



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2020 – 12:08 PM JST

PDB ID : 6LVW
Title : Polyextremophilic Beta-galactosidase from the Antarctic haloarchaeon
Halorubrum lacusprofundi
Authors : Muhammad, R.; Arold, S.T.
Deposited on : 2020-02-06
Resolution : 2.49 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

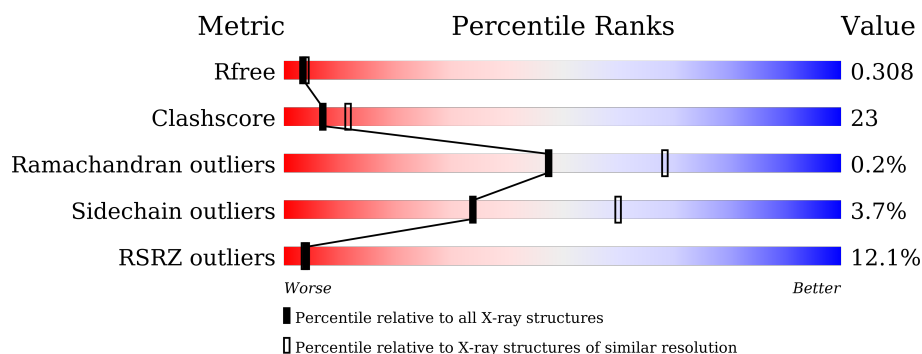
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	700	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5280 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-galactosidase Bga.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	668	Total	C	N	O	S	0	0	0
			5275	3305	926	1024	20			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

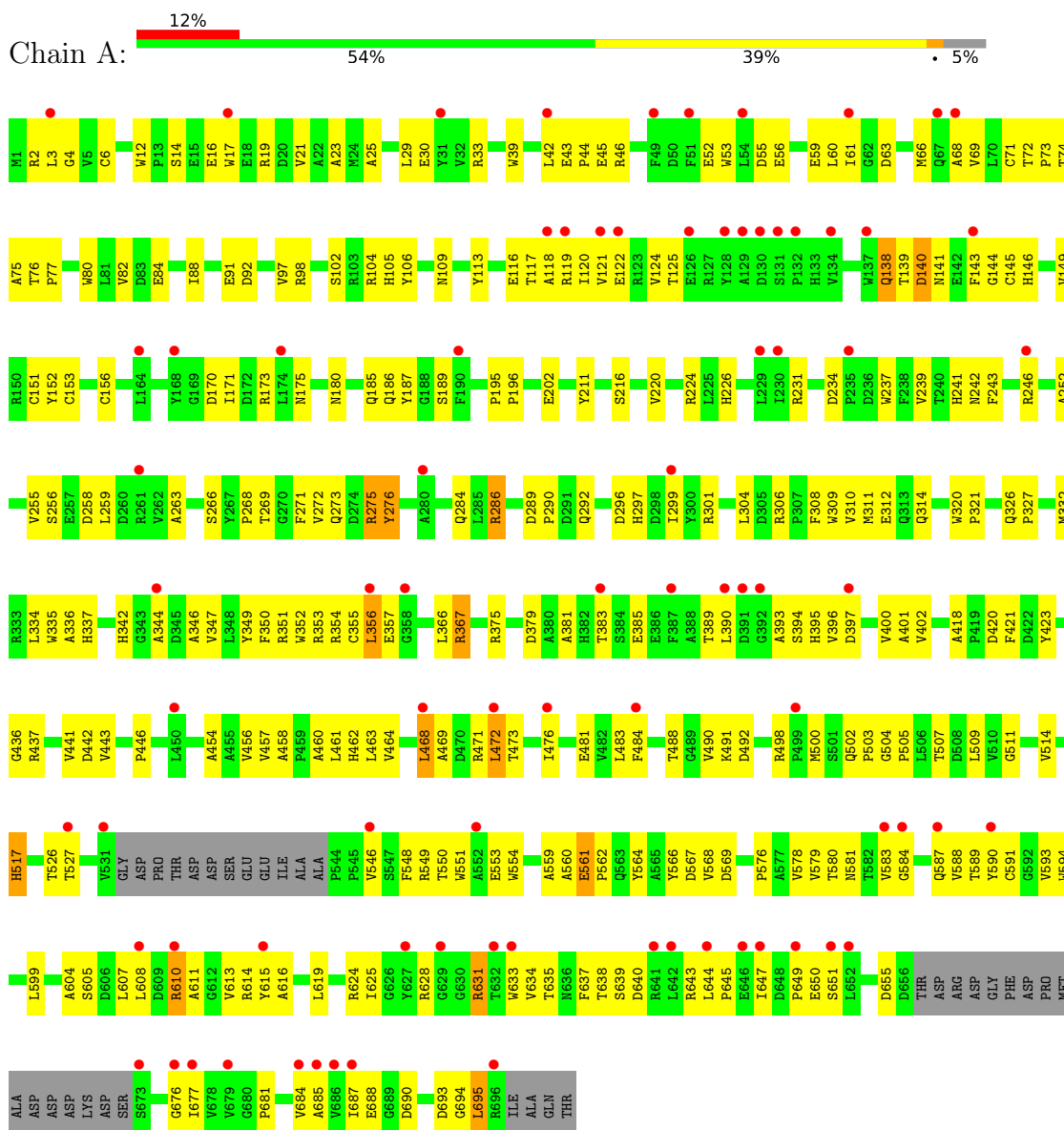
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		

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-galactosidase Bga



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	100.13Å 100.13Å 137.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.36 – 2.49 47.04 – 2.49	Depositor EDS
% Data completeness (in resolution range)	86.5 (34.36-2.49) 86.5 (47.04-2.49)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.246 , 0.307 0.246 , 0.308	Depositor DCC
R_{free} test set	1230 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	75.7	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5280	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.32	0/5434	0.57	3/7429 (0.0%)

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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	390	LEU	CA-CB-CG	6.72	130.75	115.30
1	A	695	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	468	LEU	CA-CB-CG	5.46	127.87	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	LEU	Peptide

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	5275	0	4850	233	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
All	All	5280	0	4850	233	1

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 23.

All (233) 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:481:GLU:OE2	1:A:610:ARG:HD2	1.45	1.15
1:A:19:ARG:HH22	1:A:353:ARG:NH2	1.50	1.10
1:A:481:GLU:CD	1:A:610:ARG:HD2	1.76	1.04
1:A:19:ARG:NH2	1:A:353:ARG:NH2	2.08	1.01
1:A:19:ARG:HH22	1:A:353:ARG:HH21	1.04	0.98
1:A:463:LEU:HD22	1:A:491:LYS:HB2	1.43	0.97
1:A:511:GLY:HA2	1:A:559:ALA:HB3	1.54	0.88
1:A:151:CYS:SG	1:A:156:CYS:SG	2.76	0.84
1:A:461:LEU:H	1:A:488:THR:HG22	1.44	0.82
1:A:587:GLN:HE22	1:A:610:ARG:HE	1.29	0.80
1:A:25:ALA:HA	1:A:66:MET:HE2	1.64	0.79
1:A:3:LEU:HD11	1:A:383:THR:HG23	1.64	0.78
1:A:71:CYS:SG	1:A:138:GLN:NE2	2.58	0.76
1:A:473:THR:HG22	1:A:509:LEU:HD22	1.69	0.74
1:A:25:ALA:HA	1:A:66:MET:CE	2.19	0.73
1:A:614:ARG:HH21	1:A:690:ASP:C	1.94	0.70
1:A:75:ALA:N	1:A:140:ASP:OD1	2.24	0.70
1:A:216:SER:O	1:A:220:VAL:HG23	1.91	0.70
1:A:402:VAL:HB	1:A:443:VAL:HG12	1.72	0.70
1:A:631:ARG:HH21	1:A:688:GLU:HB3	1.57	0.70
1:A:614:ARG:NH2	1:A:690:ASP:C	2.45	0.69
1:A:608:LEU:HD23	1:A:615:TYR:HB3	1.75	0.69
1:A:454:ALA:HB1	1:A:611:ALA:HB1	1.75	0.68
1:A:19:ARG:NH2	1:A:353:ARG:HH22	1.91	0.68
1:A:327:PRO:O	1:A:375:ARG:NH1	2.24	0.67
1:A:423:TYR:HE1	1:A:460:ALA:HB3	1.59	0.67
1:A:355:CYS:SG	1:A:357:GLU:HB3	2.34	0.67
1:A:457:VAL:HG12	1:A:483:LEU:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:OE1	1:A:610:ARG:HD2	1.93	0.67
1:A:152:TYR:HE2	1:A:196:PRO:HG2	1.60	0.66
1:A:289:ASP:HB3	1:A:292:GLN:HG2	1.78	0.66
1:A:401:ALA:HB3	1:A:456:VAL:HG22	1.76	0.66
1:A:638:THR:HG22	1:A:640:ASP:H	1.61	0.66
1:A:587:GLN:HE22	1:A:610:ARG:NE	1.94	0.66
1:A:468:LEU:O	1:A:472:LEU:HD12	1.96	0.65
1:A:25:ALA:CA	1:A:66:MET:CE	2.74	0.65
1:A:481:GLU:OE2	1:A:610:ARG:CD	2.33	0.65
1:A:246:ARG:HH22	1:A:276:TYR:HA	1.60	0.65
1:A:332:MET:SD	1:A:332:MET:N	2.71	0.64
1:A:286:ARG:NE	1:A:326:GLN:O	2.29	0.64
1:A:509:LEU:O	1:A:588:VAL:HG11	1.97	0.64
1:A:3:LEU:HB3	1:A:29:LEU:HD23	1.78	0.64
1:A:644:LEU:O	1:A:676:GLY:HA3	1.97	0.64
1:A:113:TYR:O	1:A:117:THR:HG23	1.99	0.63
1:A:144:GLY:HA3	1:A:149:VAL:HG23	1.81	0.63
1:A:437:ARG:HB3	1:A:615:TYR:HB2	1.78	0.63
1:A:560:ALA:HB1	1:A:561:GLU:OE1	1.99	0.62
1:A:587:GLN:NE2	1:A:610:ARG:NE	2.47	0.62
1:A:17:TRP:O	1:A:21:VAL:HG23	1.99	0.61
1:A:393:ALA:HB1	1:A:628:ARG:HD3	1.82	0.61
1:A:461:LEU:HB2	1:A:488:THR:HB	1.82	0.61
1:A:610:ARG:HH11	1:A:610:ARG:HG3	1.66	0.61
1:A:423:TYR:CE1	1:A:460:ALA:HB3	2.35	0.61
1:A:469:ALA:O	1:A:473:THR:HG23	2.00	0.61
1:A:121:VAL:HA	1:A:124:VAL:HG12	1.83	0.60
1:A:301:ARG:NH2	1:A:442:ASP:OD1	2.34	0.60
1:A:492:ASP:HB3	1:A:498:ARG:HE	1.66	0.60
1:A:46:ARG:HH21	1:A:119:ARG:HE	1.47	0.60
1:A:549:ARG:O	1:A:594:TRP:HB3	2.01	0.60
1:A:379:ASP:O	1:A:383:THR:HG22	2.02	0.59
1:A:458:ALA:HB3	1:A:484:PHE:CD1	2.37	0.59
1:A:139:THR:OG1	1:A:241:HIS:ND1	2.36	0.59
1:A:458:ALA:HB1	1:A:461:LEU:HG	1.84	0.59
1:A:562:PRO:HB3	1:A:576:PRO:HB3	1.84	0.58
1:A:171:ILE:HD11	1:A:187:TYR:HB2	1.86	0.58
1:A:117:THR:O	1:A:121:VAL:HG12	2.03	0.58
1:A:121:VAL:O	1:A:125:THR:HG23	2.04	0.58
1:A:631:ARG:NH2	1:A:688:GLU:HB3	2.18	0.57
1:A:461:LEU:H	1:A:488:THR:CG2	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG23	1:A:259:LEU:HA	1.87	0.56
1:A:19:ARG:NH2	1:A:353:ARG:HH21	1.80	0.56
1:A:23:ALA:HB1	1:A:367:ARG:HH12	1.69	0.56
1:A:337:HIS:HB2	1:A:684:VAL:HG11	1.87	0.56
1:A:299:ILE:HA	1:A:443:VAL:HG23	1.87	0.55
1:A:16:GLU:HG2	1:A:19:ARG:HH21	1.71	0.55
1:A:566:TYR:HB3	1:A:568:VAL:HG12	1.88	0.55
1:A:290:PRO:HG3	1:A:637:PHE:CG	2.42	0.54
1:A:468:LEU:HD23	1:A:471:ARG:HH21	1.71	0.54
1:A:296:ASP:HA	1:A:299:ILE:HG22	1.90	0.54
1:A:614:ARG:CZ	1:A:614:ARG:HB2	2.37	0.54
1:A:72:THR:HG21	1:A:226:HIS:CD2	2.43	0.54
1:A:458:ALA:HB3	1:A:484:PHE:HD1	1.73	0.54
1:A:613:VAL:HG12	1:A:614:ARG:H	1.72	0.53
1:A:579:VAL:HG12	1:A:590:TYR:HB3	1.91	0.53
1:A:625:ILE:HA	1:A:633:TRP:O	2.08	0.53
1:A:446:PRO:O	1:A:471:ARG:NH2	2.42	0.53
1:A:476:ILE:HD12	1:A:509:LEU:HD21	1.91	0.52
1:A:610:ARG:HG3	1:A:610:ARG:NH1	2.23	0.52
1:A:109:ASN:HD22	1:A:156:CYS:HA	1.74	0.52
1:A:396:VAL:HG12	1:A:628:ARG:HA	1.90	0.52
1:A:400:VAL:HG13	1:A:441:VAL:HG13	1.92	0.52
1:A:269:THR:OG1	1:A:314:GLN:NE2	2.33	0.52
1:A:462:HIS:C	1:A:463:LEU:HD23	2.31	0.51
1:A:170:ASP:OD1	1:A:173:ARG:HG3	2.10	0.51
1:A:91:GLU:HG2	1:A:97:VAL:HG12	1.92	0.51
1:A:60:LEU:HA	1:A:63:ASP:HB2	1.93	0.51
1:A:647:ILE:O	1:A:676:GLY:HA2	2.10	0.51
1:A:463:LEU:HA	1:A:491:LYS:O	2.11	0.51
1:A:297:HIS:HB3	1:A:342:HIS:HB3	1.93	0.50
1:A:272:VAL:HG21	1:A:284:GLN:HB3	1.93	0.50
1:A:402:VAL:O	1:A:443:VAL:HA	2.12	0.50
1:A:591:CYS:SG	1:A:593:VAL:HG12	2.52	0.50
1:A:118:ALA:O	1:A:122:GLU:HB2	2.11	0.50
1:A:420:ASP:OD1	1:A:420:ASP:N	2.40	0.50
1:A:498:ARG:NH1	1:A:505:PRO:HD3	2.27	0.50
1:A:394:SER:OG	1:A:395:HIS:N	2.45	0.50
1:A:33:ARG:HB2	1:A:69:VAL:HG13	1.94	0.49
1:A:16:GLU:O	1:A:19:ARG:HG3	2.12	0.49
1:A:4:GLY:HA2	1:A:29:LEU:HB3	1.95	0.49
1:A:647:ILE:HG22	1:A:677:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ALA:O	1:A:385:GLU:HG3	2.13	0.49
1:A:580:THR:HG22	1:A:589:THR:HB	1.95	0.49
1:A:256:SER:HA	1:A:259:LEU:HG	1.95	0.48
1:A:546:VAL:HG11	1:A:599:LEU:N	2.28	0.48
1:A:500:MET:HG3	1:A:504:GLY:HA2	1.95	0.48
1:A:320:TRP:CD2	1:A:321:PRO:HD3	2.48	0.48
1:A:351:ARG:NH1	1:A:353:ARG:O	2.45	0.48
1:A:350:PHE:HA	1:A:351:ARG:HA	1.61	0.47
1:A:334:LEU:HD21	1:A:635:THR:OG1	2.14	0.47
1:A:644:LEU:O	1:A:676:GLY:CA	2.62	0.47
1:A:549:ARG:HD3	1:A:594:TRP:CE2	2.50	0.47
1:A:171:ILE:HG13	1:A:175:ASN:ND2	2.29	0.47
1:A:490:VAL:HG12	1:A:491:LYS:HG2	1.96	0.47
1:A:25:ALA:CA	1:A:66:MET:HE2	2.36	0.47
1:A:33:ARG:HA	1:A:69:VAL:O	2.15	0.47
1:A:71:CYS:SG	1:A:138:GLN:HB3	2.54	0.47
1:A:180:ASN:HB3	1:A:185:GLN:C	2.35	0.47
1:A:52:GLU:HA	1:A:55:ASP:OD2	2.13	0.47
1:A:59:GLU:O	1:A:63:ASP:N	2.45	0.47
1:A:56:GLU:O	1:A:60:LEU:HD13	2.14	0.47
1:A:273:GLN:OE1	1:A:321:PRO:HB2	2.15	0.47
1:A:74:THR:OG1	1:A:140:ASP:CG	2.53	0.47
1:A:2:ARG:HG2	1:A:30:GLU:OE2	2.14	0.47
1:A:354:ARG:HG3	1:A:354:ARG:HH11	1.79	0.47
1:A:385:GLU:O	1:A:389:THR:HG23	2.15	0.47
1:A:402:VAL:HA	1:A:457:VAL:O	2.14	0.47
1:A:80:TRP:O	1:A:84:GLU:HB2	2.15	0.47
1:A:290:PRO:HG3	1:A:637:PHE:CD1	2.51	0.46
1:A:527:THR:OG1	1:A:567:ASP:HB3	2.16	0.46
1:A:17:TRP:HH2	1:A:53:TRP:HB2	1.79	0.46
1:A:308:PHE:CE1	1:A:344:ALA:HB2	2.50	0.46
1:A:460:ALA:HA	1:A:488:THR:HG22	1.98	0.46
1:A:39:TRP:HB2	1:A:73:PRO:HB2	1.97	0.46
1:A:437:ARG:HA	1:A:437:ARG:HD3	1.77	0.46
1:A:46:ARG:NH1	1:A:84:GLU:OE1	2.46	0.46
1:A:649:PRO:O	1:A:651:SER:N	2.48	0.46
1:A:560:ALA:HB3	1:A:581:ASN:OD1	2.16	0.45
1:A:614:ARG:NH2	1:A:690:ASP:O	2.48	0.45
1:A:220:VAL:HG13	1:A:255:VAL:HA	1.99	0.45
1:A:607:LEU:HD12	1:A:610:ARG:NH1	2.31	0.45
1:A:644:LEU:HG	1:A:695:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:NH2	1:A:106:TYR:OH	2.48	0.45
1:A:74:THR:OG1	1:A:140:ASP:OD1	2.30	0.45
1:A:171:ILE:HD11	1:A:187:TYR:CB	2.46	0.45
1:A:273:GLN:O	1:A:275:ARG:N	2.50	0.44
1:A:468:LEU:HA	1:A:471:ARG:HE	1.82	0.44
1:A:337:HIS:CB	1:A:684:VAL:HG11	2.47	0.44
1:A:402:VAL:HG22	1:A:457:VAL:HG23	1.99	0.44
1:A:195:PRO:HB3	1:A:211:TYR:CE1	2.53	0.44
1:A:310:VAL:HG22	1:A:347:VAL:HG22	1.99	0.44
1:A:564:TYR:HB2	1:A:578:VAL:HG23	1.98	0.44
1:A:23:ALA:CB	1:A:367:ARG:HH12	2.31	0.44
1:A:607:LEU:HA	1:A:607:LEU:HD12	1.82	0.44
1:A:171:ILE:HG13	1:A:175:ASN:HD21	1.82	0.44
1:A:243:PHE:HD2	1:A:263:ALA:O	2.00	0.44
1:A:337:HIS:ND1	1:A:684:VAL:HG21	2.33	0.44
1:A:481:GLU:HB3	1:A:587:GLN:H	1.82	0.44
1:A:587:GLN:HG2	1:A:588:VAL:H	1.83	0.44
1:A:61:ILE:HG21	1:A:68:ALA:HB2	1.99	0.44
1:A:616:ALA:HB1	1:A:693:ASP:O	2.18	0.43
1:A:619:LEU:HD21	1:A:625:ILE:HG12	2.00	0.43
1:A:639:SER:HA	1:A:681:PRO:HB3	2.00	0.43
1:A:337:HIS:CG	1:A:684:VAL:HG21	2.53	0.43
1:A:76:THR:HG23	1:A:105:HIS:HE1	1.83	0.43
1:A:309:TRP:CG	1:A:346:ALA:HB3	2.53	0.43
1:A:625:ILE:HG22	1:A:634:VAL:HB	2.00	0.43
1:A:116:GLU:O	1:A:120:ILE:HG22	2.19	0.43
1:A:481:GLU:HB2	1:A:587:GLN:O	2.19	0.43
1:A:604:ALA:O	1:A:608:LEU:HD13	2.18	0.43
1:A:231:ARG:NH2	1:A:258:ASP:O	2.52	0.43
1:A:607:LEU:HD12	1:A:610:ARG:HH11	1.84	0.43
1:A:6:CYS:HB3	1:A:33:ARG:HH21	1.84	0.42
1:A:624:ARG:HD3	1:A:624:ARG:HA	1.80	0.42
1:A:694:GLY:C	1:A:695:LEU:HD12	2.40	0.42
1:A:14:SER:HA	1:A:17:TRP:CG	2.55	0.42
1:A:42:LEU:O	1:A:44:PRO:HD3	2.18	0.42
1:A:461:LEU:N	1:A:488:THR:HG22	2.24	0.42
1:A:263:ALA:HB1	1:A:311:MET:HB2	2.01	0.42
1:A:310:VAL:HG22	1:A:347:VAL:HA	2.01	0.42
1:A:651:SER:OG	1:A:687:ILE:HG22	2.20	0.42
1:A:268:PRO:HG2	1:A:335:TRP:CD1	2.55	0.42
1:A:503:PRO:HD2	1:A:507:THR:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:N	1:A:66:MET:HE1	2.34	0.42
1:A:252:ALA:HA	1:A:255:VAL:HG12	2.02	0.42
1:A:418:ALA:HB3	1:A:421:PHE:HB2	2.00	0.42
1:A:352:TRP:CH2	1:A:367:ARG:NH1	2.88	0.42
1:A:436:GLY:O	1:A:619:LEU:HD12	2.20	0.42
1:A:549:ARG:HG2	1:A:550:THR:OG1	2.20	0.42
1:A:481:GLU:OE1	1:A:610:ARG:NH1	2.53	0.42
1:A:92:ASP:HB3	1:A:98:ARG:HH21	1.84	0.42
1:A:12:TRP:HH2	1:A:356:LEU:HD13	1.85	0.42
1:A:304:LEU:HB3	1:A:306:ARG:NE	2.34	0.42
1:A:180:ASN:CB	1:A:186:GLN:HA	2.50	0.41
1:A:402:VAL:HG22	1:A:457:VAL:CG2	2.50	0.41
1:A:46:ARG:NH2	1:A:116:GLU:HG2	2.35	0.41
1:A:472:LEU:O	1:A:476:ILE:HG13	2.21	0.41
1:A:580:THR:HB	1:A:587:GLN:OE1	2.19	0.41
1:A:141:ASN:OD1	1:A:242:ASN:ND2	2.47	0.41
1:A:583:VAL:HG23	1:A:584:GLY:N	2.35	0.41
1:A:349:TYR:HB2	1:A:366:LEU:HD11	2.03	0.41
1:A:502:GLN:HB3	1:A:514:VAL:HB	2.02	0.41
1:A:43:GLU:HG2	1:A:45:GLU:O	2.20	0.41
1:A:336:ALA:HB2	1:A:349:TYR:OH	2.21	0.41
1:A:46:ARG:HH21	1:A:119:ARG:NE	2.15	0.41
1:A:546:VAL:HG11	1:A:599:LEU:HB2	2.02	0.41
1:A:634:VAL:CG1	1:A:685:ALA:HB3	2.51	0.41
1:A:481:GLU:OE1	1:A:610:ARG:CD	2.67	0.41
1:A:224:ARG:HG3	1:A:224:ARG:HH11	1.86	0.41
1:A:263:ALA:HA	1:A:309:TRP:O	2.20	0.41
1:A:464:VAL:HG13	1:A:468:LEU:HD12	2.02	0.41
1:A:643:ARG:O	1:A:645:PRO:HD3	2.21	0.41
1:A:39:TRP:O	1:A:39:TRP:HD1	2.02	0.41
1:A:517:HIS:HB3	1:A:553:GLU:HG2	2.01	0.41
1:A:554:TRP:N	1:A:554:TRP:CD1	2.89	0.41
1:A:77:PRO:HG2	1:A:105:HIS:CD2	2.56	0.41
1:A:312:GLU:HG2	1:A:350:PHE:HB2	2.03	0.40
1:A:526:THR:HB	1:A:548:PHE:CZ	2.57	0.40
1:A:234:ASP:HB3	1:A:237:TRP:CD2	2.56	0.40
1:A:145:CYS:SG	1:A:146:HIS:N	2.95	0.40
1:A:551:TRP:HE1	1:A:553:GLU:HG3	1.86	0.40
1:A:61:ILE:HG22	1:A:66:MET:O	2.21	0.40
1:A:625:ILE:HG22	1:A:634:VAL:CB	2.51	0.40
1:A:82:VAL:HG22	1:A:88:ILE:HD11	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:OG	1:A:202:GLU:O[2_665]	2.14	0.06

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	662/700 (95%)	614 (93%)	47 (7%)	1 (0%)	47 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	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	542/568 (95%)	522 (96%)	20 (4%)	34 60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	143	PHE

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Mol	Chain	Res	Type
1	A	153	CYS
1	A	189	SER
1	A	266	SER
1	A	271	PHE
1	A	275	ARG
1	A	276	TYR
1	A	286	ARG
1	A	367	ARG
1	A	397	ASP
1	A	472	LEU
1	A	517	HIS
1	A	561	GLU
1	A	569	ASP
1	A	605	SER
1	A	610	ARG
1	A	631	ARG
1	A	650	GLU
1	A	655	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	587	GLN

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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	668/700 (95%)	0.73	81 (12%) 4 4	54, 97, 143, 206	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	PHE	5.7
1	A	54	LEU	5.3
1	A	687	ILE	5.2
1	A	68	ALA	5.1
1	A	642	LEU	4.9
1	A	51	PHE	4.9
1	A	450	LEU	4.9
1	A	583	VAL	4.7
1	A	121	VAL	4.7
1	A	647	ILE	4.6
1	A	652	LEU	4.5
1	A	476	ILE	4.4
1	A	590	TYR	4.3
1	A	391	ASP	4.3
1	A	651	SER	4.3
1	A	673	SER	4.3
1	A	137	TRP	4.2
1	A	546	VAL	4.2
1	A	49	PHE	4.2
1	A	131	SER	4.0
1	A	649	PRO	4.0
1	A	190	PHE	3.9
1	A	164	LEU	3.7
1	A	677	ILE	3.5
1	A	397	ASP	3.3
1	A	392	GLY	3.3
1	A	134	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	552	ALA	3.1
1	A	644	LEU	3.1
1	A	632	THR	3.0
1	A	472	LEU	3.0
1	A	42	LEU	3.0
1	A	118	ALA	2.9
1	A	3	LEU	2.9
1	A	686	VAL	2.8
1	A	344	ALA	2.7
1	A	31	TYR	2.7
1	A	168	TYR	2.7
1	A	261	ARG	2.7
1	A	679	VAL	2.7
1	A	280	ALA	2.6
1	A	685	ALA	2.6
1	A	468	LEU	2.6
1	A	235	PRO	2.6
1	A	684	VAL	2.6
1	A	119	ARG	2.5
1	A	126	GLU	2.5
1	A	356	LEU	2.5
1	A	387	PHE	2.5
1	A	122	GLU	2.5
1	A	531	VAL	2.5
1	A	629	GLY	2.5
1	A	608	LEU	2.4
1	A	130	ASP	2.4
1	A	676	GLY	2.4
1	A	610	ARG	2.4
1	A	246	ARG	2.3
1	A	627	TYR	2.3
1	A	174	LEU	2.3
1	A	230	ILE	2.3
1	A	128	TYR	2.3
1	A	696	ARG	2.3
1	A	61	ILE	2.3
1	A	132	PRO	2.2
1	A	633	TRP	2.2
1	A	646	GLU	2.2
1	A	299	ILE	2.2
1	A	390	LEU	2.2
1	A	527	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	17	TRP	2.2
1	A	67	GLN	2.2
1	A	229	LEU	2.2
1	A	641	ARG	2.1
1	A	499	PRO	2.1
1	A	143	PHE	2.1
1	A	358	GLY	2.1
1	A	587	GLN	2.1
1	A	615	TYR	2.1
1	A	584	GLY	2.1
1	A	129	ALA	2.0
1	A	383	THR	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, 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(Å ²)	Q<0.9
3	MG	A	802	1/1	0.74	0.39	78,78,78,78	0
2	ZN	A	801	1/1	0.90	0.23	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.