



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3LVT
Title : The Crystal Structure of a Protein in the Glycosyl Hydrolase Family 38 from Enterococcus faecalis to 2.55Å
Authors : Stein, A.J.; Binkowski, T.A.; Weger, A.; Borovilos, M.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-02-22
Resolution : 2.55 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

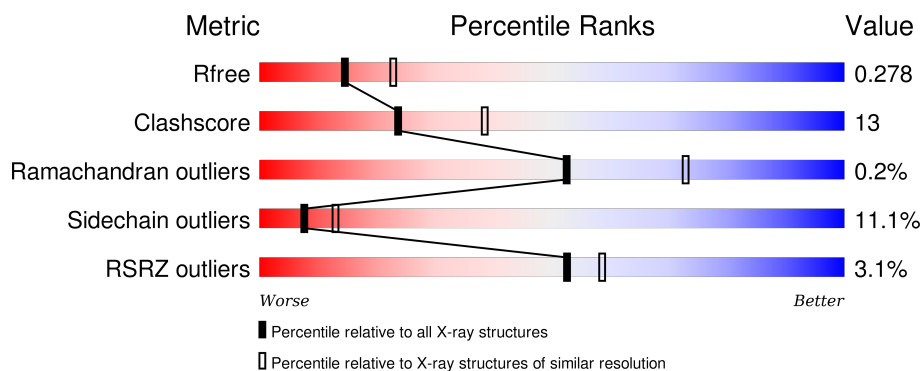
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

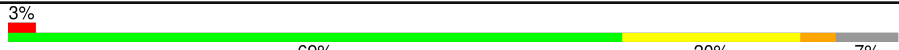
The reported resolution of this entry is 2.55 Å.

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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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. 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	899	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6466 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 Glycosyl hydrolase, family 38.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	Se	0	0	0
			6425	4087	1070	1243	6	19			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q834E8
A	-1	ASN	-	expression tag	UNP Q834E8
A	0	ALA	-	expression tag	UNP Q834E8

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

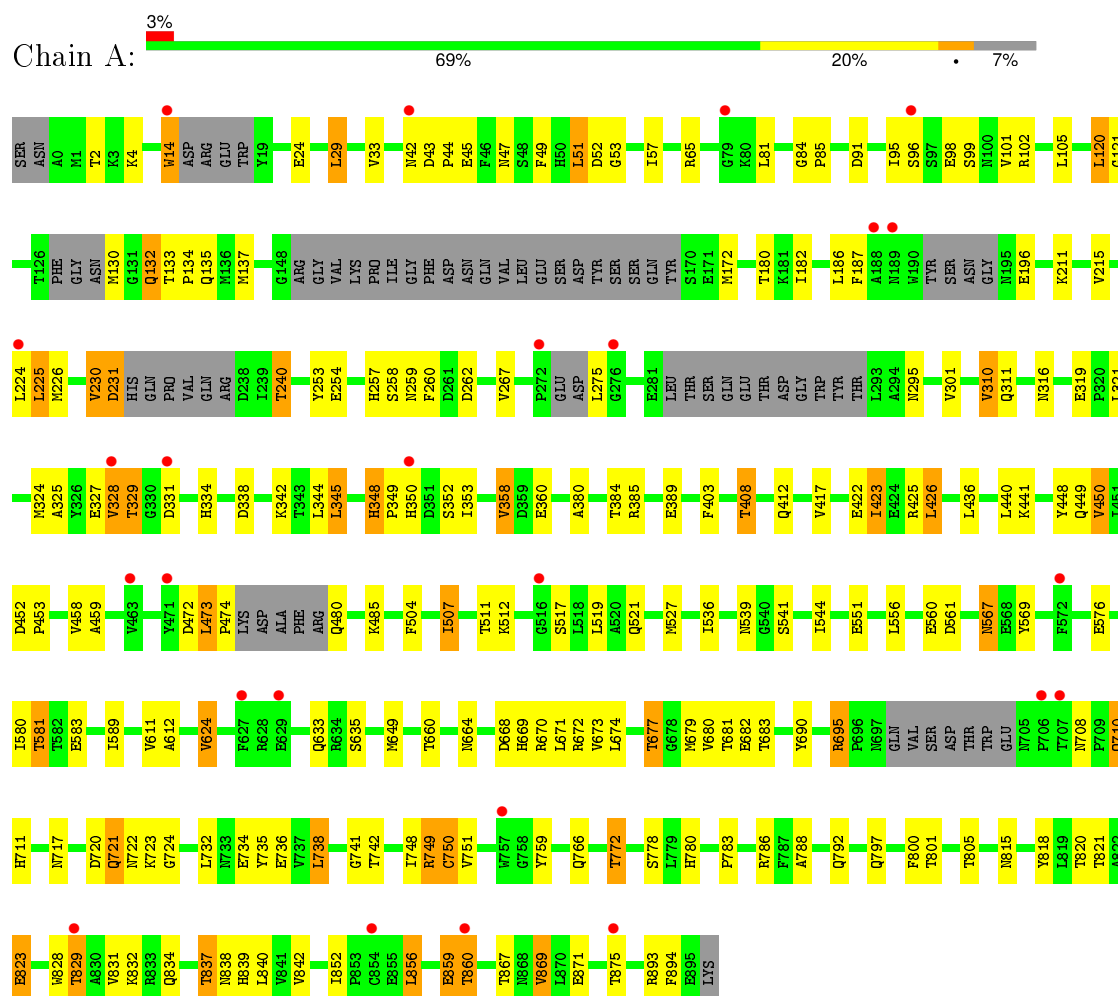
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		

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 errors 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: Glycosyl hydrolase, family 38



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.73Å 134.95Å 106.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.04 – 2.55 42.04 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.04-2.55) 99.8 (42.04-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.222 , 0.282 0.218 , 0.278	Depositor DCC
R_{free} test set	1587 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.7	EDS
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31460 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6466	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA

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	0.60	1/6553 (0.0%)	0.68	1/8909 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	750	CYS	CB-SG	-5.25	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	749	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

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	6425	0	6023	164	0
2	A	1	0	0	0	0
3	A	40	0	0	0	0
All	All	6466	0	6023	164	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 (164) 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:473:LEU:CB	1:A:474:PRO:HA	1.58	1.31
1:A:837:THR:CG2	1:A:839:HIS:H	1.62	1.13
1:A:473:LEU:CB	1:A:474:PRO:CA	2.40	0.99
1:A:98:GLU:OE2	1:A:102:ARG:NH1	2.01	0.94
1:A:837:THR:HG22	1:A:839:HIS:H	1.28	0.94
1:A:45:GLU:HB2	1:A:240:THR:HG21	1.48	0.93
1:A:720:ASP:HB3	1:A:722:ASN:H	1.38	0.87
1:A:561:ASP:OD1	1:A:669:HIS:HD2	1.62	0.82
1:A:47:ASN:H	1:A:257:HIS:HD2	1.27	0.82
1:A:45:GLU:CB	1:A:240:THR:HG21	2.09	0.81
1:A:717:ASN:HD21	1:A:780:HIS:HE1	1.25	0.81
1:A:837:THR:O	1:A:838:ASN:HB2	1.81	0.81
1:A:837:THR:HG23	1:A:839:HIS:H	1.48	0.79
1:A:380:ALA:O	1:A:384:THR:HG23	1.83	0.78
1:A:837:THR:HG22	1:A:838:ASN:N	1.97	0.77
1:A:567:ASN:O	1:A:749:ARG:NH2	2.16	0.77
1:A:423:ILE:HG22	1:A:485:LYS:O	1.86	0.75
1:A:133:THR:O	1:A:137:MSE:HG3	1.86	0.74
1:A:316:ASN:O	1:A:408:THR:HG23	1.87	0.74
1:A:425:ARG:NH2	1:A:472:ASP:OD2	2.15	0.73
1:A:49:PHE:HE1	1:A:230:VAL:HG21	1.53	0.73
1:A:677:THR:HB	1:A:741:GLY:O	1.87	0.73
1:A:49:PHE:CE1	1:A:230:VAL:HG21	2.24	0.73
1:A:230:VAL:O	1:A:231:ASP:HB3	1.88	0.73
1:A:329:THR:HG23	1:A:331:ASP:H	1.51	0.72
1:A:98:GLU:OE1	1:A:829:THR:CG2	2.39	0.71
1:A:581:THR:HG23	1:A:583:GLU:H	1.56	0.70
1:A:567:ASN:HD22	1:A:569:TYR:H	1.38	0.70
1:A:823:GLU:CD	1:A:823:GLU:H	1.95	0.70
1:A:668:ASP:H	1:A:766:GLN:HE22	1.40	0.69
1:A:14:TRP:CD1	1:A:14:TRP:N	2.61	0.68
1:A:681:THR:HG22	1:A:683:THR:H	1.58	0.67
1:A:450:VAL:HG22	1:A:458:VAL:HB	1.77	0.67
1:A:837:THR:CG2	1:A:839:HIS:N	2.48	0.67
1:A:837:THR:HG22	1:A:839:HIS:N	2.06	0.67
1:A:14:TRP:HZ2	1:A:52:ASP:OD2	1.79	0.65
1:A:348:HIS:N	1:A:349:PRO:CD	2.59	0.65
1:A:98:GLU:OE1	1:A:829:THR:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HG13	1:A:869:VAL:HG13	1.80	0.63
1:A:95:ILE:HD12	1:A:99:SER:HB2	1.80	0.62
1:A:624:VAL:O	1:A:624:VAL:HG23	1.97	0.62
1:A:519:LEU:HB3	1:A:649:MSE:CE	2.28	0.62
1:A:670:ARG:HG3	1:A:749:ARG:HG3	1.82	0.62
1:A:581:THR:CG2	1:A:583:GLU:H	2.13	0.62
1:A:519:LEU:HB3	1:A:649:MSE:HE3	1.82	0.62
1:A:14:TRP:HD1	1:A:14:TRP:H	1.47	0.62
1:A:837:THR:CG2	1:A:838:ASN:N	2.62	0.62
1:A:670:ARG:CG	1:A:749:ARG:HG3	2.30	0.61
1:A:360:GLU:CD	1:A:360:GLU:H	2.02	0.61
1:A:821:THR:HG23	1:A:828:TRP:CZ2	2.34	0.61
1:A:837:THR:CG2	1:A:839:HIS:CG	2.82	0.61
1:A:837:THR:HG23	1:A:839:HIS:CG	2.37	0.60
1:A:788:ALA:O	1:A:792:GLN:HG2	2.00	0.60
1:A:29:LEU:HD21	1:A:57:ILE:HG23	1.84	0.60
1:A:840:LEU:HB3	1:A:894:PHE:HB2	1.85	0.59
1:A:91:ASP:HB2	1:A:350:HIS:HA	1.84	0.59
1:A:95:ILE:HD12	1:A:99:SER:CB	2.33	0.59
1:A:132:GLN:HE22	1:A:135:GLN:HE21	1.51	0.59
1:A:316:ASN:O	1:A:408:THR:CG2	2.51	0.58
1:A:453:PRO:HG2	1:A:815:ASN:HD21	1.68	0.58
1:A:720:ASP:OD2	1:A:723:LYS:NZ	2.31	0.57
1:A:423:ILE:HD11	1:A:448:TYR:CE1	2.40	0.57
1:A:834:GLN:HB3	1:A:837:THR:HG22	1.86	0.57
1:A:325:ALA:O	1:A:328:VAL:HG13	2.04	0.57
1:A:417:VAL:HG11	1:A:800:PHE:CD2	2.39	0.57
1:A:132:GLN:HE22	1:A:135:GLN:NE2	2.02	0.57
1:A:519:LEU:HD13	1:A:649:MSE:HE3	1.87	0.57
1:A:695:ARG:NH2	1:A:711:HIS:O	2.38	0.56
1:A:133:THR:HB	1:A:134:PRO:HD3	1.87	0.56
1:A:348:HIS:N	1:A:349:PRO:HD2	2.20	0.56
1:A:783:PRO:O	1:A:786:ARG:HB2	2.06	0.56
1:A:321:LEU:HD13	1:A:384:THR:HG22	1.88	0.55
1:A:738:LEU:HD22	1:A:742:THR:HB	1.88	0.55
1:A:102:ARG:NH2	1:A:319:GLU:OE1	2.39	0.55
1:A:45:GLU:CB	1:A:240:THR:CG2	2.83	0.55
1:A:426:LEU:HB3	1:A:436:LEU:HD13	1.89	0.55
1:A:539:ASN:HB3	1:A:541:SER:H	1.72	0.54
1:A:681:THR:HG22	1:A:682:GLU:N	2.22	0.54
1:A:539:ASN:OD1	1:A:583:GLU:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:H	1:A:257:HIS:CD2	2.18	0.54
1:A:710:GLN:HB3	1:A:735:TYR:CE1	2.43	0.53
1:A:677:THR:HG23	1:A:679:MSE:HE3	1.89	0.53
1:A:295:ASN:HA	1:A:734:GLU:OE1	2.09	0.53
1:A:837:THR:HG21	1:A:839:HIS:CG	2.43	0.53
1:A:834:GLN:NE2	1:A:837:THR:HG21	2.24	0.53
1:A:710:GLN:HB3	1:A:735:TYR:CZ	2.44	0.53
1:A:721:GLN:H	1:A:721:GLN:CD	2.11	0.53
1:A:576:GLU:H	1:A:633:GLN:HE22	1.56	0.53
1:A:834:GLN:HB3	1:A:837:THR:CG2	2.38	0.53
1:A:14:TRP:CZ2	1:A:52:ASP:OD2	2.60	0.53
1:A:422:GLU:OE1	1:A:425:ARG:HD3	2.09	0.52
1:A:211:LYS:O	1:A:215:VAL:HG23	2.10	0.51
1:A:358:VAL:HG13	1:A:360:GLU:HG2	1.92	0.51
1:A:837:THR:HG23	1:A:839:HIS:N	2.21	0.51
1:A:664:ASN:HD21	1:A:669:HIS:CE1	2.29	0.51
1:A:132:GLN:NE2	1:A:135:GLN:HE21	2.08	0.50
1:A:717:ASN:HD21	1:A:780:HIS:CE1	2.16	0.50
1:A:834:GLN:HE21	1:A:837:THR:HG21	1.76	0.50
1:A:52:ASP:O	1:A:52:ASP:OD1	2.30	0.50
1:A:724:GLY:HA3	1:A:780:HIS:CE1	2.47	0.50
1:A:324:MSE:HE2	1:A:818:TYR:HB3	1.93	0.50
1:A:673:VAL:O	1:A:673:VAL:HG13	2.12	0.49
1:A:353:ILE:O	1:A:353:ILE:HG13	2.12	0.49
1:A:664:ASN:HD21	1:A:669:HIS:HE1	1.59	0.49
1:A:832:LYS:HE3	1:A:871:GLU:OE1	2.13	0.49
1:A:334:HIS:CE1	1:A:834:GLN:O	2.66	0.48
1:A:624:VAL:O	1:A:624:VAL:CG2	2.61	0.48
1:A:671:LEU:HB3	1:A:748:ILE:HG22	1.96	0.48
1:A:423:ILE:HG22	1:A:485:LYS:C	2.34	0.48
1:A:567:ASN:HD22	1:A:569:TYR:N	2.09	0.47
1:A:338:ASP:OD2	1:A:342:LYS:HE2	2.14	0.47
1:A:837:THR:HG21	1:A:839:HIS:CD2	2.49	0.47
1:A:670:ARG:HG2	1:A:749:ARG:HG3	1.97	0.47
1:A:120:LEU:HD21	1:A:260:PHE:CD1	2.50	0.47
1:A:259:ASN:ND2	1:A:262:ASP:H	2.13	0.47
1:A:53:GLY:HA2	1:A:84:GLY:O	2.14	0.47
1:A:536:ILE:HG21	1:A:589:ILE:HD12	1.97	0.47
1:A:672:ARG:NH2	1:A:736:GLU:OE2	2.47	0.47
1:A:403:PHE:CZ	1:A:504:PHE:HB2	2.50	0.47
1:A:612:ALA:O	1:A:635:SER:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:GLN:HE21	1:A:710:GLN:HB2	1.48	0.46
1:A:842:VAL:HG11	1:A:856:LEU:HD11	1.98	0.46
1:A:452:ASP:HB2	1:A:453:PRO:HD2	1.97	0.46
1:A:345:LEU:O	1:A:348:HIS:HB2	2.16	0.46
1:A:215:VAL:HG11	1:A:224:LEU:HB3	1.98	0.46
1:A:29:LEU:HD21	1:A:57:ILE:CG2	2.45	0.46
1:A:660:THR:O	1:A:772:THR:HA	2.16	0.45
1:A:187:PHE:CD2	1:A:187:PHE:C	2.90	0.44
1:A:96:SER:H	1:A:311:GLN:HE22	1.65	0.44
1:A:527:MSE:HB2	1:A:649:MSE:CE	2.47	0.44
1:A:551:GLU:HG3	1:A:723:LYS:HB3	2.00	0.44
1:A:310:VAL:HG22	1:A:344:LEU:HD13	1.99	0.44
1:A:45:GLU:HB3	1:A:240:THR:CG2	2.48	0.44
1:A:85:PRO:HD3	1:A:120:LEU:O	2.18	0.44
1:A:867:THR:HG21	1:A:893:ARG:HD3	1.98	0.44
1:A:452:ASP:HB2	1:A:453:PRO:CD	2.48	0.43
1:A:567:ASN:ND2	1:A:569:TYR:H	2.11	0.43
1:A:329:THR:CG2	1:A:331:ASP:H	2.27	0.43
1:A:544:ILE:HD12	1:A:556:LEU:CD1	2.48	0.43
1:A:121:GLY:HA3	1:A:137:MSE:HE1	2.01	0.43
1:A:624:VAL:HG12	1:A:759:TYR:HB2	2.00	0.43
1:A:677:THR:HG22	1:A:679:MSE:H	1.84	0.43
1:A:859:GLU:HB3	1:A:860:THR:H	1.58	0.43
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.87	0.43
1:A:837:THR:O	1:A:838:ASN:CB	2.56	0.43
1:A:96:SER:H	1:A:311:GLN:NE2	2.17	0.43
1:A:98:GLU:OE1	1:A:690:TYR:OH	2.27	0.43
1:A:527:MSE:HB2	1:A:649:MSE:HE1	2.01	0.43
1:A:449:GLN:HB3	1:A:507:ILE:HG22	2.01	0.42
1:A:51:LEU:HG	1:A:81:LEU:HD22	2.01	0.42
1:A:4:LYS:HD2	1:A:253:TYR:CE1	2.55	0.42
1:A:417:VAL:HG11	1:A:800:PHE:HD2	1.82	0.42
1:A:385:ARG:O	1:A:389:GLU:HB2	2.20	0.42
1:A:750:CYS:HB3	1:A:766:GLN:HE21	1.85	0.42
1:A:690:TYR:HE1	1:A:829:THR:HG21	1.85	0.42
1:A:29:LEU:HD22	1:A:33:VAL:HG23	2.02	0.42
1:A:327:GLU:HG3	1:A:818:TYR:HE1	1.85	0.42
1:A:43:ASP:HA	1:A:44:PRO:HD3	1.93	0.41
1:A:348:HIS:H	1:A:349:PRO:CD	2.32	0.41
1:A:258:SER:OG	1:A:259:ASN:N	2.52	0.41
1:A:544:ILE:HD12	1:A:556:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ASP:OD1	1:A:669:HIS:CD2	2.55	0.40
1:A:459:ALA:HA	1:A:512:LYS:O	2.21	0.40
1:A:225:LEU:HD23	1:A:226:MSE:H	1.85	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	813/899 (90%)	780 (96%)	31 (4%)	2 (0%)	52 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	LEU
1	A	348	HIS

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	664/766 (87%)	590 (89%)	74 (11%)	8 13

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	14	TRP
1	A	24	GLU
1	A	29	LEU
1	A	42	ASN
1	A	51	LEU
1	A	65	ARG
1	A	105	LEU
1	A	120	LEU
1	A	130	MSE
1	A	132	GLN
1	A	172	MSE
1	A	180	THR
1	A	182	ILE
1	A	186	LEU
1	A	196	GLU
1	A	225	LEU
1	A	230	VAL
1	A	231	ASP
1	A	240	THR
1	A	254	GLU
1	A	267	VAL
1	A	275	LEU
1	A	301	VAL
1	A	310	VAL
1	A	328	VAL
1	A	329	THR
1	A	345	LEU
1	A	352	SER
1	A	358	VAL
1	A	408	THR
1	A	412	GLN
1	A	423	ILE
1	A	426	LEU
1	A	440	LEU
1	A	441	LYS
1	A	450	VAL
1	A	480	GLN
1	A	507	ILE
1	A	511	THR
1	A	517	SER
1	A	521	GLN
1	A	560	GLU

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Mol	Chain	Res	Type
1	A	567	ASN
1	A	580	ILE
1	A	581	THR
1	A	611	VAL
1	A	624	VAL
1	A	674	LEU
1	A	677	THR
1	A	680	VAL
1	A	695	ARG
1	A	708	ASN
1	A	710	GLN
1	A	721	GLN
1	A	732	LEU
1	A	738	LEU
1	A	751	VAL
1	A	772	THR
1	A	778	SER
1	A	797	GLN
1	A	801	THR
1	A	805	THR
1	A	820	THR
1	A	823	GLU
1	A	829	THR
1	A	831	VAL
1	A	837	THR
1	A	852	ILE
1	A	856	LEU
1	A	859	GLU
1	A	860	THR
1	A	869	VAL
1	A	875	THR

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	11	HIS
1	A	54	GLN
1	A	119	GLN
1	A	132	GLN
1	A	257	HIS
1	A	259	ASN
1	A	305	GLN

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	412	GLN
1	A	449	GLN
1	A	539	ASN
1	A	567	ASN
1	A	591	ASN
1	A	633	GLN
1	A	664	ASN
1	A	665	GLN
1	A	669	HIS
1	A	710	GLN
1	A	766	GLN
1	A	780	HIS
1	A	815	ASN
1	A	834	GLN
1	A	838	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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	814/899 (90%)	0.19	25 (3%)	52 58	38, 57, 72, 88	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	627	PHE	4.8
1	A	706	PRO	4.3
1	A	328	VAL	4.0
1	A	14	TRP	3.9
1	A	860	THR	3.6
1	A	272	PRO	3.3
1	A	331	ASP	3.2
1	A	276	GLY	2.9
1	A	471	TYR	2.7
1	A	757	TRP	2.7
1	A	572	PHE	2.6
1	A	42	ASN	2.5
1	A	629	GLU	2.5
1	A	516	GLY	2.5
1	A	854	CYS	2.4
1	A	350	HIS	2.4
1	A	463	VAL	2.4
1	A	188	ALA	2.2
1	A	96	SER	2.2
1	A	189	ASN	2.2
1	A	707	THR	2.1
1	A	224	LEU	2.1
1	A	829	THR	2.0
1	A	79	GLY	2.0
1	A	875	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 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(\AA^2)	Q<0.9
2	CA	A	897	1/1	0.92	0.05	-3.06	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.