



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:33 AM GMT

PDB ID : 2F18  
Title : GOLGI ALPHA-MANNOSIDASE II complex with (2R,3R,4S)-2-({[(1R)-2-hydroxy-1-phenylethyl]amino}methyl)pyrrolidine-3,4-diol  
Authors : Kuntz, D.A.; Rose, D.R.  
Deposited on : 2005-11-14  
Resolution : 1.30 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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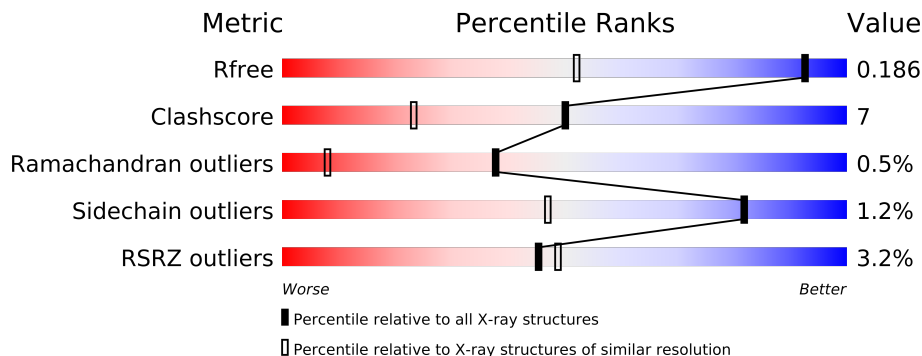
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 1.30 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))
$R_{free}$	66092	1025 (1.34-1.26)
Clashscore	79885	1140 (1.34-1.26)
Ramachandran outliers	78287	1093 (1.34-1.26)
Sidechain outliers	78261	1092 (1.34-1.26)
RSRZ outliers	66119	1025 (1.34-1.26)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1045	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PO4	A	1803	-	X
5	GB1	A	1804	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9543 atoms, of which 0 are hydrogen and 0 are deuterium.

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	33	0
			8325	5283	1454	1546	42			

There are 12 discrepancies between the modelled and reference sequences:

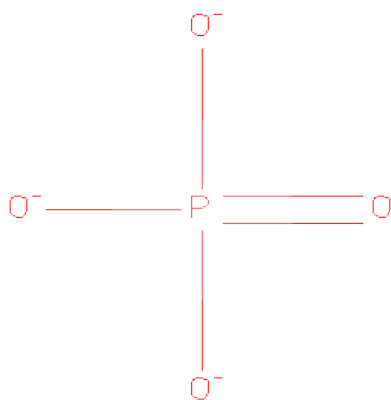
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	EXPRESSION TAG	GB 517481
A	2	SER	-	EXPRESSION TAG	GB 517481
A	3	SER	-	EXPRESSION TAG	GB 517481
A	4	HIS	-	EXPRESSION TAG	GB 517481
A	5	HIS	-	EXPRESSION TAG	GB 517481
A	6	HIS	-	EXPRESSION TAG	GB 517481
A	7	HIS	-	EXPRESSION TAG	GB 517481
A	8	HIS	-	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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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<sub>4</sub>P).

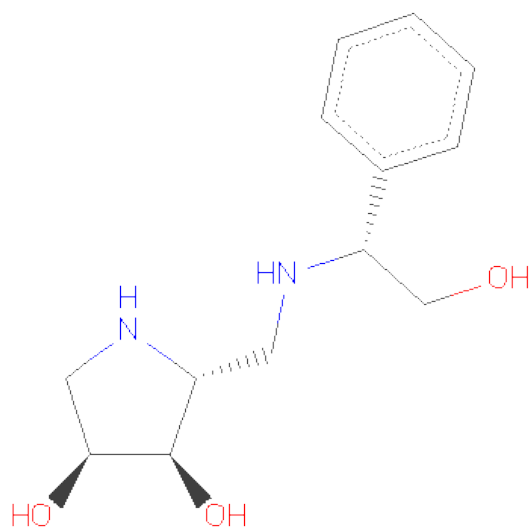


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

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

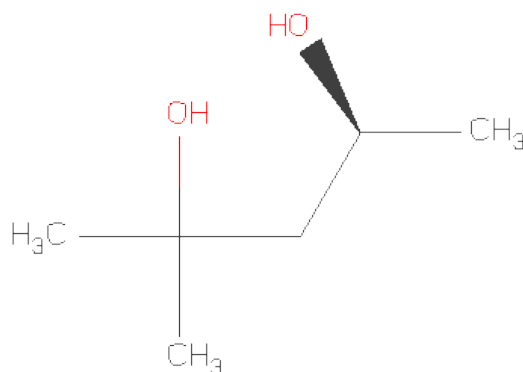
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (2R,3R,4S)-2-([(1R)-2-HYDROXY-1-PHENYLETHYL]AMINO}METHYL) PYRROLIDINE-3,4-DIOL (three-letter code: GB1) (formula: C<sub>13</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	13	2	3		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

- Molecule 7 is water.

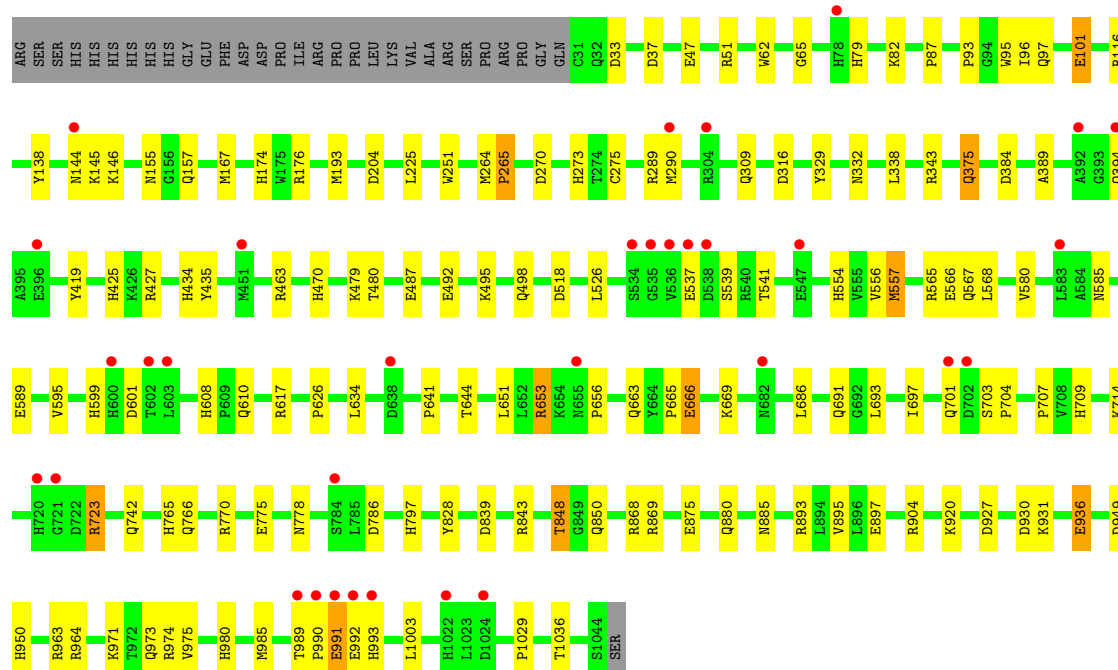
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1172	Total	O	0	0
			1172	1172		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.97Å 109.72Å 138.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 1.30 29.85 – 1.21	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.85-1.30) 93.8 (29.85-1.21)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 1.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.168 , 0.180 0.174 , 0.186	Depositor DCC
$R_{free}$ test set	5847 reflections (1.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 318061 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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, GB1

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	0.87	2/8688 (0.0%)	0.97	19/11793 (0.2%)

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	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	GLU	CB-CG	-5.59	1.41	1.52
1	A	936	GLU	CG-CD	5.42	1.60	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	963	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	963	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	565	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	843	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	839	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	868	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	384	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	265	PRO	N-CA-C	5.50	126.41	112.10
1	A	289	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	343	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	419	TYR	CB-CG-CD2	-5.43	117.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	MET	N-CA-C	-5.38	96.48	111.00
1	A	665	PRO	N-CA-C	5.27	125.81	112.10
1	A	974	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	427	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	101	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	A	949	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	518	ASP	N-CA-C	-5.02	97.45	111.00
1	A	463	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316[B]	ASP	Mainchain
1	A	766[B]	GLN	Mainchain
1	A	848[B]	THR	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8325	0	8076	122	0
2	A	14	0	13	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	18	0	18	0	0
6	A	8	0	14	3	0
7	A	1172	0	0	43	0
All	All	9543	0	8121	124	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:498[B]:GLN:HG2	1:A:526:LEU:HD12	1.15	1.11
1:A:557:MET:HE2	1:A:931:LYS:HA	1.42	1.00
1:A:557:MET:CE	1:A:931:LYS:HA	1.94	0.97
1:A:96:ILE:HG22	7:A:2654:HOH:O	1.66	0.94
1:A:82:LYS:HD2	1:A:375:GLN:HE22	1.33	0.92
1:A:47:GLU:OE2	1:A:51:ARG:HD3	1.71	0.90
1:A:567:GLN:HB2	7:A:2927:HOH:O	1.75	0.87
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.59	0.85
1:A:116:ARG:HD2	7:A:2602:HOH:O	1.79	0.81
1:A:435[B]:TYR:CE1	7:A:2245:HOH:O	2.36	0.78
1:A:989:THR:HG22	1:A:991:GLU:HG3	1.65	0.78
1:A:742:GLN:HG3	7:A:1888:HOH:O	1.84	0.77
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.33	0.77
6:A:1801:MPD:H11	7:A:2516:HOH:O	1.86	0.75
1:A:663:GLN:HG3	7:A:2451:HOH:O	1.87	0.75
1:A:786:ASP:HB3	7:A:2891:HOH:O	1.86	0.74
1:A:144:ASN:HB3	7:A:2878:HOH:O	1.88	0.74
1:A:723:ARG:HH11	1:A:723:ARG:HG2	1.54	0.73
1:A:37:ASP:HB2	7:A:2749:HOH:O	1.87	0.73
1:A:498[A]:GLN:HE21	1:A:526:LEU:H	1.34	0.73
1:A:541:THR:HG23	7:A:2259:HOH:O	1.88	0.73
1:A:155[A]:ASN:HD21	1:A:157:GLN:HE21	1.36	0.72
1:A:498[B]:GLN:HG2	1:A:526:LEU:CD1	2.09	0.72
1:A:82:LYS:HD2	1:A:375:GLN:NE2	2.05	0.72
1:A:557:MET:HE1	1:A:931:LYS:CB	2.23	0.69
1:A:435[B]:TYR:CZ	7:A:2245:HOH:O	2.46	0.68
1:A:556:VAL:O	1:A:557:MET:HE3	1.93	0.68
1:A:589:GLU:HG3	7:A:2822:HOH:O	1.95	0.66
1:A:96:ILE:CG2	7:A:2654:HOH:O	2.34	0.65
6:A:1801:MPD:H13	7:A:2362:HOH:O	1.97	0.65
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.80	0.64
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.27	0.64
1:A:693:LEU:HD13	7:A:1881:HOH:O	1.97	0.64
1:A:309[B]:GLN:NE2	7:A:2587:HOH:O	2.32	0.62
1:A:848[B]:THR:CG2	1:A:850:GLN:NE2	2.63	0.61
1:A:707:PRO:HG2	1:A:797[B]:HIS:CE1	2.36	0.60
1:A:557:MET:CE	1:A:931:LYS:CA	2.75	0.60
1:A:765:HIS:HE1	7:A:2406:HOH:O	1.85	0.60
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.85	0.60
1:A:145:LYS:HE3	7:A:2875:HOH:O	2.01	0.59
1:A:273:HIS:HE1	6:A:1801:MPD:O4	1.85	0.59
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.85	0.59
1:A:666[A]:GLU:HG2	7:A:2417:HOH:O	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:480:THR:H	1:A:880:GLN:HE22	1.50	0.58
1:A:626:PRO:O	1:A:950:HIS:HD2	1.86	0.58
1:A:568:LEU:HD12	1:A:770[A]:ARG:HD3	1.86	0.58
1:A:498[B]:GLN:NE2	7:A:2262:HOH:O	2.37	0.57
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.34	0.57
1:A:875:GLU:CD	7:A:2287:HOH:O	2.43	0.57
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.88	0.57
1:A:33:ASP:O	7:A:2749:HOH:O	2.17	0.56
1:A:980:HIS:HE1	7:A:2755:HOH:O	1.87	0.56
1:A:556:VAL:O	1:A:557:MET:CE	2.52	0.56
1:A:971:LYS:NZ	1:A:971:LYS:HB2	2.19	0.56
1:A:904:ARG:HG2	1:A:985:MET:SD	2.45	0.56
1:A:96:ILE:HG23	1:A:479:LYS:HE2	1.88	0.56
1:A:848[B]:THR:HG22	1:A:850:GLN:H	1.71	0.56
1:A:848[B]:THR:HG23	1:A:850:GLN:NE2	2.22	0.55
1:A:950:HIS:HE1	7:A:2183:HOH:O	1.91	0.54
1:A:714:LYS:HD2	7:A:1901:HOH:O	2.07	0.53
1:A:601:ASP:HB2	1:A:608:HIS:CE1	2.44	0.53
1:A:601:ASP:HB2	1:A:608:HIS:HE1	1.74	0.53
1:A:290:MET:HB2	7:A:2645:HOH:O	2.09	0.53
1:A:79:HIS:HE1	7:A:2697:HOH:O	1.92	0.52
1:A:936:GLU:HG2	7:A:2781:HOH:O	2.10	0.52
1:A:701:GLN:HE21	1:A:701:GLN:HA	1.75	0.52
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.45	0.52
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.45	0.52
1:A:434:HIS:CE1	1:A:930:ASP:OD1	2.51	0.52
1:A:425:HIS:HE1	1:A:487:GLU:OE1	1.93	0.51
1:A:537:GLU:HG2	1:A:539:SER:HB3	1.93	0.51
1:A:701:GLN:HE21	1:A:701:GLN:CA	2.23	0.50
1:A:557:MET:HE1	1:A:931:LYS:CA	2.41	0.50
1:A:557:MET:HA	1:A:557:MET:HE2	1.94	0.50
1:A:265:PRO:HD3	1:A:329:TYR:OH	2.12	0.50
1:A:557:MET:HE1	1:A:931:LYS:HG2	1.94	0.49
1:A:270:ASP:OD1	1:A:273:HIS:HD2	1.94	0.49
1:A:641:PRO:HG2	1:A:644:THR:HB	1.95	0.49
1:A:557:MET:HE1	1:A:931:LYS:HB3	1.93	0.49
1:A:138[A]:TYR:CE1	1:A:193[A]:MET:CE	2.95	0.49
1:A:498[A]:GLN:NE2	1:A:526:LEU:H	2.08	0.48
1:A:97[B]:GLN:HE21	1:A:101:GLU:HB3	1.78	0.48
1:A:653:ARG:HD2	1:A:656:PRO:HA	1.95	0.48
1:A:492:GLU:OE2	1:A:495:LYS:NZ	2.39	0.48
1:A:37:ASP:N	7:A:2749:HOH:O	2.22	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.49	0.47
1:A:251:TRP:C	1:A:251:TRP:CD1	2.87	0.47
1:A:701:GLN:NE2	1:A:701:GLN:HA	2.29	0.47
1:A:554:HIS:HD2	7:A:2002:HOH:O	1.98	0.47
1:A:991:GLU:HB3	7:A:2237:HOH:O	2.14	0.46
1:A:992:GLU:HA	1:A:992:GLU:OE1	2.16	0.46
1:A:82:LYS:NZ	7:A:2685:HOH:O	2.49	0.46
1:A:557:MET:HE1	1:A:931:LYS:CG	2.46	0.46
1:A:96:ILE:HG23	1:A:479:LYS:CE	2.45	0.45
1:A:723:ARG:NH1	1:A:723:ARG:HG2	2.28	0.45
1:A:709[A]:HIS:ND1	7:A:2403:HOH:O	2.35	0.45
1:A:541:THR:CG2	7:A:2259:HOH:O	2.56	0.45
1:A:608:HIS:HD2	7:A:2430:HOH:O	2.00	0.44
1:A:599:HIS:HD2	1:A:610:GLN:CG	2.30	0.44
1:A:599:HIS:HD2	1:A:610:GLN:HG3	1.81	0.44
1:A:37:ASP:CB	7:A:2749:HOH:O	2.55	0.44
1:A:848[B]:THR:CG2	1:A:850:GLN:HE21	2.29	0.44
1:A:389:ALA:HB1	1:A:394:GLN:HG2	2.00	0.44
1:A:770[A]:ARG:NH2	7:A:1936:HOH:O	2.51	0.44
1:A:138[B]:TYR:CE2	1:A:146[B]:LYS:HE3	2.52	0.44
1:A:116:ARG:CD	7:A:2602:HOH:O	2.50	0.43
1:A:686:LEU:HD22	1:A:697:ILE:HG12	2.01	0.43
1:A:786:ASP:CB	7:A:2891:HOH:O	2.54	0.43
1:A:332:ASN:H	1:A:394:GLN:NE2	2.17	0.42
1:A:920:LYS:HG3	7:A:2931:HOH:O	2.19	0.42
1:A:557:MET:CE	1:A:931:LYS:HG2	2.49	0.42
1:A:290:MET:N	7:A:2645:HOH:O	2.52	0.42
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.67	0.42
1:A:775:GLU:HA	1:A:893:ARG:HD2	2.02	0.41
1:A:703:SER:HB2	1:A:704:PRO:HD2	2.01	0.41
1:A:554:HIS:HE1	7:A:1997:HOH:O	2.02	0.41
1:A:580:VAL:HG22	1:A:634:LEU:HD22	2.01	0.41
1:A:895:VAL:HG12	1:A:897:GLU:CG	2.49	0.41
1:A:225:LEU:HD21	1:A:264[A]:MET:SD	2.61	0.41
1:A:389:ALA:HB1	1:A:394:GLN:CG	2.51	0.41
1:A:723:ARG:N	1:A:723:ARG:HD2	2.36	0.41
1:A:595:VAL:HG22	1:A:617:ARG:HG3	2.03	0.41
1:A:87:PRO:HA	1:A:338:LEU:O	2.21	0.41
1:A:599:HIS:CD2	1:A:610:GLN:HG3	2.55	0.41

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	1045/1045 (100%)	1016 (97%)	24 (2%)	5 (0%)	38 8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	991	GLU
1	A	993	HIS
1	A	990	PRO
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	934/929 (100%)	921 (99%)	13 (1%)	78 41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	CYS
1	A	375	GLN
1	A	557	MET
1	A	585[A]	ASN
1	A	585[B]	ASN
1	A	653	ARG
1	A	666[A]	GLU
1	A	666[B]	GLU
1	A	669	LYS

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Mol	Chain	Res	Type
1	A	691	GLN
1	A	723	ARG
1	A	828	TYR
1	A	1029	PRO

Some 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	91	ASN
1	A	148	GLN
1	A	157	GLN
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	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	608	HIS
1	A	701	GLN
1	A	765	HIS
1	A	880	GLN
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 chains 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 carbohydrates 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	1801	-	7,7,7	1.04	0	10,10,10	0.55	0
2	NAG	A	1802	1	12,14,15	0.49	0	15,19,21	0.90	0
3	PO4	A	1803	-	4,4,4	0.90	0	6,6,6	0.34	0
5	GB1	A	1804	4	19,19,19	0.68	0	25,25,25	3.46	11 (44%)

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	1801	-	1/1/2/2	0/5/5/5	0/0/0/0
2	NAG	A	1802	1	-	1/6/23/26	0/1/1/1
3	PO4	A	1803	-	-	0/0/0/0	0/0/0/0
5	GB1	A	1804	4	-	0/11/24/24	0/2/2/2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1804	GB1	C6-N7-C8	9.33	124.26	113.67
5	A	1804	GB1	C9-C8-N7	8.25	119.35	108.55
5	A	1804	GB1	O4-C4-C5	-5.45	100.56	112.29
5	A	1804	GB1	C3-C2-N1	-5.44	95.85	105.28
5	A	1804	GB1	O9-C9-C8	-3.90	104.04	111.48
5	A	1804	GB1	C2-N1-C5	3.34	114.43	106.98
5	A	1804	GB1	C13-C12-C11	3.29	125.65	120.17
5	A	1804	GB1	C10-C8-N7	-2.84	103.92	112.63
5	A	1804	GB1	O3-C3-C4	2.45	116.04	111.31
5	A	1804	GB1	C4-C5-N1	-2.33	98.05	102.48
5	A	1804	GB1	O3-C3-C2	2.31	116.06	110.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1801	MPD	C4

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1802	NAG	O7-C7-N2-C2

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 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%)	-0.11	33 (3%)	44 47	6, 12, 25, 62	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	990	PRO	8.8
1	A	993	HIS	7.5
1	A	534	SER	7.5
1	A	992	GLU	6.1
1	A	602	THR	5.9
1	A	603	LEU	5.0
1	A	78	HIS	4.8
1	A	701	GLN	4.8
1	A	682	ASN	4.7
1	A	638	ASP	4.6
1	A	702	ASP	4.4
1	A	1024	ASP	3.9
1	A	720	HIS	3.7
1	A	144	ASN	3.4
1	A	600	HIS	3.3
1	A	991	GLU	3.3
1	A	538	ASP	3.3
1	A	535	GLY	3.0
1	A	536	VAL	2.9
1	A	655	ASN	2.8
1	A	304	ARG	2.8
1	A	547	GLU	2.7
1	A	290	MET	2.6
1	A	784	SER	2.5
1	A	396	GLU	2.4
1	A	537	GLU	2.3
1	A	394	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1022	HIS	2.3
1	A	451	MET	2.2
1	A	583	LEU	2.1
1	A	392	ALA	2.1
1	A	721	GLY	2.1
1	A	989	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GB1	A	1804	18/18	0.08	3.50	8,12,16,18	0
3	PO4	A	1803	5/5	0.17	2.06	21,26,27,27	0
6	MPD	A	1801	8/8	0.10	1.77	13,16,18,20	0
4	ZN	A	1805	1/1	0.02	-3.72	7,7,7,7	0
2	NAG	A	1802	14/15	0.39	-	35,41,45,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.