



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:54 AM GMT

PDB ID : 2OKX  
Title : Crystal structure of GH78 family rhamnosidase of Bacillus SP. GL1 AT 1.9 Å  
Authors : Cui, Z.; Mikami, B.; Hashimoto, W.; Murata, K.  
Deposited on : 2007-01-17  
Resolution : 1.90 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

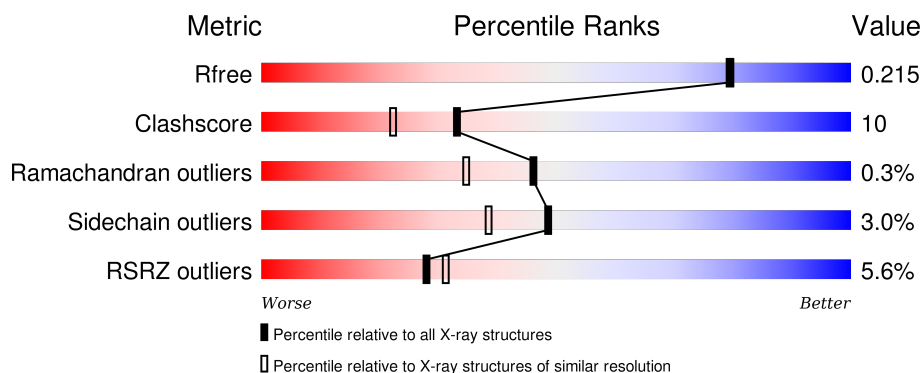
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	956	<div> <div>5%</div> <div>79%</div> <div>19%</div> </div>
1	B	956	<div> <div>6%</div> <div>81%</div> <div>18%</div> </div>

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	GOL	A	3003	-	-	-	X
3	GOL	A	3006	-	-	-	X
3	GOL	A	3007	-	-	-	X
3	GOL	A	3008	-	-	-	X
3	GOL	A	3017	-	-	-	X
3	GOL	A	3019	-	-	-	X
3	GOL	A	3022	-	-	-	X
3	GOL	A	3023	-	-	-	X
3	GOL	A	3026	-	-	-	X
3	GOL	A	3030	-	-	-	X
3	GOL	A	3033	-	-	-	X
3	GOL	A	3039	-	-	-	X
3	GOL	A	3043	-	-	-	X
3	GOL	B	3009	-	-	-	X
3	GOL	B	3010	-	-	-	X
3	GOL	B	3011	-	-	-	X
3	GOL	B	3012	-	-	-	X
3	GOL	B	3020	-	-	-	X
3	GOL	B	3021	-	-	-	X
3	GOL	B	3024	-	-	-	X
3	GOL	B	3025	-	-	-	X
3	GOL	B	3028	-	-	-	X
3	GOL	B	3029	-	-	-	X
3	GOL	B	3032	-	-	-	X
3	GOL	B	3034	-	-	-	X
3	GOL	B	3036	-	-	-	X
3	GOL	B	3037	-	-	X	X
3	GOL	B	3038	-	-	-	X
3	GOL	B	3041	-	-	-	X
3	GOL	B	3042	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17068 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 Rhamnosidase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	954	Total	C	N	O	S	0	11	0
			7531	4773	1309	1420	29			
1	B	954	Total	C	N	O	S	0	9	0
			7520	4767	1304	1420	29			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	880	Total 880	O 880	0	0
4	B	875	Total 875	O 875	0	0

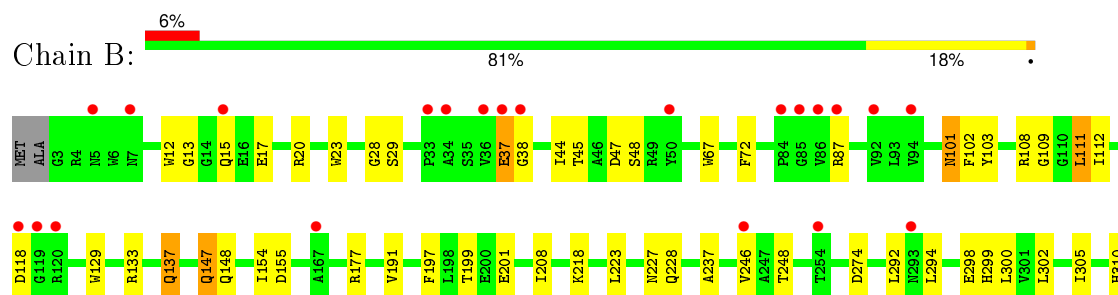
### 3 Residue-property plots

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.

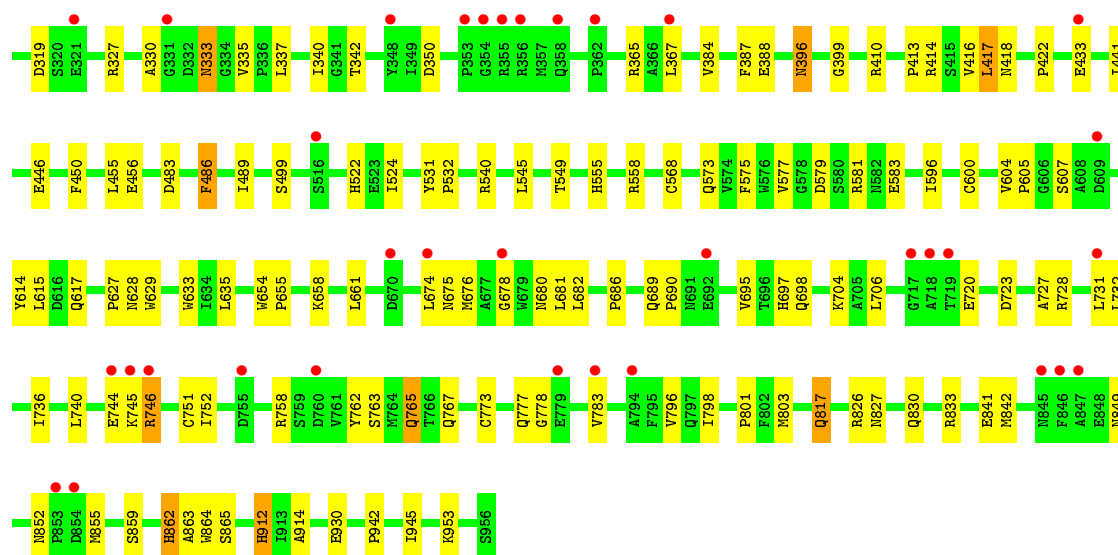
#### • Molecule 1: Rhamnosidase B



#### • Molecule 1: Rhamnosidase B







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.74Å 119.98Å 207.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 29.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-1.90) 98.7 (29.95-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.182 , 0.214 0.184 , 0.215	Depositor DCC
$R_{free}$ test set	18716 reflections (9.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.8	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 188847 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17068	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA

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	0.31	0/7782	0.61	1/10613 (0.0%)
1	B	0.31	0/7763	0.61	1/10588 (0.0%)
All	All	0.31	0/15545	0.61	2/21201 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	TRP	N-CA-C	-5.99	94.82	111.00
1	A	67	TRP	N-CA-C	-5.70	95.61	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	7531	0	7202	164	0
1	B	7520	0	7187	147	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	126	0	143	12	0
3	B	132	0	151	14	0
4	A	880	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	875	0	0	18	0
All	All	17068	0	14683	310	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 10.

All (310) 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:B:765:GLN:H	1:B:765:GLN:HE21	0.99	0.98
1:B:746:ARG:HH11	1:B:746:ARG:HB3	1.32	0.94
1:A:765:GLN:HE21	1:A:765:GLN:H	1.13	0.90
1:A:410:ARG:HH22	3:A:3033:GOL:H32	1.38	0.87
1:A:236:HIS:HD2	1:A:238:ASN:H	1.23	0.87
1:B:765:GLN:H	1:B:765:GLN:NE2	1.75	0.84
1:A:69:LYS:HG3	1:A:70:GLU:HG3	1.65	0.79
1:A:491:ARG:H	1:A:495:GLN:HE22	1.31	0.79
1:A:765:GLN:NE2	1:A:765:GLN:H	1.82	0.78
1:B:765:GLN:N	1:B:765:GLN:HE21	1.81	0.77
1:A:201:GLU:HB3	1:B:422:PRO:HG3	1.65	0.77
1:A:191:VAL:HG21	3:A:3027:GOL:H11	1.69	0.75
1:A:536:GLN:HE22	1:B:208:ILE:H	1.34	0.74
1:A:140:ASN:HD22	1:A:140:ASN:H	1.34	0.73
1:A:133[B]:ARG:HH21	1:A:137:GLN:NE2	1.87	0.73
1:B:101:ASN:HD22	1:B:103:TYR:H	1.36	0.72
1:B:413:PRO:HG2	1:B:416:VAL:HG23	1.71	0.71
1:B:689:GLN:HA	4:B:4677:HOH:O	1.89	0.70
1:A:20:ARG:HH12	1:A:227:ASN:HD22	1.40	0.70
1:B:635:LEU:HB2	3:B:3037:GOL:H31	1.74	0.70
1:A:883:ALA:CB	1:A:888[B]:THR:HG22	2.22	0.70
1:B:801:PRO:HB2	1:B:865:SER:HB3	1.74	0.69
1:A:264:THR:HG21	4:A:4303:HOH:O	1.93	0.69
1:B:101:ASN:ND2	1:B:103:TYR:H	1.91	0.68
1:B:218:LYS:HG2	1:B:319:ASP:OD1	1.93	0.68
1:B:746:ARG:HH11	1:B:746:ARG:CB	2.05	0.67
1:A:798:ILE:HG23	1:A:803:MET:HB3	1.75	0.67
1:B:801:PRO:HB2	1:B:865:SER:CB	2.26	0.66
1:A:628:ASN:HD21	1:A:698:GLN:HA	1.61	0.65
1:A:710:ARG:NH1	1:A:723:ASP:HA	2.10	0.65
1:B:555:HIS:HD2	1:B:558[B]:ARG:HH21	1.45	0.64
1:B:133:ARG:HH21	1:B:137:GLN:NE2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:LYS:HE3	4:B:4050:HOH:O	1.98	0.64
1:B:827:ASN:O	1:B:830:GLN:HG2	1.97	0.63
1:A:218:LYS:HG2	1:A:319:ASP:OD2	1.98	0.63
1:B:583:GLU:OE2	1:B:863:ALA:HB3	1.99	0.63
1:B:628:ASN:HD21	1:B:697:HIS:CD2	2.17	0.63
1:A:720:GLU:HA	1:A:723:ASP:OD1	1.98	0.62
1:A:340:ILE:HG21	1:A:367:LEU:HD21	1.81	0.62
1:A:82:LEU:HD23	1:A:83:ARG:N	2.14	0.62
1:B:342:THR:H	3:B:3038:GOL:H32	1.64	0.62
1:B:855:MET:HE2	4:B:4847:HOH:O	2.00	0.62
1:B:28:GLY:HA2	3:B:3029:GOL:H32	1.81	0.62
1:A:583:GLU:OE2	1:A:863:ALA:HB3	2.00	0.61
1:B:798:ILE:HG23	1:B:803:MET:HB3	1.82	0.61
1:A:827:ASN:O	1:A:830:GLN:HG2	2.02	0.60
1:A:414:ARG:HH22	1:A:418:ASN:ND2	2.00	0.60
1:B:841:GLU:HG2	1:B:842:MET:HG3	1.84	0.60
1:A:771:TYR:HB2	1:A:784:ILE:HG21	1.84	0.59
1:A:765:GLN:N	1:A:765:GLN:HE21	1.94	0.59
1:A:883:ALA:HB2	1:A:888[B]:THR:HG22	1.84	0.58
1:A:780:ARG:O	1:A:784:ILE:HG12	2.02	0.58
1:B:607:SER:HB2	1:B:615:LEU:HG	1.84	0.58
1:B:604:VAL:HB	1:B:605:PRO:HD3	1.85	0.58
1:A:236:HIS:CD2	1:A:238:ASN:H	2.14	0.58
1:B:689:GLN:HE21	1:B:697:HIS:HE1	1.51	0.58
1:A:533:VAL:HG12	1:A:593[A]:GLU:OE2	2.04	0.58
1:A:819:LEU:HB2	4:A:4647:HOH:O	2.04	0.57
1:B:20:ARG:HH22	1:B:227:ASN:HD22	1.51	0.57
1:A:274:ASP:OD2	1:A:299:HIS:HD2	1.87	0.57
1:B:690:PRO:HD2	4:B:4677:HOH:O	2.04	0.57
1:B:695:VAL:HG22	4:B:4677:HOH:O	2.05	0.57
1:B:555:HIS:CD2	1:B:558[B]:ARG:HH21	2.21	0.57
1:A:302:LEU:HD11	1:A:340:ILE:HD12	1.87	0.57
1:B:396:ASN:ND2	1:B:399:GLY:H	2.01	0.57
1:B:746:ARG:NH1	1:B:783:VAL:HG21	2.20	0.56
1:A:368:PRO:HB2	1:A:369:GLU:OE2	2.05	0.56
1:B:29:SER:H	3:B:3029:GOL:H12	1.69	0.56
1:B:654:TRP:HB3	1:B:655:PRO:HD3	1.86	0.56
1:B:274:ASP:OD2	1:B:299:HIS:HD2	1.88	0.56
1:A:720:GLU:CD	1:A:720:GLU:H	2.09	0.56
1:B:23:TRP:H	1:B:137:GLN:NE2	2.04	0.56
1:B:333:ASN:HD22	1:B:333:ASN:H	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ASP:O	1:B:678:GLY:HA2	2.06	0.55
1:B:177:ARG:HD2	4:B:4604:HOH:O	2.04	0.55
1:A:763:SER:HB2	1:A:765:GLN:NE2	2.22	0.55
1:A:746[B]:ARG:HH21	1:A:746[B]:ARG:HG2	1.70	0.55
1:B:727:ALA:O	1:B:731:LEU:HD23	2.07	0.55
1:A:248:THR:HB	1:A:337:LEU:HD23	1.89	0.55
1:A:848:GLU:HB2	4:A:4807:HOH:O	2.06	0.55
1:B:15:GLN:CD	1:B:15:GLN:N	2.61	0.54
1:A:252:LEU:HD23	1:A:324:PHE:HB3	1.88	0.54
1:A:819:LEU:HD22	4:A:4647:HOH:O	2.06	0.54
1:B:17:GLU:HG2	1:B:108:ARG:NH2	2.22	0.54
1:B:446:GLU:O	1:B:555:HIS:HE1	1.89	0.54
1:A:28:GLY:HA2	3:A:3030:GOL:H32	1.89	0.54
1:B:441:ILE:HD13	1:B:524:ILE:HG21	1.90	0.54
1:B:777[A]:GLN:HG3	1:B:778:GLY:N	2.23	0.54
1:A:690:PRO:C	1:A:692:GLU:H	2.11	0.53
1:A:352:ARG:NH2	1:A:610:GLU:O	2.41	0.53
1:A:140:ASN:HD22	1:A:140:ASN:N	2.04	0.53
1:A:859:SER:OG	1:A:862:HIS:HD2	1.91	0.53
1:A:159:LEU:HD12	1:A:491:ARG:HH22	1.73	0.53
1:B:728:ARG:NH2	4:B:4358:HOH:O	2.41	0.53
1:B:155:ASP:HA	1:B:489:ILE:HB	1.90	0.53
1:B:745:LYS:HG3	1:B:762:TYR:CE2	2.43	0.53
1:A:191:VAL:HG23	1:A:192:PRO:HD2	1.90	0.53
1:A:298:GLU:CD	1:A:327:ARG:HH22	2.11	0.53
1:A:267:ARG:NH2	4:A:4085:HOH:O	2.41	0.53
1:B:237:ALA:O	1:B:310:HIS:HE1	1.92	0.53
1:A:732:LEU:HD22	1:A:736:ILE:HD11	1.91	0.53
3:A:3006:GOL:H32	4:A:4111:HOH:O	2.08	0.52
1:A:779:GLU:O	1:A:783:VAL:HG23	2.09	0.52
1:A:576:TRP:CD2	3:A:3007:GOL:H32	2.44	0.52
1:A:316:PHE:HB2	3:A:3003:GOL:O1	2.09	0.52
1:B:635:LEU:HD22	3:B:3037:GOL:H11	1.91	0.52
1:B:704:LYS:HD2	1:B:773:CYS:HA	1.92	0.52
1:A:237:ALA:O	1:A:310:HIS:HE1	1.92	0.52
1:A:575:PHE:CZ	1:A:600:CYS:HB3	2.44	0.52
1:A:329:PRO:HD2	1:A:338:ALA:HB3	1.90	0.52
1:B:129:TRP:HA	3:B:3029:GOL:H31	1.92	0.52
1:A:414:ARG:HD3	4:B:4341:HOH:O	2.10	0.52
1:B:842:MET:SD	1:B:849:ASN:HB3	2.49	0.52
1:B:859:SER:OG	1:B:862:HIS:HD2	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:PRO:HB2	1:A:865:SER:CB	2.39	0.52
1:B:148:GLN:HE22	1:B:573:GLN:NE2	2.07	0.52
3:A:3007:GOL:H2	4:A:4018:HOH:O	2.10	0.52
1:A:912:HIS:HE1	4:A:4671:HOH:O	1.93	0.52
1:A:545:LEU:O	1:A:549:THR:HG23	2.09	0.51
1:B:456:GLU:OE2	1:B:522:HIS:HE1	1.93	0.51
1:B:695:VAL:HG13	4:B:4677:HOH:O	2.09	0.51
1:B:37:GLU:CD	1:B:118:ASP:HB2	2.30	0.51
1:B:37:GLU:OE2	1:B:118:ASP:HB2	2.09	0.51
1:B:228:GLN:HE22	1:B:388:GLU:H	1.57	0.51
1:B:101:ASN:C	1:B:101:ASN:HD22	2.14	0.51
1:A:72:PHE:HA	1:A:191:VAL:O	2.10	0.51
1:B:292:LEU:HB3	1:B:294:LEU:HD13	1.93	0.51
1:B:102:PHE:CE2	1:B:147:GLN:HG3	2.46	0.51
1:A:887:ARG:HD2	4:A:4551:HOH:O	2.10	0.51
1:B:327:ARG:HD2	4:B:4497:HOH:O	2.10	0.50
1:A:852:ASN:HB3	1:A:855:MET:HG3	1.93	0.50
1:A:330:ALA:HB2	1:A:384:VAL:HG12	1.93	0.50
1:B:697:HIS:CD2	1:B:698:GLN:N	2.79	0.50
1:A:325:THR:O	1:A:326:LEU:HD12	2.10	0.50
1:A:801:PRO:HB2	1:A:865:SER:HB3	1.92	0.50
1:A:456:GLU:HG2	1:A:494:ARG:HB2	1.93	0.50
1:B:37:GLU:CD	1:B:38:GLY:H	2.15	0.50
1:B:87:ARG:HG3	4:B:4221:HOH:O	2.11	0.50
1:B:340:ILE:HG21	1:B:367:LEU:HD21	1.92	0.50
1:A:455:LEU:HD12	1:A:455:LEU:C	2.33	0.50
1:B:817:GLN:NE2	1:B:817:GLN:H	2.10	0.50
1:B:545:LEU:O	1:B:549:THR:HG23	2.12	0.50
1:A:609:ASP:HB2	4:A:4328:HOH:O	2.12	0.50
1:B:777[A]:GLN:HG3	1:B:778:GLY:H	1.77	0.49
1:A:710:ARG:HH11	1:A:723:ASP:HA	1.77	0.49
1:A:654:TRP:HB3	1:A:655:PRO:HD3	1.93	0.49
1:A:133[B]:ARG:HH21	1:A:137:GLN:HE22	1.60	0.49
1:A:681:LEU:HG	1:A:682:LEU:N	2.26	0.49
1:B:575:PHE:CZ	1:B:600:CYS:HB3	2.48	0.49
1:A:367:LEU:HD13	1:A:380:PHE:CD2	2.48	0.49
1:A:646:ASN:HD22	1:A:646:ASN:C	2.14	0.49
1:B:333:ASN:ND2	1:B:335:VAL:H	2.11	0.49
1:A:932:PRO:HD2	1:A:935:ILE:HD12	1.94	0.49
1:B:736:ILE:HG23	1:B:740:LEU:HD12	1.94	0.49
1:A:486:PHE:C	1:A:486:PHE:CD2	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:PRO:HG3	1:B:201:GLU:HB2	1.94	0.49
1:A:604:VAL:HB	1:A:605:PRO:HD3	1.94	0.49
1:A:236:HIS:HD2	1:A:238:ASN:N	2.01	0.48
1:B:147:GLN:H	1:B:147:GLN:NE2	2.11	0.48
1:A:883:ALA:HB3	1:A:888[B]:THR:HG22	1.91	0.48
1:A:732:LEU:O	1:A:736:ILE:HG13	2.14	0.48
1:A:745:LYS:HG2	1:A:762:TYR:CE2	2.48	0.48
1:A:704:LYS:HD3	4:A:4874:HOH:O	2.14	0.48
1:B:661:LEU:HG	1:B:706:LEU:HD23	1.95	0.48
1:B:758:ARG:HG2	4:B:4790:HOH:O	2.12	0.48
1:B:37:GLU:CD	1:B:37:GLU:H	2.16	0.48
1:B:680:ASN:HB3	1:B:695:VAL:HG21	1.95	0.48
1:B:627:PRO:HG2	1:B:676:MET:HE3	1.96	0.48
1:A:155:ASP:HA	1:A:489:ILE:HB	1.94	0.48
1:A:20:ARG:HH12	1:A:227:ASN:ND2	2.09	0.48
1:A:894:GLN:HA	1:A:894:GLN:NE2	2.29	0.48
1:A:340:ILE:HG21	1:A:367:LEU:CD2	2.43	0.47
1:A:531:TYR:CE2	1:A:596:ILE:HB	2.49	0.47
1:B:330:ALA:HB2	1:B:384:VAL:HG12	1.96	0.47
1:B:581:ARG:C	1:B:581:ARG:HD3	2.34	0.47
1:A:333:ASN:ND2	1:A:335:VAL:H	2.12	0.47
1:A:763:SER:CB	1:A:796:VAL:HB	2.45	0.47
1:B:751:CYS:HB3	4:B:4677:HOH:O	2.14	0.47
3:B:3041:GOL:H2	4:B:4802:HOH:O	2.14	0.47
1:A:23:TRP:H	1:A:137:GLN:NE2	2.12	0.47
1:B:292:LEU:HB3	1:B:294:LEU:CD1	2.45	0.47
1:B:568:CYS:HB3	1:B:862:HIS:CD2	2.49	0.47
1:B:914:ALA:HB3	1:B:930:GLU:HB2	1.97	0.47
3:A:3023:GOL:H12	4:A:4597:HOH:O	2.14	0.47
1:B:208:ILE:HD13	1:B:416:VAL:HG12	1.96	0.46
1:A:206:ALA:HA	3:B:3024:GOL:O1	2.15	0.46
1:A:422:PRO:HG2	1:B:199:THR:HB	1.97	0.46
1:B:310:HIS:HD2	4:B:4286:HOH:O	1.98	0.46
1:A:646:ASN:HD21	1:A:648:ALA:HB3	1.80	0.46
1:A:724:ALA:HB3	4:A:4639:HOH:O	2.16	0.46
1:A:277:LEU:HD13	1:A:277:LEU:C	2.36	0.46
1:B:635:LEU:HD13	3:B:3037:GOL:H11	1.98	0.46
1:B:414:ARG:HH12	1:B:418:ASN:ND2	2.14	0.46
1:B:72:PHE:HA	1:B:191:VAL:O	2.16	0.46
1:B:486:PHE:CD2	1:B:486:PHE:C	2.89	0.46
1:B:763:SER:CB	1:B:796:VAL:HB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:HG3	4:A:4679:HOH:O	2.16	0.46
1:A:130:ARG:CZ	1:A:175:GLN:HE22	2.29	0.45
1:B:413:PRO:HG2	1:B:416:VAL:CG2	2.45	0.45
1:A:328:SER:OG	1:A:338:ALA:HB2	2.16	0.45
1:B:732:LEU:O	1:B:736:ILE:HG13	2.17	0.45
1:B:111:LEU:HD22	1:B:112:ILE:N	2.30	0.45
1:A:531:TYR:CG	1:A:532:PRO:HD2	2.51	0.45
1:A:367:LEU:HB3	1:A:368:PRO:HD3	1.99	0.45
1:B:433:GLU:HG2	3:B:3034:GOL:O1	2.17	0.45
1:B:208:ILE:CD1	1:B:416:VAL:HG12	2.47	0.45
1:A:801:PRO:HG3	1:A:843:TYR:CE2	2.52	0.45
1:A:55:ASN:HA	1:A:166:PRO:HG3	1.98	0.45
1:A:248:THR:HB	1:A:337:LEU:CD2	2.45	0.45
1:B:455:LEU:C	1:B:455:LEU:HD12	2.37	0.45
1:A:162:ASP:HB3	1:A:165:LEU:HD12	1.98	0.45
1:B:681:LEU:HG	1:B:682:LEU:N	2.32	0.44
1:B:414:ARG:O	1:B:417:LEU:HB2	2.17	0.44
1:B:246:VAL:HG23	1:B:305:ILE:HD13	2.00	0.44
1:B:680:ASN:CB	1:B:695:VAL:HG21	2.47	0.44
1:A:746[B]:ARG:NH2	1:A:746[B]:ARG:HG2	2.32	0.44
1:A:310:HIS:HD2	4:A:4188:HOH:O	1.99	0.44
1:A:159:LEU:HD13	1:A:159:LEU:C	2.38	0.44
1:A:138:ARG:HB3	1:A:140:ASN:ND2	2.32	0.44
1:A:20:ARG:NH1	1:A:227:ASN:HD22	2.11	0.44
1:A:610:GLU:HA	1:A:610:GLU:OE1	2.17	0.44
1:B:763:SER:O	1:B:767:GLN:HG2	2.18	0.44
1:B:531:TYR:CE2	1:B:596:ILE:HB	2.52	0.44
1:A:676:MET:O	1:A:692:GLU:O	2.35	0.44
1:A:326:LEU:HB3	1:A:336:PRO:HB2	2.00	0.44
1:A:247:ALA:HB2	1:A:302:LEU:HD12	2.00	0.44
1:B:228:GLN:NE2	1:B:388:GLU:H	2.16	0.44
1:B:540:ARG:HD2	4:B:4186:HOH:O	2.17	0.44
1:B:47:ASP:HA	1:B:48:SER:HA	1.78	0.44
1:B:817:GLN:HE21	1:B:817:GLN:H	1.66	0.43
1:A:581:ARG:NE	1:A:635:LEU:HD13	2.33	0.43
1:A:616:ASP:OD1	1:A:626:ILE:HG13	2.18	0.43
1:A:635:LEU:HD22	1:A:639:GLU:CD	2.39	0.43
1:B:826[A]:ARG:HB2	1:B:826[A]:ARG:NH1	2.33	0.43
1:A:199:THR:HB	1:B:422:PRO:HG2	2.01	0.43
1:B:697:HIS:HD2	1:B:698:GLN:N	2.15	0.43
1:B:396:ASN:HD22	1:B:396:ASN:C	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HG11	1:B:387:PHE:HB3	1.99	0.43
1:A:208:ILE:CD1	1:A:416:VAL:HG12	2.49	0.43
1:B:365:ARG:HH11	3:B:3018:GOL:H32	1.83	0.43
1:A:690:PRO:C	1:A:692:GLU:N	2.72	0.43
1:A:842:MET:SD	1:A:849:ASN:HB3	2.59	0.43
1:B:248:THR:HB	1:B:337:LEU:HD23	2.01	0.43
1:B:912:HIS:ND1	1:B:912:HIS:C	2.72	0.43
1:A:211:LEU:HD23	1:A:212:SER:N	2.34	0.43
1:A:302:LEU:HD11	1:A:340:ILE:CD1	2.48	0.43
1:A:272:TRP:CE2	1:A:277:LEU:HD23	2.54	0.43
1:B:44:ILE:HG12	1:B:45:THR:N	2.33	0.42
1:A:36:VAL:HG21	1:A:117:ALA:HB1	1.99	0.42
1:B:841:GLU:HB2	1:B:862:HIS:CD2	2.54	0.42
1:B:197:PHE:CZ	3:B:3021:GOL:H12	2.54	0.42
1:A:952:VAL:CG1	3:A:3043:GOL:H12	2.48	0.42
1:A:882:GLY:C	1:A:888[B]:THR:HG23	2.40	0.42
1:B:658:LYS:HE2	4:B:4667:HOH:O	2.19	0.42
1:A:576:TRP:CG	3:A:3007:GOL:H32	2.55	0.42
1:A:694:ILE:HB	1:A:752:ILE:HB	2.01	0.42
1:B:942:PRO:HG2	1:B:945:ILE:HG13	2.01	0.42
1:A:816:ARG:NH2	4:A:4647:HOH:O	2.52	0.42
1:A:197:PHE:CZ	3:A:3022:GOL:H12	2.55	0.42
1:A:44:ILE:HG12	1:A:45:THR:N	2.33	0.42
1:B:367:LEU:O	1:B:367:LEU:HD12	2.20	0.42
1:B:674:LEU:HD21	1:B:676:MET:HE1	2.01	0.42
1:A:12:TRP:CG	1:A:13:GLY:N	2.86	0.42
1:A:802:PHE:HB2	1:A:864:TRP:CE2	2.53	0.42
1:A:100:SER:HB3	1:A:621:ALA:CB	2.50	0.42
1:A:159:LEU:HD13	1:A:161:GLU:N	2.34	0.41
1:A:591:PHE:HB3	1:A:593[A]:GLU:OE2	2.20	0.41
1:A:789:SER:HB3	1:A:816:ARG:NH1	2.34	0.41
1:B:298:GLU:OE2	1:B:327:ARG:NH2	2.48	0.41
1:A:687:ILE:HD11	1:A:765:GLN:HG2	2.03	0.41
1:A:349:ILE:HG21	1:A:352:ARG:HD2	2.03	0.41
1:B:12:TRP:CE2	1:B:109:GLY:HA3	2.55	0.41
1:A:228:GLN:HE22	1:A:388:GLU:H	1.68	0.41
1:B:558[A]:ARG:NH1	4:B:4182:HOH:O	2.44	0.41
1:A:690:PRO:HB2	1:A:692:GLU:HG3	2.03	0.41
1:A:622:TRP:CE2	1:A:624:SER:HB2	2.54	0.41
1:A:687:ILE:HD11	1:A:765:GLN:CG	2.51	0.41
1:A:789:SER:HB3	1:A:816:ARG:HH12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HG22	1:A:112:ILE:CG2	2.51	0.41
1:A:246:VAL:HG23	1:A:305:ILE:HD13	2.01	0.41
1:B:340:ILE:HG21	1:B:367:LEU:CD2	2.51	0.41
1:B:577:VAL:CG1	1:B:633:TRP:HB2	2.50	0.41
1:A:129:TRP:HA	3:A:3030:GOL:H31	2.03	0.41
1:B:410:ARG:HH22	3:B:3034:GOL:H31	1.85	0.41
1:A:44:ILE:CG1	1:A:45:THR:N	2.84	0.41
1:B:720:GLU:HA	1:B:723:ASP:OD2	2.20	0.41
1:A:409:ARG:HE	1:A:409:ARG:HB3	1.69	0.41
1:A:763:SER:HB3	1:A:796:VAL:HB	2.03	0.40
1:B:852:ASN:HB3	1:B:855:MET:HG3	2.02	0.40
1:A:684:TRP:HB3	4:A:4807:HOH:O	2.20	0.40
1:B:12:TRP:CG	1:B:13:GLY:N	2.87	0.40
1:B:704:LYS:HG2	3:B:3037:GOL:H12	2.03	0.40
1:B:137:GLN:HA	1:B:154:ILE:HD13	2.04	0.40
1:B:102:PHE:N	1:B:102:PHE:CD1	2.88	0.40
1:A:211:LEU:HD23	1:A:211:LEU:C	2.41	0.40
1:A:678:GLY:O	1:A:691:ASN:HA	2.21	0.40
1:A:697:HIS:ND1	1:A:698:GLN:N	2.70	0.40
1:A:369:GLU:OE2	1:A:369:GLU:N	2.54	0.40
1:B:20:ARG:HH22	1:B:227:ASN:ND2	2.19	0.40
1:B:531:TYR:CG	1:B:532:PRO:HD2	2.56	0.40
1:A:112:ILE:O	1:A:112:ILE:HG23	2.21	0.40
1:A:882:GLY:HA3	1:A:888[B]:THR:HG23	2.03	0.40
1:A:329:PRO:HD2	1:A:338:ALA:CB	2.51	0.40
1:A:912:HIS:C	1:A:912:HIS:ND1	2.75	0.40
1:A:133[B]:ARG:NH2	1:A:139[B]:SER:OG	2.54	0.40
1:B:103:TYR:OH	1:B:148:GLN:HB3	2.22	0.40
1:B:752:ILE:HA	1:B:758:ARG:HA	2.03	0.40
1:B:450:PHE:HB3	1:B:499:SER:O	2.21	0.40

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	963/956 (101%)	929 (96%)	30 (3%)	4 (0%)	39	27
1	B	961/956 (100%)	922 (96%)	37 (4%)	2 (0%)	52	42
All	All	1924/1912 (101%)	1851 (96%)	67 (4%)	6 (0%)	46	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	692	GLU
1	B	614	TYR
1	A	614	TYR
1	A	37	GLU
1	A	686	PRO
1	B	686	PRO

### 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	787/777 (101%)	763 (97%)	24 (3%)	48	38
1	B	785/777 (101%)	761 (97%)	24 (3%)	47	37
All	All	1572/1554 (101%)	1524 (97%)	48 (3%)	48	37

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	137	GLN
1	A	140	ASN
1	A	223	LEU
1	A	333	ASN
1	A	409	ARG
1	A	483	ASP

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Mol	Chain	Res	Type
1	A	486	PHE
1	A	579	ASP
1	A	587	ASN
1	A	593[A]	GLU
1	A	593[B]	GLU
1	A	610	GLU
1	A	611	THR
1	A	617	GLN
1	A	629	TRP
1	A	635	LEU
1	A	646	ASN
1	A	732	LEU
1	A	765	GLN
1	A	833	ARG
1	A	862	HIS
1	A	864	TRP
1	A	912	HIS
1	B	37	GLU
1	B	101	ASN
1	B	111	LEU
1	B	137	GLN
1	B	147	GLN
1	B	223	LEU
1	B	300	LEU
1	B	302	LEU
1	B	333	ASN
1	B	396	ASN
1	B	417	LEU
1	B	483	ASP
1	B	486	PHE
1	B	579	ASP
1	B	617	GLN
1	B	629	TRP
1	B	675	ASN
1	B	746	ARG
1	B	765	GLN
1	B	817	GLN
1	B	833	ARG
1	B	862	HIS
1	B	864	TRP
1	B	912	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	81	GLN
1	A	137	GLN
1	A	140	ASN
1	A	148	GLN
1	A	175	GLN
1	A	209	GLN
1	A	227	ASN
1	A	228	GLN
1	A	236	HIS
1	A	278	GLN
1	A	299	HIS
1	A	310	HIS
1	A	333	ASN
1	A	358	GLN
1	A	418	ASN
1	A	478	HIS
1	A	495	GLN
1	A	522	HIS
1	A	536	GLN
1	A	602	ASN
1	A	628	ASN
1	A	646	ASN
1	A	667	HIS
1	A	680	ASN
1	A	765	GLN
1	A	862	HIS
1	A	894	GLN
1	B	71	GLN
1	B	101	ASN
1	B	137	GLN
1	B	147	GLN
1	B	148	GLN
1	B	227	ASN
1	B	228	GLN
1	B	285	GLN
1	B	299	HIS
1	B	310	HIS
1	B	333	ASN
1	B	396	ASN
1	B	418	ASN
1	B	478	HIS

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Mol	Chain	Res	Type
1	B	522	HIS
1	B	555	HIS
1	B	573	GLN
1	B	675	ASN
1	B	680	ASN
1	B	689	GLN
1	B	697	HIS
1	B	765	GLN
1	B	817	GLN
1	B	849	ASN
1	B	862	HIS
1	B	951	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](#)

Of 47 ligands modelled in this entry, 4 are monoatomic - leaving 43 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	GOL	A	3001	-	5,5,5	1.13	1 (20%)	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	3002	-	5,5,5	1.17	1 (20%)	5,5,5	0.24	0
3	GOL	A	3003	-	5,5,5	1.17	1 (20%)	5,5,5	0.31	0
3	GOL	A	3004	-	5,5,5	1.13	1 (20%)	5,5,5	0.23	0
3	GOL	A	3006	-	5,5,5	1.15	1 (20%)	5,5,5	0.31	0
3	GOL	A	3007	-	5,5,5	1.12	1 (20%)	5,5,5	0.34	0
3	GOL	A	3008	-	5,5,5	1.14	1 (20%)	5,5,5	0.22	0
3	GOL	A	3015	-	5,5,5	1.15	1 (20%)	5,5,5	0.25	0
3	GOL	A	3017	-	5,5,5	1.13	1 (20%)	5,5,5	0.24	0
3	GOL	A	3019	-	5,5,5	1.15	1 (20%)	5,5,5	0.23	0
3	GOL	A	3022	-	5,5,5	1.18	1 (20%)	5,5,5	0.36	0
3	GOL	A	3023	-	5,5,5	1.14	1 (20%)	5,5,5	0.25	0
3	GOL	A	3026	-	5,5,5	1.11	1 (20%)	5,5,5	0.23	0
3	GOL	A	3027	-	5,5,5	1.15	1 (20%)	5,5,5	0.25	0
3	GOL	A	3030	-	5,5,5	1.13	1 (20%)	5,5,5	0.22	0
3	GOL	A	3031	-	5,5,5	1.13	1 (20%)	5,5,5	0.25	0
3	GOL	A	3033	-	5,5,5	1.16	1 (20%)	5,5,5	0.29	0
3	GOL	A	3035	-	5,5,5	1.16	1 (20%)	5,5,5	0.25	0
3	GOL	A	3039	-	5,5,5	1.34	1 (20%)	5,5,5	0.49	0
3	GOL	A	3040	-	5,5,5	1.13	1 (20%)	5,5,5	0.31	0
3	GOL	A	3043	-	5,5,5	1.16	1 (20%)	5,5,5	0.32	0
3	GOL	B	3005	-	5,5,5	1.14	1 (20%)	5,5,5	0.23	0
3	GOL	B	3009	-	5,5,5	1.09	1 (20%)	5,5,5	0.23	0
3	GOL	B	3010	-	5,5,5	1.14	1 (20%)	5,5,5	0.23	0
3	GOL	B	3011	-	5,5,5	1.12	1 (20%)	5,5,5	0.23	0
3	GOL	B	3012	-	5,5,5	1.18	1 (20%)	5,5,5	0.29	0
3	GOL	B	3013	-	5,5,5	1.13	1 (20%)	5,5,5	0.24	0
3	GOL	B	3014	-	5,5,5	1.07	1 (20%)	5,5,5	0.26	0
3	GOL	B	3016	-	5,5,5	1.13	1 (20%)	5,5,5	0.22	0
3	GOL	B	3018	-	5,5,5	1.14	1 (20%)	5,5,5	0.23	0
3	GOL	B	3020	-	5,5,5	1.13	1 (20%)	5,5,5	0.22	0
3	GOL	B	3021	-	5,5,5	1.20	1 (20%)	5,5,5	0.36	0
3	GOL	B	3024	-	5,5,5	1.16	1 (20%)	5,5,5	0.27	0
3	GOL	B	3025	-	5,5,5	1.14	1 (20%)	5,5,5	0.21	0
3	GOL	B	3028	-	5,5,5	1.14	1 (20%)	5,5,5	0.26	0
3	GOL	B	3029	-	5,5,5	1.15	1 (20%)	5,5,5	0.24	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	3032	-	5,5,5	1.13	1 (20%)	5,5,5	0.23	0
3	GOL	B	3034	-	5,5,5	1.12	1 (20%)	5,5,5	0.30	0
3	GOL	B	3036	-	5,5,5	1.12	1 (20%)	5,5,5	0.21	0
3	GOL	B	3037	-	5,5,5	1.15	1 (20%)	5,5,5	0.27	0
3	GOL	B	3038	-	5,5,5	1.14	1 (20%)	5,5,5	0.25	0
3	GOL	B	3041	-	5,5,5	1.27	1 (20%)	5,5,5	0.50	0
3	GOL	B	3042	-	5,5,5	1.16	1 (20%)	5,5,5	0.30	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	GOL	A	3001	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3002	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3003	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3004	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3006	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3007	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3008	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3015	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3017	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3019	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3022	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3023	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3026	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3027	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3030	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3031	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3033	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3035	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3039	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3040	-	-	0/4/4/4	0/0/0/0
3	GOL	A	3043	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3005	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3009	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3010	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3011	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3012	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3013	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	3014	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3016	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3018	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3020	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3021	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3024	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3025	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3028	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3029	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3032	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3034	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3036	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3037	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3038	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3041	-	-	0/4/4/4	0/0/0/0
3	GOL	B	3042	-	-	0/4/4/4	0/0/0/0

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3039	GOL	O1-C1	-2.95	1.29	1.42
3	B	3041	GOL	O1-C1	-2.81	1.30	1.42
3	B	3012	GOL	O1-C1	-2.60	1.31	1.42
3	A	3003	GOL	O1-C1	-2.60	1.31	1.42
3	A	3002	GOL	O1-C1	-2.58	1.31	1.42
3	B	3021	GOL	O1-C1	-2.58	1.31	1.42
3	B	3024	GOL	O1-C1	-2.57	1.31	1.42
3	A	3043	GOL	O1-C1	-2.56	1.31	1.42
3	A	3022	GOL	O1-C1	-2.54	1.31	1.42
3	B	3042	GOL	O1-C1	-2.54	1.31	1.42
3	B	3037	GOL	O1-C1	-2.53	1.31	1.42
3	A	3035	GOL	O1-C1	-2.53	1.31	1.42
3	B	3005	GOL	O1-C1	-2.52	1.31	1.42
3	A	3006	GOL	O1-C1	-2.52	1.31	1.42
3	A	3027	GOL	O1-C1	-2.52	1.31	1.42
3	B	3010	GOL	O1-C1	-2.52	1.31	1.42
3	B	3038	GOL	O1-C1	-2.51	1.31	1.42
3	A	3015	GOL	O1-C1	-2.51	1.31	1.42
3	A	3019	GOL	O1-C1	-2.51	1.31	1.42
3	B	3029	GOL	O1-C1	-2.51	1.31	1.42
3	A	3033	GOL	O1-C1	-2.50	1.31	1.42
3	B	3028	GOL	O1-C1	-2.50	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	GOL	O1-C1	-2.50	1.31	1.42
3	B	3018	GOL	O1-C1	-2.49	1.31	1.42
3	A	3023	GOL	O1-C1	-2.49	1.31	1.42
3	B	3016	GOL	O1-C1	-2.49	1.31	1.42
3	A	3008	GOL	O1-C1	-2.49	1.31	1.42
3	B	3013	GOL	O1-C1	-2.49	1.31	1.42
3	A	3040	GOL	O1-C1	-2.48	1.31	1.42
3	A	3004	GOL	O1-C1	-2.47	1.31	1.42
3	A	3030	GOL	O1-C1	-2.47	1.31	1.42
3	A	3017	GOL	O1-C1	-2.47	1.31	1.42
3	A	3031	GOL	O1-C1	-2.46	1.31	1.42
3	B	3032	GOL	O1-C1	-2.46	1.31	1.42
3	B	3020	GOL	O1-C1	-2.46	1.31	1.42
3	B	3025	GOL	O1-C1	-2.45	1.31	1.42
3	B	3034	GOL	O1-C1	-2.44	1.31	1.42
3	B	3036	GOL	O1-C1	-2.44	1.31	1.42
3	A	3007	GOL	O1-C1	-2.43	1.31	1.42
3	A	3026	GOL	O1-C1	-2.43	1.31	1.42
3	B	3011	GOL	O1-C1	-2.43	1.31	1.42
3	B	3009	GOL	O1-C1	-2.35	1.32	1.42
3	B	3014	GOL	O1-C1	-2.29	1.32	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3003	GOL	1	0
3	A	3006	GOL	1	0
3	A	3007	GOL	3	0
3	A	3022	GOL	1	0
3	A	3023	GOL	1	0
3	A	3027	GOL	1	0
3	A	3030	GOL	2	0
3	A	3033	GOL	1	0
3	A	3043	GOL	1	0
3	B	3018	GOL	1	0
3	B	3021	GOL	1	0
3	B	3024	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3029	GOL	3	0
3	B	3034	GOL	2	0
3	B	3037	GOL	4	0
3	B	3038	GOL	1	0
3	B	3041	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	954/956 (99%)	0.19	51 (5%)	30	33	14, 26, 46, 61	0
1	B	954/956 (99%)	0.18	56 (5%)	26	29	14, 25, 49, 64	0
All	All	1908/1912 (99%)	0.18	107 (5%)	28	31	14, 26, 48, 64	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	ASP	5.4
1	B	34	ALA	4.8
1	A	853	PRO	4.4
1	A	719	THR	4.2
1	B	356	ARG	4.1
1	B	86	VAL	4.1
1	B	37	GLU	4.0
1	B	36	VAL	3.9
1	B	85	GLY	3.8
1	B	353	PRO	3.8
1	A	744	GLU	3.7
1	A	15	GLN	3.7
1	B	779	GLU	3.7
1	B	847	ALA	3.6
1	A	36	VAL	3.5
1	B	794	ALA	3.5
1	A	253	GLU	3.4
1	B	516	SER	3.4
1	B	355	ARG	3.3
1	A	34	ALA	3.2
1	A	33	PRO	3.2
1	B	354	GLY	3.2
1	B	38	GLY	3.1
1	A	93	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	256	GLY	3.1
1	B	755	ASP	3.1
1	A	367	LEU	3.0
1	B	731	LEU	3.0
1	A	516	SER	3.0
1	A	692	GLU	2.9
1	A	718	ALA	2.9
1	A	776	ALA	2.9
1	B	746	ARG	2.8
1	A	779	GLU	2.8
1	B	744[A]	GLU	2.8
1	B	5	ASN	2.7
1	A	331	GLY	2.7
1	B	331	GLY	2.7
1	A	670	ASP	2.7
1	B	846	PHE	2.7
1	B	854	ASP	2.7
1	B	609	ASP	2.7
1	B	358	GLN	2.6
1	B	692	GLU	2.6
1	B	670	ASP	2.6
1	A	846	PHE	2.6
1	B	367	LEU	2.6
1	A	92	VAL	2.6
1	B	719	THR	2.6
1	B	84	PRO	2.6
1	A	51	VAL	2.6
1	A	731	LEU	2.6
1	B	119	GLY	2.6
1	B	94	VAL	2.6
1	A	715	ALA	2.5
1	A	793	PRO	2.5
1	B	120	ARG	2.5
1	B	167	ALA	2.4
1	A	50	TYR	2.4
1	A	111	LEU	2.4
1	A	5	ASN	2.4
1	B	293	ASN	2.4
1	A	321	GLU	2.4
1	B	321	GLU	2.4
1	A	720	GLU	2.4
1	A	760	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	845	ASN	2.4
1	B	853	PRO	2.4
1	A	722	ALA	2.3
1	B	348	TYR	2.3
1	A	847	ALA	2.3
1	B	33	PRO	2.3
1	A	741	TRP	2.3
1	A	757	ARG	2.3
1	A	854	ASP	2.3
1	A	85	GLY	2.3
1	A	94	VAL	2.3
1	B	15	GLN	2.3
1	A	38	GLY	2.3
1	A	755	ASP	2.2
1	B	362	PRO	2.2
1	B	50	TYR	2.2
1	B	433	GLU	2.2
1	A	84	PRO	2.2
1	B	246	VAL	2.2
1	A	845	ASN	2.2
1	B	760	ASP	2.2
1	A	734	GLU	2.1
1	A	120	ARG	2.1
1	A	248	THR	2.1
1	A	254	THR	2.1
1	B	678	GLY	2.1
1	B	718	ALA	2.1
1	B	254	THR	2.1
1	B	783	VAL	2.1
1	A	729	ALA	2.1
1	B	92	VAL	2.1
1	B	717	GLY	2.1
1	A	730	ASP	2.1
1	B	745	LYS	2.0
1	A	37	GLU	2.0
1	B	7	ASN	2.0
1	A	44	ILE	2.0
1	A	46	ALA	2.0
1	B	87	ARG	2.0
1	A	381	ALA	2.0
1	B	674	LEU	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(Å <sup>2</sup> )	Q<0.9
3	GOL	B	3028	6/6	0.69	0.21	13.37	73,73,74,74	0
3	GOL	A	3006	6/6	0.87	0.21	13.29	34,37,39,39	0
3	GOL	A	3023	6/6	0.66	0.32	10.63	68,70,71,71	0
3	GOL	B	3021	6/6	0.87	0.22	10.19	33,34,36,36	0
3	GOL	B	3029	6/6	0.77	0.40	10.04	72,72,73,73	0
3	GOL	A	3022	6/6	0.87	0.22	8.48	34,35,36,37	0
3	GOL	A	3039	6/6	0.79	0.27	8.45	38,42,45,50	0
3	GOL	A	3007	6/6	0.88	0.16	8.39	25,29,30,31	0
3	GOL	B	3025	6/6	0.73	0.30	8.35	47,51,53,54	0
3	GOL	B	3037	6/6	0.80	0.40	7.87	67,68,69,71	0
3	GOL	B	3038	6/6	0.66	0.37	7.74	64,65,66,67	0
3	GOL	B	3024	6/6	0.64	0.29	7.58	67,68,68,69	0
3	GOL	A	3008	6/6	0.71	0.28	7.57	54,58,59,59	0
3	GOL	B	3032	6/6	0.55	0.29	6.66	74,74,75,75	0
3	GOL	B	3036	6/6	0.74	0.25	5.78	55,62,63,63	0
3	GOL	B	3042	6/6	0.80	0.20	5.17	47,49,51,54	0
3	GOL	B	3041	6/6	0.74	0.25	4.84	58,60,62,64	0
3	GOL	A	3030	6/6	0.73	0.26	4.66	68,68,68,69	0
3	GOL	A	3043	6/6	0.82	0.28	4.63	47,51,56,59	0
3	GOL	A	3033	6/6	0.77	0.32	4.48	43,47,51,55	0
3	GOL	A	3026	6/6	0.81	0.21	4.40	41,46,47,50	0
3	GOL	B	3012	6/6	0.85	0.23	3.97	42,44,45,50	0
3	GOL	B	3020	6/6	0.66	0.28	3.69	41,48,48,49	0
3	GOL	A	3019	6/6	0.70	0.27	3.40	67,67,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	3009	6/6	0.89	0.14	3.38	27,34,34,35	0
3	GOL	A	3003	6/6	0.87	0.27	3.36	47,48,51,51	0
3	GOL	A	3017	6/6	0.74	0.17	2.62	66,67,67,67	0
3	GOL	B	3034	6/6	0.82	0.32	2.49	36,41,45,51	0
3	GOL	B	3011	6/6	0.88	0.21	2.06	44,47,48,48	0
3	GOL	B	3010	6/6	0.88	0.16	2.06	45,46,46,47	0
2	CA	B	4003	1/1	1.00	0.09	1.76	30,30,30,30	0
3	GOL	B	3018	6/6	0.71	0.21	1.74	74,75,75,75	0
3	GOL	A	3040	6/6	0.88	0.15	1.70	48,51,51,52	0
3	GOL	B	3014	6/6	0.93	0.11	1.45	22,26,26,26	0
3	GOL	A	3002	6/6	0.89	0.19	1.42	43,45,47,47	0
3	GOL	B	3005	6/6	0.91	0.14	0.86	39,42,43,46	0
3	GOL	A	3001	6/6	0.93	0.12	0.13	33,35,38,43	0
2	CA	A	4001	1/1	0.99	0.04	-2.98	29,29,29,29	0
3	GOL	B	3016	6/6	0.85	0.23	-	50,55,56,57	0
3	GOL	A	3027	6/6	0.72	0.32	-	72,73,73,75	0
3	GOL	A	3031	6/6	0.59	0.41	-	84,85,85,86	0
2	CA	B	4002	1/1	0.99	0.09	-	31,31,31,31	0
3	GOL	A	3015	6/6	0.89	0.25	-	50,53,53,55	0
3	GOL	A	3035	6/6	0.84	0.24	-	51,54,55,56	0
2	CA	A	4004	1/1	0.99	0.07	-	28,28,28,28	0
3	GOL	A	3004	6/6	0.89	0.16	-	42,43,44,44	0
3	GOL	B	3013	6/6	0.88	0.20	-	42,44,45,46	0

## 6.5 Other polymers

There are no such residues in this entry.