



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:11 AM BST

PDB ID : 1H49  
Title : CRYSTAL STRUCTURE OF THE INACTIVE DOUBLE MUTANT OF THE MAIZE BETA-GLUCOSIDASE ZMGLU1-E191D-F198V IN COMPLEX WITH DIMBOA-GLUCOSIDE  
Authors : Czjzek, M.; Moriniere, J.; Verdoucq, L.; Bevan, D.R.; Henrissat, B.; Esen, A.  
Deposited on : 2003-02-25  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

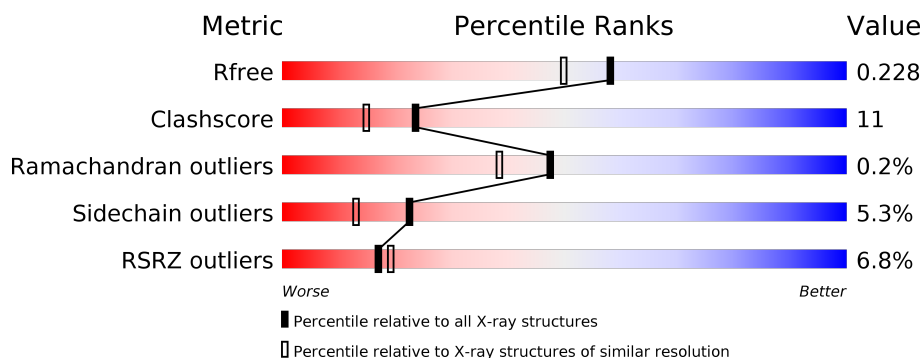
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	512	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	512	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>• •</div> </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
2	HBO	A	1502	-	-	-	X
2	HBO	B	1502	-	-	-	X
3	BGC	A	1503	-	-	X	-
3	BGC	B	1503	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8469 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.

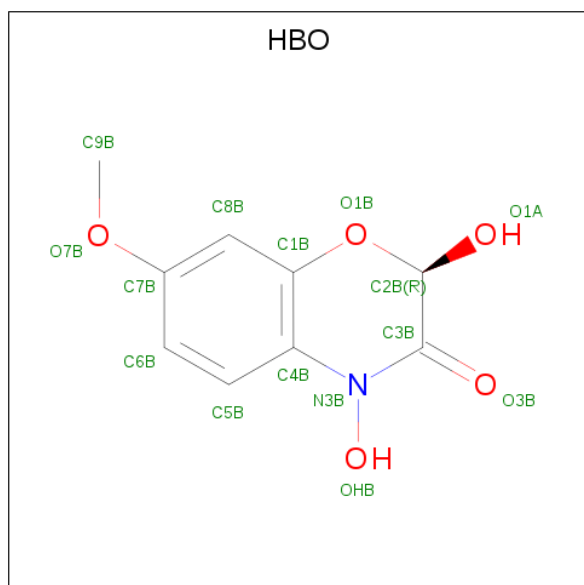
- Molecule 1 is a protein called BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	1
			3963	2539	657	749	18			
1	B	491	Total	C	N	O	S	0	0	1
			3963	2539	657	749	18			

There are 4 discrepancies between the modelled and reference sequences:

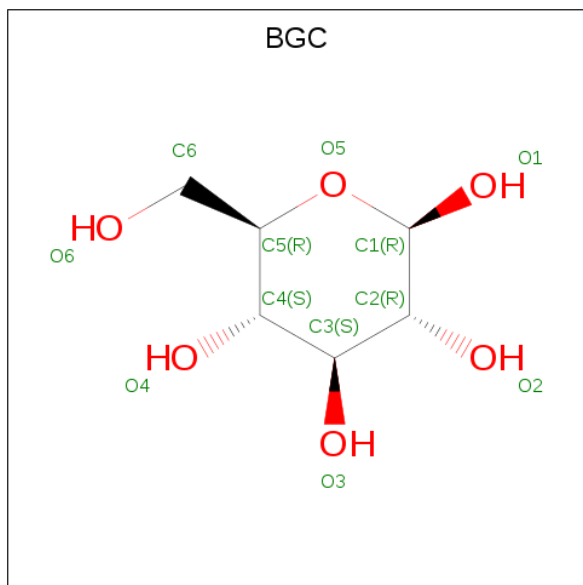
Chain	Residue	Modelled	Actual	Comment	Reference
A	191	ASP	GLU	engineered mutation	UNP P49235
A	198	VAL	PHE	engineered mutation	UNP P49235
B	191	ASP	GLU	engineered mutation	UNP P49235
B	198	VAL	PHE	engineered mutation	UNP P49235

- Molecule 2 is 2,4-DIHYDROXY-7-(METHYLOXY)-2H-1,4-BENZOXAZIN-3(4H)-ONE (three-letter code: HBO) (formula: C<sub>9</sub>H<sub>9</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	9	1	5		
2	B	1	Total	C	N	O	0	0
			15	9	1	5		

- Molecule 3 is beta-D-glucopyranose (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

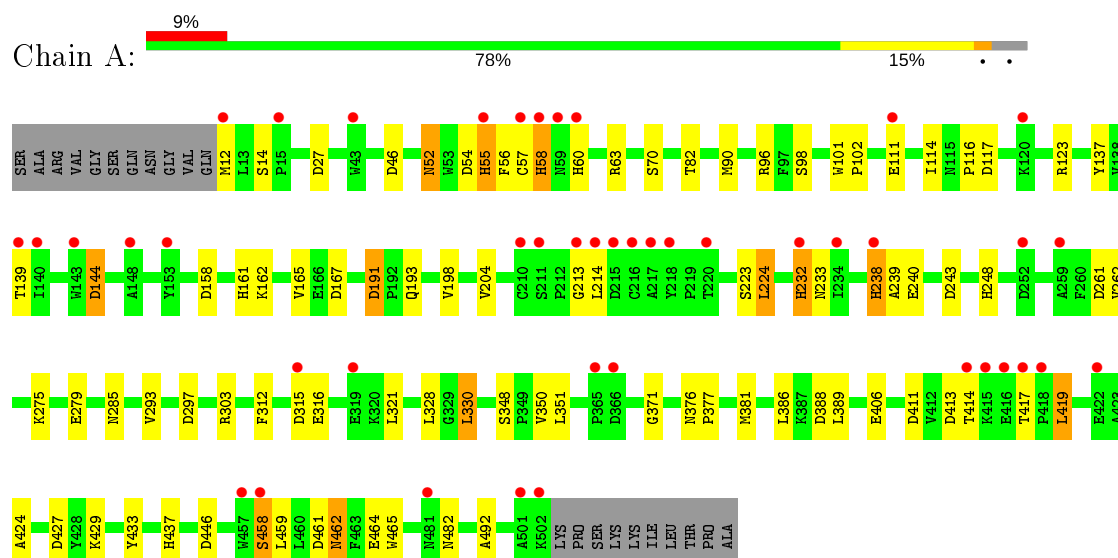
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	276	Total	O	0	0
			276	276		

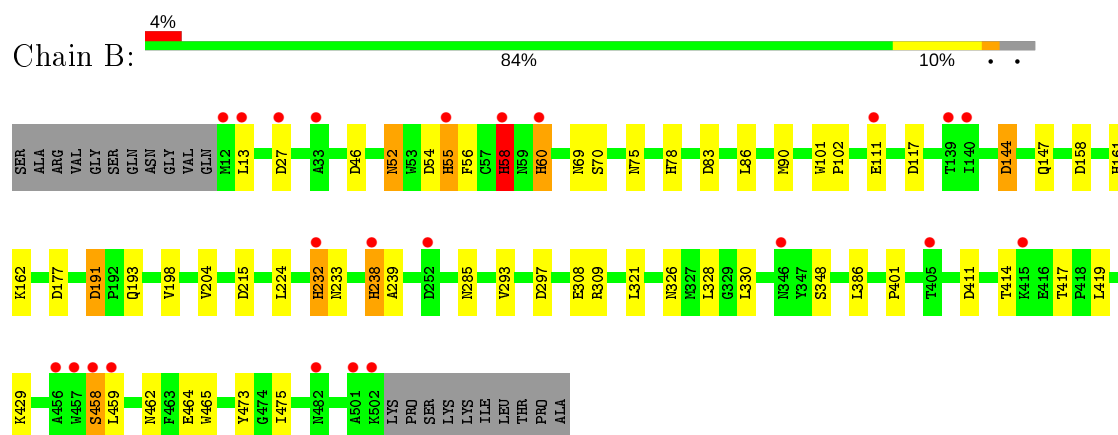
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: BETA-GLUCOSIDASE



#### • Molecule 1: BETA-GLUCOSIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.15Å 114.09Å 80.13Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	79.06 – 1.90 31.80 – 1.90	Depositor EDS
% Data completeness (in resolution range)	86.5 (79.06-1.90) 86.5 (31.80-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.184 , 0.221 0.193 , 0.228	Depositor DCC
$R_{free}$ test set	3518 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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

### 5.1 Standard geometry

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

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	0.53	0/4083	0.82	17/5545 (0.3%)
1	B	0.58	0/4083	0.81	13/5545 (0.2%)
All	All	0.55	0/8166	0.81	30/11090 (0.3%)

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	B	0	1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ASP	CB-CG-OD2	8.07	125.57	118.30
1	B	297	ASP	CB-CG-OD2	7.54	125.08	118.30
1	B	177	ASP	CB-CG-OD2	7.45	125.00	118.30
1	B	58	HIS	CB-CA-C	7.41	125.22	110.40
1	A	411	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	144	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	461	ASP	CB-CG-OD2	6.76	124.38	118.30
1	B	117	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	158	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	27	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	243	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	388	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	144	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	54	ASP	CB-CG-OD2	5.94	123.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	411	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	158	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	54	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	413	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	297	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	27	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	215	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	315	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	46	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	83	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	58	HIS	CA-CB-CG	-5.37	104.47	113.60
1	A	427	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	446	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	46	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	58	HIS	CB-CA-C	5.09	120.59	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	HIS	Sidechain

## 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	3963	0	3757	84	0
1	B	3963	0	3757	76	0
2	A	15	0	8	1	0
2	B	15	0	8	0	0
3	A	11	0	10	17	0
3	B	11	0	10	17	0
4	A	215	0	0	21	0
4	B	276	0	0	17	0
All	All	8469	0	7550	173	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 11.

All (173) 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:161:HIS:CE1	1:A:232:HIS:CE1	2.04	1.46
1:A:161:HIS:ND1	1:A:232:HIS:CE1	1.84	1.43
1:A:56:PHE:O	1:A:60:HIS:CE1	1.72	1.43
1:B:238:HIS:HD2	1:B:239:ALA:N	1.17	1.38
1:A:161:HIS:CE1	1:A:232:HIS:HE1	1.38	1.38
1:B:56:PHE:O	1:B:60:HIS:NE2	1.59	1.33
1:B:55:HIS:NE2	4:B:2029:HOH:O	1.62	1.27
1:B:56:PHE:CD1	1:B:60:HIS:HE1	1.55	1.23
1:B:238:HIS:CD2	1:B:239:ALA:N	2.08	1.21
1:A:232:HIS:HD2	1:A:233:ASN:N	1.41	1.17
1:B:161:HIS:ND1	1:B:232:HIS:NE2	1.95	1.12
1:A:55:HIS:NE2	4:A:2020:HOH:O	1.82	1.10
1:B:458:SER:HA	4:B:2250:HOH:O	1.49	1.09
1:A:56:PHE:C	1:A:60:HIS:HE1	1.57	1.07
1:B:55:HIS:HD2	1:B:56:PHE:N	1.52	1.05
1:B:56:PHE:CD1	1:B:60:HIS:CE1	2.43	1.05
1:B:56:PHE:O	1:B:60:HIS:CD2	2.09	1.04
1:B:161:HIS:ND1	1:B:232:HIS:CE1	2.28	1.02
1:A:161:HIS:ND1	1:A:232:HIS:NE2	1.94	1.02
1:A:232:HIS:CD2	1:A:233:ASN:N	2.31	0.98
1:A:56:PHE:O	1:A:60:HIS:ND1	1.95	0.98
1:B:58:HIS:HE1	1:B:69:ASN:CB	1.77	0.97
1:B:238:HIS:CD2	1:B:238:HIS:C	2.37	0.96
1:A:232:HIS:CD2	1:A:232:HIS:C	2.39	0.91
1:B:238:HIS:HE1	1:B:293:VAL:HG12	1.34	0.91
1:A:56:PHE:O	1:A:60:HIS:HE1	1.30	0.90
1:B:60:HIS:CD2	1:B:60:HIS:O	2.25	0.90
1:B:232:HIS:HB2	4:B:2174:HOH:O	1.72	0.89
1:B:58:HIS:HE1	1:B:69:ASN:HB3	1.35	0.89
1:B:55:HIS:CD2	1:B:56:PHE:N	2.40	0.88
1:B:161:HIS:CE1	1:B:232:HIS:NE2	2.45	0.83
1:B:238:HIS:CE1	1:B:293:VAL:HG12	2.13	0.83
1:A:232:HIS:HB2	4:A:2093:HOH:O	1.79	0.82
1:B:161:HIS:CE1	1:B:232:HIS:HE2	1.97	0.82
3:B:1503:BGC:H4	4:B:2276:HOH:O	1.76	0.81
1:B:55:HIS:C	1:B:55:HIS:CD2	2.53	0.81
3:A:1503:BGC:O2	4:A:2215:HOH:O	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:C	1:A:232:HIS:HD2	1.81	0.81
1:A:56:PHE:C	1:A:60:HIS:CE1	2.41	0.81
1:A:465:TRP:CD1	3:A:1503:BGC:O6	2.33	0.80
1:B:238:HIS:HD2	1:B:238:HIS:C	1.79	0.79
1:B:58:HIS:CE1	1:B:69:ASN:ND2	2.51	0.79
3:B:1503:BGC:C4	4:B:2276:HOH:O	2.18	0.78
1:B:60:HIS:CD2	1:B:60:HIS:C	2.54	0.78
1:A:161:HIS:ND1	1:A:232:HIS:HE1	1.44	0.77
1:B:191:ASP:OD2	3:B:1503:BGC:C2	2.33	0.76
1:A:57:CYS:C	1:A:58:HIS:HD2	1.89	0.76
1:B:56:PHE:CE1	1:B:60:HIS:CE1	2.73	0.75
3:A:1503:BGC:O2	4:A:2213:HOH:O	1.94	0.75
1:A:464:GLU:CD	3:A:1503:BGC:O6	2.24	0.75
1:B:465:TRP:CD1	3:B:1503:BGC:O6	2.39	0.75
1:B:56:PHE:C	1:B:60:HIS:NE2	2.40	0.74
1:A:238:HIS:C	1:A:238:HIS:ND1	2.41	0.74
1:B:414:THR:HG23	1:B:417:THR:H	1.52	0.73
1:B:58:HIS:CE1	1:B:69:ASN:HB3	2.22	0.73
1:B:60:HIS:HD2	1:B:60:HIS:C	1.92	0.72
1:B:56:PHE:CE1	1:B:60:HIS:HE1	2.06	0.71
1:B:58:HIS:CE1	1:B:69:ASN:CB	2.69	0.70
1:B:238:HIS:HD2	1:B:239:ALA:CA	2.05	0.69
1:B:232:HIS:C	1:B:232:HIS:ND1	2.46	0.69
1:A:465:TRP:HD1	3:A:1503:BGC:H6	1.30	0.69
1:B:238:HIS:HD2	1:B:239:ALA:H	1.32	0.69
3:A:1503:BGC:C4	4:A:2214:HOH:O	2.38	0.69
3:A:1503:BGC:H4	4:A:2214:HOH:O	1.92	0.68
1:B:238:HIS:CD2	1:B:239:ALA:CA	2.76	0.68
3:B:1503:BGC:O2	4:B:2273:HOH:O	2.07	0.67
1:B:238:HIS:NE2	1:B:321:LEU:HD23	2.09	0.67
1:A:191:ASP:OD2	3:A:1503:BGC:H2	1.95	0.67
3:B:1503:BGC:O2	4:B:2274:HOH:O	2.12	0.65
1:B:56:PHE:CG	1:B:60:HIS:CE1	2.85	0.65
1:A:191:ASP:OD2	3:A:1503:BGC:C2	2.45	0.65
1:B:191:ASP:OD2	3:B:1503:BGC:H2	1.96	0.65
1:B:58:HIS:CE1	1:B:69:ASN:HD22	2.13	0.64
3:B:1503:BGC:H5	4:B:2254:HOH:O	1.99	0.63
1:A:238:HIS:NE2	1:A:321:LEU:HD23	2.13	0.63
1:B:191:ASP:OD2	3:B:1503:BGC:O2	2.17	0.63
1:B:198:VAL:HG13	1:B:204:VAL:HG22	1.80	0.62
1:A:238:HIS:ND1	1:A:239:ALA:N	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:CD2	1:A:63:ARG:HB2	2.34	0.61
1:B:464:GLU:OE1	3:B:1503:BGC:H6C2	2.00	0.61
1:A:238:HIS:CE1	1:A:321:LEU:HD23	2.36	0.61
1:A:60:HIS:O	1:A:60:HIS:CG	2.53	0.61
1:B:58:HIS:NE2	1:B:69:ASN:ND2	2.49	0.60
1:B:465:TRP:NE1	3:B:1503:BGC:O6	2.35	0.60
1:A:161:HIS:HE1	1:A:232:HIS:CE1	2.07	0.60
1:A:57:CYS:C	1:A:58:HIS:CD2	2.75	0.59
1:A:57:CYS:O	1:A:58:HIS:HD2	1.84	0.59
1:B:90:MET:HE1	1:B:475:ILE:HD12	1.84	0.59
1:A:198:VAL:HG13	1:A:204:VAL:HG22	1.85	0.58
1:A:238:HIS:NE2	1:A:321:LEU:CD2	2.66	0.58
1:A:458:SER:HA	4:A:2189:HOH:O	2.02	0.57
1:A:191:ASP:OD2	3:A:1503:BGC:O2	2.22	0.57
1:A:238:HIS:NE2	1:A:293:VAL:HG12	2.19	0.57
3:A:1503:BGC:H6C1	4:A:2214:HOH:O	2.04	0.56
1:B:60:HIS:CD2	1:B:60:HIS:N	2.68	0.56
1:B:308:GLU:HB3	4:B:2080:HOH:O	2.06	0.56
1:B:58:HIS:CE1	4:B:2030:HOH:O	2.57	0.56
1:A:465:TRP:HE1	3:A:1503:BGC:H6C1	1.71	0.56
1:B:58:HIS:HE1	1:B:69:ASN:CG	2.10	0.55
1:A:238:HIS:HD1	1:A:238:HIS:C	2.07	0.55
1:B:55:HIS:HD2	1:B:56:PHE:CA	2.18	0.55
1:B:464:GLU:OE1	3:B:1503:BGC:C6	2.55	0.55
2:A:1502:HBO:O3B	4:A:2213:HOH:O	2.18	0.54
1:B:198:VAL:CG1	1:B:204:VAL:HG22	2.36	0.53
1:A:60:HIS:CD2	1:A:60:HIS:O	2.61	0.53
1:A:60:HIS:HB3	4:A:2022:HOH:O	2.09	0.53
1:A:414:THR:HG23	1:A:417:THR:H	1.73	0.52
1:B:58:HIS:CE1	1:B:69:ASN:CG	2.82	0.52
1:A:419:LEU:HD13	1:A:424:ALA:HB2	1.91	0.52
1:B:75:ASN:HD21	1:B:78:HIS:HD2	1.58	0.52
1:A:52:ASN:N	1:A:52:ASN:HD22	2.08	0.52
3:B:1503:BGC:C1	4:B:2275:HOH:O	2.58	0.52
1:B:55:HIS:ND1	1:B:147:GLN:NE2	2.58	0.51
1:B:232:HIS:CE1	1:B:233:ASN:OD1	2.63	0.51
1:B:52:ASN:HD21	1:B:144:ASP:HA	1.74	0.51
1:A:465:TRP:HD1	3:A:1503:BGC:O6	1.81	0.51
1:A:198:VAL:CG1	1:A:204:VAL:HG22	2.40	0.51
1:B:52:ASN:N	1:B:52:ASN:HD22	2.09	0.51
1:B:198:VAL:CG1	1:B:204:VAL:CG2	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:MET:HE1	1:A:492:ALA:HA	1.93	0.50
1:B:58:HIS:HB2	4:B:2026:HOH:O	2.11	0.50
1:A:240:GLU:HG2	4:A:2095:HOH:O	2.10	0.50
1:A:351:LEU:HD23	4:A:2072:HOH:O	2.12	0.50
1:A:406:GLU:OE2	3:A:1503:BGC:O3	2.28	0.49
1:A:55:HIS:CD2	4:A:2020:HOH:O	2.45	0.49
1:B:60:HIS:CG	1:B:60:HIS:O	2.66	0.49
1:A:330:LEU:HG	1:A:389:LEU:HD21	1.94	0.48
1:B:55:HIS:CD2	4:B:2029:HOH:O	2.39	0.47
1:B:464:GLU:OE2	3:B:1503:BGC:C6	2.62	0.47
1:A:60:HIS:HD2	1:A:63:ARG:HG3	1.79	0.47
1:B:326:ASN:O	1:B:401:PRO:HG2	2.14	0.47
1:A:482:ASN:ND2	4:A:2197:HOH:O	2.47	0.47
1:B:101:TRP:HB3	1:B:102:PRO:HD3	1.96	0.47
1:A:464:GLU:OE1	3:A:1503:BGC:H6C2	2.15	0.47
1:A:371:GLY:HA3	1:A:381:MET:O	2.15	0.47
3:B:1503:BGC:O4	4:B:2276:HOH:O	1.72	0.46
1:A:52:ASN:HD21	1:A:144:ASP:HA	1.80	0.46
1:A:351:LEU:CD2	4:A:2072:HOH:O	2.63	0.46
1:A:223:SER:CB	4:A:2072:HOH:O	2.63	0.46
1:A:56:PHE:CG	1:A:60:HIS:CE1	3.04	0.45
1:A:464:GLU:OE1	3:A:1503:BGC:O6	2.34	0.45
1:A:275:LYS:NZ	1:A:279:GLU:OE2	2.49	0.45
1:B:458:SER:HB2	1:B:473:TYR:O	2.16	0.45
1:A:165:VAL:CG1	1:A:240:GLU:HG3	2.46	0.45
1:A:60:HIS:ND1	1:A:60:HIS:N	2.65	0.45
1:A:376:ASN:HB2	1:A:377:PRO:CD	2.47	0.45
1:A:60:HIS:HD2	1:A:63:ARG:CG	2.30	0.44
1:B:238:HIS:HB2	4:B:2135:HOH:O	2.18	0.44
1:B:58:HIS:CB	4:B:2026:HOH:O	2.65	0.44
1:A:56:PHE:CE1	1:A:60:HIS:NE2	2.85	0.44
1:A:213:GLY:HA3	4:A:2079:HOH:O	2.17	0.44
1:A:464:GLU:OE1	3:A:1503:BGC:C6	2.66	0.43
1:A:191:ASP:OD1	1:A:261:ASP:HB3	2.19	0.43
1:A:248:HIS:HB3	4:A:2099:HOH:O	2.19	0.43
1:A:58:HIS:CD2	1:A:58:HIS:N	2.83	0.43
1:A:56:PHE:CA	1:A:60:HIS:HE1	2.29	0.43
1:B:238:HIS:CG	4:B:2135:HOH:O	2.72	0.43
1:A:98:SER:HA	1:A:139:THR:O	2.18	0.43
1:A:462:ASN:ND2	4:A:2190:HOH:O	2.42	0.43
1:A:303:ARG:HH22	1:A:312:PHE:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:GLU:CD	3:B:1503:BGC:H6C2	2.39	0.42
1:A:82:THR:HG23	4:A:2011:HOH:O	2.19	0.41
1:A:433:TYR:CE2	1:A:437:HIS:HE1	2.39	0.41
1:B:308:GLU:HG2	1:B:309:ARG:N	2.35	0.41
1:A:101:TRP:HB3	1:A:102:PRO:HD3	2.03	0.41
1:A:214:LEU:CD1	4:A:2072:HOH:O	2.68	0.41
1:A:262:VAL:HG11	1:A:389:LEU:HD21	2.01	0.41
1:B:464:GLU:OE2	3:B:1503:BGC:H6C2	2.21	0.41
1:A:224:LEU:HD13	1:A:350:VAL:O	2.19	0.41
1:B:60:HIS:O	1:B:60:HIS:HD2	1.87	0.41
1:A:114:ILE:O	1:A:116:PRO:HD3	2.21	0.40
1:A:96:ARG:HA	1:A:137:TYR:O	2.21	0.40
1:A:56:PHE:CA	1:A:60:HIS:CE1	3.04	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	489/512 (96%)	468 (96%)	20 (4%)	1 (0%)	47	38
1	B	489/512 (96%)	470 (96%)	18 (4%)	1 (0%)	47	38
All	All	978/1024 (96%)	938 (96%)	38 (4%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	SER
1	B	458	SER

### 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	423/441 (96%)	400 (95%)	23 (5%)	22	13
1	B	423/441 (96%)	401 (95%)	22 (5%)	23	14
All	All	846/882 (96%)	801 (95%)	45 (5%)	22	13

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	14	SER
1	A	52	ASN
1	A	55	HIS
1	A	70	SER
1	A	111	GLU
1	A	123	ARG
1	A	162	LYS
1	A	191	ASP
1	A	193	GLN
1	A	224	LEU
1	A	232	HIS
1	A	238	HIS
1	A	285	ASN
1	A	316	GLU
1	A	328	LEU
1	A	330	LEU
1	A	348	SER
1	A	386	LEU
1	A	419	LEU
1	A	429	LYS
1	A	459	LEU
1	A	462	ASN
1	B	13	LEU
1	B	52	ASN
1	B	55	HIS
1	B	60	HIS

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Mol	Chain	Res	Type
1	B	70	SER
1	B	86	LEU
1	B	111	GLU
1	B	162	LYS
1	B	191	ASP
1	B	193	GLN
1	B	224	LEU
1	B	232	HIS
1	B	238	HIS
1	B	285	ASN
1	B	328	LEU
1	B	330	LEU
1	B	348	SER
1	B	386	LEU
1	B	419	LEU
1	B	429	LYS
1	B	459	LEU
1	B	462	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	75	ASN
1	A	132	ASN
1	A	246	ASN
1	A	276	GLN
1	A	452	GLN
1	A	462	ASN
1	B	52	ASN
1	B	58	HIS
1	B	75	ASN
1	B	132	ASN
1	B	238	HIS
1	B	246	ASN
1	B	452	GLN
1	B	462	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are 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	HBO	B	1502	3	14,16,16	2.34	3 (21%)	18,23,23	3.62	8 (44%)
2	HBO	A	1502	3	14,16,16	2.11	3 (21%)	18,23,23	4.52	8 (44%)
3	BGC	A	1503	1,2	11,11,12	0.84	0	15,15,17	2.12	6 (40%)
3	BGC	B	1503	2	11,11,12	1.41	2 (18%)	15,15,17	3.47	8 (53%)

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	HBO	B	1502	3	-	2/2/18/18	0/2/2/2
2	HBO	A	1502	3	-	2/2/18/18	0/2/2/2
3	BGC	A	1503	1,2	-	2/2/19/22	0/1/1/1
3	BGC	B	1503	2	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1502	HBO	C4B-C1B	6.37	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1502	HBO	C4B-C1B	6.26	1.50	1.40
2	B	1502	HBO	O1A-C2B	4.22	1.49	1.38
2	B	1502	HBO	O1B-C1B	3.09	1.42	1.38
2	A	1502	HBO	O1A-C2B	3.02	1.46	1.38
3	B	1503	BGC	O3-C3	-2.23	1.37	1.43
2	A	1502	HBO	O1B-C1B	2.20	1.41	1.38
3	B	1503	BGC	C4-C5	-2.09	1.48	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1502	HBO	C4B-N3B-C3B	-12.51	109.96	126.20
2	B	1502	HBO	C4B-N3B-C3B	-9.77	113.51	126.20
2	A	1502	HBO	O1A-C2B-O1B	7.64	122.73	110.91
2	A	1502	HBO	C1B-O1B-C2B	-7.39	106.50	116.25
2	A	1502	HBO	OHB-N3B-C3B	7.28	124.19	116.94
3	B	1503	BGC	C1-C2-C3	6.25	117.34	109.67
3	B	1503	BGC	O3-C3-C4	-5.39	97.89	110.35
2	B	1502	HBO	OHB-N3B-C3B	5.34	122.26	116.94
3	B	1503	BGC	O5-C5-C6	5.33	115.56	107.20
2	B	1502	HBO	C1B-O1B-C2B	-5.15	109.45	116.25
2	B	1502	HBO	O3B-C3B-C2B	4.73	125.64	119.29
3	B	1503	BGC	O2-C2-C3	-4.57	100.98	110.14
3	B	1503	BGC	C3-C4-C5	-4.53	102.15	110.24
2	B	1502	HBO	O1A-C2B-O1B	4.52	117.91	110.91
2	B	1502	HBO	O1B-C1B-C8B	4.50	123.46	116.38
2	A	1502	HBO	O1B-C1B-C8B	4.36	123.24	116.38
3	B	1503	BGC	O5-C1-C2	-3.67	105.10	110.77
3	A	1503	BGC	C1-O5-C5	3.57	117.02	112.19
3	A	1503	BGC	C6-C5-C4	-3.32	105.22	113.00
3	A	1503	BGC	C1-C2-C3	3.06	113.42	109.67
3	A	1503	BGC	O4-C4-C3	2.88	117.01	110.35
3	A	1503	BGC	O5-C5-C6	2.84	111.65	107.20
3	A	1503	BGC	C3-C4-C5	-2.81	105.22	110.24
2	B	1502	HBO	C1B-C4B-N3B	-2.80	116.33	118.33
2	A	1502	HBO	O3B-C3B-C2B	2.74	122.97	119.29
2	A	1502	HBO	C1B-C4B-N3B	-2.56	116.50	118.33
3	B	1503	BGC	O5-C5-C4	-2.55	104.62	110.83
2	B	1502	HBO	C8B-C1B-C4B	-2.51	117.13	120.42
2	A	1502	HBO	C8B-C1B-C4B	-2.41	117.27	120.42
3	B	1503	BGC	O2-C2-C1	2.12	113.50	109.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1502	HBO	C8B-C7B-O7B-C9B
2	A	1502	HBO	C6B-C7B-O7B-C9B
2	B	1502	HBO	C6B-C7B-O7B-C9B
2	B	1502	HBO	C8B-C7B-O7B-C9B
3	A	1503	BGC	O5-C5-C6-O6
3	A	1503	BGC	C4-C5-C6-O6
3	B	1503	BGC	O5-C5-C6-O6
3	B	1503	BGC	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1502	HBO	1	0
3	A	1503	BGC	17	0
3	B	1503	BGC	17	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	491/512 (95%)	0.43	44 (8%) 9 10	7, 15, 26, 44	1 (0%)
1	B	491/512 (95%)	0.21	23 (4%) 31 34	7, 15, 26, 39	1 (0%)
All	All	982/1024 (95%)	0.32	67 (6%) 17 19	7, 15, 26, 44	2 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	HIS	7.5
1	A	55	HIS	6.8
1	A	60	HIS	6.2
1	B	60	HIS	5.7
1	B	58	HIS	5.1
1	B	55	HIS	5.1
1	A	238	HIS	4.8
1	A	232	HIS	4.7
1	B	238	HIS	4.7
1	B	232	HIS	4.4
1	B	501	ALA	4.1
1	B	457	TRP	3.6
1	B	458	SER	3.6
1	A	210	CYS	3.4
1	A	217	ALA	3.3
1	A	501	ALA	3.2
1	A	418	PRO	3.1
1	A	218	TYR	3.1
1	A	214	LEU	3.1
1	A	417	THR	3.0
1	B	459	LEU	3.0
1	A	59	ASN	3.0
1	B	252	ASP	3.0
1	A	414	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	33	ALA	2.9
1	B	13	LEU	2.9
1	A	259	ALA	2.9
1	A	57	CYS	2.8
1	B	111	GLU	2.8
1	A	457	TRP	2.8
1	A	148	ALA	2.8
1	A	140	ILE	2.7
1	B	456	ALA	2.7
1	B	502	LYS	2.7
1	B	482	ASN	2.7
1	A	319	GLU	2.6
1	A	502	LYS	2.6
1	B	346	ASN	2.5
1	A	481	ASN	2.5
1	A	213	GLY	2.5
1	A	153	TYR	2.5
1	A	315	ASP	2.4
1	B	12	MET	2.4
1	A	216	CYS	2.4
1	A	458	SER	2.4
1	A	12	MET	2.4
1	B	27	ASP	2.3
1	A	416	GLU	2.3
1	A	415	LYS	2.3
1	A	143	TRP	2.2
1	B	139	THR	2.2
1	A	111	GLU	2.2
1	A	365	PRO	2.2
1	A	220	THR	2.2
1	A	120	LYS	2.2
1	A	139	THR	2.1
1	A	15	PRO	2.1
1	A	252	ASP	2.1
1	A	366	ASP	2.1
1	B	405	THR	2.1
1	B	415	LYS	2.1
1	A	211	SER	2.1
1	B	140	ILE	2.1
1	A	422	GLU	2.0
1	A	43	TRP	2.0
1	A	215	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	234	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HBO	B	1502	15/15	0.53	0.44	42,47,48,50	0
2	HBO	A	1502	15/15	0.59	0.46	39,44,47,48	0
3	BGC	A	1503	11/12	0.71	0.31	19,33,38,42	0
3	BGC	B	1503	11/12	0.78	0.30	19,31,36,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.