



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:41 pm GMT

PDB ID : 3BVX  
Title : GOLGI MANNOSIDASE II D204A catalytic nucleophile mutant complex with Methyl (2-deoxy-2-acetamido-beta-D-glucopyranosyl)-(1->2)-(alpha-D-mannopyranosyl)-(1->3)-[(alpha-D-mannopyranosyl)-(1->6)-(alpha-D-mannopyranosyl)-(1->6)]-beta-D-mannopyranoside  
Authors : Kuntz, D.A.; Rose, D.R.  
Deposited on : 2008-01-07  
Resolution : 1.10 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

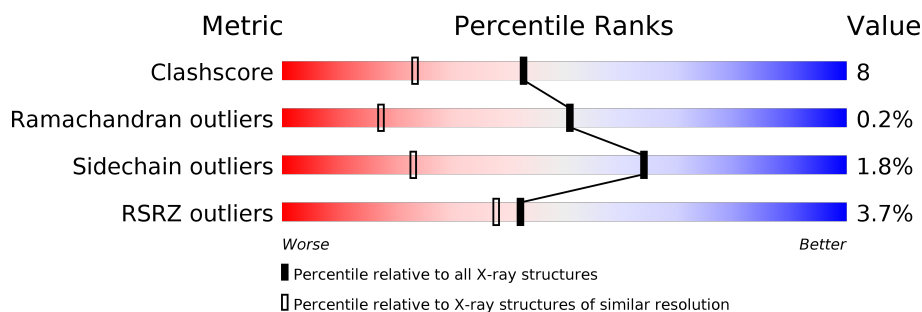
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1244 (1.14-1.06)
Ramachandran outliers	110173	1198 (1.14-1.06)
Sidechain outliers	110143	1196 (1.14-1.06)
RSRZ outliers	101464	1197 (1.14-1.06)

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. 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	

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
3	WZ5	A	1047	-	-	-	X
4	MPD	A	1048	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10180 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	45	0
			8585	5446	1518	1577	44			

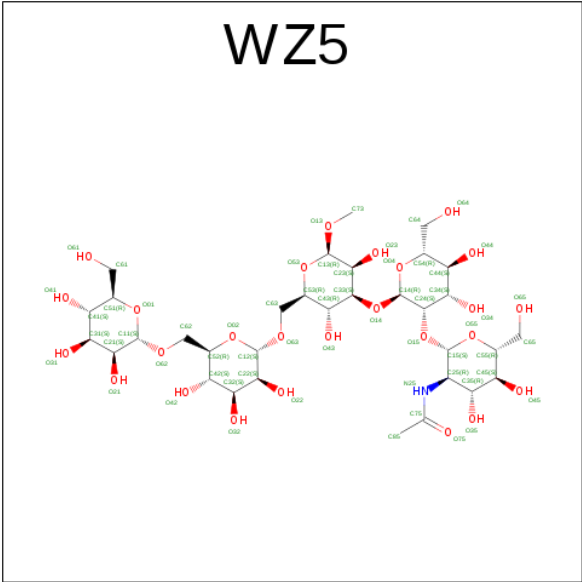
There are 14 discrepancies between the modelled and reference sequences:

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	204	ALA	ASP	ENGINEERED	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

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

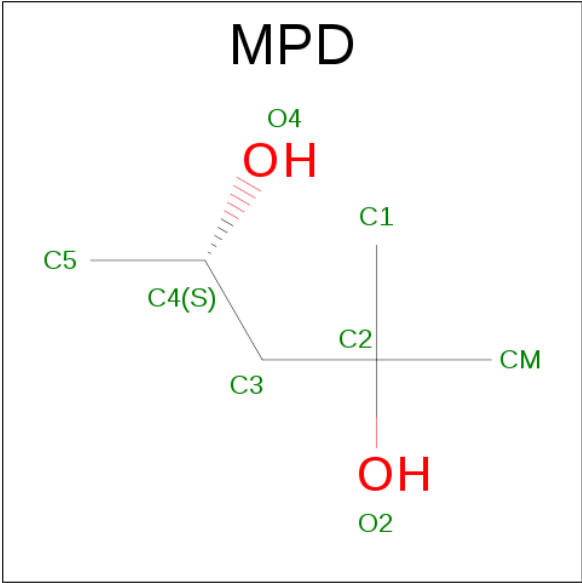
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is METHYL 2-(ACETYLAMINO)-2-DEOXY-BETA-D-GLUCOPYRANOSYL-(1->2)-ALPHA-D-MANNOPYRANOSYL-(1->3)-[ALPHA-D-MANNOPYRANOSYL-(1->6)-ALPHA-D-MANNOPYRANOSYL-(1->6)]-BETA-D-MANNOPYRANOSIDE (three-letter code: WZ5) (formula: C<sub>33</sub>H<sub>57</sub>NO<sub>26</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			60	33	1	26		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			8	6	2		

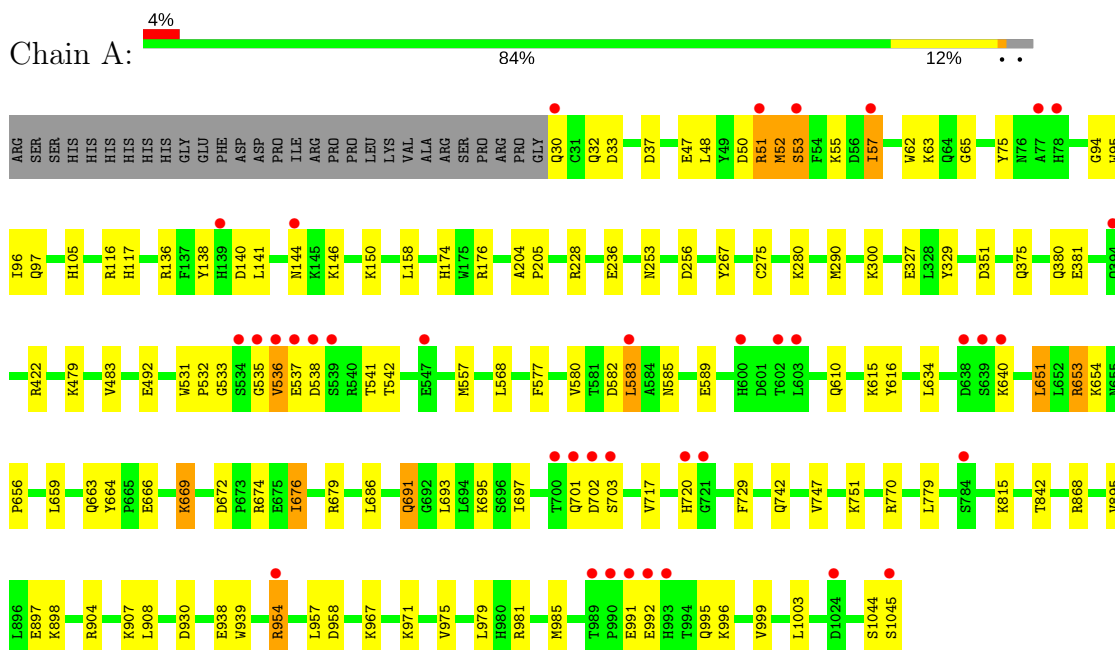
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1500	Total 1526	O 1526	0	26

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Alpha-mannosidase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.81Å 109.55Å 138.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.10 19.99 – 1.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-1.10) 73.9 (19.99-1.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 1.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.153 , 0.190 0.137 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	10.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: ZN, WZ5, MPD

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	0.73	1/8824 (0.0%)	1.13	21/11971 (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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	GLU	CD-OE2	-5.89	1.19	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	868	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	267	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	A	267	TYR	CB-CG-CD1	5.77	124.46	121.00
1	A	676	ILE	CA-CB-CG2	5.73	122.36	110.90
1	A	50	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	672	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	664	TYR	CG-CD1-CE1	-5.47	116.92	121.30
1	A	729	PHE	CB-CG-CD1	-5.45	116.98	120.80
1	A	958	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	531	TRP	NE1-CE2-CZ2	-5.41	124.45	130.40
1	A	381	GLU	OE1-CD-OE2	-5.39	116.84	123.30
1	A	140	ASP	CB-CG-OD2	-5.34	113.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	939	TRP	CB-CG-CD1	5.33	133.93	127.00
1	A	422	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	717	VAL	CA-CB-CG1	5.25	118.77	110.90
1	A	329	TYR	CG-CD1-CE1	-5.21	117.13	121.30
1	A	815	LYS	CD-CE-NZ	-5.18	99.78	111.70
1	A	616	TYR	CG-CD1-CE1	-5.14	117.19	121.30
1	A	674	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	674	ARG	CD-NE-CZ	5.09	130.72	123.60
1	A	577	PHE	CB-CG-CD1	-5.04	117.28	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	583	LEU	Peptide
1	A	992	GLU	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8585	0	8334	128	0
2	A	1	0	0	0	0
3	A	60	0	55	5	0
4	A	8	0	14	1	0
5	A	1526	0	0	62	0
All	All	10180	0	8403	134	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 8.

All (134) 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:532:PRO:HB2	1:A:536:VAL:CG1	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:PRO:C	1:A:536:VAL:HG11	1.65	1.15
3:A:1047:WZ5:H32	5:A:2544:HOH:O	1.50	1.08
1:A:136[B]:ARG:HD2	1:A:136[B]:ARG:O	1.55	1.07
1:A:532:PRO:HB2	1:A:536:VAL:HG13	1.40	1.01
1:A:96:ILE:HG22	5:A:2330:HOH:O	1.59	0.99
1:A:380:GLN:HG2	5:A:2186:HOH:O	1.63	0.96
1:A:532:PRO:CB	1:A:536:VAL:CG1	2.45	0.94
1:A:532:PRO:CB	1:A:536:VAL:HG11	1.98	0.94
1:A:532:PRO:O	1:A:536:VAL:HG11	1.71	0.91
1:A:57:ILE:HG12	5:A:2158:HOH:O	1.73	0.86
1:A:532:PRO:C	1:A:536:VAL:CG1	2.45	0.85
1:A:136[B]:ARG:HG2	1:A:136[B]:ARG:HH21	1.40	0.84
3:A:1047:WZ5:H62	5:A:2142[B]:HOH:O	1.79	0.81
1:A:654:LYS:HD2	1:A:742[A]:GLN:HE22	1.44	0.81
1:A:954:ARG:NH2	1:A:981[B]:ARG:HH21	1.79	0.81
1:A:136[B]:ARG:HD2	1:A:136[B]:ARG:C	2.01	0.80
1:A:954:ARG:NH2	1:A:981[B]:ARG:NH2	2.31	0.78
1:A:971[B]:LYS:HZ2	1:A:1045:SER:H	1.30	0.78
1:A:532:PRO:CA	1:A:536:VAL:HG11	2.15	0.77
1:A:742[A]:GLN:HG3	5:A:1786:HOH:O	1.85	0.76
1:A:96:ILE:CG2	5:A:2330:HOH:O	2.24	0.76
1:A:659:LEU:HB3	5:A:2047:HOH:O	1.85	0.76
1:A:136[A]:ARG:HD3	5:A:1065[A]:HOH:O	1.88	0.74
1:A:116:ARG:HD2	5:A:2420:HOH:O	1.87	0.73
1:A:693:LEU:HD13	5:A:1949:HOH:O	1.88	0.73
1:A:679:ARG:HH12	1:A:701:GLN:HG2	1.53	0.73
1:A:666:GLU:HB2	5:A:1837:HOH:O	1.88	0.71
1:A:47[B]:GLU:HG3	5:A:1169:HOH:O	1.91	0.70
1:A:770[B]:ARG:NE	5:A:1465:HOH:O	2.24	0.70
1:A:971[B]:LYS:HZ2	1:A:1045:SER:N	1.88	0.69
1:A:533:GLY:O	1:A:536:VAL:HG12	1.90	0.69
1:A:651:LEU:HD13	1:A:653:ARG:HG2	1.74	0.69
1:A:653:ARG:HD2	1:A:656:PRO:HA	1.76	0.68
1:A:300:LYS:NZ	5:A:2487:HOH:O	2.27	0.67
1:A:53:SER:OG	1:A:55:LYS:HG2	1.96	0.66
1:A:610:GLN:HB3	5:A:2241:HOH:O	1.94	0.66
1:A:136[B]:ARG:HH21	1:A:136[B]:ARG:CG	2.09	0.66
1:A:742[B]:GLN:HG3	5:A:2442:HOH:O	1.95	0.65
1:A:904:ARG:HG2	1:A:985[A]:MET:SD	2.38	0.64
4:A:1048:MPD:HM2	5:A:1365:HOH:O	1.96	0.64
1:A:583:LEU:HA	5:A:2059:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105[B]:HIS:ND1	5:A:1955:HOH:O	2.31	0.62
1:A:256:ASP:HB2	5:A:1961:HOH:O	1.99	0.61
1:A:720:HIS:CE1	5:A:2526:HOH:O	2.52	0.61
1:A:1044:SER:HB3	5:A:2490:HOH:O	2.01	0.61
3:A:1047:WZ5:H52	5:A:2544:HOH:O	2.01	0.60
1:A:532:PRO:CB	1:A:536:VAL:HG13	2.22	0.59
1:A:663:GLN:HG3	5:A:2043:HOH:O	2.02	0.58
1:A:380:GLN:CG	5:A:2186:HOH:O	2.36	0.58
1:A:654:LYS:HD2	1:A:742[A]:GLN:NE2	2.17	0.57
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.40	0.57
1:A:96:ILE:HG23	1:A:479:LYS:HE2	1.85	0.57
1:A:538:ASP:HA	5:A:2475:HOH:O	2.03	0.57
1:A:535:GLY:HA3	1:A:779:LEU:HD21	1.87	0.57
1:A:691:GLN:NE2	5:A:1117:HOH:O	2.29	0.57
1:A:75[A]:TYR:HD1	5:A:1266:HOH:O	1.87	0.56
1:A:770[B]:ARG:NH2	5:A:1465:HOH:O	2.38	0.56
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.34	0.56
1:A:30:GLN:N	5:A:2450:HOH:O	2.38	0.56
1:A:117[B]:HIS:HE1	1:A:351:ASP:OD1	1.88	0.56
1:A:720:HIS:HB3	5:A:2319:HOH:O	2.04	0.55
1:A:967:LYS:HE2	5:A:2507:HOH:O	2.04	0.55
1:A:116:ARG:CD	5:A:2420:HOH:O	2.48	0.55
1:A:536:VAL:CG1	1:A:537:GLU:N	2.69	0.55
1:A:938:GLU:HG3	5:A:2402:HOH:O	2.06	0.55
1:A:532:PRO:O	1:A:536:VAL:CG1	2.50	0.55
1:A:954:ARG:HH22	1:A:981[B]:ARG:NH2	2.02	0.55
1:A:280:LYS:HB2	1:A:280:LYS:NZ	2.22	0.55
1:A:589:GLU:OE2	1:A:751:LYS:HE3	2.07	0.55
1:A:483:VAL:HG11	5:A:2136:HOH:O	2.07	0.54
1:A:653:ARG:HD3	1:A:654:LYS:O	2.06	0.54
1:A:51[B]:ARG:NH2	5:A:1162:HOH:O	2.42	0.52
1:A:583:LEU:HG	5:A:1918:HOH:O	2.09	0.52
1:A:770[B]:ARG:CZ	5:A:1465:HOH:O	2.58	0.52
1:A:492:GLU:HG3	5:A:2263:HOH:O	2.08	0.51
1:A:37:ASP:HB2	5:A:2444:HOH:O	2.11	0.51
1:A:96:ILE:HG23	1:A:479:LYS:CE	2.40	0.50
1:A:535:GLY:N	5:A:2408:HOH:O	2.29	0.50
1:A:995:GLN:HG3	5:A:1502:HOH:O	2.10	0.50
1:A:48:LEU:HG	1:A:52[A]:MET:HE2	1.94	0.50
1:A:96:ILE:O	1:A:96:ILE:HG22	2.11	0.50
1:A:538:ASP:OD1	1:A:538:ASP:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136[B]:ARG:CG	1:A:136[B]:ARG:NH2	2.69	0.49
1:A:907:LYS:HD3	5:A:2454:HOH:O	2.12	0.49
1:A:954:ARG:CZ	1:A:981[B]:ARG:NH2	2.75	0.49
1:A:537:GLU:CD	5:A:2359:HOH:O	2.50	0.49
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.47	0.49
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.93	0.49
1:A:138[A]:TYR:OH	1:A:150:LYS:HE2	2.13	0.49
1:A:51[A]:ARG:NH2	5:A:1162:HOH:O	2.46	0.49
1:A:908:LEU:HG	5:A:2485:HOH:O	2.13	0.49
1:A:32:GLN:HG3	5:A:2203:HOH:O	2.13	0.49
1:A:679:ARG:NH1	1:A:701:GLN:HG2	2.24	0.49
1:A:536:VAL:HG12	1:A:537:GLU:N	2.28	0.48
1:A:37:ASP:HB2	1:A:253[B]:ASN:ND2	2.29	0.48
1:A:290:MET:HE1	5:A:1951[B]:HOH:O	2.13	0.48
1:A:47[A]:GLU:HG2	5:A:1067:HOH:O	2.14	0.48
1:A:533:GLY:O	1:A:536:VAL:CG1	2.61	0.47
1:A:954:ARG:HD2	1:A:991:GLU:OE2	2.15	0.47
1:A:640:LYS:HE3	5:A:2497:HOH:O	2.14	0.47
1:A:48:LEU:HD11	1:A:236:GLU:HG2	1.96	0.47
1:A:33:ASP:O	5:A:2444:HOH:O	2.21	0.46
1:A:542:THR:OG1	1:A:615:LYS:HE3	2.16	0.45
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.98	0.45
1:A:676:ILE:HD13	1:A:747:VAL:HG21	1.99	0.45
1:A:141:LEU:O	1:A:146:LYS:NZ	2.49	0.45
1:A:979[B]:LEU:HD21	1:A:999:VAL:HG11	1.98	0.45
1:A:615:LYS:HD2	5:A:1847:HOH:O	2.17	0.45
1:A:582:ASP:O	1:A:585:ASN:N	2.36	0.45
3:A:1047:WZ5:C32	5:A:2544:HOH:O	2.29	0.44
1:A:63:LYS:HE2	5:A:1947:HOH:O	2.17	0.44
1:A:702:ASP:OD2	1:A:703:SER:N	2.50	0.44
1:A:280:LYS:NZ	5:A:1681:HOH:O	2.50	0.44
1:A:996[B]:LYS:HA	1:A:996[B]:LYS:HE3	1.98	0.44
1:A:568:LEU:HD12	1:A:770[A]:ARG:HD3	2.00	0.44
1:A:907:LYS:NZ	5:A:2459:HOH:O	2.50	0.44
1:A:536:VAL:HG12	1:A:537:GLU:H	1.82	0.44
1:A:663:GLN:HG2	5:A:2422:HOH:O	2.17	0.44
1:A:57:ILE:H	1:A:57:ILE:HG12	1.69	0.43
1:A:656:PRO:HB3	5:A:1074:HOH:O	2.18	0.43
1:A:720:HIS:HB3	5:A:2271:HOH:O	2.18	0.43
1:A:535:GLY:HA3	1:A:779:LEU:CD2	2.49	0.43
1:A:48:LEU:O	1:A:52[A]:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ASP:C	1:A:582:ASP:OD2	2.58	0.42
1:A:957:LEU:HD11	1:A:979[A]:LEU:HG	2.02	0.42
1:A:94:GLY:HA2	1:A:97[B]:GLN:O	2.21	0.41
3:A:1047:WZ5:C42	5:A:2544:HOH:O	2.64	0.41
1:A:669:LYS:HG3	1:A:669:LYS:HZ3	1.53	0.41
1:A:205:PRO:O	1:A:228:ARG:HB2	2.21	0.40
1:A:615:LYS:HD2	5:A:1848:HOH:O	2.20	0.40
1:A:842:THR:OG1	1:A:898:LYS:NZ	2.54	0.40
1:A:557:MET:HA	1:A:930:ASP:O	2.21	0.40
1:A:580:VAL:HG22	1:A:634:LEU:HD22	2.03	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	1059/1045 (101%)	1030 (97%)	27 (2%)	2 (0%)	51 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	204	ALA

### 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	946/928 (102%)	926 (98%)	20 (2%)	59 17

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51[A]	ARG
1	A	51[B]	ARG
1	A	52[A]	MET
1	A	52[B]	MET
1	A	53	SER
1	A	57	ILE
1	A	144	ASN
1	A	158[A]	LEU
1	A	158[B]	LEU
1	A	275	CYS
1	A	375[A]	GLN
1	A	375[B]	GLN
1	A	536	VAL
1	A	541	THR
1	A	651	LEU
1	A	653	ARG
1	A	669	LYS
1	A	691	GLN
1	A	695	LYS
1	A	954	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	WZ5	A	1047	2	64,64,64	0.58	1 (1%)	93,94,94	1.50	16 (17%)
4	MPD	A	1048	-	7,7,7	0.64	0	9,10,10	0.58	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
3	WZ5	A	1047	2	-	0/30/130/130	0/5/5/5
4	MPD	A	1048	-	-	0/5/5/5	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1047	WZ5	O13-C13	2.93	1.45	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1047	WZ5	O02-C52-C62	-3.91	98.82	106.64
3	A	1047	WZ5	C64-C54-C44	-3.16	105.61	113.00
3	A	1047	WZ5	C14-O14-C33	-3.10	110.44	118.00
3	A	1047	WZ5	O53-C13-O13	-2.86	104.22	110.92
3	A	1047	WZ5	O53-C13-C23	-2.46	105.55	110.30
3	A	1047	WZ5	C23-C33-C43	-2.44	107.32	110.83
3	A	1047	WZ5	C63-O63-C12	-2.40	108.83	113.76
3	A	1047	WZ5	C15-O15-C24	-2.24	112.53	118.00
3	A	1047	WZ5	C65-C55-C45	-2.17	107.92	113.00
3	A	1047	WZ5	O02-C52-C42	-2.00	105.97	109.66
3	A	1047	WZ5	C11-C21-C31	2.01	113.71	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1047	WZ5	C62-C52-C42	2.03	116.33	112.00
3	A	1047	WZ5	O13-C13-C23	2.37	110.96	108.14
3	A	1047	WZ5	O35-C35-C25	2.46	114.61	109.61
3	A	1047	WZ5	O62-C62-C52	3.12	114.17	108.94
3	A	1047	WZ5	O63-C12-C22	5.25	116.81	108.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1047	WZ5	5	0
4	A	1048	MPD	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	1016/1045 (97%)	-0.01	38 (3%) 42 38	8, 14, 33, 97	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	VAL	19.1
1	A	538	ASP	12.0
1	A	537	GLU	11.2
1	A	535	GLY	10.3
1	A	539	SER	8.3
1	A	993	HIS	7.0
1	A	701	GLN	7.0
1	A	702	ASP	6.4
1	A	534	SER	5.6
1	A	990	PRO	5.3
1	A	602	THR	4.5
1	A	30	GLN	4.4
1	A	638	ASP	4.2
1	A	78	HIS	4.2
1	A	992	GLU	4.1
1	A	720	HIS	4.0
1	A	989	THR	3.4
1	A	1024	ASP	3.2
1	A	991	GLU	3.2
1	A	53	SER	3.2
1	A	144	ASN	2.9
1	A	954	ARG	2.9
1	A	721	GLY	2.9
1	A	784	SER	2.8
1	A	600	HIS	2.7
1	A	583	LEU	2.7
1	A	139[A]	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	57	ILE	2.5
1	A	51[A]	ARG	2.5
1	A	603	LEU	2.5
1	A	547	GLU	2.4
1	A	1045	SER	2.4
1	A	77	ALA	2.3
1	A	394	GLN	2.3
1	A	640	LYS	2.2
1	A	639	SER	2.2
1	A	700	THR	2.1
1	A	703	SER	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MPD	A	1048	8/8	0.78	0.16	8.84	23,33,40,40	0
3	WZ5	A	1047	60/60	0.94	0.13	4.95	10,27,59,81	0
2	ZN	A	1046	1/1	1.00	0.03	-2.74	9,9,9,9	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.