



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:02 AM GMT

PDB ID : 3NUK  
Title : THE CRYSTAL STRUCTURE OF THE W169Y mutant of ALPHA-GLUCOSIDASE (FAMILY 31) from RUMINOCOCCUS OBEUM ATCC 29174  
Authors : Tan, K.; Tesar, C.; Wilton, R.; Keigher, L.; Babnigg, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2010-07-07  
Resolution : 2.06 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

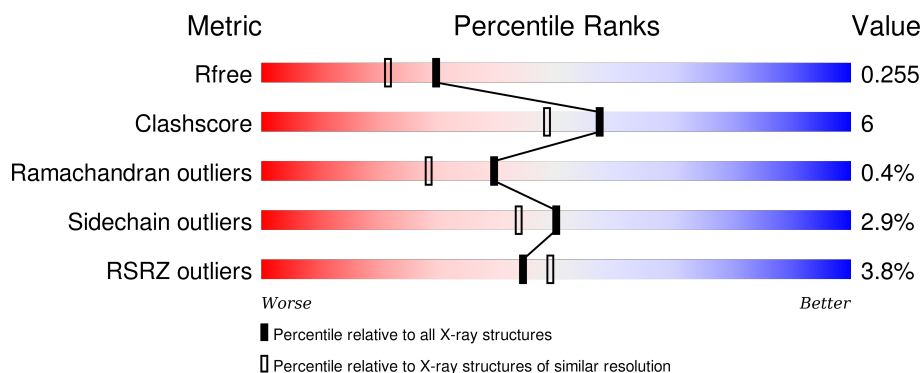
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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))
$R_{free}$	91344	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	666	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>•</div> </div>
1	B	666	<div> <div>4%</div> <div>81%</div> <div>15%</div> <div>••</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11119 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-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	1	0
			5444	3491	893	1025	35			
1	B	650	Total	C	N	O	S	0	2	0
			5343	3436	871	1001	35			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A5ZY13
A	-1	ASN	-	expression tag	UNP A5ZY13
A	0	ALA	-	expression tag	UNP A5ZY13
A	169	TYR	TRP	engineered	UNP A5ZY13
B	-2	SER	-	expression tag	UNP A5ZY13
B	-1	ASN	-	expression tag	UNP A5ZY13
B	0	ALA	-	expression tag	UNP A5ZY13
B	169	TYR	TRP	engineered	UNP A5ZY13

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

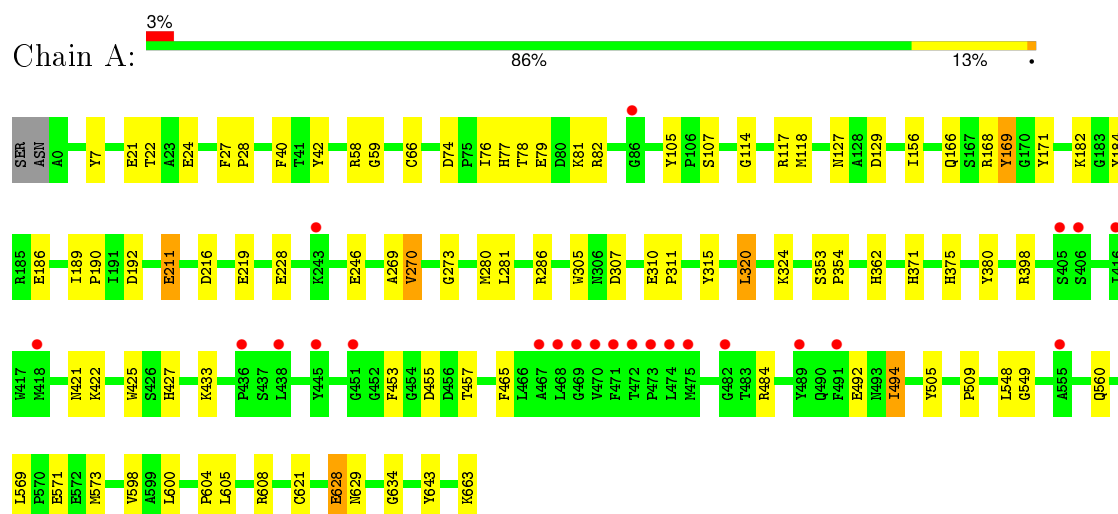
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total	O	0	0
			174	174		
3	B	152	Total	O	0	0
			152	152		

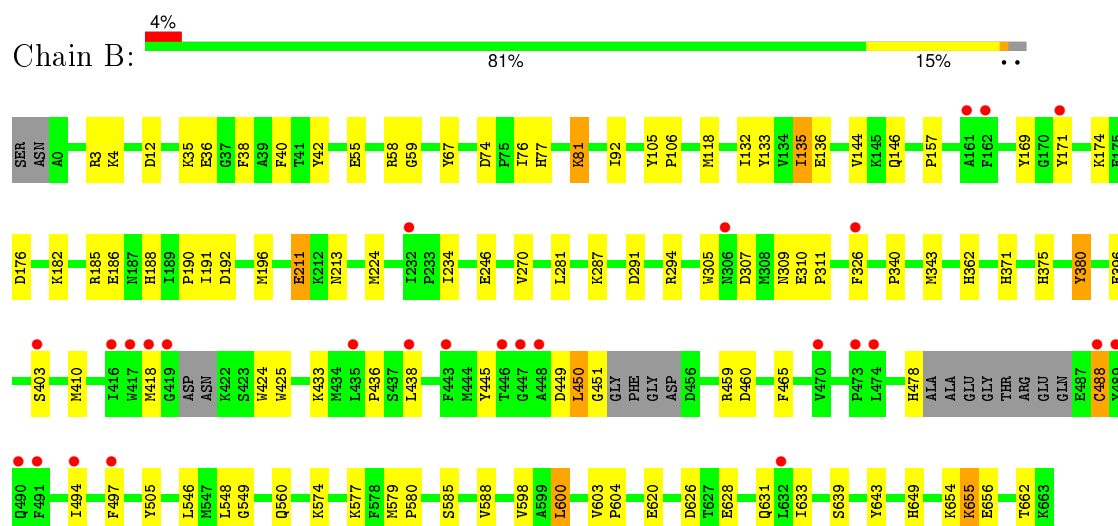
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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-GLUCOSIDASE



#### • Molecule 1: ALPHA-GLUCOSIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.80 Å 125.53 Å 88.30 Å 90.00° 107.82° 90.00°	Depositor
Resolution (Å)	34.70 – 2.06 34.70 – 2.05	Depositor EDS
% Data completeness (in resolution range)	86.4 (34.70-2.06) 97.4 (34.70-2.05)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.05 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.195 , 0.247 0.203 , 0.255	Depositor DCC
$R_{free}$ test set	4387 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 38.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 86453 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL

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	0.40	0/5589	0.53	0/7534
1	B	0.38	0/5487	0.52	0/7394
All	All	0.39	0/11076	0.53	0/14928

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	5444	0	5215	53	0
1	B	5343	0	5135	75	0
2	A	6	0	8	1	0
3	A	174	0	0	4	0
3	B	152	0	0	4	0
All	All	11119	0	10358	126	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 6.

All (126) 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:422:LYS:H	1:A:427:HIS:HD2	1.09	0.98
1:A:422:LYS:H	1:A:427:HIS:CD2	1.89	0.89
1:B:598:VAL:HG11	1:B:604:PRO:HG3	1.65	0.77
1:B:655:LYS:HE2	1:B:656:GLU:HG2	1.69	0.75
1:A:189:ILE:HD11	1:A:494:ILE:HD11	1.67	0.74
1:B:459:ARG:HG3	1:B:497:PHE:HZ	1.55	0.69
1:A:59:GLY:HA2	1:A:433:LYS:HD3	1.75	0.69
1:B:310:GLU:N	1:B:311:PRO:HA	2.07	0.69
1:B:362:HIS:NE2	1:B:371:HIS:HD2	1.90	0.69
1:B:655:LYS:HD3	1:B:656:GLU:N	2.08	0.68
1:A:66:CYS:SG	3:A:832:HOH:O	2.51	0.67
1:B:38:PHE:CZ	1:B:132:ILE:HD11	2.30	0.66
1:B:655:LYS:HD3	1:B:656:GLU:H	1.61	0.66
1:A:629:ASN:HB2	3:A:814:HOH:O	1.98	0.64
1:B:488:CYS:SG	1:B:497:PHE:HB3	2.38	0.63
1:B:654:LYS:HZ2	1:B:656:GLU:HB2	1.63	0.61
1:B:135[A]:ILE:HD11	1:B:146:GLN:HB2	1.82	0.61
1:B:36:GLU:HG2	1:B:36:GLU:O	2.01	0.61
1:B:135[A]:ILE:CD1	1:B:146:GLN:HB2	2.30	0.60
1:B:188:HIS:HA	1:B:620:GLU:OE1	2.03	0.59
1:A:571:GLU:OE2	1:A:608:ARG:HD2	2.03	0.59
1:A:605:LEU:C	1:A:605:LEU:HD12	2.23	0.59
1:A:310:GLU:N	1:A:311:PRO:HA	2.18	0.58
1:A:371:HIS:HE1	1:A:375:HIS:ND1	2.02	0.58
1:B:371:HIS:HE1	1:B:375:HIS:ND1	2.01	0.58
1:B:246:GLU:HG2	3:B:806:HOH:O	2.05	0.57
1:A:421:ASN:HB2	1:A:427:HIS:CD2	2.40	0.56
1:A:21:GLU:HG2	1:A:22:THR:N	2.20	0.56
1:A:598:VAL:HG11	1:A:604:PRO:HG3	1.85	0.56
1:A:371:HIS:CE1	1:A:375:HIS:ND1	2.73	0.56
1:A:494:ILE:HG22	3:A:756:HOH:O	2.05	0.56
1:B:577:LYS:HB2	1:B:585:SER:OG	2.06	0.56
1:A:634:GLY:O	1:A:663:LYS:HE2	2.07	0.55
1:A:114:GLY:HA2	1:A:117:ARG:O	2.07	0.55
1:B:548:LEU:HD23	1:B:549:GLY:N	2.22	0.55
1:A:74:ASP:OD1	1:A:81:LYS:HE3	2.07	0.55
1:B:291:ASP:O	1:B:294:ARG:HG3	2.07	0.54
1:A:425:TRP:CE2	1:A:560:GLN:HB2	2.44	0.53
1:B:185:ARG:NH1	1:B:191:ILE:HG22	2.24	0.53
1:B:309:ASN:ND2	1:B:403:SER:OG	2.37	0.52
1:B:626:ASP:OD1	1:B:628:GLU:HB2	2.09	0.52
1:A:281:LEU:HD12	1:A:362:HIS:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:SER:HB3	1:B:662:THR:HG22	1.92	0.51
1:B:436:PRO:HG3	1:B:546:LEU:HD22	1.92	0.51
1:A:280:MET:O	1:A:286:ARG:HD3	2.10	0.51
1:B:4:LYS:HB2	1:B:133:TYR:CE1	2.46	0.51
1:A:281:LEU:HD12	1:A:362:HIS:CG	2.48	0.49
1:B:654:LYS:NZ	1:B:654:LYS:HB3	2.27	0.49
1:B:460:ASP:HB3	1:B:600:LEU:HD11	1.94	0.49
1:B:654:LYS:NZ	1:B:656:GLU:HG3	2.28	0.49
1:A:166:GLN:NE2	1:A:184:TYR:OH	2.46	0.49
1:B:418:MET:HB3	3:B:760:HOH:O	2.12	0.49
1:B:157:PRO:HG3	1:B:445:TYR:CD1	2.48	0.49
1:B:450:LEU:HD12	1:B:465:PHE:CD1	2.48	0.48
1:B:310:GLU:N	1:B:311:PRO:CA	2.77	0.48
1:A:74:ASP:O	1:A:77:HIS:CE1	2.67	0.48
1:A:7:TYR:O	1:A:129:ASP:HA	2.14	0.48
1:A:269:ALA:HA	1:A:273:GLY:O	2.13	0.48
1:A:569:LEU:HD13	1:A:573:MET:HB2	1.96	0.48
1:B:436:PRO:HG3	1:B:546:LEU:CD2	2.43	0.48
1:A:76:ILE:O	1:A:81:LYS:HE2	2.15	0.47
1:A:320:LEU:HD13	1:A:324:LYS:HE3	1.96	0.47
1:A:307:ASP:OD2	2:A:664:GOL:H31	2.15	0.47
1:A:189:ILE:HD11	1:A:494:ILE:CD1	2.38	0.46
1:B:494:ILE:HG12	1:B:494:ILE:O	2.15	0.46
1:B:380:TYR:HA	1:B:410:MET:HG3	1.97	0.46
1:B:371:HIS:CE1	1:B:375:HIS:ND1	2.83	0.46
1:A:168:ARG:HB3	1:A:171:TYR:CZ	2.51	0.46
1:B:326:PHE:HE2	1:B:343:MET:HA	1.82	0.45
1:A:182:LYS:HD2	1:A:186:GLU:OE1	2.17	0.45
1:A:105:TYR:CZ	1:A:107:SER:HB3	2.51	0.45
1:A:422:LYS:HD3	1:A:455:ASP:OD2	2.17	0.45
1:A:548:LEU:HD23	1:A:549:GLY:N	2.31	0.45
1:B:450:LEU:O	1:B:451:GLY:C	2.55	0.45
1:B:55:GLU:HB2	1:B:438:LEU:HD21	1.97	0.45
1:B:631:GLN:NE2	1:B:633:ILE:HD11	2.31	0.45
1:B:92:ILE:HD11	1:B:144:VAL:HG22	1.99	0.45
1:A:79:GLU:OE2	1:B:424:TRP:HB3	2.17	0.45
1:B:425:TRP:CE2	1:B:560:GLN:HB2	2.52	0.45
1:B:81:LYS:HD2	1:B:81:LYS:HA	1.73	0.44
1:A:628:GLU:HA	1:A:628:GLU:OE2	2.16	0.44
1:B:309:ASN:HD21	1:B:403:SER:HG	1.58	0.44
1:B:603:VAL:HA	1:B:604:PRO:HD3	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:PRO:HD2	3:A:741:HOH:O	2.17	0.44
1:B:459:ARG:HG3	1:B:497:PHE:CZ	2.45	0.44
1:A:40:PHE:CZ	1:A:42:TYR:HB2	2.52	0.44
1:B:171:TYR:HD1	1:B:176:ASP:HB3	1.83	0.43
1:A:211:GLU:H	1:A:211:GLU:HG3	1.54	0.43
1:B:190:PRO:HB2	1:B:505:TYR:CE1	2.52	0.43
1:B:234:ILE:HD11	1:B:307:ASP:CB	2.48	0.43
1:B:38:PHE:HZ	1:B:132:ILE:HD11	1.82	0.43
1:B:396:GLU:O	1:B:649:HIS:HA	2.18	0.43
1:B:224:MET:HE2	1:B:224:MET:HA	1.99	0.43
1:B:459:ARG:CG	1:B:497:PHE:HZ	2.29	0.43
1:B:182:LYS:HE2	1:B:186:GLU:OE1	2.18	0.43
1:B:59:GLY:HA2	1:B:433:LYS:HD3	2.01	0.43
1:B:234:ILE:HD11	1:B:307:ASP:HB2	2.01	0.42
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.85	0.42
1:A:156:ILE:HG22	1:A:398:ARG:HD3	2.01	0.42
1:B:185:ARG:HH12	1:B:191:ILE:HG22	1.83	0.42
1:A:76:ILE:HG22	1:A:78:THR:HG23	2.01	0.42
1:A:228:GLU:HG3	1:A:621:CYS:SG	2.59	0.42
1:A:216:ASP:OD2	1:A:219:GLU:HB2	2.20	0.42
1:B:174:LYS:HD3	1:B:213:ASN:O	2.21	0.41
1:A:74:ASP:O	1:A:77:HIS:HE1	2.02	0.41
1:A:190:PRO:HB2	1:A:505:TYR:CE1	2.56	0.41
1:A:27:PHE:HA	1:A:28:PRO:HD3	1.61	0.41
1:B:655:LYS:HG3	3:B:814:HOH:O	2.20	0.41
1:B:654:LYS:HZ1	1:B:656:GLU:HG3	1.85	0.41
1:A:353:SER:HA	1:A:354:PRO:HD3	1.91	0.41
1:B:287:LYS:HA	3:B:807:HOH:O	2.20	0.41
1:B:3:ARG:NH2	1:B:136:GLU:OE2	2.53	0.41
1:B:211:GLU:HG3	1:B:211:GLU:H	1.55	0.41
1:B:643:TYR:CD2	1:B:643:TYR:C	2.94	0.41
1:A:643:TYR:CD2	1:A:643:TYR:C	2.93	0.40
1:B:38:PHE:C	1:B:38:PHE:CD2	2.95	0.40
1:A:315:TYR:CD2	1:B:340:PRO:HG2	2.56	0.40
1:B:67:TYR:N	1:B:67:TYR:CD2	2.89	0.40
1:A:421:ASN:O	1:A:453:PHE:HB3	2.22	0.40
1:B:579:MET:HA	1:B:580:PRO:HD3	1.90	0.40
1:B:105:TYR:HA	1:B:106:PRO:HD3	1.74	0.40
1:B:574:LYS:HG2	1:B:588:VAL:HG22	2.03	0.40
1:A:457:THR:O	1:A:484:ARG:HD3	2.21	0.40
1:B:74:ASP:O	1:B:77:HIS:NE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:PHE:CZ	1:B:42:TYR:HB2	2.57	0.40
1:B:449:ASP:HB3	1:B:478:HIS:HB3	2.04	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	663/666 (100%)	625 (94%)	35 (5%)	3 (0%)	34	22
1	B	644/666 (97%)	609 (95%)	33 (5%)	2 (0%)	46	36
All	All	1307/1332 (98%)	1234 (94%)	68 (5%)	5 (0%)	39	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	TYR
1	B	35	LYS
1	B	58	ARG
1	A	58	ARG
1	A	270	VAL

### 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	574/575 (100%)	557 (97%)	17 (3%)	48	42
1	B	566/575 (98%)	549 (97%)	17 (3%)	48	42
All	All	1140/1150 (99%)	1106 (97%)	34 (3%)	50	42

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	82	ARG
1	A	118	MET
1	A	127	ASN
1	A	169	TYR
1	A	192	ASP
1	A	211	GLU
1	A	246	GLU
1	A	270	VAL
1	A	305	TRP
1	A	320	LEU
1	A	380	TYR
1	A	465	PHE
1	A	492	GLU
1	A	494	ILE
1	A	600	LEU
1	A	628	GLU
1	B	12	ASP
1	B	76	ILE
1	B	81	LYS
1	B	118	MET
1	B	135[A]	ILE
1	B	135[B]	ILE
1	B	169	TYR
1	B	192	ASP
1	B	196	MET
1	B	211	GLU
1	B	270	VAL
1	B	305	TRP
1	B	380	TYR
1	B	450	LEU
1	B	488	CYS
1	B	600	LEU
1	B	655	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	127	ASN
1	A	166	GLN
1	A	306	ASN
1	A	371	HIS
1	A	427	HIS
1	A	431	ASN
1	A	631	GLN
1	B	89	ASN
1	B	371	HIS
1	B	490	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z  > 2$
2	GOL	A	664	-	5,5,5	0.25	0	5,5,5	0.53	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
2	GOL	A	664	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	664	GOL	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	664/666 (99%)	-0.07	23 (3%)	48 53	35, 50, 79, 122	2 (0%)
1	B	650/666 (97%)	-0.00	27 (4%)	40 44	38, 53, 92, 168	3 (0%)
All	All	1314/1332 (98%)	-0.03	50 (3%)	44 49	35, 52, 86, 168	5 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	PHE	5.1
1	B	490	GLN	4.8
1	B	419	GLY	4.8
1	B	418	MET	4.3
1	B	417	TRP	4.3
1	B	494	ILE	3.7
1	B	474	LEU	3.7
1	A	482	GLY	3.6
1	B	435	LEU	3.6
1	B	489	TYR	3.6
1	A	471	PHE	3.5
1	B	161	ALA	3.4
1	A	451	GLY	3.4
1	A	472	THR	3.3
1	B	488	CYS	3.2
1	A	468	LEU	3.2
1	B	443	PHE	3.2
1	A	406	SER	3.1
1	B	497	PHE	3.1
1	A	470	VAL	2.9
1	B	473	PRO	2.9
1	B	403	SER	2.8
1	A	474	LEU	2.7
1	B	470	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	446	THR	2.6
1	A	418	MET	2.6
1	B	438	LEU	2.6
1	A	473	PRO	2.6
1	A	491	PHE	2.5
1	A	469	GLY	2.5
1	B	448	ALA	2.5
1	B	162	PHE	2.5
1	A	438	LEU	2.5
1	A	436	PRO	2.5
1	A	467	ALA	2.4
1	B	416	ILE	2.4
1	A	475	MET	2.4
1	A	405	SER	2.4
1	A	445	TYR	2.3
1	B	447	GLY	2.3
1	A	243	LYS	2.2
1	B	326	PHE	2.2
1	A	416	ILE	2.2
1	A	489	TYR	2.2
1	B	632	LEU	2.1
1	A	86	GLY	2.1
1	B	232	ILE	2.1
1	A	555	ALA	2.1
1	B	306	ASN	2.1
1	B	171	TYR	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. 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( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	664	6/6	0.84	0.13	-0.12	48,61,64,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.