



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:59 pm GMT

PDB ID : 1E56
Title : Crystal structure of the inactive mutant Monocot (Maize ZMGlu1) beta-glucosidase ZMGluE191D in complex with the natural substrate DIMBOA -beta-D-glucoside
Authors : Czjzek, M.; Cicek, M.; Bevan, D.R.; Zamboni, V.; Henrissat, B.; Esen, A.
Deposited on : 2000-07-18
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

A user guide is available at

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

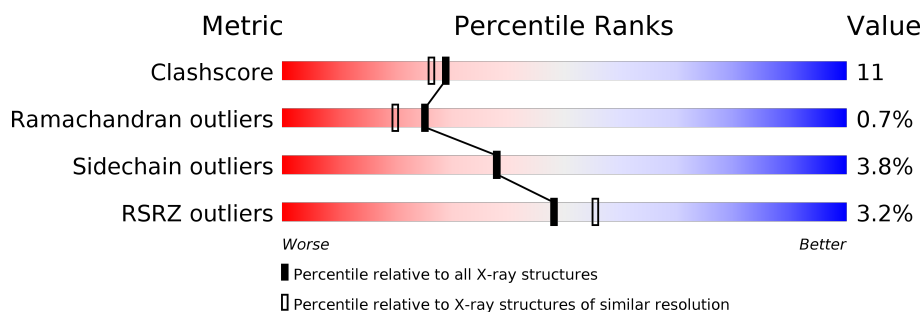
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 ≥ 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	512	<div> <div>3%</div> <div>74%</div> <div>19%</div> <div>• •</div> </div>
1	B	512	<div> <div>3%</div> <div>77%</div> <div>16%</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	BGC	A	513[A]	-	-	-	X
2	BGC	A	513[B]	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	B	513	-	-	-	X
3	HBO	A	514[A]	X	-	X	X
3	HBO	A	514[B]	X	-	-	X
3	HBO	B	514	X	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8316 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.

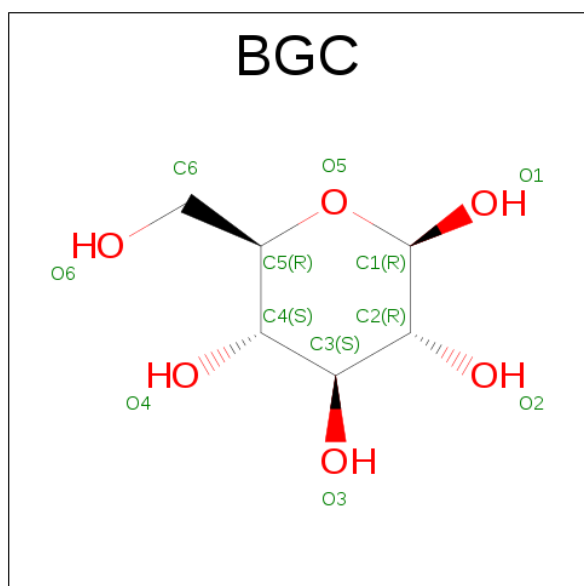
- Molecule 1 is a protein called BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	2	1
			3959	2538	656	748	17			
1	B	490	Total	C	N	O	S	0	2	1
			3959	2538	656	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 SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C₆H₁₂O₆).



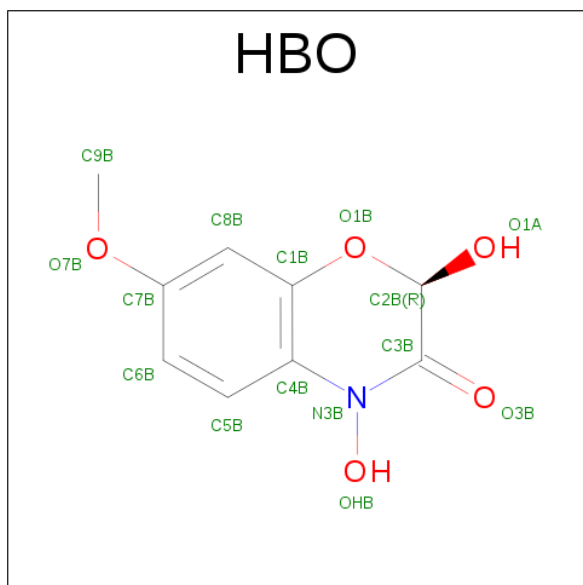
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			24	12	12		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 2,4-DIHYDROXY-7-(METHYLOXY)-2H-1,4-BENZOXAZIN-3(4H)-ONE (three-letter code: HBO) (formula: C₉H₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			28	18	2	8		
3	B	1	Total	C	N	O	0	0
			14	9	1	4		

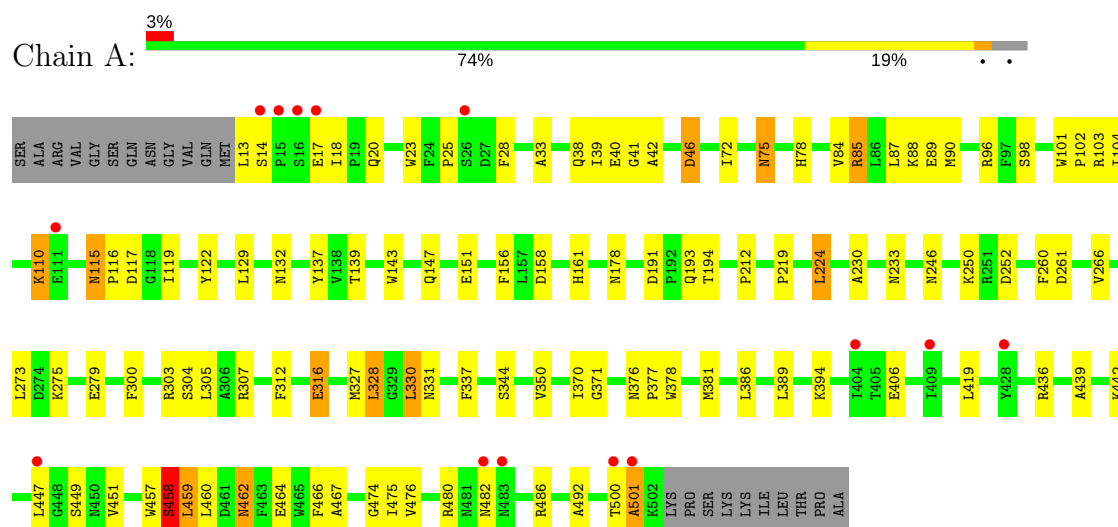
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	168	Total	O	0	0
			168	168		
4	B	152	Total	O	0	0
			152	152		

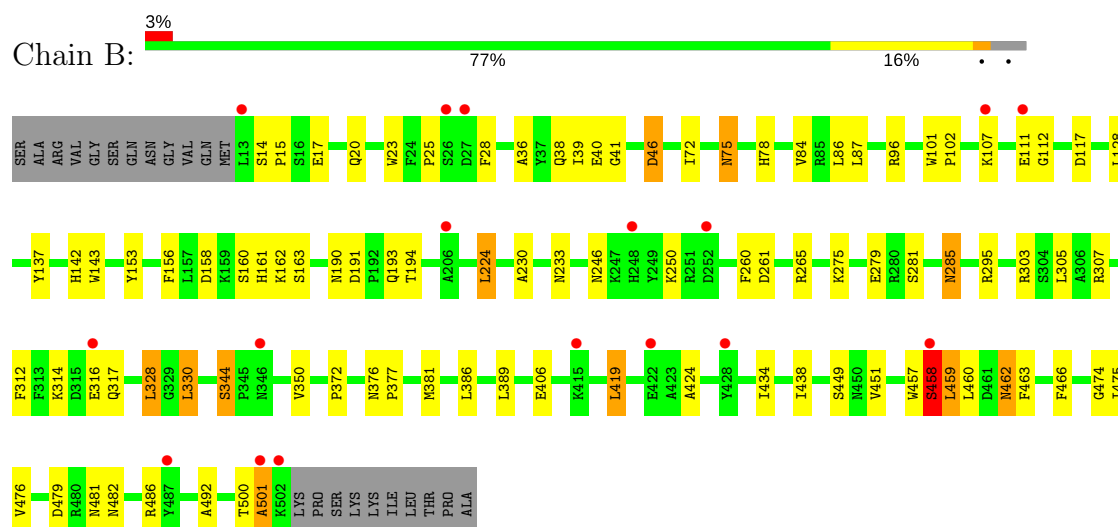
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, α , β , γ	93.10Å 95.30Å 119.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.10 19.74 – 1.99	Depositor EDS
% Data completeness (in resolution range)	93.6 (29.00-2.10) 91.6 (19.74-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.99Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.267 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8316	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.43	0/4080	0.60	0/5541
1	B	0.42	0/4080	0.60	0/5541
All	All	0.42	0/8160	0.60	0/11082

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	3959	0	3744	97	0
1	B	3959	0	3744	69	0
2	A	24	0	20	4	0
2	B	12	0	11	2	0
3	A	28	0	14	13	0
3	B	14	0	7	4	0
4	A	168	0	0	7	0
4	B	152	0	0	7	0
All	All	8316	0	7540	169	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 (169) 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)
2:A:513[B]:BGC:O1	2:A:513[B]:BGC:C1	1.70	1.37
1:B:406:GLU:OE1	2:B:513:BGC:O2	1.66	1.13
1:A:85:ARG:HE	1:A:85:ARG:HA	1.24	1.00
3:A:514[B]:HBO:H9B1	4:A:2163:HOH:O	1.75	0.86
1:A:304:SER:HB2	4:B:2103:HOH:O	1.77	0.83
3:B:514:HBO:H9B1	4:B:2148:HOH:O	1.78	0.82
3:A:514[A]:HBO:C9B	4:A:2163:HOH:O	2.28	0.81
1:A:191:ASP:OD1	1:A:194:THR:HB	1.82	0.79
3:A:514[A]:HBO:H9B2	4:A:2163:HOH:O	1.83	0.77
1:A:376:ASN:HB2	1:A:377:PRO:HD2	1.66	0.76
1:A:85:ARG:NE	1:A:85:ARG:HA	2.02	0.75
1:A:191:ASP:OD1	1:A:194:THR:CB	2.37	0.73
1:A:14:SER:HB3	1:A:17:GLU:CD	2.10	0.71
1:A:406:GLU:OE1	2:A:513[A]:BGC:H3	1.91	0.71
1:B:449:SER:OG	1:B:451:VAL:HG23	1.91	0.70
1:A:457:TRP:O	1:A:458:SER:HB2	1.93	0.68
1:B:261:ASP:HB2	4:B:2086:HOH:O	1.94	0.67
1:B:75:ASN:HD21	1:B:78:HIS:HD2	1.41	0.66
1:A:378:TRP:CD2	3:A:514[A]:HBO:OHB	2.49	0.65
1:B:457:TRP:O	1:B:458:SER:HB2	1.98	0.64
1:B:191:ASP:OD1	1:B:261:ASP:HB3	1.99	0.63
1:A:406:GLU:OE1	2:A:513[B]:BGC:O2	2.11	0.61
1:A:300:PHE:HB3	4:B:2097:HOH:O	2.01	0.61
1:B:275:LYS:O	1:B:279:GLU:HG3	2.00	0.61
1:A:449:SER:OG	1:A:451:VAL:HG23	2.01	0.61
2:A:513[A]:BGC:HA	3:A:514[A]:HBO:C2B	2.07	0.60
3:A:514[A]:HBO:H9B1	4:A:2163:HOH:O	1.96	0.60
1:A:90:MET:HE1	1:A:475:ILE:HD12	1.84	0.60
1:B:246:ASN:ND2	1:B:250:LYS:HD2	2.16	0.60
1:A:330:LEU:HG	1:A:389:LEU:HD21	1.83	0.59
1:B:38:GLN:HG2	1:B:463:PHE:O	2.02	0.59
1:A:110:LYS:NZ	1:A:110:LYS:HB2	2.17	0.59
1:A:459:LEU:HD13	1:A:460:LEU:HG	1.84	0.59
1:A:458:SER:HB3	1:A:474:GLY:HA2	1.85	0.57
1:B:458:SER:HB3	1:B:474:GLY:HA2	1.85	0.57
1:A:115:ASN:HD22	1:A:116:PRO:HD2	1.68	0.57
1:B:142:HIS:CE1	2:B:513:BGC:O3	2.57	0.57
1:B:75:ASN:HD21	1:B:78:HIS:CD2	2.22	0.57
1:A:115:ASN:HD22	1:A:116:PRO:CD	2.17	0.57
1:B:305:LEU:HG	4:B:2103:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:HB2	1:B:112:GLY:HA3	1.88	0.56
1:A:110:LYS:HG2	4:A:2048:HOH:O	2.05	0.56
1:A:344:SER:HA	1:B:312:PHE:CE1	2.42	0.55
1:B:87:LEU:HD21	1:B:459:LEU:HG	1.87	0.55
1:A:191:ASP:OD1	1:A:191:ASP:O	2.24	0.55
1:A:378:TRP:CE3	3:A:514[A]:HBO:OHB	2.59	0.55
1:B:458:SER:O	1:B:474:GLY:HA2	2.07	0.55
1:B:38:GLN:O	1:B:462:ASN:HB2	2.06	0.55
1:A:38:GLN:O	1:A:462:ASN:HB2	2.06	0.54
1:A:191:ASP:OD1	1:A:261:ASP:OD1	2.24	0.54
1:B:376:ASN:HB2	1:B:377:PRO:CD	2.37	0.54
1:A:246:ASN:ND2	1:A:250:LYS:HD2	2.23	0.54
1:A:459:LEU:O	1:A:476:VAL:HB	2.08	0.54
1:B:459:LEU:HD13	1:B:460:LEU:HG	1.90	0.54
1:B:156:PHE:O	1:B:230:ALA:HA	2.08	0.54
1:A:191:ASP:CG	1:A:194:THR:HB	2.28	0.53
1:B:142:HIS:CE1	1:B:190:ASN:HD22	2.27	0.53
1:A:14:SER:HB3	1:A:17:GLU:CG	2.38	0.52
1:A:467:ALA:HB3	3:A:514[A]:HBO:H9B3	1.91	0.52
1:A:371:GLY:HA3	1:A:381:MET:O	2.09	0.52
1:A:275:LYS:O	1:A:279:GLU:HG3	2.09	0.52
3:B:514:HBO:C9B	4:B:2148:HOH:O	2.46	0.52
1:B:14:SER:HB3	1:B:17:GLU:CD	2.29	0.52
1:A:394:LYS:HE3	1:A:447:LEU:O	2.10	0.51
1:B:160:SER:O	1:B:162:LYS:HG2	2.10	0.51
1:B:372:PRO:HG2	1:B:381:MET:HB3	1.92	0.51
1:B:314:LYS:HB2	1:B:317:GLN:HG3	1.93	0.51
1:B:246:ASN:HD22	1:B:250:LYS:HD2	1.76	0.51
1:A:337:PHE:CE2	1:A:370:ILE:HB	2.46	0.50
1:A:500:THR:HG22	1:A:501:ALA:N	2.25	0.50
1:B:419:LEU:HD13	1:B:424:ALA:HB2	1.91	0.50
1:A:14:SER:O	1:A:17:GLU:HB2	2.11	0.50
1:A:464:GLU:HB3	3:A:514[B]:HBO:H9B3	1.93	0.50
1:A:104:ILE:HD11	1:A:122:TYR:CD2	2.47	0.50
1:A:212:PRO:HA	1:A:219:PRO:O	2.12	0.50
1:A:191:ASP:OD1	1:A:194:THR:N	2.42	0.50
1:B:86:LEU:HD11	1:B:486:ARG:HB3	1.94	0.50
1:A:104:ILE:HD11	1:A:122:TYR:HD2	1.77	0.49
1:A:224:LEU:HD13	1:A:350:VAL:O	2.13	0.49
1:A:312:PHE:CE2	1:B:344:SER:HA	2.46	0.49
1:B:500:THR:HG22	1:B:501:ALA:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASP:HB3	1:A:117:ASP:CB	2.43	0.49
1:A:75:ASN:HD21	1:A:78:HIS:HD2	1.60	0.49
1:B:153:TYR:CE2	1:B:163:SER:HB3	2.48	0.49
1:B:86:LEU:HD11	1:B:486:ARG:HG2	1.94	0.49
1:A:13:LEU:HD23	1:A:18:ILE:HD13	1.93	0.48
1:B:194:THR:OG1	3:B:514:HBO:O3B	2.28	0.48
1:A:458:SER:O	1:A:474:GLY:HA2	2.13	0.48
1:B:303[B]:ARG:HH22	1:B:312:PHE:HA	1.79	0.48
1:B:101:TRP:HB3	1:B:102:PRO:CD	2.44	0.48
1:A:147:GLN:O	1:A:151:GLU:HG3	2.13	0.48
1:B:36:ALA:O	1:B:40:GLU:HG3	2.14	0.48
1:A:96:ARG:HA	1:A:137:TYR:O	2.14	0.47
1:A:303[A]:ARG:NH2	1:A:312:PHE:HA	2.29	0.47
1:A:161:HIS:HA	1:A:233:ASN:OD1	2.15	0.47
1:A:480:ARG:HB2	1:A:480:ARG:NH1	2.29	0.47
1:B:46:ASP:HB3	1:B:117:ASP:CB	2.45	0.47
1:A:41:GLY:O	1:A:42:ALA:C	2.53	0.47
1:A:90:MET:HE1	1:A:492:ALA:HA	1.97	0.47
1:B:25:PRO:HG2	1:B:28:PHE:HB2	1.97	0.46
1:B:303[B]:ARG:NH2	1:B:312:PHE:HA	2.31	0.46
1:A:261:ASP:HB2	4:A:2166:HOH:O	2.15	0.46
1:A:475:ILE:O	1:A:492:ALA:HB2	2.16	0.46
1:A:467:ALA:CB	3:A:514[A]:HBO:H9B3	2.45	0.46
1:B:101:TRP:HB3	1:B:102:PRO:HD3	1.98	0.46
1:A:305:LEU:HA	1:B:307:ARG:NH2	2.30	0.46
1:A:101:TRP:N	1:A:102:PRO:HD2	2.31	0.45
1:A:119:ILE:HG21	1:A:178:ASN:HD22	1.81	0.45
1:A:303[A]:ARG:HH22	1:A:312:PHE:HA	1.81	0.45
1:A:90:MET:CE	1:A:475:ILE:HD12	2.44	0.45
1:B:84:VAL:HG11	1:B:128:LEU:HG	1.97	0.45
1:B:475:ILE:O	1:B:492:ALA:HB2	2.16	0.45
1:B:260:PHE:HE2	1:B:328:LEU:HG	1.82	0.45
1:A:260:PHE:HE2	1:A:328:LEU:HG	1.82	0.45
1:A:98:SER:HA	1:A:139:THR:O	2.17	0.45
1:A:88:LYS:O	1:A:88:LYS:HD3	2.17	0.45
1:B:330:LEU:HG	1:B:389:LEU:HD21	1.97	0.44
1:A:101:TRP:HB3	1:A:102:PRO:CD	2.47	0.44
1:A:103:ARG:HH11	1:A:103:ARG:HG3	1.83	0.44
1:A:25:PRO:HG2	1:A:28:PHE:HB2	1.99	0.44
1:A:156:PHE:O	1:A:230:ALA:HA	2.17	0.44
1:A:191:ASP:CG	1:A:261:ASP:OD1	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG22	1:A:129:LEU:CD2	2.48	0.44
1:B:143:TRP:N	1:B:143:TRP:CD1	2.84	0.44
1:B:86:LEU:HD13	1:B:476:VAL:HG11	1.98	0.44
1:A:85:ARG:O	1:A:89:GLU:HG3	2.18	0.43
1:B:14:SER:HA	1:B:15:PRO:HD3	1.87	0.43
1:B:285:ASN:HB3	4:B:2100:HOH:O	2.18	0.43
1:A:273:LEU:HD11	1:B:295:ARG:HD2	2.00	0.43
1:A:307:ARG:NH2	1:B:305:LEU:HA	2.33	0.43
1:A:84:VAL:HA	1:A:87:LEU:HD12	2.01	0.43
1:B:466:PHE:CZ	3:B:514:HBO:O7B	2.71	0.43
1:A:33:ALA:HA	1:A:96:ARG:O	2.18	0.43
1:B:41:GLY:HA3	1:B:72:ILE:O	2.18	0.43
1:A:119:ILE:HG21	1:A:178:ASN:ND2	2.34	0.42
1:B:142:HIS:CE1	1:B:190:ASN:ND2	2.87	0.42
1:B:434:ILE:O	1:B:438:ILE:HG13	2.19	0.42
1:A:110:LYS:HZ2	1:A:110:LYS:HB2	1.84	0.42
1:A:85:ARG:NH2	1:A:132:ASN:OD1	2.52	0.42
1:A:143:TRP:N	1:A:143:TRP:CD1	2.85	0.42
1:B:14:SER:HB3	1:B:17:GLU:OE1	2.20	0.42
1:A:466:PHE:CZ	3:A:514[B]:HBO:C6B	3.03	0.42
1:B:86:LEU:HD11	1:B:486:ARG:CB	2.49	0.42
1:B:20:GLN:HB2	1:B:23:TRP:CD1	2.55	0.42
1:A:266:VAL:O	1:A:337:PHE:HA	2.19	0.42
1:A:20:GLN:HB2	1:A:23:TRP:CD1	2.55	0.42
1:A:13:LEU:HD13	1:A:436:ARG:NH1	2.34	0.42
1:A:39:ILE:HG13	1:A:40:GLU:N	2.35	0.42
1:B:479:ASP:OD1	1:B:481:ASN:HB2	2.20	0.42
1:A:327:MET:O	1:A:328:LEU:HD13	2.20	0.42
1:A:261:ASP:HA	1:A:331:ASN:HB2	2.02	0.41
1:B:86:LEU:CD1	1:B:486:ARG:HG2	2.50	0.41
1:B:101:TRP:N	1:B:102:PRO:HD2	2.36	0.41
1:B:39:ILE:HG13	1:B:40:GLU:N	2.35	0.41
1:B:265:ARG:HD2	1:B:281:SER:HB3	2.03	0.41
1:A:378:TRP:NE1	3:A:514[A]:HBO:C5B	2.84	0.41
1:A:96:ARG:NH1	4:A:2044:HOH:O	2.53	0.41
1:A:439:ALA:O	1:A:442:LYS:HB3	2.21	0.41
1:A:467:ALA:HB3	3:A:514[B]:HBO:H9B3	2.02	0.41
1:A:41:GLY:HA3	1:A:72:ILE:O	2.21	0.41
1:B:161:HIS:HA	1:B:233:ASN:OD1	2.20	0.41
1:B:96:ARG:HA	1:B:137:TYR:O	2.21	0.41
1:A:46:ASP:HB3	1:A:117:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:SER:O	1:B:17:GLU:HB2	2.22	0.40
1:A:115:ASN:HD22	1:A:116:PRO:N	2.20	0.40
1:B:224:LEU:HD13	1:B:350:VAL:O	2.20	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	488/512 (95%)	459 (94%)	25 (5%)	4 (1%)	22	17
1	B	488/512 (95%)	459 (94%)	26 (5%)	3 (1%)	28	24
All	All	976/1024 (95%)	918 (94%)	51 (5%)	7 (1%)	25	20

All (7) 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
1	A	252	ASP
1	A	501	ALA
1	B	501	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/441 (96%)	405 (96%)	17 (4%)	36	36
1	B	422/441 (96%)	407 (96%)	15 (4%)	40	41
All	All	844/882 (96%)	812 (96%)	32 (4%)	38	38

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	75	ASN
1	A	85	ARG
1	A	110	LYS
1	A	115	ASN
1	A	193	GLN
1	A	224	LEU
1	A	316[A]	GLU
1	A	328	LEU
1	A	330	LEU
1	A	386	LEU
1	A	419	LEU
1	A	458	SER
1	A	459	LEU
1	A	462	ASN
1	A	482	ASN
1	A	486	ARG
1	B	46	ASP
1	B	75	ASN
1	B	111	GLU
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	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	55	HIS
1	A	59	ASN
1	A	78	HIS
1	A	115	ASN
1	A	124	ASN
1	A	142	HIS
1	A	178	ASN
1	A	246	ASN
1	A	276	GLN
1	A	426	ASN
1	A	462	ASN
1	A	481	ASN
1	A	482	ASN
1	A	499	ASN
1	B	75	ASN
1	B	190	ASN
1	B	246	ASN
1	B	276	GLN
1	B	426	ASN
1	B	462	ASN
1	B	481	ASN
1	B	482	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](#)

6 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	BGC	A	513[A]	3	12,12,12	1.66	3 (25%)	17,17,17	1.65	5 (29%)
2	BGC	A	513[B]	3	12,12,12	3.36	4 (33%)	17,17,17	3.27	8 (47%)
3	HBO	A	514[A]	2	14,15,16	4.20	6 (42%)	18,21,23	2.27	4 (22%)
3	HBO	A	514[B]	2	14,15,16	4.24	6 (42%)	18,21,23	2.27	4 (22%)
2	BGC	B	513	3	12,12,12	1.10	1 (8%)	17,17,17	2.35	5 (29%)
3	HBO	B	514	2	14,15,16	4.35	7 (50%)	18,21,23	2.29	6 (33%)

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	BGC	A	513[A]	3	-	0/2/22/22	0/1/1/1
2	BGC	A	513[B]	3	1/1/5/5	0/2/22/22	0/1/1/1
3	HBO	A	514[A]	2	1/1/2/3	0/2/15/18	0/2/2/2
3	HBO	A	514[B]	2	1/1/2/3	0/2/15/18	0/2/2/2
2	BGC	B	513	3	-	0/2/22/22	0/1/1/1
3	HBO	B	514	2	1/1/2/3	0/2/15/18	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	514	HBO	C2B-C3B	-4.65	1.45	1.51
3	A	514[B]	HBO	C2B-C3B	-3.85	1.46	1.51
3	A	514[A]	HBO	C2B-C3B	-3.79	1.46	1.51
2	A	513[B]	BGC	C4-C3	-3.63	1.43	1.52
2	A	513[A]	BGC	O4-C4	-3.27	1.35	1.43
2	B	513	BGC	O5-C1	-2.67	1.38	1.43
2	A	513[A]	BGC	O6-C6	-2.30	1.32	1.42
2	A	513[B]	BGC	O3-C3	-2.26	1.37	1.43
3	B	514	HBO	O7B-C9B	2.09	1.48	1.42
2	A	513[A]	BGC	C6-C5	2.18	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	514[A]	HBO	O7B-C7B	4.73	1.47	1.37
3	A	514[B]	HBO	O7B-C7B	4.78	1.47	1.37
3	B	514	HBO	O7B-C7B	4.97	1.48	1.37
3	A	514[B]	HBO	C4B-N3B	5.49	1.47	1.39
3	A	514[A]	HBO	C4B-N3B	5.53	1.47	1.39
2	A	513[B]	BGC	O4-C4	5.63	1.55	1.43
3	B	514	HBO	C4B-N3B	5.64	1.47	1.39
3	A	514[A]	HBO	O1B-C1B	6.35	1.44	1.37
3	B	514	HBO	OHB-N3B	6.53	1.48	1.40
3	A	514[B]	HBO	O1B-C1B	6.54	1.45	1.37
3	A	514[A]	HBO	OHB-N3B	6.64	1.48	1.40
3	A	514[B]	HBO	OHB-N3B	6.72	1.48	1.40
3	B	514	HBO	O1B-C1B	7.04	1.45	1.37
2	A	513[B]	BGC	O1-C1	8.94	1.70	1.39
3	B	514	HBO	O3B-C3B	9.21	1.44	1.23
3	A	514[A]	HBO	O3B-C3B	9.28	1.44	1.23
3	A	514[B]	HBO	O3B-C3B	9.34	1.44	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	514	HBO	OHB-N3B-C3B	-6.25	109.85	116.80
3	A	514[B]	HBO	OHB-N3B-C3B	-6.21	109.89	116.80
3	A	514[A]	HBO	OHB-N3B-C3B	-6.07	110.05	116.80
2	B	513	BGC	C4-C3-C2	-4.17	103.49	110.84
2	B	513	BGC	O3-C3-C2	-3.97	101.72	110.36
2	A	513[B]	BGC	O4-C4-C3	-3.85	101.98	110.36
3	A	514[B]	HBO	C9B-O7B-C7B	-3.12	110.68	117.50
3	A	514[A]	HBO	C9B-O7B-C7B	-3.12	110.68	117.50
2	A	513[B]	BGC	C4-C3-C2	-3.00	105.54	110.84
2	A	513[B]	BGC	O3-C3-C4	-2.88	104.10	110.36
3	B	514	HBO	C9B-O7B-C7B	-2.82	111.34	117.50
2	A	513[A]	BGC	C1-C2-C3	-2.41	106.30	110.65
2	A	513[B]	BGC	O6-C6-C5	-2.33	103.49	111.34
2	A	513[A]	BGC	O5-C1-C2	-2.27	106.27	110.04
2	B	513	BGC	O2-C2-C1	-2.11	105.37	109.75
2	A	513[A]	BGC	O4-C4-C3	-2.09	105.81	110.36
3	B	514	HBO	C5B-C4B-N3B	-2.09	120.08	121.88
2	B	513	BGC	O4-C4-C3	-2.06	105.88	110.36
2	A	513[A]	BGC	C4-C3-C2	-2.01	107.29	110.84
3	B	514	HBO	C1B-C4B-N3B	2.09	119.84	118.27
3	B	514	HBO	O1B-C1B-C8B	2.25	120.11	116.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	513[A]	BGC	O5-C5-C6	2.48	112.35	106.41
3	A	514[B]	HBO	O1B-C1B-C8B	2.54	120.55	116.81
2	A	513[B]	BGC	O1-C1-O5	2.56	117.78	110.20
3	A	514[A]	HBO	O1B-C1B-C8B	2.60	120.63	116.81
3	B	514	HBO	C2B-C3B-N3B	5.20	121.11	116.31
3	A	514[B]	HBO	C2B-C3B-N3B	5.41	121.31	116.31
3	A	514[A]	HBO	C2B-C3B-N3B	5.52	121.42	116.31
2	A	513[B]	BGC	O2-C2-C1	5.87	121.95	109.75
2	B	513	BGC	O5-C1-C2	5.91	119.84	110.04
2	A	513[B]	BGC	O5-C5-C6	6.22	121.31	106.41
2	A	513[B]	BGC	O1-C1-C2	7.41	130.33	109.42

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	513[B]	BGC	C1
3	A	514[A]	HBO	C2B
3	A	514[B]	HBO	C2B
3	B	514	HBO	C2B

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	513[A]	BGC	2	0
2	A	513[B]	BGC	2	0
3	A	514[A]	HBO	9	0
3	A	514[B]	HBO	4	0
2	B	513	BGC	2	0
3	B	514	HBO	4	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, 95th 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 ²)	Q < 0.9
1	A	490/512 (95%)	0.16	14 (2%)	52	59	27, 43, 60, 72	1 (0%)
1	B	490/512 (95%)	0.12	17 (3%)	44	51	28, 43, 59, 73	1 (0%)
All	All	980/1024 (95%)	0.14	31 (3%)	48	55	27, 43, 60, 73	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	TYR	4.4
1	A	500	THR	3.9
1	A	501	ALA	3.7
1	B	501	ALA	3.6
1	A	482	ASN	3.6
1	B	26	SER	3.5
1	B	428	TYR	3.3
1	A	111	GLU	3.3
1	B	415	LYS	3.3
1	A	26	SER	3.0
1	B	316[B]	GLU	3.0
1	B	252	ASP	2.9
1	B	502	LYS	2.9
1	A	16	SER	2.8
1	A	483	ASN	2.7
1	B	111	GLU	2.7
1	B	107	LYS	2.7
1	B	458	SER	2.6
1	A	15	PRO	2.5
1	B	248	HIS	2.5
1	B	422	GLU	2.3
1	B	487	TYR	2.2
1	A	14	SER	2.2
1	B	206	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	447	LEU	2.1
1	B	27	ASP	2.1
1	A	17	GLU	2.1
1	A	404	ILE	2.1
1	B	346	ASN	2.1
1	B	13	LEU	2.0
1	A	409	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 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, 95th 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 ²)	Q<0.9
2	BGC	B	513	12/12	0.44	0.61	20.35	14,20,24,25	12
3	HBO	B	514	14/15	0.36	0.46	14.03	51,52,52,52	14
2	BGC	A	513[B]	12/12	0.47	0.49	9.76	56,57,59,59	12
2	BGC	A	513[A]	12/12	0.47	0.49	8.52	59,60,61,62	12
3	HBO	A	514[B]	14/15	0.75	0.38	6.30	54,55,56,56	14
3	HBO	A	514[A]	14/15	0.75	0.38	6.30	56,58,59,59	14

6.5 Other polymers [i](#)

There are no such residues in this entry.