 R176 L203 D204 F206 E236 Q239 T250 W251 D256 P265 Y269 D270 H273 H274 C275 K280 K288 P289 W290
- P302 P303 R304 R314 L317 T331 N332 D340 E349 H363 Q367 Q375 Q394 Y418 R422 H425 H434 Y435 S447 E456 F468 Q469 H470 H471 I474 E487 Q488 Q498 D518 T525 L526 S534 G546 I549 W550
- L568 V569 D570 V580 N585 E589 V595 W596 H600 D601 T602 L603 T604 K605 T606 T607 H608 P609 R617 L618 P626 L634 P641 T644 S645 F646 L651 L652 K654 M655 L659 Q663 E666 K669 L676 S677 L678 M682 L686
- Q691 L694 K695 S696 P697 Q698 T700 Q701 W702 S703 P704 H705 V706 P707 W708 H709 K714 H720 R723 E739 Q742 L746 V747 K751 S761 P762 V763 W764 H765 W769 K770 N778 L785 T788 Y828 R869 N885 W895 E897 S1044 SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.81Å 108.64Å 137.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 1.90 29.60 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.0 (29.60-1.90) 94.2 (29.60-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.162 , 0.212 0.160 , 0.210	Depositor DCC
$R_{free}$ test set	1967 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.4	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: PO4, ZN, MPD, NAG, W72

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	0.95	4/8493 (0.0%)	0.92	8/11534 (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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	GLU	CG-CD	5.30	1.59	1.51
1	A	828	TYR	CD1-CE1	5.13	1.47	1.39
1	A	580	VAL	CB-CG1	5.10	1.63	1.52
1	A	132	SER	CB-OG	5.07	1.48	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	167	MET	N-CA-C	-6.44	93.62	111.00
1	A	422	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	518	ASP	N-CA-C	-5.83	95.27	111.00
1	A	607	ILE	N-CA-C	-5.73	95.54	111.00
1	A	678	LEU	CA-CB-CG	5.73	128.47	115.30
1	A	763	VAL	CB-CA-C	-5.20	101.52	111.40
1	A	954	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	646	TYR	Sidechain

## 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	8216	0	7995	153	0
2	A	14	0	13	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	21	0	20	1	0
6	A	8	0	14	1	0
7	A	1048	0	0	33	0
All	All	9313	0	8042	153	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 9.

All (153) 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:256:ASP:HB2	7:A:2871:HOH:O	1.46	1.15
1:A:954:ARG:HD3	1:A:981:ARG:HH21	1.06	1.08
1:A:954:ARG:HD3	1:A:981:ARG:NH2	1.70	1.06
1:A:40:ASN:HB2	7:A:2015:HOH:O	1.67	0.92
1:A:116:ARG:HD3	7:A:3035:HOH:O	1.72	0.90
1:A:954:ARG:CD	1:A:981:ARG:HH21	1.86	0.88
1:A:996:LYS:HE2	7:A:2896:HOH:O	1.75	0.85
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.60	0.84
1:A:332:ASN:H	1:A:394:GLN:HE22	1.25	0.83
1:A:701:GLN:HA	1:A:701:GLN:HE21	1.42	0.83
1:A:53[A]:SER:OG	1:A:55:LYS:HG2	1.81	0.80
1:A:742:GLN:HG3	7:A:2756:HOH:O	1.82	0.80
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ASP:HB2	1:A:608:HIS:CE1	2.19	0.76
1:A:989:THR:HG22	1:A:991:GLU:HG3	1.67	0.76
1:A:488:GLN:HB3	7:A:2270:HOH:O	1.86	0.75
1:A:698:GLN:HB2	1:A:705:HIS:ND1	2.03	0.74
1:A:666:GLU:HB2	7:A:2964:HOH:O	1.87	0.73
1:A:40:ASN:CB	7:A:2015:HOH:O	2.32	0.73
1:A:332:ASN:H	1:A:394:GLN:NE2	1.89	0.69
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.23	0.68
1:A:304:ARG:HH21	1:A:314:ARG:CZ	2.06	0.68
1:A:331:THR:HA	1:A:394:GLN:HE21	1.59	0.68
1:A:608:HIS:HD2	7:A:2977:HOH:O	1.78	0.67
1:A:954:ARG:CD	1:A:981:ARG:NH2	2.51	0.66
1:A:723:ARG:HH11	1:A:723:ARG:HG3	1.60	0.65
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.26	0.65
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.79	0.65
1:A:651:LEU:HD11	1:A:653:ARG:HG2	1.80	0.64
1:A:155:ASN:HD21	1:A:157:GLN:HE21	1.45	0.64
1:A:498:GLN:HE21	1:A:526:LEU:H	1.45	0.63
1:A:739:GLU:OE1	1:A:739:GLU:HA	1.97	0.63
1:A:549:ILE:HG23	1:A:550:LEU:H	1.64	0.62
1:A:75:TYR:HE2	7:A:3027:HOH:O	1.81	0.62
1:A:139:HIS:HB2	7:A:2254:HOH:O	1.99	0.62
1:A:57:ILE:C	1:A:57:ILE:HD12	2.21	0.61
1:A:280:LYS:HE3	7:A:2669:HOH:O	2.01	0.61
1:A:950:HIS:HE1	7:A:2107:HOH:O	1.82	0.60
1:A:304:ARG:NH2	1:A:314:ARG:CZ	2.64	0.60
1:A:765:HIS:HE1	7:A:2980:HOH:O	1.84	0.59
1:A:525:THR:HG23	7:A:2302:HOH:O	2.02	0.59
1:A:141:LEU:O	1:A:146:LYS:NZ	2.31	0.58
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.86	0.57
1:A:273:HIS:HE1	6:A:2001:MPD:O4	1.88	0.57
1:A:290:MET:HG2	1:A:303:PRO:HG2	1.86	0.57
1:A:549:ILE:HG23	1:A:550:LEU:N	2.19	0.57
1:A:125:LYS:HE2	7:A:2201:HOH:O	2.03	0.56
1:A:678:LEU:HD12	1:A:769:MET:HE1	1.87	0.56
1:A:290:MET:CG	1:A:303:PRO:HG2	2.36	0.56
1:A:695:LYS:HA	1:A:709[B]:HIS:HD2	1.70	0.56
1:A:981:ARG:NH1	1:A:1031:VAL:O	2.39	0.55
1:A:761:PRO:O	1:A:762:SER:HB2	2.07	0.55
1:A:250:ILE:HB	1:A:910:PRO:HG2	1.89	0.55
1:A:435[A]:TYR:HE2	1:A:526:LEU:HD13	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:HIS:HE1	7:A:2917:HOH:O	1.91	0.54
1:A:723:ARG:NH1	7:A:2583:HOH:O	2.40	0.53
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.55	0.53
1:A:904:ARG:HG2	1:A:985:MET:SD	2.48	0.53
1:A:602:THR:C	1:A:603:LEU:HD22	2.30	0.53
1:A:641:PRO:HG2	1:A:644:THR:HB	1.91	0.52
1:A:723:ARG:NH1	1:A:723:ARG:HG3	2.25	0.52
1:A:57:ILE:HD12	1:A:58:ASP:C	2.29	0.52
1:A:1009:CYS:HB3	1:A:1026:MET:HA	1.92	0.51
1:A:714:LYS:HD2	7:A:2751:HOH:O	2.10	0.51
1:A:695:LYS:HA	1:A:709[B]:HIS:CD2	2.44	0.51
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.94	0.51
1:A:989:THR:CG2	1:A:991:GLU:HG3	2.38	0.51
1:A:435[A]:TYR:CE2	1:A:526:LEU:HD13	2.45	0.51
1:A:155:ASN:ND2	1:A:157:GLN:HE21	2.10	0.50
1:A:79:HIS:HE1	7:A:2046:HOH:O	1.95	0.49
1:A:314:ARG:HH21	1:A:317:LEU:HD12	1.78	0.49
1:A:1018:GLN:NE2	7:A:2080:HOH:O	2.37	0.48
1:A:57:ILE:HD12	1:A:58:ASP:N	2.27	0.48
1:A:663:GLN:NE2	7:A:2813:HOH:O	2.36	0.48
1:A:626:PRO:O	1:A:950:HIS:HD2	1.96	0.48
1:A:995:GLN:HB3	7:A:2845:HOH:O	2.14	0.48
1:A:595:VAL:HG22	1:A:617:ARG:HG3	1.96	0.48
1:A:957:LEU:HD13	1:A:981:ARG:NH1	2.29	0.48
1:A:340:ASP:OD1	5:A:2000:W72:O13	2.32	0.47
1:A:57:ILE:HD12	1:A:58:ASP:O	2.14	0.47
1:A:98:THR:OG1	1:A:101:GLU:HG3	2.15	0.47
1:A:270:ASP:OD1	1:A:273:HIS:HD2	1.98	0.47
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.49	0.47
1:A:456:GLU:HB2	7:A:2280:HOH:O	2.15	0.47
1:A:993:HIS:O	1:A:993:HIS:CD2	2.67	0.47
1:A:332:ASN:N	1:A:394:GLN:NE2	2.59	0.47
1:A:676:ILE:HD13	1:A:747:VAL:HG21	1.97	0.47
1:A:363:HIS:O	1:A:367:GLN:HG2	2.15	0.46
1:A:288:LYS:HD2	1:A:349:GLU:CD	2.35	0.46
1:A:470:HIS:CD2	1:A:471:HIS:N	2.83	0.46
1:A:869:ARG:NH1	1:A:885:ASN:HD22	2.13	0.46
1:A:608:HIS:HB2	1:A:609:PRO:HD2	1.97	0.46
1:A:145:LYS:HE3	7:A:3042:HOH:O	2.15	0.46
1:A:75:TYR:CE2	7:A:3027:HOH:O	2.56	0.46
1:A:251:TRP:C	1:A:251:TRP:CD1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:NH2	1:A:314:ARG:NH2	2.64	0.46
1:A:69:LYS:HA	7:A:2677:HOH:O	2.17	0.45
1:A:331:THR:CA	1:A:394:GLN:HE21	2.28	0.45
1:A:698:GLN:HG2	1:A:700:THR:O	2.17	0.45
1:A:678:LEU:HD12	1:A:769:MET:CE	2.46	0.45
1:A:990:PRO:O	1:A:991:GLU:C	2.55	0.45
1:A:885:ASN:ND2	1:A:885:ASN:H	2.15	0.45
1:A:964:ARG:HH11	1:A:973:GLN:NE2	2.09	0.44
1:A:304:ARG:HH21	1:A:314:ARG:NH1	2.15	0.44
1:A:703:SER:HB2	1:A:704:PRO:HD2	1.99	0.44
1:A:601:ASP:HB2	1:A:608:HIS:ND1	2.33	0.44
1:A:651:LEU:HD13	1:A:651:LEU:C	2.38	0.44
1:A:1008:ARG:CZ	1:A:1022:HIS:CD2	3.01	0.44
1:A:602:THR:O	1:A:603:LEU:HD22	2.18	0.43
1:A:66:TRP:CZ3	1:A:239:GLN:HG3	2.53	0.43
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.53	0.43
1:A:655:ASN:CG	1:A:655:ASN:O	2.57	0.43
1:A:314:ARG:NH2	1:A:317:LEU:HD12	2.33	0.43
1:A:549:ILE:HG12	1:A:550:LEU:H	1.82	0.43
1:A:570:ASP:HA	1:A:618:ILE:O	2.18	0.43
1:A:901:ASN:HB2	7:A:2908:HOH:O	2.19	0.43
1:A:686:LEU:HD22	1:A:697:ILE:HG12	2.00	0.43
1:A:701:GLN:CA	1:A:701:GLN:HE21	2.17	0.43
1:A:568:LEU:HD12	1:A:770:ARG:HD2	2.00	0.43
1:A:785:LEU:O	1:A:788:THR:HB	2.19	0.42
1:A:765:HIS:HD2	1:A:778:ASN:OD1	2.02	0.42
1:A:425:HIS:HE1	1:A:487:GLU:OE1	2.03	0.42
1:A:601:ASP:OD1	1:A:603:LEU:HB2	2.19	0.42
1:A:206:PHE:CD1	1:A:206:PHE:N	2.87	0.42
1:A:206:PHE:HB2	1:A:418:TYR:CE1	2.54	0.42
1:A:654:LYS:O	1:A:655:ASN:HB3	2.20	0.42
1:A:1008:ARG:CZ	1:A:1022:HIS:NE2	2.83	0.42
1:A:40:ASN:CG	7:A:2015:HOH:O	2.56	0.42
1:A:601:ASP:C	1:A:603:LEU:H	2.23	0.42
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.54	0.42
1:A:468:PHE:CZ	1:A:474:ILE:HA	2.55	0.42
1:A:546:GLY:HA3	1:A:549:ILE:HG22	2.00	0.42
1:A:601:ASP:N	1:A:606:THR:O	2.51	0.42
1:A:608:HIS:CD2	7:A:2977:HOH:O	2.62	0.42
1:A:236:GLU:OE2	7:A:2029:HOH:O	2.22	0.41
1:A:981:ARG:NE	7:A:2867:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589[A]:GLU:OE2	1:A:751:LYS:HD3	2.20	0.41
1:A:919:HIS:HE1	7:A:2355:HOH:O	2.04	0.41
1:A:981:ARG:HH11	1:A:981:ARG:HB2	1.84	0.41
1:A:435[A]:TYR:HE2	1:A:526:LEU:CD1	2.33	0.41
1:A:580:VAL:HG22	1:A:634:LEU:HD22	2.02	0.41
1:A:468:PHE:CE2	1:A:474:ILE:HA	2.56	0.41
1:A:55:LYS:HA	1:A:55:LYS:HD3	1.76	0.41
1:A:434:HIS:CE1	1:A:930:ASP:OD1	2.53	0.41
1:A:706:VAL:HA	1:A:707:PRO:HD3	1.93	0.41
1:A:1009:CYS:SG	1:A:1023:LEU:HD12	2.61	0.41
1:A:596:TRP:CZ3	1:A:659:LEU:HD13	2.55	0.41
1:A:203:ILE:HD12	1:A:269:TYR:CG	2.56	0.41
1:A:596:TRP:CG	1:A:746:LEU:HD21	2.56	0.40
1:A:152:ILE:O	1:A:155:ASN:OD1	2.40	0.40
1:A:723:ARG:CG	1:A:723:ARG:NH1	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1022/1045 (98%)	987 (97%)	31 (3%)	4 (0%)	34	24

All (4) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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	911/929 (98%)	890 (98%)	21 (2%)	50 45

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

Mol	Chain	Res	Type
1	A	57	ILE
1	A	69	LYS
1	A	82	LYS
1	A	96	ILE
1	A	158	LEU
1	A	265	PRO
1	A	275	CYS
1	A	302	PRO
1	A	447	SER
1	A	585	ASN
1	A	653	ARG
1	A	669	LYS
1	A	691	GLN
1	A	701	GLN
1	A	723	ARG
1	A	828	TYR
1	A	906	SER
1	A	954	ARG
1	A	981	ARG
1	A	1004	PRO
1	A	1044	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	91	ASN
1	A	121	ASN
1	A	157	GLN

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Mol	Chain	Res	Type
1	A	191	GLN
1	A	240	GLN
1	A	249	GLN
1	A	253	ASN
1	A	273	HIS
1	A	347	ASN
1	A	369	HIS
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	498	GLN
1	A	554	HIS
1	A	701	GLN
1	A	765	HIS
1	A	809	ASN
1	A	885	ASN
1	A	901	ASN
1	A	919	HIS
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	986	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 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
6	MPD	A	2001	-	7,7,7	0.54	0	9,10,10	0.65	0
2	NAG	A	1047	1	14,14,15	0.88	0	17,19,21	0.93	1 (5%)
3	PO4	A	2002	-	4,4,4	2.59	2 (50%)	6,6,6	0.83	0
5	W72	A	2000	4	18,21,21	0.87	1 (5%)	22,30,30	3.01	8 (36%)

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
6	MPD	A	2001	-	1/1/2/2	2/5/5/5	-
2	NAG	A	1047	1	-	2/6/23/26	0/1/1/1
5	W72	A	2000	4	1/1/9/9	4/18/38/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2002	PO4	P-O1	4.57	1.61	1.50
5	A	2000	W72	C3-N4	2.49	1.51	1.47
3	A	2002	PO4	P-O3	2.36	1.61	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2000	W72	C9-C10-C11	7.32	126.48	113.58
5	A	2000	W72	O2-C2-C1	5.63	121.93	111.27
5	A	2000	W72	O1-C1-C5	5.42	125.28	111.70
5	A	2000	W72	C3-N4-C5	-4.82	96.26	105.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2000	W72	O1-C1-C2	3.70	120.98	112.04
5	A	2000	W72	C1-C5-N4	3.55	110.39	103.83
5	A	2000	W72	C7-C8-C9	3.00	118.17	109.79
5	A	2000	W72	O10-C10-C9	-2.99	102.52	109.47
2	A	1047	NAG	C2-N2-C7	-2.85	118.85	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	2001	MPD	C4
5	A	2000	W72	C11

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2001	MPD	C2-C3-C4-O4
5	A	2000	W72	C7-C8-C9-C10
2	A	1047	NAG	C4-C5-C6-O6
2	A	1047	NAG	O5-C5-C6-O6
5	A	2000	W72	O10-C10-C11-C12
5	A	2000	W72	C9-C10-C11-C12
5	A	2000	W72	C9-C10-C11-O11
6	A	2001	MPD	C2-C3-C4-C5

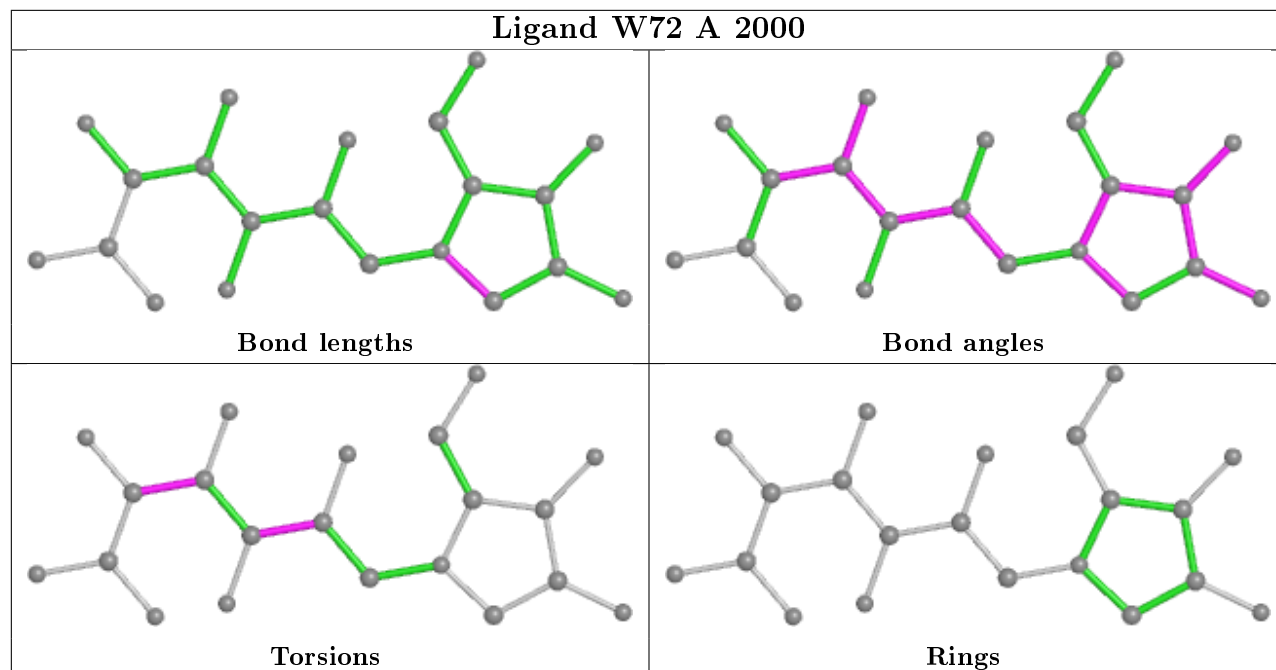
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2001	MPD	1	0
5	A	2000	W72	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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, 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%)	-0.24	20 (1%) 65 68	4, 13, 31, 66	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	603	LEU	5.9
1	A	993	HIS	5.7
1	A	601	ASP	5.2
1	A	602	THR	5.2
1	A	991	GLU	5.2
1	A	604	THR	5.1
1	A	600	HIS	4.2
1	A	990	PRO	4.0
1	A	720	HIS	3.6
1	A	78	HIS	3.5
1	A	742	GLN	3.0
1	A	701	GLN	2.8
1	A	702	ASP	2.8
1	A	1024	ASP	2.8
1	A	1022	HIS	2.8
1	A	682	ASN	2.4
1	A	992	GLU	2.4
1	A	534	SER	2.3
1	A	549	ILE	2.1
1	A	73	LEU	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](#)

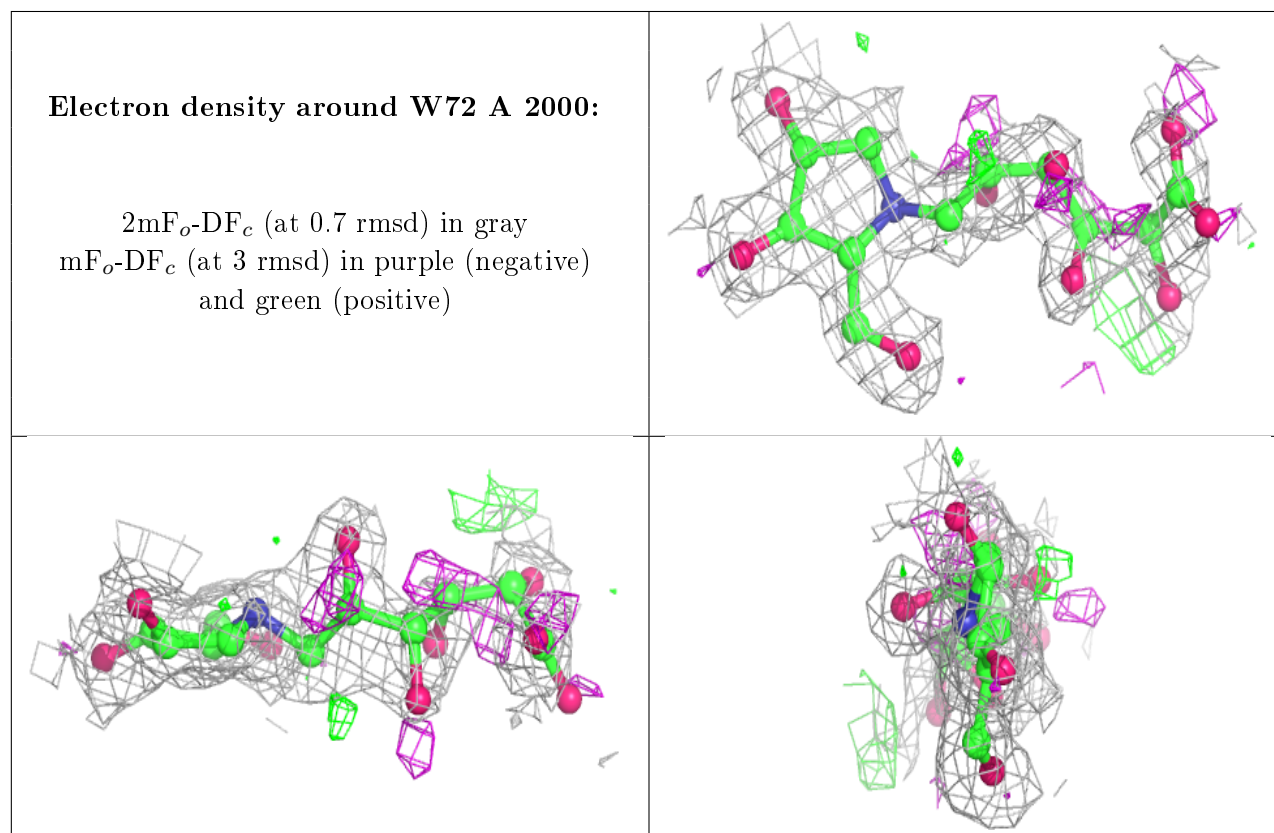
There are no monosaccharides in this entry.

## 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	1047	14/15	0.78	0.33	38,44,46,46	0
3	PO4	A	2002	5/5	0.89	0.14	41,41,43,43	0
5	W72	A	2000	21/21	0.92	0.18	9,19,42,44	0
6	MPD	A	2001	8/8	0.93	0.16	19,20,23,23	0
4	ZN	A	2003	1/1	1.00	0.04	10,10,10,10	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.