



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:36 AM GMT

PDB ID : 2RDY
Title : Crystal structure of a putative glycoside hydrolase family protein from *Bacillus halodurans*
Authors : Sugadev, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-09-25
Resolution : 2.03 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

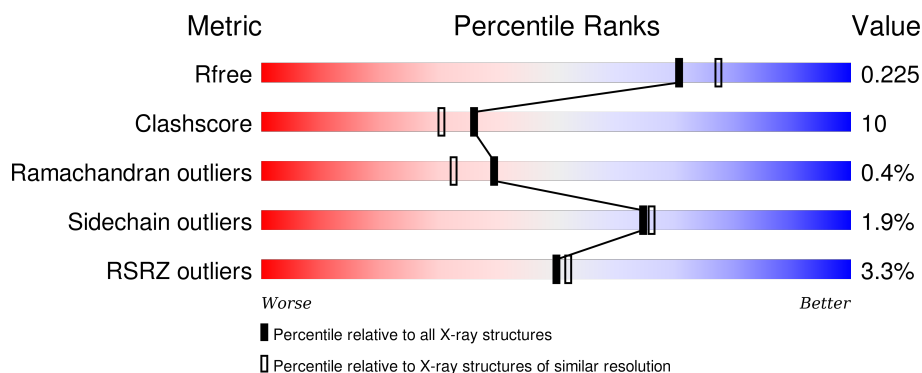
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


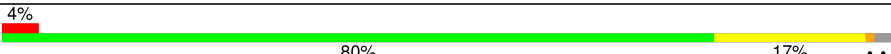
The reported resolution of this entry is 2.03 Å.

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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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	803	 3% 79% 18% ..
1	B	803	 4% 80% 17% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13037 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 BH0842 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	Se	0	0	0
			6239	3955	1076	1181	9	18			
1	B	787	Total	C	N	O	S	Se	0	0	0
			6239	3955	1076	1181	9	18			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q9KEL0
A	2	SER	-	EXPRESSION TAG	UNP Q9KEL0
A	3	LEU	-	EXPRESSION TAG	UNP Q9KEL0
A	796	GLU	-	EXPRESSION TAG	UNP Q9KEL0
A	797	GLY	-	EXPRESSION TAG	UNP Q9KEL0
A	798	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	799	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	800	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	801	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	802	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	803	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	1	MSE	-	EXPRESSION TAG	UNP Q9KEL0
B	2	SER	-	EXPRESSION TAG	UNP Q9KEL0
B	3	LEU	-	EXPRESSION TAG	UNP Q9KEL0
B	796	GLU	-	EXPRESSION TAG	UNP Q9KEL0
B	797	GLY	-	EXPRESSION TAG	UNP Q9KEL0
B	798	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	799	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	800	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	801	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	802	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	803	HIS	-	EXPRESSION TAG	UNP Q9KEL0

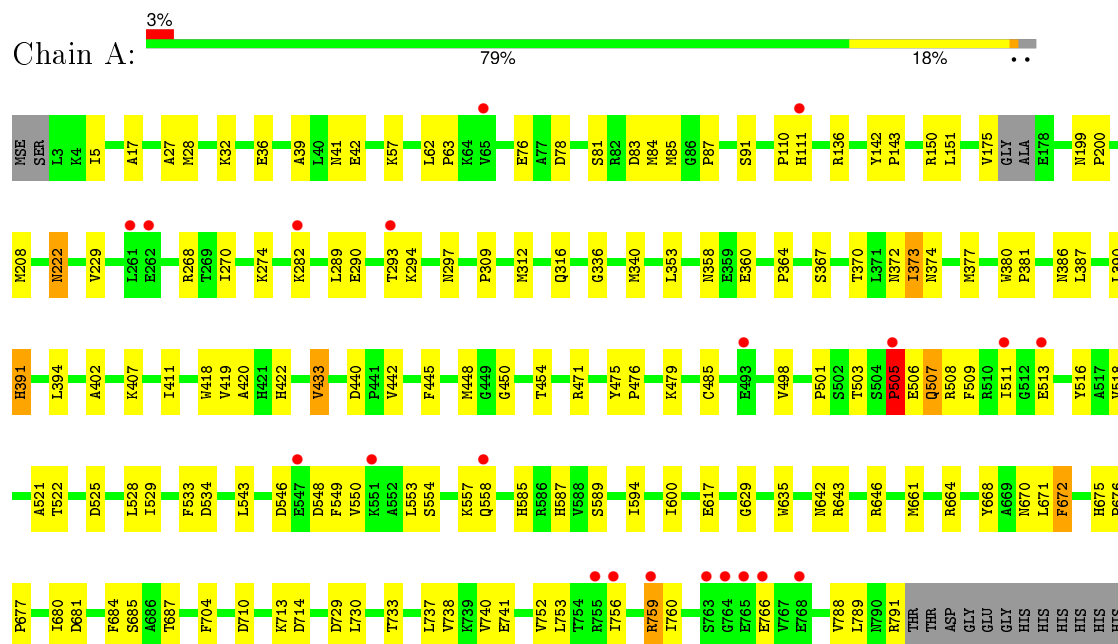
- Molecule 2 is water.

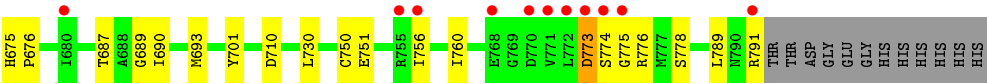
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	275	Total 275	O 275	0	0
2	B	284	Total 284	O 284	0	0

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 ($\text{RSRZ} > 2$). 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: BH0842 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.61Å 149.07Å 164.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 2.03 47.57 – 2.03	Depositor EDS
% Data completeness (in resolution range)	93.6 (47.57-2.03) 93.8 (47.57-2.03)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 2.03Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.225 0.197 , 0.225	Depositor DCC
R_{free} test set	6536 reflections (6.01%)	DCC
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 116001 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13037	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.94 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.4057e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

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	0.33	0/6378	0.60	2/8621 (0.0%)
1	B	0.34	0/6378	0.60	1/8621 (0.0%)
All	All	0.33	0/12756	0.60	3/17242 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	ILE	N-CA-C	-5.28	96.75	111.00
1	A	42	GLU	N-CA-C	-5.14	97.13	111.00
1	A	5	ILE	N-CA-C	-5.10	97.23	111.00

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	6239	0	6036	123	0
1	B	6239	0	6036	112	0
2	A	275	0	0	5	0
2	B	284	0	0	2	0
All	All	13037	0	12072	235	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 10.

All (235) 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:448:MSE:HE2	1:A:525:ASP:HA	1.22	1.17
1:B:690:ILE:HA	1:B:693:MSE:HE3	1.43	0.97
1:B:407:LYS:HE3	1:B:411:ILE:HD11	1.49	0.93
1:B:84:MSE:HE1	1:B:501:PRO:HG2	1.48	0.93
1:A:448:MSE:HE3	1:A:528:LEU:HB2	1.53	0.91
1:B:690:ILE:CA	1:B:693:MSE:HE3	2.02	0.88
1:A:661:MSE:HE2	1:A:664:ARG:HD2	1.56	0.88
1:A:642:ASN:HD21	1:A:710:ASP:H	1.23	0.85
1:A:81:SER:HA	1:A:84:MSE:HE2	1.60	0.83
1:A:448:MSE:HE2	1:A:525:ASP:CA	2.08	0.83
1:B:642:ASN:HD21	1:B:710:ASP:H	1.28	0.82
1:B:632:ILE:CG2	1:B:693:MSE:HE2	2.11	0.80
1:B:81:SER:HA	1:B:84:MSE:HE2	1.65	0.79
1:B:136:ARG:HD3	2:B:821:HOH:O	1.81	0.79
1:A:41:ASN:HD21	1:A:358:ASN:H	1.32	0.77
1:A:506:GLU:HG3	1:A:587:HIS:NE2	2.00	0.77
1:A:407:LYS:HE2	1:A:411:ILE:HD11	1.68	0.75
1:A:448:MSE:CE	1:A:528:LEU:HB2	2.16	0.75
1:B:690:ILE:N	1:B:693:MSE:HE3	2.01	0.74
1:A:222:ASN:HD22	1:A:222:ASN:H	1.37	0.72
1:A:642:ASN:ND2	1:A:710:ASP:H	1.88	0.71
1:A:737:LEU:HB3	1:A:756:ILE:HD11	1.73	0.71
1:B:751:GLU:OE2	1:B:776:ARG:HD2	1.92	0.70
1:A:661:MSE:HE3	1:A:664:ARG:HB2	1.73	0.69
1:B:701:TYR:CD2	1:B:776:ARG:HD3	2.27	0.69
1:A:635:TRP:CD2	1:A:643:ARG:HG2	2.28	0.69
1:B:642:ASN:ND2	1:B:710:ASP:H	1.90	0.68
1:A:340:MSE:HG2	1:A:390:LEU:HD23	1.75	0.68
1:B:324:ARG:HH11	1:B:324:ARG:HG3	1.61	0.66
1:B:340:MSE:HG2	1:B:390:LEU:HD23	1.78	0.66
1:A:81:SER:CA	1:A:84:MSE:HE2	2.26	0.66
1:A:136:ARG:HD3	2:A:904:HOH:O	1.96	0.66
1:A:525:ASP:O	1:A:529:ILE:HG12	1.95	0.65
1:B:507:GLN:HB2	1:B:585:HIS:CD2	2.31	0.65
1:A:546:ASP:HB3	1:A:549:PHE:HB3	1.79	0.64
1:B:142:TYR:HB3	1:B:143:PRO:HD3	1.79	0.63
1:B:41:ASN:HD21	1:B:358:ASN:H	1.46	0.63
1:A:41:ASN:ND2	1:A:358:ASN:H	1.96	0.62
1:B:62:LEU:O	1:B:65:VAL:HG12	2.00	0.61
1:B:689:GLY:C	1:B:693:MSE:HE3	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ASP:HB3	1:B:549:PHE:HB3	1.81	0.61
1:B:32:LYS:HB2	1:B:36:GLU:HA	1.83	0.60
1:A:142:TYR:HB3	1:A:143:PRO:HD3	1.81	0.60
1:A:738:VAL:HG12	1:A:791:ARG:CZ	2.31	0.60
1:B:222:ASN:HD22	1:B:222:ASN:H	1.51	0.59
1:A:222:ASN:ND2	1:A:222:ASN:H	2.01	0.59
1:A:136:ARG:HD2	1:A:151:LEU:CD2	2.33	0.59
1:A:293:THR:OG1	1:A:297:ASN:ND2	2.36	0.58
1:B:479:LYS:HG3	1:B:549:PHE:CE2	2.39	0.58
1:B:632:ILE:HG21	1:B:693:MSE:HE2	1.85	0.58
1:B:293:THR:OG1	1:B:297:ASN:ND2	2.36	0.57
1:A:312:MSE:HE2	1:A:316:GLN:NE2	2.19	0.57
1:B:632:ILE:HD13	1:B:648:LEU:HD13	1.87	0.57
1:B:136:ARG:HD2	1:B:151:LEU:CD2	2.35	0.57
1:A:554:SER:O	1:A:558:GLN:HG3	2.04	0.56
1:B:309:PRO:HG2	1:B:312:MSE:HB2	1.85	0.56
1:A:450:GLY:O	1:A:454:THR:HG23	2.04	0.56
1:A:643:ARG:HD3	1:A:646:ARG:HH11	1.70	0.56
1:A:546:ASP:O	1:A:550:VAL:HG23	2.06	0.56
1:A:585:HIS:CD2	1:A:587:HIS:HB2	2.41	0.56
1:A:617:GLU:OE2	1:A:643:ARG:NH2	2.38	0.56
1:B:136:ARG:HD2	1:B:151:LEU:HD22	1.87	0.55
1:B:41:ASN:ND2	1:B:358:ASN:H	2.04	0.55
1:B:222:ASN:ND2	1:B:222:ASN:H	2.04	0.55
1:A:81:SER:CB	1:A:84:MSE:HE2	2.36	0.55
1:B:690:ILE:HA	1:B:693:MSE:CE	2.27	0.55
1:B:585:HIS:CD2	1:B:587:HIS:HB2	2.42	0.54
1:B:760:ILE:HG12	1:B:789:LEU:CD2	2.36	0.54
1:B:199:ASN:ND2	1:B:202:ARG:HG2	2.23	0.54
1:A:507:GLN:HB2	1:A:585:HIS:CD2	2.43	0.54
1:A:505:PRO:HB2	1:A:589:SER:OG	2.08	0.54
1:A:57:LYS:HE3	1:A:83:ASP:HB3	1.90	0.54
1:A:309:PRO:HG2	1:A:312:MSE:HB2	1.89	0.54
1:B:179:HIS:HD2	1:B:217:ARG:HH11	1.56	0.54
1:A:534:ASP:OD1	1:A:557:LYS:HE2	2.09	0.53
1:A:78:ASP:OD1	1:A:518:VAL:HG22	2.09	0.53
1:B:81:SER:CA	1:B:84:MSE:HE2	2.38	0.53
1:A:81:SER:HB2	1:A:84:MSE:HE2	1.89	0.53
1:A:675:HIS:N	1:A:676:PRO:HA	2.23	0.53
1:A:377:MSE:SE	1:A:685:SER:HB3	2.58	0.53
1:B:566:GLY:HA2	1:B:572:GLN:HE21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASP:OD1	1:B:518:VAL:HG22	2.09	0.52
1:A:448:MSE:HE1	1:A:529:ILE:HG12	1.92	0.52
1:B:546:ASP:O	1:B:550:VAL:HG23	2.09	0.52
1:B:312:MSE:HE2	1:B:316:GLN:NE2	2.24	0.52
1:A:373:ILE:HG23	1:A:374:ASN:N	2.24	0.52
1:B:510:ARG:HD2	1:B:581:GLU:HG3	1.92	0.52
1:B:506:GLU:HG3	1:B:587:HIS:NE2	2.25	0.51
1:B:523:THR:HG23	1:B:563:LEU:HD22	1.92	0.51
1:B:547:GLU:CD	1:B:547:GLU:H	2.14	0.51
1:A:17:ALA:HB3	1:A:28:MSE:HG3	1.93	0.51
1:B:399:GLU:HG2	1:B:477:ILE:HD11	1.93	0.51
1:B:394:LEU:O	1:B:398:ILE:HG13	2.11	0.50
1:A:675:HIS:H	1:A:676:PRO:HA	1.76	0.50
1:A:675:HIS:HB3	1:A:676:PRO:C	2.31	0.50
1:A:508:ARG:HB3	1:A:516:TYR:O	2.11	0.50
1:B:450:GLY:O	1:B:454:THR:HG23	2.12	0.50
1:B:510:ARG:HH21	1:B:513:GLU:C	2.15	0.50
1:A:336:GLY:HA3	1:A:687:THR:OG1	2.12	0.50
1:A:760:ILE:HG12	1:A:789:LEU:HD22	1.94	0.50
1:B:27:ALA:HA	1:B:39:ALA:O	2.12	0.50
1:A:506:GLU:HG3	1:A:587:HIS:CD2	2.46	0.49
1:A:268:ARG:HB3	1:A:268:ARG:HH11	1.77	0.49
1:A:729:ASP:HB2	1:A:741:GLU:HB2	1.94	0.49
1:B:402:ALA:HA	1:B:418:TRP:CD2	2.48	0.49
1:B:498:VAL:HB	1:B:521:ALA:HB2	1.94	0.49
1:A:360:GLU:OE1	1:A:364:PRO:HD3	2.12	0.49
1:A:84:MSE:HE3	1:A:445:PHE:CE1	2.48	0.49
1:A:372:ASN:O	1:A:373:ILE:HB	2.13	0.48
1:B:756:ILE:CD1	1:B:791:ARG:HG2	2.43	0.48
1:B:261:LEU:HD23	1:B:261:LEU:O	2.13	0.48
1:B:675:HIS:HB3	1:B:676:PRO:C	2.33	0.48
1:B:324:ARG:NH1	1:B:324:ARG:HG3	2.27	0.48
1:A:199:ASN:N	1:A:200:PRO:HD3	2.28	0.48
1:A:402:ALA:HA	1:A:418:TRP:CD2	2.48	0.48
1:B:533:PHE:O	1:B:537:ILE:HG13	2.13	0.48
1:A:643:ARG:HA	1:A:646:ARG:NH1	2.29	0.48
1:A:136:ARG:HD2	1:A:151:LEU:HD22	1.96	0.48
1:B:774:SER:OG	1:B:775:GLY:N	2.44	0.48
1:A:200:PRO:HG3	2:A:813:HOH:O	2.13	0.48
1:A:84:MSE:HE3	1:A:445:PHE:CD1	2.50	0.47
1:B:675:HIS:N	1:B:676:PRO:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:PRO:HB2	1:B:589:SER:OG	2.14	0.47
1:A:440:ASP:OD1	1:A:442:VAL:HG12	2.15	0.47
1:B:756:ILE:HD12	1:B:791:ARG:HG2	1.96	0.47
1:A:738:VAL:HG12	1:A:791:ARG:NH2	2.30	0.47
1:B:290:GLU:O	1:B:293:THR:HG22	2.15	0.47
1:B:268:ARG:HB3	1:B:268:ARG:HH11	1.79	0.47
1:A:629:GLY:HA3	1:A:685:SER:OG	2.16	0.46
1:B:205:HIS:ND1	1:B:207:ASP:HB2	2.29	0.46
1:B:81:SER:HA	1:B:84:MSE:CE	2.42	0.46
1:B:336:GLY:HA3	1:B:687:THR:OG1	2.15	0.46
1:A:62:LEU:N	1:A:63:PRO:HD2	2.30	0.46
1:A:377:MSE:SE	1:A:681:ASP:HB2	2.65	0.46
1:A:290:GLU:O	1:A:293:THR:HG22	2.15	0.46
1:A:509:PHE:CE1	1:A:516:TYR:HB2	2.50	0.46
1:B:603:GLN:CD	1:B:603:GLN:N	2.69	0.46
1:B:760:ILE:HG12	1:B:789:LEU:HD22	1.97	0.46
1:A:440:ASP:OD2	1:A:508:ARG:NH1	2.45	0.46
1:A:448:MSE:HE3	1:A:528:LEU:CB	2.36	0.45
1:A:668:TYR:OH	1:A:677:PRO:HA	2.16	0.45
1:A:270:ILE:HG12	1:A:274:LYS:HE3	1.99	0.45
1:B:264:ASP:HB3	1:B:267:LEU:HD12	1.98	0.45
1:A:353:LEU:HB2	1:A:367:SER:HA	1.98	0.45
1:A:289:LEU:O	1:A:293:THR:HG22	2.16	0.45
1:B:28:MSE:HB2	1:B:39:ALA:HB3	1.98	0.45
1:B:750:CYS:O	1:B:778:SER:HA	2.17	0.45
1:A:136:ARG:HA	1:A:150:ARG:O	2.17	0.45
1:A:479:LYS:HG3	1:A:549:PHE:CE2	2.52	0.45
1:B:179:HIS:CD2	1:B:217:ARG:HD3	2.52	0.45
1:B:635:TRP:CG	1:B:643:ARG:HG2	2.52	0.45
1:A:175:VAL:HG21	1:A:229:VAL:HG13	1.99	0.45
1:A:27:ALA:HA	1:A:39:ALA:O	2.16	0.45
1:A:475:TYR:HB3	1:A:476:PRO:HD3	1.99	0.45
1:B:555:ASP:O	1:B:559:ARG:HG3	2.16	0.45
1:B:373:ILE:HD11	1:B:377:MSE:HE3	1.99	0.45
1:A:282:LYS:HG3	2:A:1006:HOH:O	2.16	0.45
1:A:661:MSE:CE	1:A:664:ARG:HB2	2.46	0.45
1:B:730:LEU:HD12	1:B:730:LEU:C	2.38	0.45
1:B:189:HIS:HD2	2:B:950:HOH:O	1.99	0.45
1:A:380:TRP:N	1:A:381:PRO:CD	2.80	0.45
1:A:87:PRO:O	1:A:433:VAL:HA	2.17	0.44
1:B:635:TRP:CD2	1:B:643:ARG:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:TRP:N	1:B:381:PRO:CD	2.80	0.44
1:B:774:SER:C	1:B:776:ARG:H	2.20	0.44
1:B:17:ALA:HB3	1:B:28:MSE:HE3	1.99	0.44
1:A:714:ASP:OD1	1:A:733:THR:HA	2.18	0.44
1:B:670:ASN:OD1	1:B:672:PHE:HB2	2.17	0.44
1:B:73:LYS:HD3	1:B:76:GLU:OE2	2.18	0.44
1:A:594:ILE:HD13	1:A:600:ILE:HB	1.99	0.44
1:A:485:CYS:SG	1:A:529:ILE:HD12	2.58	0.44
1:A:370:THR:CG2	1:A:374:ASN:HD22	2.31	0.44
1:B:390:LEU:O	1:B:393:PRO:HD2	2.18	0.44
1:B:475:TYR:HB3	1:B:476:PRO:HD3	2.00	0.44
1:A:76:GLU:HG3	2:A:1052:HOH:O	2.17	0.44
1:B:510:ARG:HG3	1:B:581:GLU:HA	2.00	0.43
1:A:741:GLU:HG2	1:A:788:VAL:HG22	2.00	0.43
1:B:613:LYS:O	1:B:617:GLU:HG3	2.19	0.43
1:A:222:ASN:HD22	1:A:222:ASN:N	2.10	0.43
1:B:175:VAL:HG21	1:B:229:VAL:HG13	2.00	0.43
1:A:110:PRO:O	1:A:111:HIS:HB2	2.18	0.43
1:A:84:MSE:HE1	1:A:501:PRO:HG2	1.99	0.43
1:A:710:ASP:O	1:A:713:LYS:HD2	2.19	0.43
1:A:737:LEU:HD21	1:A:740:VAL:CG2	2.49	0.43
1:B:586:ARG:HG2	1:B:586:ARG:HH11	1.82	0.43
1:B:351:ALA:HB1	1:B:355:GLY:HA2	2.01	0.42
1:A:635:TRP:CG	1:A:643:ARG:HG2	2.55	0.42
1:A:387:LEU:HD22	1:A:390:LEU:HD22	2.02	0.42
1:A:759:ARG:O	1:A:789:LEU:HA	2.19	0.42
1:A:391:HIS:HE1	1:A:394:LEU:HD23	1.85	0.42
1:B:689:GLY:O	1:B:693:MSE:HG3	2.19	0.42
1:B:483:LEU:HD23	1:B:486:LEU:HD12	2.01	0.42
1:B:502:SER:OG	1:B:522:THR:HG23	2.19	0.42
1:A:670:ASN:OD1	1:A:672:PHE:HB2	2.19	0.42
1:B:383:GLU:OE2	1:B:391:HIS:HD2	2.02	0.42
1:B:75:GLU:OE1	1:B:514:LYS:HE2	2.18	0.42
1:B:22:ASN:HB3	1:B:140:VAL:HG12	2.01	0.42
1:B:509:PHE:CE1	1:B:516:TYR:HB2	2.55	0.42
1:A:753:LEU:HD23	1:A:753:LEU:C	2.39	0.42
1:A:680:ILE:HG12	1:A:684:PHE:CE2	2.55	0.42
1:A:293:THR:HG23	1:A:294:LYS:N	2.34	0.42
1:B:341:ILE:HA	1:B:390:LEU:HD21	2.02	0.42
1:B:372:ASN:O	1:B:373:ILE:HB	2.20	0.42
1:A:380:TRP:N	1:A:381:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:TRP:N	1:B:381:PRO:HD2	2.35	0.42
1:A:498:VAL:HB	1:A:521:ALA:HB2	2.02	0.42
1:A:471:ARG:HB2	1:A:543:LEU:HD22	2.02	0.42
1:A:671:LEU:HD12	1:A:671:LEU:HA	1.86	0.41
1:A:533:PHE:CD1	1:A:553:LEU:HD22	2.55	0.41
1:A:511:ILE:HB	1:A:516:TYR:HE2	1.85	0.41
1:B:628:LEU:O	1:B:632:ILE:HG13	2.20	0.41
1:A:32:LYS:HE2	1:A:32:LYS:HB3	1.83	0.41
1:A:222:ASN:ND2	1:A:222:ASN:N	2.68	0.41
1:B:773:ASP:CG	1:B:774:SER:N	2.75	0.41
1:B:585:HIS:NE2	1:B:587:HIS:HB2	2.36	0.41
1:B:537:ILE:HG23	1:B:550:VAL:HG13	2.03	0.41
1:A:419:VAL:HG22	1:A:420:ALA:N	2.36	0.41
1:A:759:ARG:HG2	2:A:1050:HOH:O	2.20	0.41
1:B:372:ASN:HA	1:B:446:TRP:CH2	2.56	0.41
1:A:85:MSE:HB3	1:A:433:VAL:O	2.19	0.41
1:A:32:LYS:HB2	1:A:36:GLU:HA	2.02	0.41
1:B:228:LYS:HG2	1:B:235:HIS:HB2	2.03	0.41
1:B:282:LYS:HA	1:B:285:VAL:HG12	2.03	0.41
1:B:470:LEU:HA	1:B:474:ALA:HB3	2.03	0.40
1:A:704:PHE:HE1	1:A:752:VAL:HB	1.85	0.40
1:B:282:LYS:O	1:B:285:VAL:HG12	2.21	0.40
1:A:664:ARG:O	1:A:676:PRO:HD3	2.21	0.40
1:B:773:ASP:CG	1:B:774:SER:H	2.24	0.40
1:A:635:TRP:CE2	1:A:643:ARG:HG2	2.56	0.40
1:A:420:ALA:HB3	1:A:450:GLY:N	2.36	0.40
1:B:142:TYR:N	1:B:143:PRO:CD	2.85	0.40
1:A:759:ARG:HH11	1:A:759:ARG:HG3	1.86	0.40
1:A:503:THR:C	1:A:522:THR:HG21	2.41	0.40
1:A:387:LEU:HB3	1:A:390:LEU:HD22	2.03	0.40
1:B:730:LEU:HD12	1:B:730:LEU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	783/803 (98%)	749 (96%)	31 (4%)	3 (0%)	39	32
1	B	783/803 (98%)	750 (96%)	29 (4%)	4 (0%)	34	26
All	All	1566/1606 (98%)	1499 (96%)	60 (4%)	7 (0%)	39	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	ILE
1	B	373	ILE
1	A	505	PRO
1	B	505	PRO
1	B	773	ASP
1	A	433	VAL
1	B	433	VAL

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	661/654 (101%)	647 (98%)	14 (2%)	61	62
1	B	661/654 (101%)	650 (98%)	11 (2%)	68	70
All	All	1322/1308 (101%)	1297 (98%)	25 (2%)	65	66

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	208	MSE
1	A	222	ASN
1	A	386	ASN
1	A	391	HIS
1	A	422	HIS

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Mol	Chain	Res	Type
1	A	505	PRO
1	A	507	GLN
1	A	513	GLU
1	A	548	ASP
1	A	672	PHE
1	A	730	LEU
1	A	759	ARG
1	A	766	GLU
1	B	91	SER
1	B	222	ASN
1	B	290	GLU
1	B	386	ASN
1	B	391	HIS
1	B	422	HIS
1	B	505	PRO
1	B	506	GLU
1	B	507	GLN
1	B	558	GLN
1	B	672	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	41	ASN
1	A	104	HIS
1	A	179	HIS
1	A	222	ASN
1	A	288	HIS
1	A	297	ASN
1	A	374	ASN
1	A	386	ASN
1	A	391	HIS
1	A	423	ASN
1	A	642	ASN
1	A	679	GLN
1	A	699	GLN
1	B	24	ASN
1	B	41	ASN
1	B	133	GLN
1	B	179	HIS
1	B	189	HIS

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Mol	Chain	Res	Type
1	B	222	ASN
1	B	288	HIS
1	B	297	ASN
1	B	316	GLN
1	B	386	ASN
1	B	391	HIS
1	B	507	GLN
1	B	558	GLN
1	B	572	GLN
1	B	642	ASN
1	B	662	GLN
1	B	679	GLN
1	B	699	GLN

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](#)

There are no ligands in this entry.

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	769/803 (95%)	0.14	21 (2%) 58 59	7, 14, 28, 42	0
1	B	769/803 (95%)	0.21	30 (3%) 43 45	6, 14, 30, 49	0
All	All	1538/1606 (95%)	0.18	51 (3%) 50 52	6, 14, 28, 49	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	775	GLY	6.7
1	B	261	LEU	5.2
1	B	773	ASP	5.2
1	B	774	SER	5.0
1	B	756	ILE	4.7
1	A	759	ARG	4.0
1	B	207	ASP	3.9
1	A	763	SER	3.9
1	B	206	PRO	3.7
1	B	205	HIS	3.7
1	B	755	ARG	3.4
1	A	768	GLU	3.3
1	A	755	ARG	3.2
1	A	765	GLU	3.2
1	A	261	LEU	3.1
1	B	513	GLU	3.0
1	A	766	GLU	3.0
1	A	756	ILE	2.9
1	B	542	ARG	2.8
1	A	511	ILE	2.8
1	B	510	ARG	2.8
1	A	764	GLY	2.7
1	B	324	ARG	2.7
1	B	772	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	513	GLU	2.6
1	B	603	GLN	2.5
1	A	547	GLU	2.4
1	A	493	GLU	2.4
1	B	293	THR	2.3
1	B	262	GLU	2.3
1	A	262	GLU	2.3
1	B	547	GLU	2.2
1	B	311	ASP	2.2
1	B	771	VAL	2.2
1	B	791	ARG	2.2
1	A	551	LYS	2.2
1	B	514	LYS	2.2
1	B	768	GLU	2.2
1	A	111	HIS	2.2
1	B	770	ASP	2.2
1	A	505	PRO	2.2
1	A	293	THR	2.1
1	B	282	LYS	2.1
1	A	558	GLN	2.1
1	B	680	ILE	2.1
1	B	111	HIS	2.1
1	B	175	VAL	2.1
1	B	505	PRO	2.1
1	A	282	LYS	2.1
1	B	512	GLY	2.0
1	A	65	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.