



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:14 AM UTC

PDB ID : 1E4N / pdb_00001e4n
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

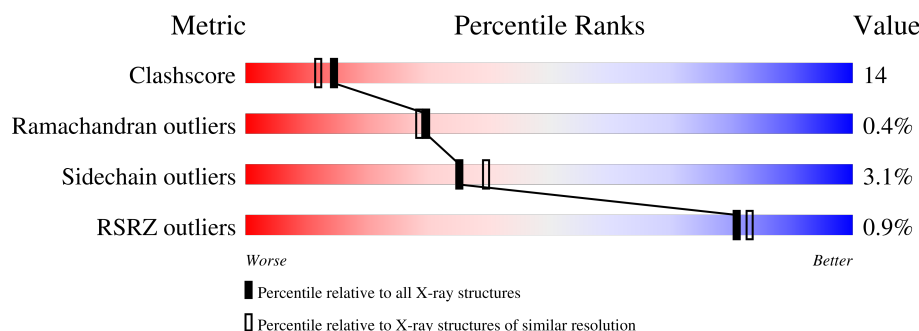
1 Overall quality at a glance

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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	% 65% 28% ..
1	B	512	% 70% 23% .

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.

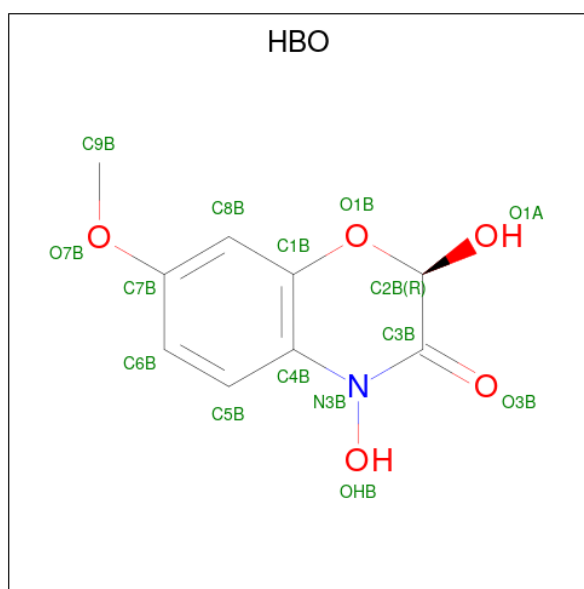
- Molecule 1 is a protein called BETA-GLUCOSIDASE.

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 (CCD ID: HBO) (formula: C₉H₉NO₅).



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

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

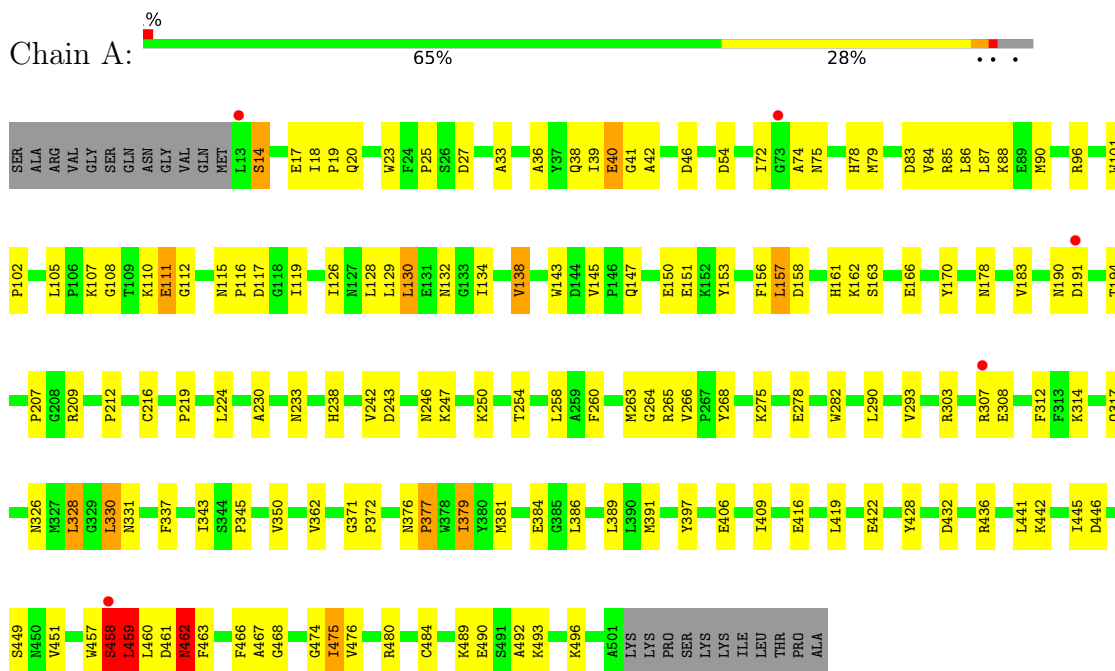
- Molecule 3 is water.

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

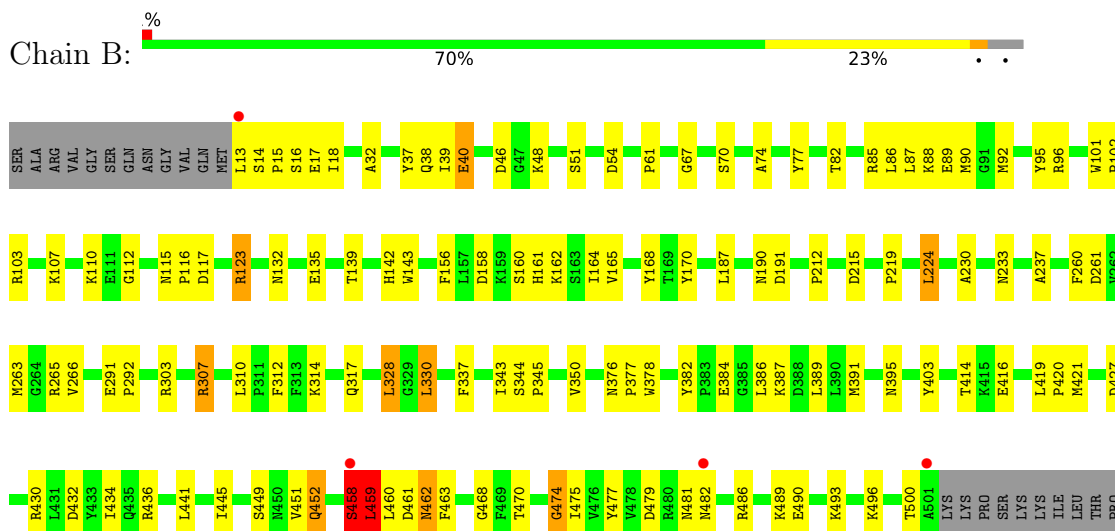
3 Residue-property plots

These plots are drawn for all protein, RNA, 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



ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.57Å 95.31Å 117.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.10 29.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.00-2.10) 96.1 (29.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.223 , 0.269 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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

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	0.46	0/4079	0.94	20/5539 (0.4%)
1	B	0.45	0/4079	0.96	17/5539 (0.3%)
All	All	0.46	0/8158	0.95	37/11078 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	GLU	N-CA-C	9.75	122.92	111.02
1	A	459	LEU	N-CA-C	-8.43	102.17	111.36
1	B	459	LEU	N-CA-C	-8.39	102.21	111.36
1	A	475	ILE	N-CA-C	-7.94	102.19	113.07
1	B	475	ILE	N-CA-C	-7.86	102.30	113.07
1	A	40	GLU	N-CA-C	7.26	119.88	111.02
1	B	54	ASP	N-CA-C	-7.04	103.54	111.07
1	B	461	ASP	N-CA-C	-6.96	99.97	110.28
1	A	461	ASP	N-CA-C	-6.96	99.99	110.28
1	A	397	TYR	N-CA-C	6.87	120.33	112.57
1	A	350	VAL	N-CA-C	-6.40	106.74	112.12
1	B	500	THR	N-CA-C	6.27	121.00	113.23
1	A	138	VAL	N-CA-C	6.26	117.81	108.23
1	B	307	ARG	CB-CA-C	-6.25	109.35	116.54
1	B	343	ILE	N-CA-C	-6.11	101.66	109.30
1	A	74	ALA	N-CA-C	-5.94	105.22	112.88
1	A	14	SER	CA-C-N	5.80	126.19	119.47
1	A	14	SER	C-N-CA	5.80	126.19	119.47
1	B	395	ASN	N-CA-C	5.69	119.40	112.23
1	B	74	ALA	N-CA-C	-5.67	105.57	112.88
1	B	16	SER	N-CA-C	-5.45	106.13	112.89
1	A	343	ILE	N-CA-C	-5.45	102.48	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ASP	N-CA-C	-5.40	105.29	111.07
1	A	145	VAL	CB-CA-C	-5.39	105.92	110.94
1	A	379	ILE	N-CA-C	5.36	115.91	108.84
1	A	362	VAL	N-CA-C	-5.30	105.22	111.00
1	B	310	LEU	CA-C-N	5.30	125.30	119.89
1	B	310	LEU	C-N-CA	5.30	125.30	119.89
1	A	462	ASN	N-CA-C	5.29	115.22	108.24
1	A	326	ASN	N-CA-C	-5.28	106.79	114.12
1	B	215	ASP	N-CA-C	5.20	117.79	108.17
1	A	474	GLY	N-CA-C	5.18	118.82	112.14
1	B	378	TRP	N-CA-C	5.16	121.11	114.56
1	B	474	GLY	N-CA-C	5.08	118.69	112.14
1	A	157	LEU	N-CA-C	-5.02	107.15	113.28
1	B	123	ARG	N-CA-C	-5.02	105.72	111.14
1	A	377	PRO	N-CA-C	5.01	120.20	114.03

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	128	0
1	B	3958	0	3748	91	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	217	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 14.

All (217) 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:191:ASP:CG	1:A:194:THR:HB	1.93	0.91
1:A:90:MET:HE1	1:A:475:ILE:HD12	1.53	0.90
1:A:406:GLU:OE2	3:A:2192:HOH:O	1.91	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:191:ASP:CG	1:A:194:THR:CB	2.60	0.71
1:A:150:GLU:HG2	3:A:2067:HOH:O	1.90	0.71
1:A:75:ASN:OD1	1:A:79:MET:HE3	1.91	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:88:LYS:CD	1:B:132:ASN:HD22	2.06	0.69
1:B:135:GLU:OE1	3:B:2057:HOH:O	2.11	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: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: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: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: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
1:B:82:THR:O	1:B:86:LEU:HD23	2.02	0.59
1:A:14:SER:HB3	1:A:17:GLU:CD	2.28	0.59
1:B:38:GLN:O	1:B:462:ASN:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:NH2	1:A:190:ASN:CG	2.61	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:90:MET:HE3	1:A:492:ALA:HA	1.85	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:90:MET:O	1:B:496:LYS:HA	2.05	0.56
1:B:156:PHE:O	1:B:230:ALA:HA	2.06	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:B:462:ASN:HD22	1:B:462:ASN:C	2.16	0.54
1:A:246:ASN:ND2	3:A:2099:HOH:O	2.41	0.54
1:B:263:MET:HE2	3:B:2075:HOH:O	2.06	0.54
1:A:86:LEU:O	1:A:90:MET:HG3	2.08	0.54
1:A:90:MET:HE3	1:A:492:ALA:CA	2.38	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:OE1	1:A:384:GLU:HA	2.08	0.53
1:B:161:HIS:HA	1:B:233:ASN:OD1	2.09	0.53
1:B:263:MET:HE3	1:B:265:ARG:HH22	1.73	0.53
1:B:382:TYR:CE2	1:B:384:GLU:HB3	2.43	0.53
1:A:263:MET:HE3	1:A:265:ARG:HH22	1.72	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:CD1	1:B:143:TRP:N	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:MET:HE1	3:A:2109:HOH:O	2.10	0.51
1:B:260:PHE:HE1	1:B:328:LEU:HG	1.75	0.51
1:A:191:ASP:CG	1:A:194:THR:OG1	2.53	0.51
1:A:238:HIS:CE1	1:A:258:LEU:HD22	2.45	0.51
1:A:96:ARG:NH2	1:A:190:ASN:OD1	2.44	0.51
1:A:496:LYS:HE3	3:A:2049:HOH:O	2.10	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:462:ASN:C	1:A:462:ASN:HD22	2.20	0.50
1:A:88:LYS:HD3	1:A:132:ASN:HB3	1.94	0.50
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:96:ARG:HD2	1:B:187:LEU:HD12	1.95	0.48
1:B:382:TYR:CZ	1:B:384:GLU:HB3	2.48	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:A:191:ASP:OD2	1:A:191:ASP:C	2.56	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:14:SER:HB3	1:A:17:GLU:CG	2.44	0.47
1:A:153:TYR:CE2	1:A:163:SER:HB3	2.50	0.47
1:A:307:ARG:NH2	1:B:307:ARG:HG3	2.29	0.47
1:A:466:PHE:CZ	2:A:514:HBO:H9B1	2.49	0.47
1:A:33:ALA:HB2	1:A:96:ARG:HB3	1.96	0.47
1:A:263:MET:HE3	1:A:265:ARG:NH2	2.28	0.47
1:A:312:PHE:CD2	1:B:345:PRO:HD3	2.50	0.47
1:A:331:ASN:HB3	1:A:406:GLU:HB2	1.96	0.47
1:A:105:LEU:O	1:A:108:GLY:N	2.42	0.47
1:A:111:GLU:H	1:A:111:GLU:CD	2.23	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: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:A:263:MET:HE2	3:A:2110:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:14:SER:HB3	1:B:17:GLU:CD	2.41	0.46
1:B:330:LEU:HG	1:B:389:LEU:HD21	1.97	0.46
1:A:41:GLY:O	1:A:42:ALA:C	2.59	0.46
1:A:480:ARG:NH1	1:A:480:ARG:HB2	2.30	0.46
1:A:143:TRP:CD1	1:A:143:TRP:N	2.82	0.45
1:A:266:VAL:O	1:A:337:PHE:HA	2.16	0.45
1:B:421:MET:HE2	1:B:477:TYR:CE2	2.51	0.45
1:A:308:GLU:CD	1:A:308:GLU:H	2.24	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:46:ASP:HB3	1:B:117:ASP:CB	2.46	0.45
1:B:224:LEU:HD13	1:B:350:VAL:O	2.16	0.45
1:B:85:ARG:O	1:B:89:GLU:HG3	2.16	0.45
1:A:416:GLU:CD	1:A:416:GLU:N	2.75	0.45
1:B:32:ALA:HB2	1:B:92:MET:HE3	1.99	0.45
1:A:212:PRO:HA	1:A:219:PRO:O	2.18	0.44
1:A:416:GLU:CD	1:A:416:GLU:H	2.25	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:B:420:PRO:O	1:B:421:MET:C	2.61	0.44
1:A:345:PRO:HD3	1:B:312:PHE:CD2	2.52	0.44
1:A:449:SER:OG	1:A:451:VAL:HG23	2.17	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:B:414:THR:C	1:B:416:GLU:H	2.26	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:B:263:MET:HE3	1:B:265:ARG:NH2	2.32	0.43
1:A:331:ASN:CB	1:A:406:GLU:HB2	2.48	0.43
1:A:96:ARG:HH21	1:A:190:ASN:CG	2.26	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:B:427:ASP:OD2	1:B:430:ARG:HD2	2.18	0.43
1:A:84:VAL:HG22	1:A:129:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ALA:HB2	2:A:514:HBO:C9B	2.27	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:39:ILE:HG13	1:A:40:GLU:N	2.32	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:A:46:ASP:HB3	1:A:117:ASP:CG	2.45	0.42
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.90	0.42
1:B:14:SER:O	1:B:17:GLU:HB2	2.20	0.42
1:B:139:THR:HA	1:B:187:LEU:HB2	2.01	0.42
1:B:61:PRO:O	1:B:67:GLY:HA2	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
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:25:PRO:HB2	1:A:27:ASP:OD1	2.20	0.41
1:A:38:GLN:HG2	1:A:463:PHE:O	2.21	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: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:A:432:ASP:CG	1:A:436:ARG:HE	2.29	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:421:MET:HE2	1:B:477:TYR:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	30	28
1	B	487/512 (95%)	461 (95%)	24 (5%)	2 (0%)	30	28
All	All	974/1024 (95%)	926 (95%)	44 (4%)	4 (0%)	30	28

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 ⓘ

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%)	409 (97%)	13 (3%)	35	39
1	B	422/441 (96%)	409 (97%)	13 (3%)	35	39
All	All	844/882 (96%)	818 (97%)	26 (3%)	35	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ARG
1	A	111	GLU
1	A	130	LEU
1	A	224	LEU
1	A	328	LEU
1	A	330	LEU
1	A	386	LEU
1	A	391	MET
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	224	LEU
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	452	GLN
1	B	458	SER
1	B	459	LEU
1	B	462	ASN
1	B	482	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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	193	GLN
1	A	246	ASN
1	A	248	HIS
1	A	407	ASN
1	A	426	ASN
1	A	452	GLN
1	A	462	ASN
1	A	481	ASN
1	A	499	ASN
1	B	20	GLN
1	B	59	ASN
1	B	75	ASN
1	B	115	ASN
1	B	124	ASN
1	B	132	ASN
1	B	142	HIS
1	B	193	GLN
1	B	246	ASN
1	B	360	GLN
1	B	407	ASN
1	B	426	ASN
1	B	435	GLN
1	B	452	GLN
1	B	462	ASN
1	B	481	ASN
1	B	499	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 [i](#)

There are no oligosaccharides 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	-	15,16,16	3.81	9 (60%)	16,23,23	2.55	3 (18%)
2	HBO	A	514	-	15,16,16	3.73	7 (46%)	16,23,23	2.21	3 (18%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	514	HBO	OHB-N3B	8.15	1.49	1.39
2	B	514	HBO	OHB-N3B	7.44	1.49	1.39
2	A	514	HBO	O1B-C1B	6.55	1.46	1.38
2	B	514	HBO	O1B-C1B	6.42	1.46	1.38
2	B	514	HBO	C4B-N3B	6.29	1.47	1.40
2	B	514	HBO	O7B-C7B	6.27	1.50	1.37
2	A	514	HBO	C4B-N3B	6.03	1.47	1.40
2	A	514	HBO	O7B-C7B	5.64	1.48	1.37
2	A	514	HBO	C2B-C3B	-3.58	1.46	1.51
2	B	514	HBO	C2B-C3B	-3.55	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	514	HBO	O1A-C2B	2.52	1.44	1.38
2	B	514	HBO	O1A-C2B	2.37	1.43	1.38
2	B	514	HBO	C8B-C7B	2.36	1.42	1.39
2	A	514	HBO	O7B-C9B	2.21	1.49	1.42
2	B	514	HBO	C6B-C5B	2.15	1.42	1.38
2	B	514	HBO	O7B-C9B	2.09	1.48	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	514	HBO	OHB-N3B-C3B	-8.62	109.64	116.88
2	A	514	HBO	OHB-N3B-C3B	-6.28	111.61	116.88
2	A	514	HBO	C1B-C4B-N3B	4.84	121.91	118.20
2	B	514	HBO	C1B-C4B-N3B	3.10	120.57	118.20
2	A	514	HBO	C9B-O7B-C7B	-2.91	111.25	117.50
2	B	514	HBO	C9B-O7B-C7B	-2.44	112.27	117.50

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	489/512 (95%)	0.20	5 (1%) 79 81	25, 40, 54, 68	1 (0%)
1	B	489/512 (95%)	0.18	4 (0%) 82 84	28, 39, 54, 63	1 (0%)
All	All	978/1024 (95%)	0.19	9 (0%) 81 83	25, 40, 55, 68	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ASP	5.1
1	B	13	LEU	3.4
1	B	501	ALA	2.9
1	A	307	ARG	2.8
1	B	458	SER	2.7
1	A	458	SER	2.6
1	A	13	LEU	2.4
1	B	482	ASN	2.3
1	A	73	GLY	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	HBO	A	514	15/15	0.75	0.20	53,55,56,57	15
2	HBO	B	514	15/15	0.82	0.17	59,61,61,61	15

6.5 Other polymers [i](#)

There are no such residues in this entry.