



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:51 am BST

PDB ID : 1E4N  
Title : Crystal structure of the inactive mutant Monocot (Maize ZMGlu1) beta-glucosidase ZMGluE191D in complex with the natural aglycone DIMBOA  
Authors : Czjzek, M.; Cicek, M.; Bevan, D.R.; Zamboni, V.; Henrissat, B.; Esen, A.  
Deposited on : 2000-07-11  
Resolution : 2.10 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

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

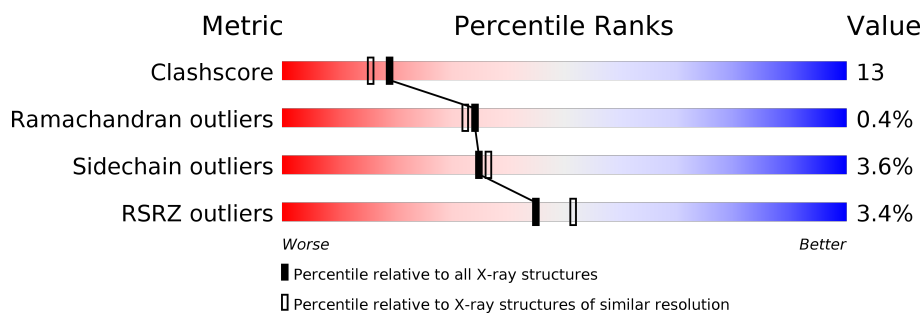
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	
1	B	512	

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	514	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8382 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.

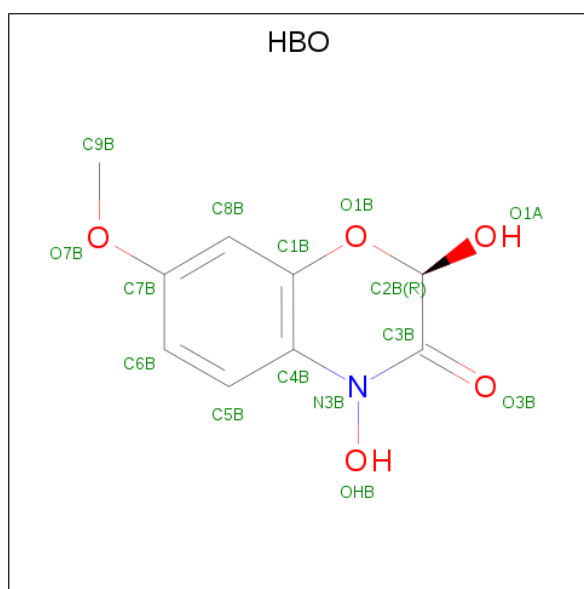
- Molecule 1 is a protein called BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3958	2538	655	748	17			
1	B	489	Total	C	N	O	S	0	0	0
			3958	2538	655	748	17			

There are 2 discrepancies between the modelled and reference sequences:

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

Continued on next page...

*Continued from previous page...*

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

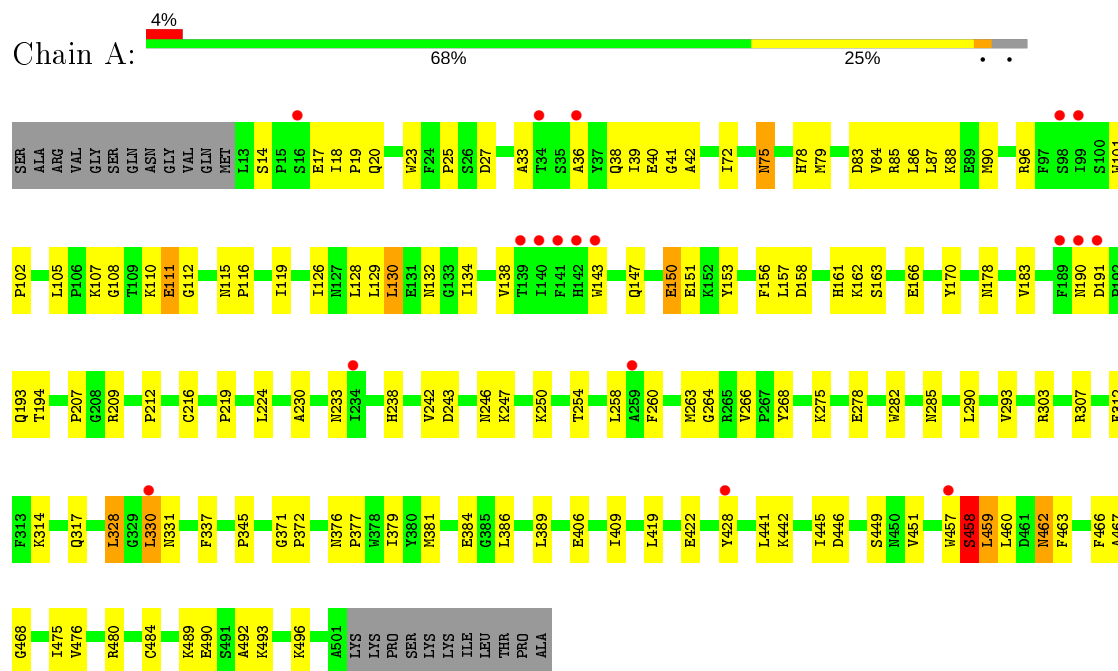
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	229	Total	O	0	0
			229	229		
3	B	207	Total	O	0	0
			207	207		

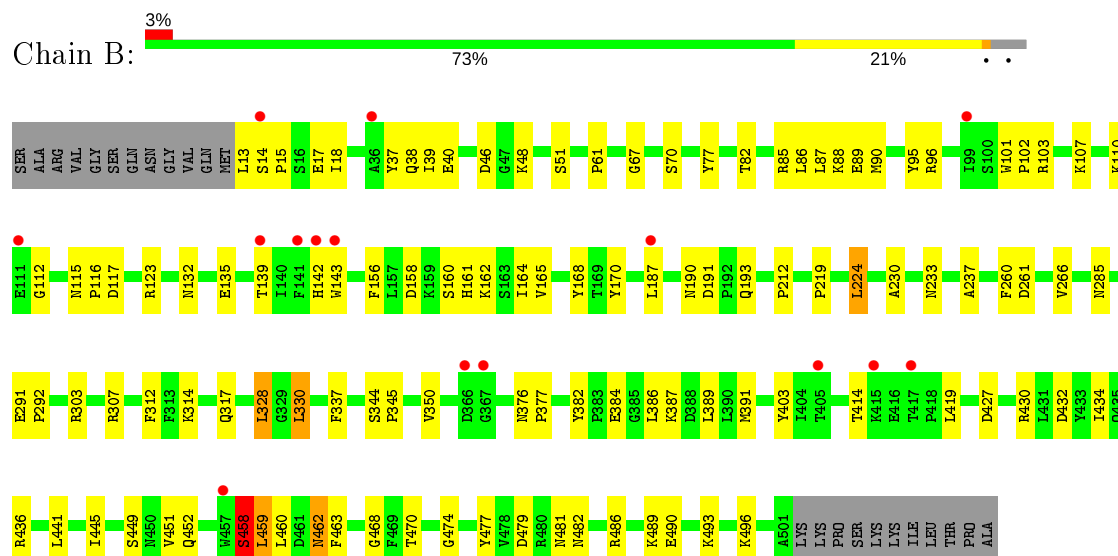
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.57Å 95.31Å 117.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.10 29.08 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.00-2.10) 96.2 (29.08-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.223 , 0.269 0.210 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.42	0/4079	0.61	0/5539
1	B	0.40	0/4079	0.61	0/5539
All	All	0.41	0/8158	0.61	0/11078

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	3958	0	3748	119	0
1	B	3958	0	3748	84	0
2	A	15	0	9	9	0
2	B	15	0	9	0	0
3	A	229	0	0	11	0
3	B	207	0	0	11	0
All	All	8382	0	7514	201	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 13.

All (201) 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:191:ASP:OD2	1:A:194:THR:HB	1.43	1.19
1:A:467:ALA:HB2	2:A:514:HBO:H9B3	1.38	1.04
1:A:191:ASP:OD2	1:A:194:THR:CB	2.06	1.03
1:A:406:GLU:OE2	3:A:2192:HOH:O	1.91	0.87
1:A:191:ASP:CG	1:A:194:THR:HB	1.93	0.87
1:B:376:ASN:HB2	1:B:377:PRO:HD2	1.57	0.86
1:A:376:ASN:HB2	1:A:377:PRO:HD2	1.58	0.85
1:A:191:ASP:OD2	1:A:191:ASP:O	1.95	0.85
1:A:79:MET:SD	3:A:2218:HOH:O	2.37	0.83
1:A:466:PHE:CZ	2:A:514:HBO:H6B	2.16	0.81
1:B:160:SER:OG	3:B:2066:HOH:O	2.01	0.78
1:A:467:ALA:CB	2:A:514:HBO:H9B3	2.12	0.78
1:B:162:LYS:HB2	3:B:2066:HOH:O	1.85	0.74
1:B:88:LYS:HD2	1:B:132:ASN:HD22	1.53	0.73
1:B:427:ASP:HA	3:B:2183:HOH:O	1.89	0.73
1:A:150:GLU:HG2	3:A:2067:HOH:O	1.90	0.71
1:A:263:MET:HE3	3:A:2109:HOH:O	1.89	0.71
1:A:489:LYS:O	1:A:493:LYS:HG2	1.91	0.70
1:A:466:PHE:HZ	2:A:514:HBO:H6B	1.56	0.69
1:B:135:GLU:OE1	3:B:2057:HOH:O	2.11	0.69
1:B:88:LYS:CD	1:B:132:ASN:HD22	2.06	0.69
1:B:77:TYR:HB3	3:B:2015:HOH:O	1.93	0.69
1:A:84:VAL:HG11	1:A:128:LEU:HG	1.75	0.68
1:B:13:LEU:HD13	1:B:436:ARG:NH1	2.09	0.68
1:A:126:ILE:O	1:A:130:LEU:HD22	1.94	0.67
1:A:191:ASP:CG	1:A:194:THR:CB	2.60	0.67
1:B:101:TRP:HB3	1:B:102:PRO:HD3	1.76	0.66
1:A:442:LYS:HE2	1:A:446:ASP:OD2	1.95	0.66
1:A:191:ASP:OD1	1:A:194:THR:OG1	2.14	0.65
1:A:147:GLN:O	1:A:151:GLU:HG3	1.96	0.65
1:A:90:MET:HE1	1:A:492:ALA:HA	1.77	0.65
1:B:13:LEU:HD13	1:B:436:ARG:HH12	1.64	0.63
1:A:107:LYS:HD2	1:A:112:GLY:HA2	1.80	0.63
1:A:466:PHE:CZ	2:A:514:HBO:C6B	2.81	0.63
1:A:90:MET:HE1	1:A:475:ILE:HD12	1.79	0.62
1:B:449:SER:OG	1:B:451:VAL:HG23	2.00	0.62
1:A:38:GLN:O	1:A:462:ASN:HB2	2.00	0.61
1:B:441:LEU:O	1:B:445:ILE:HG13	2.00	0.61
1:A:263:MET:HE2	3:A:2110:HOH:O	2.00	0.61
1:B:414:THR:HG22	1:B:470:THR:HB	1.83	0.61
1:A:330:LEU:HG	1:A:389:LEU:HD21	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:THR:O	1:B:86:LEU:HD23	2.02	0.59
1:B:38:GLN:O	1:B:462:ASN:HB2	2.03	0.59
1:B:432:ASP:O	1:B:436:ARG:HG3	2.03	0.59
1:A:75:ASN:HD21	1:A:78:HIS:HD2	1.49	0.58
1:B:384:GLU:HG2	3:B:2163:HOH:O	2.02	0.58
1:A:459:LEU:HD13	1:A:460:LEU:HG	1.84	0.58
1:A:459:LEU:O	1:A:476:VAL:HB	2.04	0.58
1:A:303:ARG:NH2	1:A:312:PHE:HA	2.19	0.57
1:B:88:LYS:HD2	1:B:132:ASN:HB3	1.85	0.57
1:B:142:HIS:CE1	1:B:190:ASN:HD22	2.23	0.57
1:A:191:ASP:OD1	1:A:194:THR:CB	2.53	0.57
1:A:260:PHE:HE1	1:A:328:LEU:HG	1.71	0.56
1:A:441:LEU:O	1:A:445:ILE:HG13	2.05	0.56
1:A:307:ARG:NH1	3:A:2136:HOH:O	2.38	0.56
1:B:156:PHE:O	1:B:230:ALA:HA	2.06	0.56
1:B:90:MET:O	1:B:496:LYS:HA	2.05	0.56
1:A:238:HIS:O	1:A:242:VAL:HG23	2.05	0.56
1:A:314:LYS:HB2	1:A:317:GLN:HG3	1.87	0.56
1:B:489:LYS:O	1:B:493:LYS:HG2	2.05	0.55
1:A:14:SER:HB3	1:A:17:GLU:CD	2.28	0.54
1:A:246:ASN:ND2	3:A:2099:HOH:O	2.41	0.54
1:A:96:ARG:NH2	1:A:190:ASN:CG	2.61	0.54
1:A:86:LEU:O	1:A:90:MET:HG3	2.08	0.54
1:A:161:HIS:HA	1:A:233:ASN:OD1	2.08	0.54
1:B:110:LYS:HE2	1:B:170:TYR:CE1	2.43	0.54
1:A:384:GLU:HA	1:A:384:GLU:OE1	2.08	0.53
1:B:161:HIS:HA	1:B:233:ASN:OD1	2.09	0.53
1:B:382:TYR:CE2	1:B:384:GLU:HB3	2.43	0.53
1:A:463:PHE:CE1	1:A:468:GLY:HA2	2.44	0.53
1:B:165:VAL:HG23	1:B:237:ALA:HA	1.89	0.53
1:B:191:ASP:OD1	1:B:261:ASP:HB3	2.08	0.53
1:A:101:TRP:N	1:A:102:PRO:HD2	2.24	0.53
1:B:143:TRP:N	1:B:143:TRP:CD1	2.76	0.52
1:A:466:PHE:CE2	2:A:514:HBO:H9B1	2.44	0.52
1:A:90:MET:CE	1:A:475:ILE:HD12	2.40	0.51
1:A:90:MET:CE	1:A:492:ALA:HA	2.39	0.51
1:A:119:ILE:HG21	1:A:178:ASN:ND2	2.25	0.51
1:B:110:LYS:HG3	1:B:170:TYR:CZ	2.45	0.51
1:B:303:ARG:NH2	1:B:312:PHE:HA	2.25	0.51
1:B:260:PHE:HE1	1:B:328:LEU:HG	1.75	0.51
1:A:238:HIS:CE1	1:A:258:LEU:HD22	2.45	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LYS:HE3	3:A:2049:HOH:O	2.10	0.51
1:A:96:ARG:NH2	1:A:190:ASN:OD1	2.44	0.51
1:A:480:ARG:HG2	1:A:484:CYS:SG	2.51	0.51
1:A:156:PHE:O	1:A:230:ALA:HA	2.10	0.50
1:B:107:LYS:HB2	1:B:112:GLY:HA3	1.92	0.50
1:A:88:LYS:HD3	1:A:132:ASN:HB3	1.94	0.50
1:B:462:ASN:HD22	1:B:462:ASN:C	2.16	0.49
1:B:463:PHE:CE1	1:B:468:GLY:HA2	2.47	0.49
1:A:303:ARG:HH22	1:A:312:PHE:HA	1.77	0.49
1:A:459:LEU:HD13	1:A:460:LEU:CD2	2.43	0.49
1:A:20:GLN:HB2	1:A:23:TRP:CD1	2.47	0.49
1:A:162:LYS:O	1:A:166:GLU:HG3	2.13	0.48
1:B:382:TYR:CZ	1:B:384:GLU:HB3	2.48	0.48
1:B:96:ARG:HD2	1:B:187:LEU:HD12	1.95	0.48
1:B:212:PRO:HA	1:B:219:PRO:O	2.14	0.48
1:A:84:VAL:HG22	1:A:129:LEU:CD2	2.43	0.48
1:B:164:ILE:HG23	1:B:165:VAL:N	2.29	0.48
1:A:268:TYR:HA	1:A:337:PHE:HB3	1.95	0.47
1:A:87:LEU:HD21	1:A:459:LEU:HG	1.95	0.47
1:A:153:TYR:CE2	1:A:163:SER:HB3	2.50	0.47
1:A:14:SER:HB3	1:A:17:GLU:CG	2.44	0.47
1:A:466:PHE:CZ	2:A:514:HBO:H9B1	2.49	0.47
1:A:307:ARG:NH2	1:B:307:ARG:HG3	2.29	0.47
1:A:33:ALA:HB2	1:A:96:ARG:HB3	1.96	0.47
1:A:331:ASN:HB3	1:A:406:GLU:HB2	1.96	0.47
1:A:312:PHE:CD2	1:B:345:PRO:HD3	2.50	0.47
1:A:105:LEU:O	1:A:108:GLY:N	2.42	0.47
1:A:138:VAL:HG21	1:A:183:VAL:HG21	1.96	0.47
1:A:216:CYS:O	1:A:219:PRO:HD3	2.15	0.47
1:A:41:GLY:HA3	1:A:72:ILE:O	2.15	0.46
1:B:38:GLN:HG2	1:B:463:PHE:O	2.15	0.46
1:A:191:ASP:CG	1:A:194:THR:OG1	2.53	0.46
1:B:458:SER:O	1:B:474:GLY:HA2	2.15	0.46
1:A:191:ASP:OD2	1:A:194:THR:N	2.48	0.46
1:B:477:TYR:O	1:B:486:ARG:HA	2.15	0.46
1:A:110:LYS:HA	1:A:170:TYR:CE2	2.50	0.46
1:A:475:ILE:O	1:A:492:ALA:HB2	2.16	0.46
1:B:142:HIS:CE1	1:B:190:ASN:ND2	2.83	0.46
1:B:330:LEU:HG	1:B:389:LEU:HD21	1.97	0.46
1:A:462:ASN:C	1:A:462:ASN:HD22	2.20	0.46
1:A:480:ARG:NH1	1:A:480:ARG:HB2	2.30	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:TRP:N	1:A:143:TRP:CD1	2.82	0.45
1:A:266:VAL:O	1:A:337:PHE:HA	2.16	0.45
1:B:162:LYS:N	3:B:2066:HOH:O	2.49	0.45
1:A:83:ASP:O	1:A:87:LEU:HG	2.17	0.45
1:B:224:LEU:HD13	1:B:350:VAL:O	2.16	0.45
1:B:46:ASP:HB3	1:B:117:ASP:CB	2.46	0.45
1:B:85:ARG:O	1:B:89:GLU:HG3	2.16	0.45
1:A:212:PRO:HA	1:A:219:PRO:O	2.18	0.44
2:A:514:HBO:H9B2	3:A:2216:HOH:O	2.16	0.44
1:A:101:TRP:HB2	3:A:2066:HOH:O	2.17	0.44
1:A:115:ASN:HA	1:A:116:PRO:HD2	1.86	0.44
1:A:449:SER:OG	1:A:451:VAL:HG23	2.17	0.44
1:A:345:PRO:HD3	1:B:312:PHE:CD2	2.52	0.44
1:A:441:LEU:HD22	1:A:451:VAL:HG11	2.00	0.44
1:B:266:VAL:O	1:B:337:PHE:HA	2.17	0.44
1:A:191:ASP:OD2	1:A:194:THR:OG1	2.36	0.44
1:A:14:SER:HB3	1:A:17:GLU:OE2	2.17	0.43
1:B:87:LEU:HD13	1:B:95:TYR:HB2	2.00	0.43
1:A:331:ASN:CB	1:A:406:GLU:HB2	2.48	0.43
1:A:371:GLY:HA3	1:A:381:MET:O	2.18	0.43
1:B:37:TYR:CZ	1:B:70:SER:HB3	2.53	0.43
1:B:490:GLU:O	1:B:493:LYS:HB2	2.17	0.43
1:A:191:ASP:OD2	1:A:191:ASP:C	2.56	0.43
1:B:427:ASP:OD2	1:B:430:ARG:HD2	2.18	0.43
1:A:39:ILE:HG13	1:A:40:GLU:N	2.32	0.43
1:A:467:ALA:HB2	2:A:514:HBO:C9B	2.27	0.43
1:A:84:VAL:HG22	1:A:129:LEU:HD23	2.00	0.43
1:B:88:LYS:HD3	1:B:132:ASN:HD22	1.83	0.43
1:B:414:THR:HB	3:B:2181:HOH:O	2.18	0.43
1:B:51:SER:HB3	1:B:102:PRO:HG2	2.00	0.42
1:A:250:LYS:HE3	3:A:2099:HOH:O	2.18	0.42
1:B:430:ARG:O	1:B:434:ILE:HG13	2.19	0.42
1:B:479:ASP:OD2	1:B:481:ASN:HB2	2.19	0.42
1:A:33:ALA:HA	1:A:96:ARG:O	2.20	0.42
1:B:387:LYS:NZ	3:B:2190:HOH:O	2.49	0.42
1:A:111:GLU:CD	1:A:111:GLU:H	2.23	0.42
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.90	0.42
1:B:139:THR:HA	1:B:187:LEU:HB2	2.01	0.42
1:B:14:SER:O	1:B:17:GLU:HB2	2.20	0.42
1:B:291:GLU:N	1:B:292:PRO:CD	2.83	0.42
1:B:314:LYS:HB2	1:B:317:GLN:HG3	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PRO:O	1:B:67:GLY:HA2	2.20	0.42
1:A:36:ALA:O	1:A:40:GLU:HB2	2.20	0.42
1:A:87:LEU:HB3	1:A:134:ILE:HD13	2.02	0.42
1:A:18:ILE:HA	1:A:19:PRO:HD3	1.89	0.41
1:A:428:TYR:CZ	1:A:490:GLU:HG3	2.54	0.41
1:B:303:ARG:HH22	1:B:312:PHE:HA	1.84	0.41
1:A:243:ASP:OD2	1:A:247:LYS:HE3	2.21	0.41
1:B:459:LEU:HD13	1:B:460:LEU:HG	2.02	0.41
1:A:264:GLY:HA2	1:A:282:TRP:CH2	2.55	0.41
1:B:168:TYR:CD2	1:B:237:ALA:HB1	2.55	0.41
1:B:115:ASN:HA	1:B:116:PRO:HD2	1.88	0.41
1:A:191:ASP:OD2	1:A:194:THR:CA	2.67	0.41
1:A:459:LEU:HD13	1:A:460:LEU:CG	2.48	0.41
1:B:260:PHE:CE1	1:B:328:LEU:HG	2.53	0.41
1:B:376:ASN:HB2	1:B:377:PRO:CD	2.40	0.41
1:A:41:GLY:O	1:A:42:ALA:C	2.59	0.41
1:B:14:SER:HB3	1:B:17:GLU:CD	2.41	0.41
1:A:25:PRO:HB2	1:A:27:ASP:OD1	2.20	0.41
1:A:372:PRO:HG2	1:A:381:MET:HB3	2.02	0.41
1:A:376:ASN:HB2	1:A:377:PRO:CD	2.38	0.41
1:A:38:GLN:HG2	1:A:463:PHE:O	2.21	0.41
1:A:207:PRO:HG2	1:A:209:ARG:HG3	2.02	0.41
1:A:250:LYS:HE2	1:A:254:THR:O	2.20	0.41
1:B:387:LYS:HG2	3:B:2164:HOH:O	2.20	0.41
1:B:403:TYR:CZ	1:B:452:GLN:HB2	2.56	0.41
1:B:39:ILE:HG13	1:B:40:GLU:N	2.34	0.41
1:B:458:SER:HB3	1:B:474:GLY:HA2	2.03	0.41
1:A:290:LEU:O	1:A:293:VAL:HG22	2.21	0.40
1:B:15:PRO:HA	1:B:18:ILE:HG12	2.03	0.40
1:A:275:LYS:HD2	1:A:278:GLU:OE1	2.22	0.40
1:B:436:ARG:HH11	1:B:436:ARG:HG2	1.85	0.40
1:B:87:LEU:HD21	1:B:459:LEU:HG	2.03	0.40
1:A:379:ILE:CD1	1:A:409:ILE:HA	2.51	0.40
1:A:457:TRP:O	1:A:458:SER:CB	2.68	0.40
1:B:14:SER:HB3	1:B:17:GLU:CG	2.52	0.40
1:B:48:LYS:HE3	3:B:2020:HOH:O	2.21	0.40
1:B:48:LYS:HG3	1:B:103:ARG:HA	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	487/512 (95%)	465 (96%)	20 (4%)	2 (0%)	34	32
1	B	487/512 (95%)	461 (95%)	24 (5%)	2 (0%)	34	32
All	All	974/1024 (95%)	926 (95%)	44 (4%)	4 (0%)	34	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	ASP
1	A	458	SER
1	B	458	SER
1	A	158	ASP

### 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	422/441 (96%)	406 (96%)	16 (4%)	33	34
1	B	422/441 (96%)	408 (97%)	14 (3%)	38	40
All	All	844/882 (96%)	814 (96%)	30 (4%)	35	36

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	85	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	111	GLU
1	A	130	LEU
1	A	150	GLU
1	A	193	GLN
1	A	224	LEU
1	A	285	ASN
1	A	328	LEU
1	A	330	LEU
1	A	386	LEU
1	A	419	LEU
1	A	422	GLU
1	A	458	SER
1	A	459	LEU
1	A	462	ASN
1	B	123	ARG
1	B	193	GLN
1	B	224	LEU
1	B	285	ASN
1	B	328	LEU
1	B	330	LEU
1	B	344	SER
1	B	386	LEU
1	B	391	MET
1	B	419	LEU
1	B	458	SER
1	B	459	LEU
1	B	462	ASN
1	B	482	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	59	ASN
1	A	78	HIS
1	A	178	ASN
1	A	246	ASN
1	A	276	GLN
1	A	426	ASN
1	A	452	GLN
1	A	462	ASN
1	A	481	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	499	ASN
1	B	20	GLN
1	B	59	ASN
1	B	75	ASN
1	B	124	ASN
1	B	132	ASN
1	B	246	ASN
1	B	276	GLN
1	B	426	ASN
1	B	452	GLN
1	B	462	ASN
1	B	481	ASN
1	B	499	ASN

### 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](#)

2 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	514	-	14,16,16	3.78	6 (42%)	18,23,23	3.10	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HBO	A	514	-	14,16,16	3.70	6 (42%)	18,23,23	3.17	4 (22%)

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	514	-	-	2/2/18/18	0/2/2/2
2	HBO	A	514	-	-	2/2/18/18	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	514	HBO	OHB-N3B	8.02	1.49	1.39
2	B	514	HBO	OHB-N3B	7.32	1.49	1.39
2	B	514	HBO	C4B-N3B	6.59	1.47	1.39
2	A	514	HBO	O1B-C1B	6.56	1.46	1.38
2	B	514	HBO	O1B-C1B	6.43	1.46	1.38
2	A	514	HBO	C4B-N3B	6.33	1.47	1.39
2	B	514	HBO	O7B-C7B	5.97	1.50	1.37
2	A	514	HBO	O7B-C7B	5.38	1.48	1.37
2	A	514	HBO	O1A-C2B	2.35	1.44	1.38
2	B	514	HBO	C8B-C7B	2.25	1.42	1.38
2	B	514	HBO	O1A-C2B	2.21	1.43	1.38
2	A	514	HBO	O7B-C9B	2.08	1.49	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	514	HBO	C4B-N3B-C3B	-10.55	112.50	126.20
2	B	514	HBO	C4B-N3B-C3B	-9.56	113.78	126.20
2	B	514	HBO	OHB-N3B-C3B	-7.33	109.64	116.94
2	A	514	HBO	OHB-N3B-C3B	-5.36	111.61	116.94
2	A	514	HBO	C1B-C4B-N3B	5.00	121.91	118.33
2	B	514	HBO	C1B-C4B-N3B	3.14	120.57	118.33
2	A	514	HBO	C9B-O7B-C7B	-2.89	111.25	117.51
2	B	514	HBO	C9B-O7B-C7B	-2.42	112.27	117.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	514	HBO	C6B-C7B-O7B-C9B
2	B	514	HBO	C8B-C7B-O7B-C9B
2	A	514	HBO	C8B-C7B-O7B-C9B
2	A	514	HBO	C6B-C7B-O7B-C9B

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	514	HBO	9	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	489/512 (95%)	0.07	18 (3%)	41 48	28, 40, 54, 68	1 (0%)
1	B	489/512 (95%)	0.04	15 (3%)	49 55	28, 39, 54, 63	1 (0%)
All	All	978/1024 (95%)	0.05	33 (3%)	45 51	28, 40, 55, 68	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ASP	3.6
1	A	428	TYR	3.4
1	A	141	PHE	3.1
1	B	415	LYS	3.0
1	B	139	THR	2.9
1	B	14	SER	2.9
1	A	140	ILE	2.8
1	A	457	TRP	2.7
1	B	457	TRP	2.7
1	A	189	PHE	2.7
1	A	142	HIS	2.7
1	B	99	ILE	2.7
1	A	143	TRP	2.6
1	A	190	ASN	2.6
1	B	143	TRP	2.6
1	A	139	THR	2.5
1	A	34	THR	2.5
1	A	98	SER	2.5
1	A	259	ALA	2.4
1	B	367	GLY	2.4
1	B	141	PHE	2.4
1	A	36	ALA	2.3
1	B	417	THR	2.3
1	A	16	SER	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	142	HIS	2.1
1	A	234	ILE	2.1
1	B	366	ASP	2.1
1	B	36	ALA	2.1
1	A	99	ILE	2.0
1	A	330	LEU	2.0
1	B	405	THR	2.0
1	B	111	GLU	2.0
1	B	187	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. 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	A	514	15/15	0.61	0.29	53,55,56,57	15
2	HBO	B	514	15/15	0.75	0.24	59,61,61,61	15

## 6.5 Other polymers [i](#)

There are no such residues in this entry.