



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:42 am BST

PDB ID : 3R4Y
Title : Crystal structure of alpha-neoagarobiose hydrolase (ALPHA-NABH) from Saccharophagus degradans 2-40
Authors : Lee, S.; Lee, J.Y.; Ha, S.C.; Shin, D.H.; Kim, K.H.; Bang, W.G.; Kim, S.H.; Choi, I.G.
Deposited on : 2011-03-18
Resolution : 2.00 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	:	2.11
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)	:	2.11

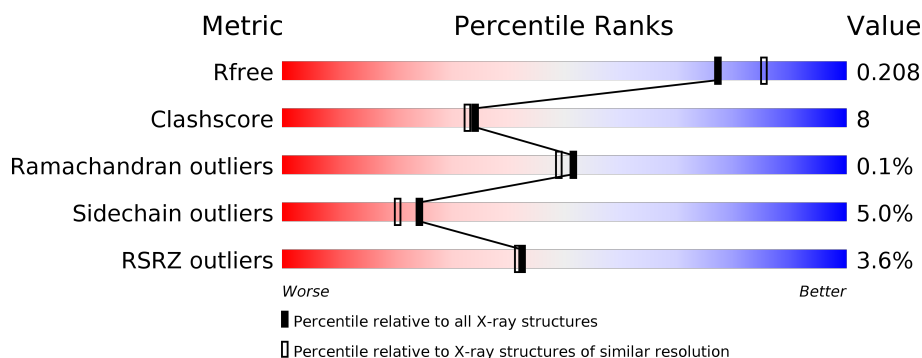
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	374	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	374	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6058 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 32, N terminal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2881	1835	482	554	10			
1	B	359	Total	C	N	O	S	0	0	0
			2874	1832	481	551	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	HIS	-	EXPRESSION TAG	UNP Q21HB2
A	370	HIS	-	EXPRESSION TAG	UNP Q21HB2
A	371	HIS	-	EXPRESSION TAG	UNP Q21HB2
A	372	HIS	-	EXPRESSION TAG	UNP Q21HB2
A	373	HIS	-	EXPRESSION TAG	UNP Q21HB2
A	374	HIS	-	EXPRESSION TAG	UNP Q21HB2
B	369	HIS	-	EXPRESSION TAG	UNP Q21HB2
B	370	HIS	-	EXPRESSION TAG	UNP Q21HB2
B	371	HIS	-	EXPRESSION TAG	UNP Q21HB2
B	372	HIS	-	EXPRESSION TAG	UNP Q21HB2
B	373	HIS	-	EXPRESSION TAG	UNP Q21HB2
B	374	HIS	-	EXPRESSION TAG	UNP Q21HB2

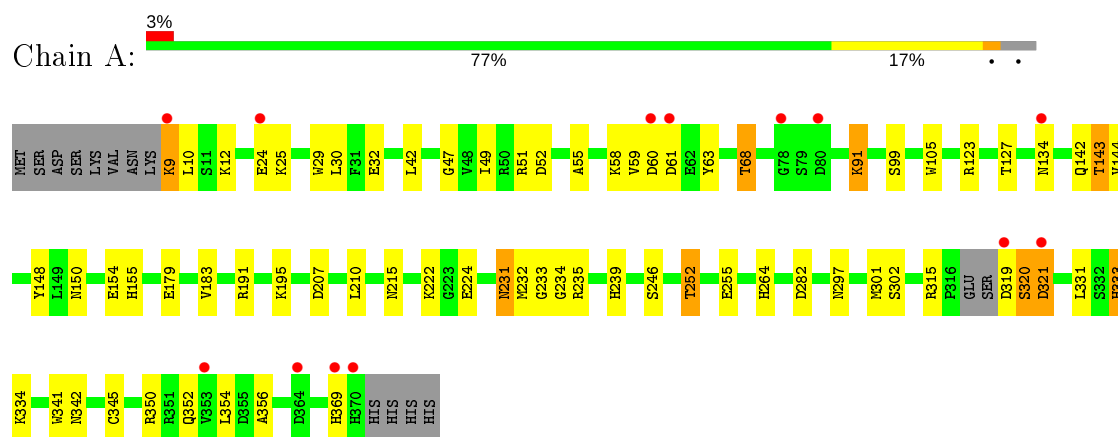
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	164	Total	O	0	0
			164	164		
2	B	139	Total	O	0	0
			139	139		

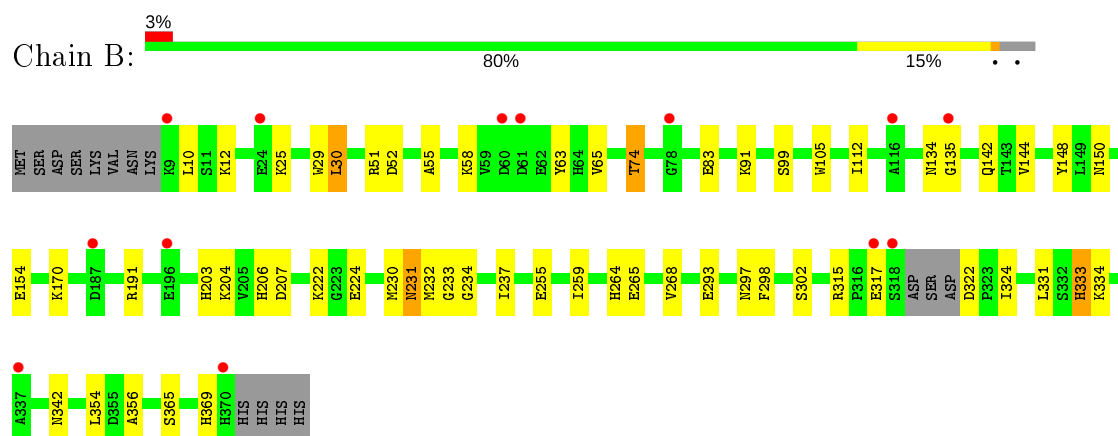
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Glycosyl hydrolase family 32, N terminal



- Molecule 1: Glycosyl hydrolase family 32, N terminal



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.87Å 76.81Å 90.11Å 90.00° 101.86° 90.00°	Depositor
Resolution (Å)	19.69 – 2.00 19.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.69-2.00) 90.1 (19.70-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.161 , 0.206 0.164 , 0.208	Depositor DCC
R_{free} test set	2710 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6058	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.77	0/2971	0.80	1/4035 (0.0%)
1	B	0.73	0/2964	0.75	1/4025 (0.0%)
All	All	0.75	0/5935	0.77	2/8060 (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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	135	GLY	N-CA-C	-6.18	97.66	113.10
1	A	301	MET	CG-SD-CE	5.03	108.25	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ASN	Peptide
1	A	59	VAL	Peptide
1	B	134	ASN	Peptide

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	2881	0	2694	61	0
1	B	2874	0	2692	45	0
2	A	164	0	0	9	0
2	B	139	0	0	2	0
All	All	6058	0	5386	93	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 8.

All (93) 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:52:ASP:H	1:A:333:HIS:HD2	1.02	1.02
1:A:30:LEU:HD11	1:B:234:GLY:HA2	1.45	0.96
1:B:52:ASP:H	1:B:333:HIS:HD2	1.01	0.95
1:A:319:ASP:HA	1:A:320:SER:CB	2.00	0.91
1:A:142:GLN:NE2	1:A:207:ASP:H	1.70	0.90
1:B:142:GLN:HE21	1:B:207:ASP:H	1.19	0.90
1:A:319:ASP:HA	1:A:320:SER:HB2	1.54	0.89
1:A:297:ASN:HD22	1:B:12:LYS:H	1.23	0.84
1:B:52:ASP:H	1:B:333:HIS:CD2	1.93	0.82
1:A:68:THR:HG21	2:A:388:HOH:O	1.78	0.81
1:A:142:GLN:HE21	1:A:207:ASP:H	1.28	0.80
1:B:222:LYS:HD3	1:B:264:HIS:O	1.81	0.80
1:A:68:THR:HG22	1:A:127:THR:H	1.48	0.79
1:A:52:ASP:H	1:A:333:HIS:CD2	1.95	0.78
1:B:142:GLN:NE2	1:B:207:ASP:H	1.83	0.76
1:A:12:LYS:H	1:B:297:ASN:HD22	1.33	0.74
1:B:150:ASN:ND2	1:B:191:ARG:H	1.88	0.72
1:B:224:GLU:HG2	1:B:237:ILE:HD12	1.71	0.71
1:A:144:VAL:HG22	1:A:154:GLU:HG2	1.74	0.70
1:B:74:THR:HG22	2:B:379:HOH:O	1.91	0.69
1:A:68:THR:CG2	1:A:127:THR:H	2.05	0.69
1:A:252:THR:CG2	2:A:407:HOH:O	2.41	0.68
1:B:52:ASP:N	1:B:333:HIS:HD2	1.85	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD11	1:B:234:GLY:CA	2.24	0.66
1:B:334:LYS:CE	1:B:369:HIS:CD2	2.80	0.65
1:B:150:ASN:HD22	1:B:191:ARG:H	1.43	0.65
1:A:231:ASN:C	1:A:231:ASN:HD22	2.02	0.63
1:A:143:THR:HG23	2:A:389:HOH:O	2.00	0.61
1:A:234:GLY:HA2	1:B:30:LEU:HD11	1.83	0.61
1:A:252:THR:HG23	2:A:407:HOH:O	2.01	0.60
1:A:319:ASP:CA	1:A:320:SER:HB2	2.30	0.59
1:A:52:ASP:N	1:A:333:HIS:HD2	1.87	0.58
1:B:154:GLU:OE1	1:B:206:HIS:HE1	1.85	0.58
1:A:319:ASP:HA	1:A:320:SER:HB3	1.86	0.57
1:B:334:LYS:HE3	1:B:369:HIS:CD2	2.39	0.57
1:A:297:ASN:ND2	1:B:12:LYS:H	1.99	0.56
1:A:264:HIS:HD2	1:A:282:ASP:OD2	1.88	0.56
1:B:51:ARG:HH11	1:B:342:ASN:HD21	1.54	0.55
1:A:51:ARG:HH11	1:A:342:ASN:HD21	1.55	0.54
1:A:58:LYS:HE2	1:A:61:ASP:HA	1.88	0.54
1:A:231:ASN:ND2	1:A:233:GLY:H	2.06	0.54
1:A:321:ASP:HA	2:A:479:HOH:O	2.09	0.53
1:B:144:VAL:HG22	1:B:154:GLU:HG2	1.90	0.53
1:A:143:THR:CG2	2:A:389:HOH:O	2.57	0.52
1:A:99:SER:HB2	1:A:105:TRP:CD2	2.45	0.52
1:A:150:ASN:ND2	1:A:191:ARG:H	2.09	0.51
1:A:334:LYS:NZ	1:A:369:HIS:CD2	2.78	0.51
1:A:235:ARG:HG2	1:B:354:LEU:HD11	1.93	0.51
1:A:25:LYS:HB3	1:B:232:MET:HB3	1.93	0.51
1:A:9:LYS:HE3	1:B:255:GLU:HB3	1.93	0.51
1:A:319:ASP:CA	1:A:320:SER:CB	2.80	0.51
1:B:65:VAL:HG21	1:B:331:LEU:HD12	1.93	0.51
1:A:246:SER:HB3	2:A:461:HOH:O	2.11	0.50
1:B:222:LYS:NZ	1:B:224:GLU:OE2	2.45	0.49
1:B:99:SER:HB2	1:B:105:TRP:CD2	2.48	0.49
1:B:112:ILE:HG23	1:B:170:LYS:HD3	1.94	0.49
1:B:206:HIS:HD2	1:B:222:LYS:NZ	2.10	0.49
1:A:150:ASN:HD22	1:A:191:ARG:H	1.59	0.49
1:B:74:THR:CG2	2:B:379:HOH:O	2.54	0.49
1:B:231:ASN:C	1:B:231:ASN:HD22	2.17	0.48
1:A:58:LYS:HD3	1:A:63:TYR:CE1	2.49	0.47
1:A:232:MET:HB3	1:B:25:LYS:HB3	1.96	0.47
1:A:29:TRP:HB2	1:A:302:SER:HB3	1.97	0.46
1:A:55:ALA:HB1	1:A:315:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HD12	1:B:298:PHE:HE2	1.81	0.46
1:B:51:ARG:HH11	1:B:342:ASN:ND2	2.14	0.46
1:A:51:ARG:HD2	1:A:342:ASN:ND2	2.31	0.46
1:B:58:LYS:HD3	1:B:63:TYR:CE1	2.51	0.46
1:A:356:ALA:HB1	1:B:150:ASN:ND2	2.31	0.45
1:A:350:ARG:HD2	2:A:511:HOH:O	2.17	0.45
1:A:32:GLU:CD	1:A:352:GLN:HG3	2.37	0.45
1:B:231:ASN:ND2	1:B:233:GLY:H	2.14	0.45
1:B:154:GLU:OE1	1:B:206:HIS:CE1	2.69	0.44
1:B:203:HIS:CE1	1:B:204:LYS:HE2	2.52	0.44
1:A:222:LYS:NZ	1:A:224:GLU:OE2	2.50	0.44
1:A:150:ASN:ND2	1:B:356:ALA:HB1	2.33	0.44
1:B:322:ASP:OD1	1:B:324:ILE:HG22	2.17	0.44
1:B:29:TRP:HB2	1:B:302:SER:HB3	2.00	0.43
1:A:183:VAL:HG11	1:A:195:LYS:HE3	1.99	0.42
1:A:47:GLY:HA2	1:A:341:TRP:CH2	2.55	0.42
1:A:239:HIS:HE1	1:A:264:HIS:O	2.01	0.42
1:A:32:GLU:OE1	1:A:350:ARG:NH1	2.53	0.41
1:A:49:ILE:HG23	1:A:342:ASN:HD22	1.85	0.41
1:A:334:LYS:HZ2	1:A:369:HIS:CD2	2.39	0.41
1:B:55:ALA:HB1	1:B:315:ARG:HG2	2.03	0.41
1:A:143:THR:HG22	1:A:155:HIS:HB2	2.03	0.41
1:A:334:LYS:HZ3	1:A:369:HIS:CD2	2.39	0.41
2:A:477:HOH:O	1:B:230:MET:HE1	2.20	0.41
1:A:331:LEU:HA	1:A:345:CYS:O	2.20	0.40
1:A:142:GLN:HE21	1:A:207:ASP:N	2.07	0.40
1:A:91:LYS:HA	1:A:123:ARG:O	2.22	0.40
1:A:12:LYS:H	1:B:297:ASN:ND2	2.10	0.40
1:A:42:LEU:HD22	1:A:105:TRP:CB	2.52	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	356/374 (95%)	340 (96%)	15 (4%)	1 (0%)	41	37
1	B	355/374 (95%)	344 (97%)	11 (3%)	0	100	100
All	All	711/748 (95%)	684 (96%)	26 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	SER

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	303/317 (96%)	286 (94%)	17 (6%)	21	17
1	B	302/317 (95%)	289 (96%)	13 (4%)	29	26
All	All	605/634 (95%)	575 (95%)	30 (5%)	24	20

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	10	LEU
1	A	24	GLU
1	A	60	ASP
1	A	68	THR
1	A	91	LYS
1	A	143	THR
1	A	148	TYR
1	A	179	GLU
1	A	210	LEU
1	A	215	ASN
1	A	231	ASN
1	A	252	THR
1	A	255	GLU
1	A	321	ASP

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Mol	Chain	Res	Type
1	A	333	HIS
1	A	354	LEU
1	B	10	LEU
1	B	30	LEU
1	B	74	THR
1	B	83	GLU
1	B	91	LYS
1	B	148	TYR
1	B	231	ASN
1	B	265	GLU
1	B	268	VAL
1	B	293	GLU
1	B	317	GLU
1	B	333	HIS
1	B	365	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	142	GLN
1	A	150	ASN
1	A	231	ASN
1	A	239	HIS
1	A	264	HIS
1	A	297	ASN
1	A	333	HIS
1	A	342	ASN
1	A	352	GLN
1	A	369	HIS
1	B	133	HIS
1	B	142	GLN
1	B	150	ASN
1	B	206	HIS
1	B	231	ASN
1	B	239	HIS
1	B	264	HIS
1	B	297	ASN
1	B	333	HIS
1	B	342	ASN
1	B	369	HIS

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	360/374 (96%)	-0.08	13 (3%) 42 42	9, 20, 42, 59	0
1	B	359/374 (95%)	-0.02	13 (3%) 42 42	10, 24, 38, 50	0
All	All	719/748 (96%)	-0.05	26 (3%) 42 42	9, 22, 41, 59	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	SER	5.1
1	A	80	ASP	4.7
1	B	60	ASP	4.5
1	B	61	ASP	4.4
1	A	319	ASP	4.1
1	A	61	ASP	4.1
1	B	317	GLU	4.0
1	A	370	HIS	4.0
1	B	24	GLU	3.8
1	A	60	ASP	3.7
1	A	353	VAL	3.7
1	B	78	GLY	3.5
1	A	369	HIS	3.4
1	A	78	GLY	3.4
1	A	9	LYS	3.3
1	B	187	ASP	2.9
1	A	24	GLU	2.9
1	A	364	ASP	2.9
1	A	134	ASN	2.7
1	B	9	LYS	2.7
1	B	370	HIS	2.6
1	B	116	ALA	2.5
1	B	337	ALA	2.4
1	B	196	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	135	GLY	2.1
1	A	321	ASP	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.