



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:22 PM BST

PDB ID : 1HTY  
Title : GOLGI ALPHA-MANNOSIDASE II  
Authors : van den Elsen, J.M.H.; Kuntz, D.A.; Rose, D.R.  
Deposited on : 2001-01-02  
Resolution : 1.40 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  
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

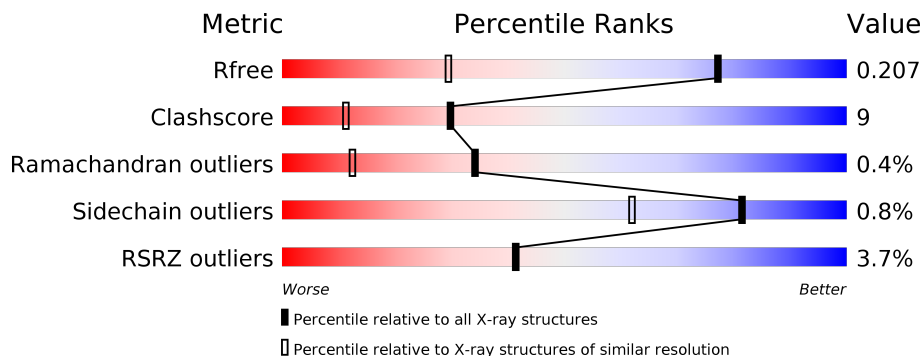
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	1015	<p>4% 81% 19%</p>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9193 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALPHA-MANNOSIDASE II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	1014	8181	5202	1434	1506	13	26	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	MSE	MET	modified residue	UNP Q24451
A	52	MSE	MET	modified residue	UNP Q24451
A	124	MSE	MET	modified residue	UNP Q24451
A	149	MSE	MET	modified residue	UNP Q24451
A	167	MSE	MET	modified residue	UNP Q24451
A	193	MSE	MET	modified residue	UNP Q24451
A	212	MSE	MET	modified residue	UNP Q24451
A	263	MSE	MET	modified residue	UNP Q24451
A	264	MSE	MET	modified residue	UNP Q24451
A	290	MSE	MET	modified residue	UNP Q24451
A	428	MSE	MET	modified residue	UNP Q24451
A	433	MSE	MET	modified residue	UNP Q24451
A	441	MSE	MET	modified residue	UNP Q24451
A	490	MSE	MET	modified residue	UNP Q24451
A	499	MSE	MET	modified residue	UNP Q24451
A	501	MSE	MET	modified residue	UNP Q24451
A	557	MSE	MET	modified residue	UNP Q24451
A	627	MSE	MET	modified residue	UNP Q24451
A	769	MSE	MET	modified residue	UNP Q24451
A	792	MSE	MET	modified residue	UNP Q24451
A	835	MSE	MET	modified residue	UNP Q24451
A	865	MSE	MET	modified residue	UNP Q24451
A	962	MSE	MET	modified residue	UNP Q24451
A	985	MSE	MET	modified residue	UNP Q24451
A	1026	MSE	MET	modified residue	UNP Q24451
A	1034	MSE	MET	modified residue	UNP Q24451

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

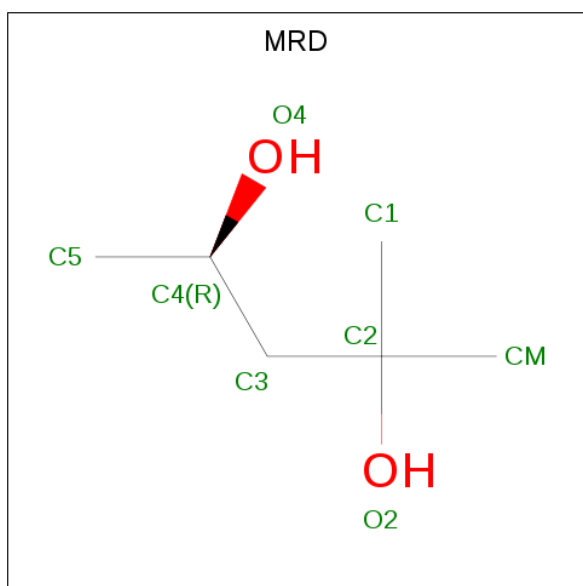
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	8	4	1	3	0	0

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	981	Total 981	O 981	0	0

### 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-MANNOSEDASE II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.86Å 109.72Å 138.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.30 – 1.40 69.30 – 1.40	Depositor EDS
% Data completeness (in resolution range)	71.0 (69.30-1.40) 70.9 (69.30-1.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 1.40Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.193 , 0.210 0.189 , 0.207	Depositor DCC
$R_{free}$ test set	7379 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtrriage
Anisotropy	0.069	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.30	1/8380 (0.0%)	0.61	2/11338 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	CYS	CB-SG	-6.29	1.71	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	MSE	N-CA-C	-5.43	96.33	111.00
1	A	518	ASP	N-CA-C	-5.19	96.98	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	8181	0	7971	152	0
2	A	14	0	13	0	0
3	A	1	0	0	0	0
4	A	8	0	10	0	0
5	A	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	981	0	0	51	0
All	All	9193	0	8008	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:290:MSE:HG2	1:A:303:PRO:HG2	1.45	0.97
1:A:297:CYS:HB3	6:A:1771:HOH:O	1.68	0.91
1:A:441:MSE:HB3	6:A:1762:HOH:O	1.72	0.87
1:A:904:ARG:HG2	1:A:985:MSE:SE	2.28	0.82
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.63	0.81
1:A:979:LEU:HD21	1:A:999:VAL:HG11	1.62	0.80
1:A:883:LEU:HD23	6:A:1616:HOH:O	1.86	0.75
1:A:641:PRO:HG2	1:A:644:THR:HB	1.67	0.74
1:A:824:LEU:HB2	6:A:2084:HOH:O	1.85	0.74
1:A:185:GLY:HA2	6:A:1632:HOH:O	1.86	0.73
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.33	0.73
1:A:155:ASN:HD21	1:A:157:GLN:HE21	1.37	0.72
1:A:439:ALA:HB2	1:A:497:CYS:SG	2.30	0.71
1:A:435:TYR:O	1:A:497:CYS:SG	2.49	0.71
1:A:630:ALA:HB3	6:A:1584:HOH:O	1.90	0.70
1:A:153:VAL:HG22	1:A:158:LEU:HD12	1.75	0.67
1:A:954:ARG:HH12	1:A:981:ARG:HH21	1.42	0.65
1:A:947:GLY:HA3	6:A:1730:HOH:O	1.96	0.65
1:A:954:ARG:HH12	1:A:981:ARG:NH2	1.94	0.65
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.45	0.65
1:A:498:GLN:HE21	1:A:526:LEU:H	1.44	0.64
1:A:284:GLN:HA	6:A:1689:HOH:O	1.96	0.64
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.80	0.64
1:A:435:TYR:HB3	1:A:497:CYS:SG	2.38	0.63
1:A:203:ILE:HG12	6:A:1714:HOH:O	1.99	0.62
1:A:870:LEU:N	6:A:1616:HOH:O	2.33	0.62
1:A:986:GLN:HG2	6:A:1267:HOH:O	2.00	0.62
1:A:695:LYS:HG3	1:A:709:HIS:CE1	2.35	0.62
1:A:1009:CYS:SG	1:A:1023:LEU:HD12	2.40	0.61
1:A:565:ARG:HG2	6:A:1543:HOH:O	2.00	0.60
1:A:235:LYS:O	1:A:239:GLN:HG3	2.01	0.60
1:A:441:MSE:HE2	1:A:627:MSE:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.84	0.59
1:A:470:HIS:CE1	1:A:472:ASP:HB2	2.37	0.59
1:A:765:HIS:HE1	6:A:1784:HOH:O	1.85	0.59
1:A:678:LEU:HD12	1:A:769:MSE:HE1	1.84	0.58
1:A:299:TRP:HE3	6:A:1771:HOH:O	1.86	0.58
1:A:1008:ARG:HG2	1:A:1042:SER:HB2	1.85	0.58
1:A:628:GLY:HA2	6:A:1730:HOH:O	2.04	0.57
1:A:480:THR:H	1:A:880:GLN:HE22	1.52	0.57
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.86	0.56
1:A:96:ILE:HA	1:A:479:LYS:HG3	1.87	0.56
1:A:438:ALA:HA	6:A:1762:HOH:O	2.04	0.56
1:A:950:HIS:HE1	6:A:1789:HOH:O	1.89	0.56
1:A:222:LYS:HD2	6:A:2068:HOH:O	2.06	0.55
1:A:69:LYS:HE2	6:A:1590:HOH:O	2.05	0.55
1:A:254:LYS:HD3	1:A:256:ASP:OD2	2.06	0.55
1:A:287:PHE:HB3	1:A:352:VAL:HG22	1.87	0.55
1:A:699:LEU:HG	6:A:1647:HOH:O	2.05	0.55
1:A:299:TRP:HB2	6:A:1771:HOH:O	2.05	0.55
1:A:116:ARG:HG3	6:A:1326:HOH:O	2.07	0.55
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.37	0.55
1:A:488:GLN:O	1:A:492:GLU:HG3	2.07	0.54
1:A:740:LEU:HD22	1:A:760:LEU:HD22	1.89	0.54
1:A:154:LYS:NZ	1:A:154:LYS:HB3	2.23	0.54
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.89	0.54
1:A:572:TYR:CD2	1:A:615:LYS:HD3	2.44	0.53
1:A:653:ARG:HD3	1:A:744:VAL:HG22	1.89	0.53
1:A:425:HIS:HE1	1:A:487:GLU:OE1	1.92	0.53
1:A:835:MSE:HE2	1:A:862:LEU:HD22	1.91	0.52
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.44	0.52
1:A:301:VAL:O	1:A:301:VAL:HG23	2.10	0.52
1:A:595:VAL:HG21	1:A:615:LYS:HG2	1.92	0.52
1:A:250:ILE:HD11	6:A:1708:HOH:O	2.09	0.52
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.40	0.52
1:A:992:GLU:O	1:A:994:THR:HG23	2.09	0.52
1:A:203:ILE:N	6:A:1714:HOH:O	2.27	0.51
1:A:980:HIS:HE1	6:A:1184:HOH:O	1.92	0.51
1:A:138:TYR:CE1	1:A:193:MSE:HE1	2.45	0.51
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.93	0.51
1:A:96:ILE:HG12	1:A:102:TYR:OH	2.10	0.51
1:A:264:MSE:HE3	6:A:1533:HOH:O	2.11	0.51
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HE2	6:A:2003:HOH:O	2.12	0.50
1:A:48:LEU:HG	1:A:52:MSE:SE	2.62	0.50
1:A:995:GLN:HG3	6:A:1727:HOH:O	2.11	0.50
1:A:934:PHE:CE2	1:A:936:GLU:HB2	2.46	0.50
1:A:551:PRO:HG2	6:A:1375:HOH:O	2.12	0.50
1:A:419:TYR:CE2	1:A:830:PRO:HG3	2.47	0.50
5:A:1104:MRD:H1C3	6:A:1873:HOH:O	2.12	0.49
1:A:154:LYS:HB3	1:A:154:LYS:HZ3	1.77	0.49
1:A:624:VAL:HG22	6:A:1584:HOH:O	2.11	0.49
1:A:883:LEU:CD2	6:A:1616:HOH:O	2.54	0.49
1:A:158:LEU:HD13	1:A:158:LEU:C	2.32	0.49
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.47	0.49
1:A:954:ARG:NH1	1:A:981:ARG:NH2	2.59	0.49
1:A:57:ILE:HD11	6:A:1587:HOH:O	2.13	0.49
1:A:654:LYS:HE3	1:A:672:ASP:OD1	2.13	0.49
1:A:583:LEU:HD22	1:A:944:GLY:N	2.28	0.48
1:A:290:MSE:CG	1:A:303:PRO:HG2	2.31	0.48
1:A:480:THR:HG23	6:A:1739:HOH:O	2.13	0.48
1:A:869:ARG:HG2	6:A:1616:HOH:O	2.14	0.48
1:A:434:HIS:CE1	1:A:930:ASP:OD1	2.55	0.48
1:A:626:PRO:O	1:A:950:HIS:HD2	1.97	0.48
1:A:441:MSE:HE3	6:A:1716:HOH:O	2.13	0.48
1:A:499:MSE:HG3	6:A:2025:HOH:O	2.12	0.48
1:A:929:LEU:HD11	6:A:1543:HOH:O	2.14	0.48
1:A:37:ASP:HB3	1:A:253:ASN:ND2	2.29	0.47
1:A:229:THR:HG21	1:A:263:MSE:HE2	1.97	0.47
1:A:378:THR:OG1	1:A:381:GLU:HG3	2.15	0.47
1:A:568:LEU:HD12	1:A:770:ARG:HD3	1.97	0.47
1:A:396:GLU:N	1:A:396:GLU:OE1	2.47	0.46
1:A:160:PHE:CE1	1:A:193:MSE:HG3	2.51	0.46
1:A:177:ASN:HD21	1:A:433:MSE:HB2	1.81	0.46
1:A:778:ASN:HD21	1:A:792:MSE:SE	2.49	0.46
1:A:389:ALA:O	1:A:394:GLN:HG2	2.17	0.45
1:A:761:PRO:O	1:A:762:SER:HB2	2.16	0.45
1:A:837:ILE:HG23	1:A:862:LEU:HD21	1.99	0.45
1:A:265:PRO:HD3	1:A:329:TYR:OH	2.16	0.45
1:A:678:LEU:CD1	1:A:769:MSE:HE1	2.47	0.45
1:A:144:ASN:HB3	6:A:1687:HOH:O	2.17	0.44
1:A:325:LYS:HE2	6:A:1334:HOH:O	2.17	0.44
1:A:434:HIS:CD2	1:A:927:ASP:HA	2.52	0.44
1:A:549:ILE:HG23	1:A:550:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ASP:HB2	1:A:608:HIS:HE1	1.82	0.44
1:A:1008:ARG:CG	1:A:1042:SER:HB2	2.47	0.44
1:A:580:VAL:HG22	1:A:634:LEU:CD2	2.47	0.44
1:A:1039:TYR:HE2	6:A:1745:HOH:O	2.00	0.44
1:A:782:ILE:O	1:A:785:LEU:HD13	2.17	0.44
1:A:807:ASP:OD1	1:A:832:PRO:HG2	2.18	0.43
1:A:603:LEU:N	1:A:603:LEU:HD22	2.34	0.43
1:A:1029:PRO:HD2	6:A:1745:HOH:O	2.18	0.43
1:A:975:VAL:HG21	1:A:1003:LEU:HD12	2.00	0.43
1:A:807:ASP:CG	1:A:832:PRO:HG2	2.39	0.43
1:A:954:ARG:HG2	1:A:956:ASP:OD1	2.19	0.43
1:A:558:HIS:CE1	6:A:1762:HOH:O	2.72	0.42
1:A:610:GLN:HG2	6:A:1638:HOH:O	2.19	0.42
1:A:909:HIS:HA	1:A:910:PRO:HD3	1.91	0.42
1:A:497:CYS:SG	1:A:501:MSE:SE	3.28	0.42
1:A:583:LEU:HD22	1:A:944:GLY:CA	2.49	0.42
1:A:601:ASP:HB2	1:A:608:HIS:CE1	2.55	0.42
1:A:812:GLN:HB2	6:A:1708:HOH:O	2.18	0.42
1:A:498:GLN:NE2	1:A:526:LEU:H	2.14	0.41
1:A:155:ASN:HB3	6:A:1465:HOH:O	2.19	0.41
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.85	0.41
1:A:679:ARG:HH12	1:A:701:GLN:CD	2.23	0.41
1:A:721:GLY:O	1:A:723:ARG:HD2	2.19	0.41
1:A:1011:ARG:NH2	6:A:1745:HOH:O	2.54	0.41
1:A:446:HIS:HE1	1:A:508:LEU:HD23	1.85	0.41
1:A:344:PHE:HB3	1:A:350:TRP:CE2	2.54	0.41
1:A:188:TRP:CB	6:A:1632:HOH:O	2.69	0.41
1:A:206:PHE:CD1	1:A:206:PHE:N	2.86	0.41
1:A:554:HIS:HE1	6:A:2006:HOH:O	2.04	0.41
1:A:435:TYR:C	1:A:497:CYS:SG	2.98	0.41
1:A:785:LEU:N	1:A:785:LEU:HD12	2.36	0.41
1:A:624:VAL:HA	1:A:625:PRO:HD3	1.94	0.41
1:A:869:ARG:NH1	1:A:885:ASN:HD22	2.16	0.41
1:A:188:TRP:HB3	6:A:1632:HOH:O	2.21	0.41
1:A:566:GLU:HA	1:A:622:ALA:O	2.20	0.41
1:A:301:VAL:CG2	6:A:1220:HOH:O	2.69	0.40
1:A:558:HIS:HA	1:A:629:LEU:HD23	2.02	0.40
1:A:652:LEU:O	1:A:653:ARG:HB3	2.22	0.40
1:A:557:MSE:HA	1:A:930:ASP:O	2.20	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	1012/1015 (100%)	975 (96%)	33 (3%)	4 (0%)	34 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	993	HIS
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	901/876 (103%)	894 (99%)	7 (1%)	81 62

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	PHE
1	A	275	CYS
1	A	396	GLU
1	A	585	ASN
1	A	710	PHE
1	A	828	TYR
1	A	993	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
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	309	GLN
1	A	347	ASN
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	608	HIS
1	A	682	ASN
1	A	698	GLN
1	A	709	HIS
1	A	765	HIS
1	A	778	ASN
1	A	809	ASN
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	986	GLN
1	A	993	HIS
1	A	995	GLN
1	A	1018	GLN
1	A	1022	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	MRD	A	1104	-	7,7,7	0.50	0	9,10,10	0.32	0
4	TRS	A	1103	3	7,7,7	1.71	2 (28%)	9,9,9	1.41	2 (22%)
2	NAG	A	1101	1	14,14,15	0.49	0	17,19,21	0.64	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	1104	-	-	2/5/5/5	-
4	TRS	A	1103	3	-	0/9/9/9	-
2	NAG	A	1101	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	TRS	C2-C	-3.72	1.41	1.53
4	A	1103	TRS	O1-C1	-2.12	1.35	1.42

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	1103	TRS	O2-C2-C	2.55	119.08	111.00
4	A	1103	TRS	C3-C-C1	-2.01	104.58	110.81

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1104	MRD	C2-C3-C4-O4
2	A	1101	NAG	C8-C7-N2-C2
2	A	1101	NAG	O7-C7-N2-C2
2	A	1101	NAG	O5-C5-C6-O6
2	A	1101	NAG	C4-C5-C6-O6
5	A	1104	MRD	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1104	MRD	1	0

## 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

### 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	988/1015 (97%)	0.11	37 (3%) 41 41	6, 13, 27, 47	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	991	GLU	7.2
1	A	993	HIS	6.8
1	A	992	GLU	6.1
1	A	497	CYS	4.7
1	A	720	HIS	4.7
1	A	682	ASN	4.5
1	A	990	PRO	4.1
1	A	583	LEU	4.1
1	A	702	ASP	3.9
1	A	701	GLN	3.7
1	A	600	HIS	3.5
1	A	986	GLN	3.3
1	A	78	HIS	3.3
1	A	785	LEU	3.2
1	A	116	ARG	3.1
1	A	994	THR	3.1
1	A	638	ASP	3.1
1	A	1008	ARG	3.0
1	A	534	SER	3.0
1	A	1024	ASP	3.0
1	A	537	GLU	3.0
1	A	538	ASP	3.0
1	A	396	GLU	2.9
1	A	301	VAL	2.9
1	A	547	GLU	2.6
1	A	602	THR	2.5
1	A	676	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	655	ASN	2.4
1	A	666	GLU	2.4
1	A	75	TYR	2.3
1	A	599	HIS	2.3
1	A	665	PRO	2.2
1	A	988	GLY	2.1
1	A	603	LEU	2.1
1	A	667	ASP	2.1
1	A	723	ARG	2.1
1	A	784	SER	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(Å <sup>2</sup> )	Q<0.9
2	NAG	A	1101	14/15	0.66	0.23	47,52,56,57	0
5	MRD	A	1104	8/8	0.85	0.12	16,18,19,20	0
4	TRS	A	1103	8/8	0.89	0.13	13,15,16,17	0
3	ZN	A	1102	1/1	1.00	0.04	9,9,9,9	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.