



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:18 pm BST

PDB ID : 3DX2  
Title : Golgi mannosidase II complex with MANNOSTATIN B  
Authors : Kuntz, D.A.; Zhong, W.; Guo, J.; Rose, D.R.; Boons, G.-J.  
Deposited on : 2008-07-23  
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 : 2.11  
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) : 2.11

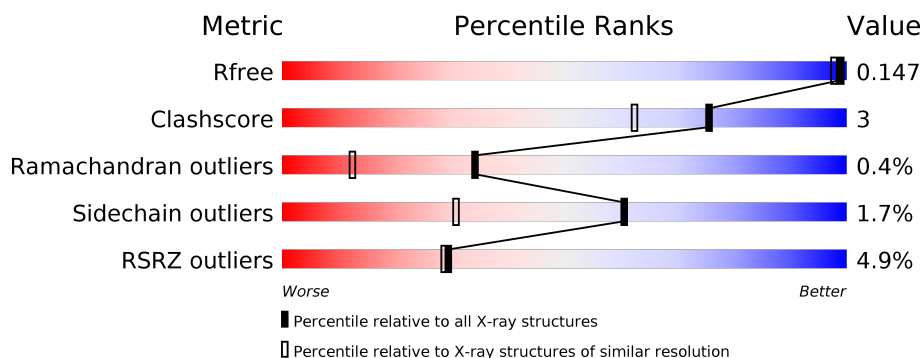
# 1 Overall quality at a glance

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	1045	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Alpha-mannosidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	0	22	0
			8348	5317	1460	1529	42			

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	SEE REMARK 999	UNP Q24451

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

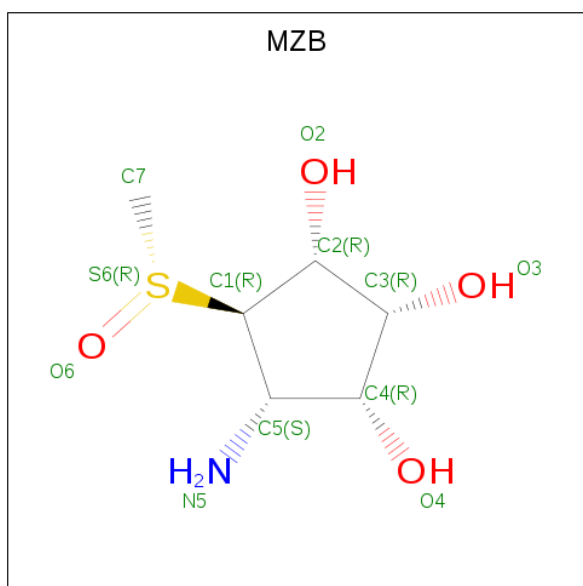
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is (1R,2R,3R,4S,5R)-4-amino-5-[(R)-methylsulfinyl]cyclopentane-1,2,3-triol (three-letter code: MZB) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



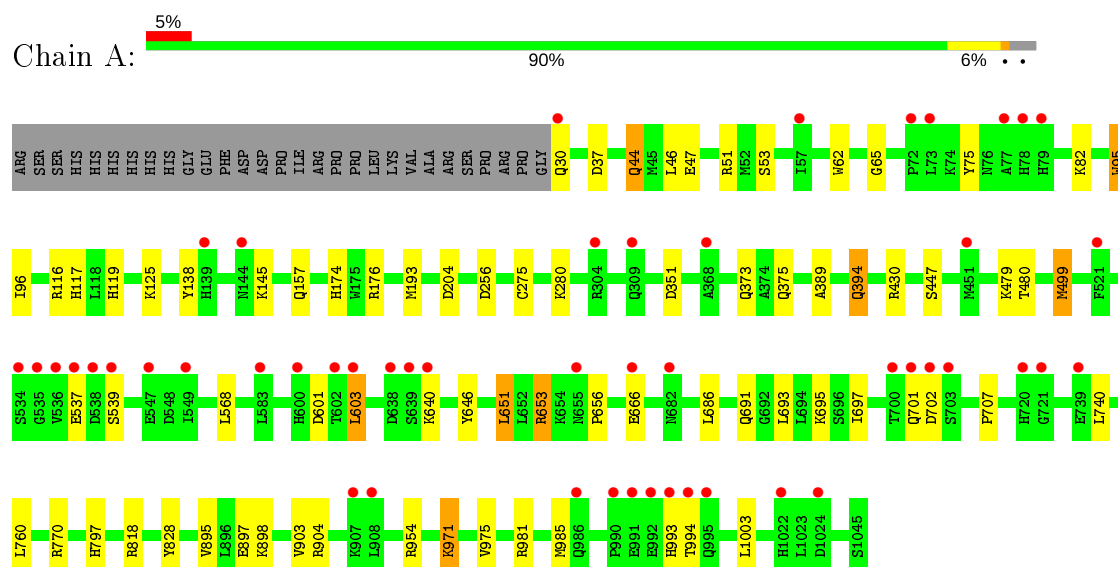
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1141	Total	O	0	21
			1162	1162		



- 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, $\alpha$ , $\beta$ , $\gamma$	68.63Å 109.28Å 137.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.90 – 1.40 24.90 – 1.40	Depositor EDS
% Data completeness (in resolution range)	95.0 (24.90-1.40) 95.1 (24.90-1.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 1.40Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, $R_{free}$	0.142 , 0.164 0.145 , 0.147	Depositor DCC
$R_{free}$ test set	2916 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 58.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, ZN, MPD, MZB

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	0.57	0/8624	0.72	4/11702 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	430	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	499	MET	CG-SD-CE	-5.37	91.62	100.20
1	A	53	SER	N-CA-C	5.18	124.98	111.00
1	A	818	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	8348	0	8169	51	0
2	A	1	0	0	0	0
3	A	8	0	14	0	0
4	A	12	0	11	2	0
5	A	16	0	28	1	0
6	A	1162	0	0	16	0
All	All	9547	0	8222	52	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 3.

All (52) 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:954:ARG:NH2	1:A:981[A]:ARG:HH21	1.36	1.22
1:A:954:ARG:NH2	1:A:981[A]:ARG:NH2	2.22	0.87
1:A:75[B]:TYR:HD2	6:A:1499:HOH:O	1.59	0.85
1:A:280:LYS:HE3	6:A:1565:HOH:O	1.80	0.81
1:A:82[A]:LYS:HD3	1:A:373:GLN:HB3	1.72	0.71
1:A:37:ASP:HB2	6:A:1739:HOH:O	1.94	0.67
1:A:82[B]:LYS:HD2	1:A:375:GLN:HE22	1.61	0.65
1:A:954:ARG:HH21	1:A:981[A]:ARG:HH21	1.41	0.64
1:A:47[B]:GLU:OE1	1:A:51:ARG:NH1	2.30	0.62
1:A:256:ASP:HB2	6:A:1406:HOH:O	2.01	0.60
1:A:116:ARG:HD2	6:A:2130:HOH:O	2.01	0.60
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.33	0.58
1:A:389:ALA:HB1	1:A:394:GLN:HG2	1.85	0.58
1:A:904:ARG:HG2	1:A:985[A]:MET:SD	2.47	0.55
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.36	0.54
1:A:971:LYS:NZ	1:A:971:LYS:HB2	2.23	0.54
1:A:666:GLU:CG	6:A:1777:HOH:O	2.58	0.52
1:A:537:GLU:HG2	1:A:539:SER:HB3	1.91	0.52
1:A:653:ARG:HD2	1:A:656:PRO:HA	1.91	0.51
1:A:75[B]:TYR:CD2	6:A:1499:HOH:O	2.46	0.51
1:A:651:LEU:HD13	1:A:653:ARG:HG2	1.93	0.50
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.47	0.49
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.47	0.49
1:A:693:LEU:HD13	6:A:1906:HOH:O	2.12	0.48
1:A:37:ASP:N	6:A:1739:HOH:O	2.29	0.47
1:A:119:HIS:HD2	6:A:2115:HOH:O	1.98	0.47
1:A:47[B]:GLU:OE2	1:A:51:ARG:HD3	2.16	0.46
1:A:51:ARG:HG3	6:A:1346:HOH:O	2.16	0.46
1:A:96:ILE:O	1:A:96:ILE:HG22	2.15	0.46
1:A:96:ILE:HD12	1:A:479:LYS:HE2	1.97	0.46
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.97	0.45
5:A:1049:MPD:O4	5:A:1049:MPD:H12	2.16	0.45
1:A:138:TYR:CE1	1:A:193[A]:MET:CE	3.00	0.45
1:A:125:LYS:HD3	1:A:157:GLN:HA	1.99	0.45
1:A:117[B]:HIS:HE1	1:A:351:ASP:OD1	2.00	0.45
1:A:44:GLN:HE22	1:A:46:LEU:H	1.65	0.44
1:A:707:PRO:HG2	1:A:797:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:HE3	6:A:2128:HOH:O	2.17	0.43
1:A:895:VAL:HG12	1:A:897:GLU:HG3	2.01	0.42
1:A:95:TRP:CZ2	4:A:1048:MZB:H2	2.56	0.41
1:A:37:ASP:CB	6:A:1739:HOH:O	2.58	0.41
1:A:96:ILE:O	1:A:96:ILE:CG2	2.68	0.41
1:A:740:LEU:HD22	1:A:760:LEU:HD22	2.03	0.41
1:A:480:THR:HG23	6:A:1221:HOH:O	2.20	0.41
1:A:640:LYS:HD2	1:A:646:TYR:CE2	2.56	0.41
1:A:537:GLU:HB2	6:A:1806:HOH:O	2.20	0.41
1:A:389:ALA:HB1	1:A:394:GLN:CG	2.50	0.40
1:A:601:ASP:OD1	1:A:603:LEU:HB2	2.21	0.40
1:A:499:MET:HE2	6:A:1262:HOH:O	2.21	0.40
1:A:568:LEU:HD12	1:A:770:ARG:HD3	2.03	0.40
1:A:95:TRP:CE2	4:A:1048:MZB:H2	2.57	0.40
1:A:903:VAL:O	1:A:985[B]:MET:HE1	2.21	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	1036/1045 (99%)	1010 (98%)	22 (2%)	4 (0%)	34 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	993	HIS
1	A	994	THR
1	A	95	TRP
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	925/929 (100%)	910 (98%)	15 (2%)	62 33

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	44	GLN
1	A	275	CYS
1	A	394	GLN
1	A	447	SER
1	A	603	LEU
1	A	651	LEU
1	A	653	ARG
1	A	691	GLN
1	A	695	LYS
1	A	701	GLN
1	A	702	ASP
1	A	828	TYR
1	A	898	LYS
1	A	971	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	44	GLN
1	A	119	HIS
1	A	144	ASN
1	A	186	GLN
1	A	488	GLN
1	A	742	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 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	$\# Z  > 2$
3	MRD	A	1047	-	7,7,7	0.48	0	9,10,10	0.77	0
5	MPD	A	1050	-	7,7,7	0.26	0	9,10,10	0.23	0
5	MPD	A	1049	-	7,7,7	0.28	0	9,10,10	0.74	0
4	MZB	A	1048	2	9,12,12	5.02	2 (22%)	10,18,18	1.80	2 (20%)

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
3	MRD	A	1047	-	-	1/5/5/5	-
5	MPD	A	1050	-	-	0/5/5/5	-
5	MPD	A	1049	-	-	3/5/5/5	-
4	MZB	A	1048	2	-	1/4/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1048	MZB	O6-S6	14.29	1.68	1.50
4	A	1048	MZB	C7-S6	-4.39	1.76	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1048	MZB	O6-S6-C7	-4.75	101.92	106.18
4	A	1048	MZB	C3-C4-C5	2.36	105.98	102.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1047	MRD	C2-C3-C4-O4
5	A	1049	MPD	C1-C2-C3-C4
5	A	1049	MPD	O2-C2-C3-C4
4	A	1048	MZB	C2-C1-S6-C7
5	A	1049	MPD	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1049	MPD	1	0
4	A	1048	MZB	2	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	1016/1045 (97%)	0.06	50 (4%)	29 29	8, 15, 28, 47	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	VAL	10.2
1	A	537	GLU	8.3
1	A	539	SER	7.4
1	A	702	ASP	6.6
1	A	534	SER	6.5
1	A	701	GLN	6.0
1	A	30	GLN	5.9
1	A	78	HIS	5.8
1	A	721	GLY	5.6
1	A	603	LEU	5.4
1	A	538	ASP	5.3
1	A	602	THR	5.1
1	A	535	GLY	4.7
1	A	638	ASP	4.7
1	A	720	HIS	4.7
1	A	700	THR	4.2
1	A	993	HIS	4.2
1	A	139	HIS	4.0
1	A	1024	ASP	3.9
1	A	600[A]	HIS	3.6
1	A	682	ASN	3.6
1	A	309	GLN	3.5
1	A	77	ALA	3.4
1	A	703	SER	3.3
1	A	994	THR	3.2
1	A	655	ASN	3.2
1	A	639	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	3.0
1	A	995[A]	GLN	3.0
1	A	992	GLU	2.9
1	A	640	LYS	2.9
1	A	547	GLU	2.9
1	A	144	ASN	2.8
1	A	990	PRO	2.7
1	A	908	LEU	2.7
1	A	521[A]	PHE	2.6
1	A	549	ILE	2.6
1	A	583	LEU	2.5
1	A	991	GLU	2.4
1	A	739	GLU	2.3
1	A	1022	HIS	2.3
1	A	907	LYS	2.3
1	A	451	MET	2.2
1	A	79	HIS	2.1
1	A	986	GLN	2.1
1	A	57	ILE	2.1
1	A	72	PRO	2.0
1	A	666	GLU	2.0
1	A	304	ARG	2.0
1	A	368	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MPD	A	1050	8/8	0.76	0.17	47,49,50,50	0
5	MPD	A	1049	8/8	0.78	0.25	24,30,33,34	0
3	MRD	A	1047	8/8	0.92	0.09	15,20,22,22	0
4	MZB	A	1048	12/12	0.99	0.06	9,10,13,14	0
2	ZN	A	1046	1/1	1.00	0.04	9,9,9,9	0

## 6.5 Other polymers

There are no such residues in this entry.