



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:29 PM UTC

PDB ID : 2RDY / pdb_00002rdy
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

<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

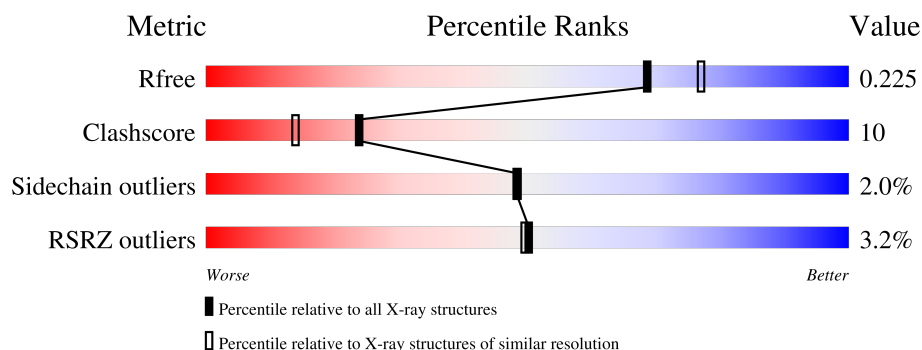
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (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 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	803	
1	B	803	

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

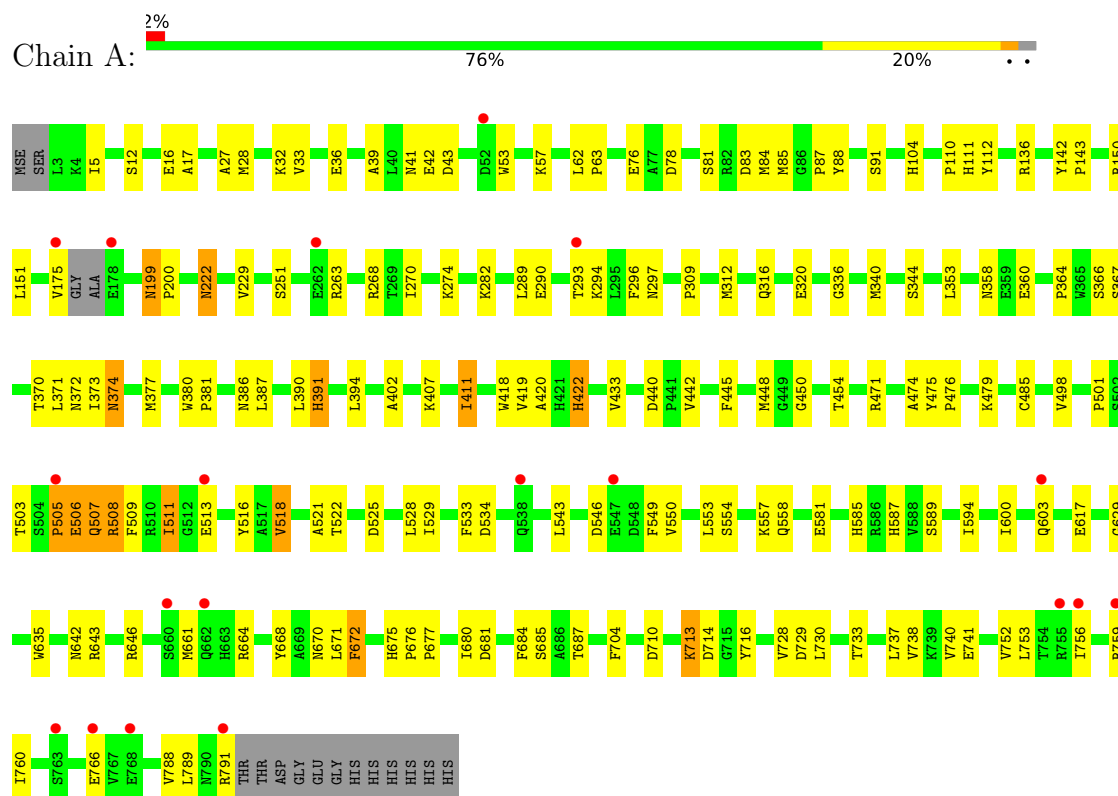
- Molecule 2 is water.

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

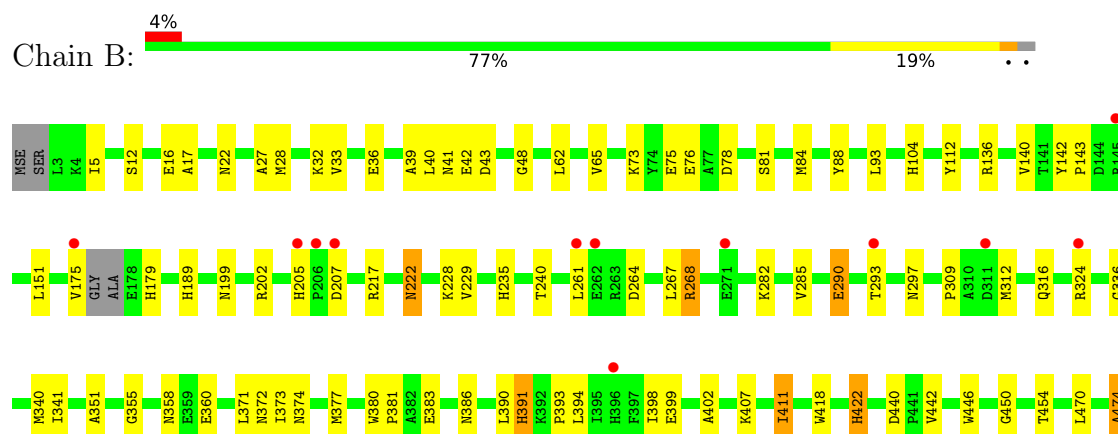
3 Residue-property plots [i](#)

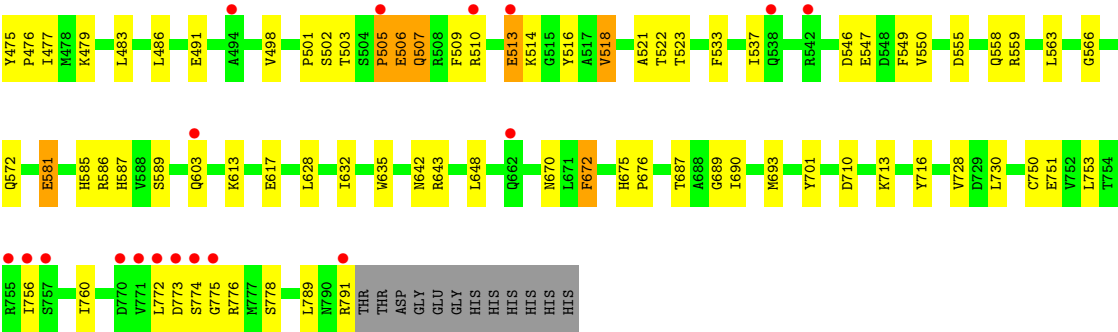
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BH0842 protein



• 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) 93.7 (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 (5.63%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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

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	0.37	0/6378	0.90	25/8621 (0.3%)
1	B	0.37	0/6378	0.89	23/8621 (0.3%)
All	All	0.37	0/12756	0.89	48/17242 (0.3%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	ILE	N-CA-C	8.43	118.46	110.53
1	A	33	VAL	N-CA-C	7.75	117.81	110.53
1	B	374	ASN	N-CA-C	7.46	119.05	111.07
1	A	5	ILE	N-CA-C	-7.29	97.23	107.80
1	B	5	ILE	N-CA-C	-7.17	96.75	107.37
1	A	42	GLU	N-CA-C	-6.70	97.13	108.26
1	A	411	ILE	N-CA-C	6.69	116.82	110.53
1	B	43	ASP	N-CA-C	6.56	120.74	112.87
1	A	199	ASN	CA-C-N	6.35	126.27	119.28
1	A	199	ASN	C-N-CA	6.35	126.27	119.28
1	B	104	HIS	N-CA-C	6.28	119.96	112.93
1	B	42	GLU	N-CA-C	-6.24	98.10	108.34
1	B	728	VAL	N-CA-C	6.19	117.40	108.48
1	A	728	VAL	N-CA-C	6.09	118.23	108.85
1	A	374	ASN	N-CA-C	6.04	118.36	111.11
1	A	53	TRP	N-CA-C	6.02	120.62	113.28
1	A	12	SER	N-CA-C	-5.96	106.34	113.97
1	A	474	ALA	N-CA-C	5.96	117.46	110.97
1	A	104	HIS	N-CA-C	5.93	119.48	112.72
1	A	713	LYS	N-CA-C	5.88	117.36	111.07
1	B	112	TYR	N-CA-C	-5.85	102.39	110.35
1	B	713	LYS	N-CA-C	5.81	117.42	111.14
1	B	518	VAL	N-CA-C	5.78	117.33	108.71
1	B	581	GLU	N-CA-C	-5.78	104.95	112.23
1	B	33	VAL	N-CA-C	5.70	115.83	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	TYR	N-CA-C	-5.69	102.61	110.35
1	B	371	LEU	N-CA-C	5.67	119.83	113.02
1	B	240	THR	N-CA-C	-5.62	106.36	113.43
1	B	88	TYR	N-CA-C	-5.59	102.62	110.50
1	A	581	GLU	N-CA-C	-5.48	105.33	112.23
1	B	48	GLY	N-CA-C	5.47	121.74	112.22
1	A	43	ASP	N-CA-C	5.46	119.42	112.87
1	B	16	GLU	N-CA-C	-5.45	106.63	113.72
1	B	360	GLU	N-CA-C	5.44	118.11	109.24
1	B	12	SER	N-CA-C	-5.42	107.22	113.88
1	B	422	HIS	N-CA-C	5.36	119.83	113.28
1	A	88	TYR	N-CA-C	-5.35	102.57	110.48
1	B	93	LEU	N-CA-C	5.30	117.61	110.29
1	B	474	ALA	N-CA-C	5.30	116.74	110.97
1	A	371	LEU	N-CA-C	5.26	119.69	113.16
1	A	422	HIS	N-CA-C	5.20	119.63	113.28
1	A	320	GLU	N-CA-C	5.16	118.74	112.23
1	A	344	SER	N-CA-C	5.16	116.61	109.54
1	A	296	PHE	N-CA-C	5.16	116.90	111.28
1	A	16	GLU	N-CA-C	-5.14	107.03	113.72
1	B	40	LEU	N-CA-C	5.12	118.10	109.95
1	A	518	VAL	N-CA-C	5.10	116.88	108.97
1	A	511	ILE	N-CA-C	-5.06	98.82	109.34

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	6239	0	6036	128	0
1	B	6239	0	6036	120	0
2	A	275	0	0	5	0
2	B	284	0	0	2	0
All	All	13037	0	12072	248	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 (248) 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:HG3	1:B:324:ARG:HH11	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:B:689:GLY:C	1:B:693:MSE:HE3	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H	1:A:222:ASN:ND2	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:136:ARG:HD2	1:B:151:LEU:CD2	2.35	0.57
1:B:632:ILE:HD13	1:B:648:LEU:HD13	1.87	0.57
1:A:554:SER:O	1:A:558:GLN:HG3	2.04	0.56
1:A:450:GLY:O	1:A:454:THR:HG23	2.04	0.56
1:B:309:PRO:HG2	1:B:312:MSE:HB2	1.85	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:B:547:GLU:CD	1:B:547:GLU:H	2.14	0.56
1:A:675:HIS:HB3	1:A:676:PRO:C	2.31	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:H	1:B:222:ASN:ND2	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:510:ARG:HH21	1:B:513:GLU:C	2.15	0.54
1:B:199:ASN:ND2	1:B:202:ARG:HG2	2.23	0.54
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:A:505:PRO:HB2	1:A:589:SER:OG	2.08	0.54
1:A:507:GLN:HB2	1:A:585:HIS:CD2	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASP:OD1	1:A:518:VAL:HG22	2.09	0.53
1:A:81:SER:HB2	1:A:84:MSE:HE2	1.89	0.53
1:B:81:SER:CA	1:B:84:MSE:HE2	2.38	0.53
1:A:675:HIS:N	1:A:676:PRO:HA	2.23	0.53
1:B:675:HIS:HB3	1:B:676:PRO:C	2.33	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
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:312:MSE:HE2	1:B:316:GLN:NE2	2.24	0.52
1:B:546:ASP:O	1:B:550:VAL:HG23	2.09	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:A:17:ALA:HB3	1:A:28:MSE:HG3	1.93	0.51
1:B:523:THR:HG23	1:B:563:LEU:HD22	1.92	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:508:ARG:HB3	1:A:516:TYR:O	2.11	0.50
1:A:675:HIS:H	1:A:676:PRO:HA	1.76	0.50
1:B:450:GLY:O	1:B:454:THR:HG23	2.12	0.50
1:A:336:GLY:HA3	1:A:687:THR:OG1	2.12	0.50
1:B:603:GLN:N	1:B:603:GLN:CD	2.69	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:B:730:LEU:C	1:B:730:LEU:HD12	2.38	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:A:360:GLU:OE1	1:A:364:PRO:HD3	2.12	0.49
1:B:498:VAL:HB	1:B:521:ALA:HB2	1.94	0.49
1:B:774:SER:C	1:B:776:ARG:H	2.20	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:A:199:ASN:N	1:A:200:PRO:HD3	2.28	0.48
1:B:324:ARG:HG3	1:B:324:ARG:NH1	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:HD2	1:A:151:LEU:HD22	1.96	0.48
1:A:643:ARG:HA	1:A:646:ARG:NH1	2.29	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
1:B:505:PRO:HB2	1:B:589:SER:OG	2.14	0.47
1:B:774:SER:OG	1:B:775:GLY:N	2.44	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:A:753:LEU:C	1:A:753:LEU:HD23	2.39	0.47
1:B:290:GLU:O	1:B:293:THR:HG22	2.15	0.47
1:B:268:ARG:HH11	1:B:268:ARG:HB3	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:A:62:LEU:N	1:A:63:PRO:HD2	2.30	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: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:A:440:ASP:OD2	1:A:508:ARG:NH1	2.45	0.46
1:B:760:ILE:HG12	1:B:789:LEU:HD22	1.97	0.46
1:A:448:MSE:HE3	1:A:528:LEU:CB	2.36	0.45
1:A:270:ILE:HG12	1:A:274:LYS:HE3	1.99	0.45
1:A:668:TYR:OH	1:A:677:PRO:HA	2.16	0.45
1:B:264:ASP:HB3	1:B:267:LEU:HD12	1.98	0.45
1:B:773:ASP:CG	1:B:774:SER:N	2.75	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:B:773:ASP:CG	1:B:774:SER:H	2.24	0.45
1:A:27:ALA:HA	1:A:39:ALA:O	2.16	0.45
1:A:175:VAL:HG21	1:A:229:VAL:HG13	1.99	0.45
1:A:503:THR:C	1:A:522:THR:HG21	2.41	0.45
1:A:475:TYR:HB3	1:A:476:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ILE:HD11	1:B:377:MSE:HE3	1.99	0.45
1:B:555:ASP:O	1:B:559:ARG:HG3	2.16	0.45
1:A:282:LYS:HG3	2:A:1006:HOH:O	2.16	0.45
1:A:380:TRP:N	1:A:381:PRO:CD	2.80	0.45
1:A:661:MSE:CE	1:A:664:ARG:HB2	2.46	0.45
1:B:189:HIS:HD2	2:B:950:HOH:O	1.99	0.45
1:A:87:PRO:O	1:A:433:VAL:HA	2.17	0.44
1:B:380:TRP:N	1:B:381:PRO:CD	2.80	0.44
1:B:635:TRP:CD2	1:B:643:ARG:HG2	2.52	0.44
1:B:261:LEU:HD23	1:B:261:LEU:C	2.42	0.44
1:A:714:ASP:OD1	1:A:733:THR:HA	2.18	0.44
1:B:17:ALA:HB3	1:B:28:MSE:HE3	1.99	0.44
1:B:689:GLY:C	1:B:693:MSE:CE	2.89	0.44
1:B:670:ASN:OD1	1:B:672:PHE:HB2	2.17	0.44
1:A:594:ILE:HD13	1:A:600:ILE:HB	1.99	0.44
1:B:73:LYS:HD3	1:B:76:GLU:OE2	2.18	0.44
1:A:370:THR:CG2	1:A:374:ASN:HD22	2.31	0.44
1:A:485:CYS:SG	1:A:529:ILE:HD12	2.58	0.44
1:A:76:GLU:HG3	2:A:1052:HOH:O	2.17	0.44
1:A:716:TYR:CD1	1:A:716:TYR:C	2.96	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:741:GLU:HG2	1:A:788:VAL:HG22	2.00	0.43
1:B:510:ARG:HG3	1:B:581:GLU:HA	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:HH11	1:B:586:ARG:HG2	1.82	0.43
1:B:351:ALA:HB1	1:B:355:GLY:HA2	2.01	0.42
1:B:503:THR:C	1:B:522:THR:HG21	2.44	0.42
1:A:387:LEU:HD22	1:A:390:LEU:HD22	2.02	0.42
1:A:391:HIS:HE1	1:A:394:LEU:HD23	1.85	0.42
1:A:635:TRP:CG	1:A:643:ARG:HG2	2.55	0.42
1:A:759:ARG:O	1:A:789:LEU:HA	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:B:689:GLY:O	1:B:693:MSE:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ASN:OD1	1:A:672:PHE:HB2	2.19	0.42
1:B:22:ASN:HB3	1:B:140:VAL:HG12	2.01	0.42
1:B:75:GLU:OE1	1:B:514:LYS:HE2	2.18	0.42
1:B:383:GLU:OE2	1:B:391:HIS:HD2	2.02	0.42
1:B:509:PHE:CE1	1:B:516:TYR:HB2	2.55	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:A:380:TRP:N	1:A:381:PRO:HD2	2.34	0.42
1:A:471:ARG:HB2	1:A:543:LEU:HD22	2.02	0.42
1:A:498:VAL:HB	1:A:521:ALA:HB2	2.02	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:B:380:TRP:N	1:B:381:PRO:HD2	2.35	0.42
1:A:671:LEU:HD12	1:A:671:LEU:HA	1.86	0.41
1:A:366:SER:O	1:A:367:SER:C	2.62	0.41
1:A:533:PHE:CD1	1:A:553:LEU:HD22	2.55	0.41
1:A:603:GLN:N	1:A:603:GLN:CD	2.78	0.41
1:A:440:ASP:CG	1:A:442:VAL:HG12	2.45	0.41
1:A:511:ILE:HB	1:A:516:TYR:HE2	1.85	0.41
1:A:32:LYS:HB3	1:A:32:LYS:HE2	1.83	0.41
1:B:491:GLU:CD	1:B:559:ARG:HH22	2.27	0.41
1:B:628:LEU:O	1:B:632:ILE:HG13	2.20	0.41
1:A:222:ASN:ND2	1:A:222:ASN:N	2.68	0.41
1:A:251:SER:C	1:A:263:ARG:HD3	2.46	0.41
1:B:774:SER:C	1:B:776:ARG:N	2.78	0.41
1:A:32:LYS:HB2	1:A:36:GLU:HA	2.02	0.41
1:A:85:MSE:HB3	1:A:433:VAL:O	2.19	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:228:LYS:HG2	1:B:235:HIS:HB2	2.03	0.41
1:B:372:ASN:HA	1:B:446:TRP:CH2	2.56	0.41
1:B:537:ILE:HG23	1:B:550:VAL:HG13	2.03	0.41
1:B:585:HIS:NE2	1:B:587:HIS:HB2	2.36	0.41
1:B:282:LYS:HA	1:B:285:VAL:HG12	2.03	0.41
1:B:440:ASP:CG	1:B:442:VAL:HG12	2.46	0.41
1:A:704:PHE:HE1	1:A:752:VAL:HB	1.85	0.40
1:B:470:LEU:HA	1:B:474:ALA:HB3	2.03	0.40
1:B:716:TYR:CD1	1:B:716:TYR:C	2.99	0.40
1:B:282:LYS:O	1:B:285:VAL:HG12	2.21	0.40
1:A:420:ALA:HB3	1:A:450:GLY:N	2.36	0.40
1:A:635:TRP:CE2	1:A:643:ARG:HG2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ARG:O	1:A:676:PRO:HD3	2.21	0.40
1:A:759:ARG:HH11	1:A:759:ARG:HG3	1.86	0.40
1:B:142:TYR:N	1:B:143:PRO:CD	2.85	0.40
1:B:772:LEU:O	1:B:773:ASP:C	2.64	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 [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	638/654 (98%)	625 (98%)	13 (2%)	48	48
1	B	661/654 (101%)	648 (98%)	13 (2%)	48	48
All	All	1299/1308 (99%)	1273 (98%)	26 (2%)	48	48

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

Mol	Chain	Res	Type
1	A	91	SER
1	A	222	ASN
1	A	386	ASN
1	A	391	HIS
1	A	422	HIS
1	A	505	PRO
1	A	506	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	507	GLN
1	A	508	ARG
1	A	513	GLU
1	A	672	PHE
1	A	730	LEU
1	A	766	GLU
1	B	222	ASN
1	B	268	ARG
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	513	GLU
1	B	558	GLN
1	B	672	PHE
1	B	753	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	41	ASN
1	A	79	GLN
1	A	104	HIS
1	A	179	HIS
1	A	222	ASN
1	A	349	GLN
1	A	374	ASN
1	A	386	ASN
1	A	391	HIS
1	A	396	HIS
1	A	423	ASN
1	A	642	ASN
1	A	679	GLN
1	B	41	ASN
1	B	99	ASN
1	B	133	GLN
1	B	179	HIS
1	B	189	HIS

Continued on next page...

Continued from previous page...

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	584	HIS
1	B	642	ASN
1	B	662	GLN
1	B	679	GLN
1	B	699	GLN
1	B	790	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	769/803 (95%)	-0.09	19 (2%) 58 58	7, 14, 28, 42	0
1	B	769/803 (95%)	-0.06	30 (3%) 43 43	6, 14, 30, 49	0
All	All	1538/1606 (95%)	-0.07	49 (3%) 50 49	6, 14, 28, 49	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	774	SER	5.0
1	B	775	GLY	4.9
1	B	773	ASP	4.7
1	A	755	ARG	4.2
1	B	261	LEU	4.0
1	B	206	PRO	3.9
1	B	756	ILE	3.7
1	A	766	GLU	3.4
1	A	763	SER	3.4
1	A	759	ARG	3.3
1	B	755	ARG	3.3
1	B	324	ARG	3.2
1	B	293	THR	3.0
1	A	768	GLU	2.9
1	B	207	ASP	2.9
1	A	175	VAL	2.8
1	B	175	VAL	2.8
1	A	513	GLU	2.8
1	A	603	GLN	2.7
1	B	770	ASP	2.7
1	B	311	ASP	2.7
1	B	603	GLN	2.6
1	B	772	LEU	2.6
1	A	756	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	771	VAL	2.5
1	A	262	GLU	2.5
1	A	662	GLN	2.5
1	B	205	HIS	2.4
1	B	262	GLU	2.4
1	A	538	GLN	2.4
1	B	542	ARG	2.4
1	B	396	HIS	2.4
1	B	791	ARG	2.4
1	B	757	SER	2.4
1	A	660	SER	2.3
1	B	513	GLU	2.3
1	A	505	PRO	2.3
1	B	662	GLN	2.3
1	B	538	GLN	2.2
1	A	178	GLU	2.2
1	B	494	ALA	2.2
1	B	505	PRO	2.2
1	B	271	GLU	2.2
1	A	547	GLU	2.1
1	A	791	ARG	2.1
1	A	52	ASP	2.1
1	A	293	THR	2.1
1	B	510	ARG	2.1
1	B	145	ARG	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.