



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:43 am BST

PDB ID : 3TA9  
Title : beta-Glucosidase A from the halothermophile H. orenii  
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Deposited on : 2011-08-03  
Resolution : 3.00 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](mailto: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.

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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

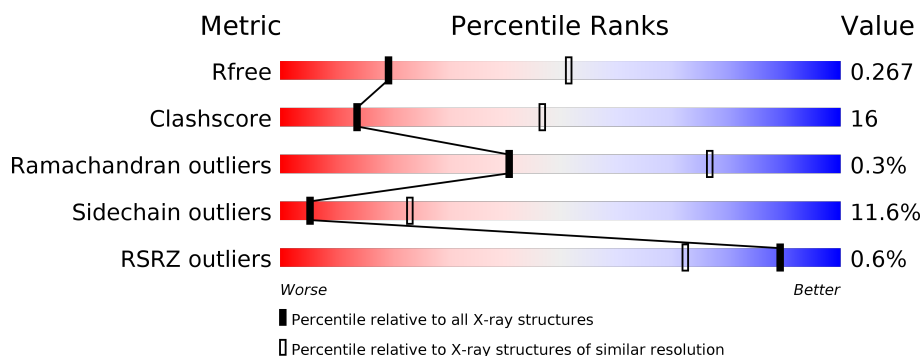
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	458	<div> <div></div> <div>62% 29% 7% .</div> </div>
1	B	458	<div> <div></div> <div>62% 29% 5% .</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7315 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 Glycoside hydrolase family 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3621	2330	607	674	10			
1	B	441	Total	C	N	O	S	0	0	0
			3565	2298	597	660	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP B8CYA8
A	-5	HIS	-	EXPRESSION TAG	UNP B8CYA8
A	-4	HIS	-	EXPRESSION TAG	UNP B8CYA8
A	-3	HIS	-	EXPRESSION TAG	UNP B8CYA8
A	-2	HIS	-	EXPRESSION TAG	UNP B8CYA8
A	-1	HIS	-	EXPRESSION TAG	UNP B8CYA8
A	0	HIS	-	EXPRESSION TAG	UNP B8CYA8
B	-6	MET	-	EXPRESSION TAG	UNP B8CYA8
B	-5	HIS	-	EXPRESSION TAG	UNP B8CYA8
B	-4	HIS	-	EXPRESSION TAG	UNP B8CYA8
B	-3	HIS	-	EXPRESSION TAG	UNP B8CYA8
B	-2	HIS	-	EXPRESSION TAG	UNP B8CYA8
B	-1	HIS	-	EXPRESSION TAG	UNP B8CYA8
B	0	HIS	-	EXPRESSION TAG	UNP B8CYA8

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

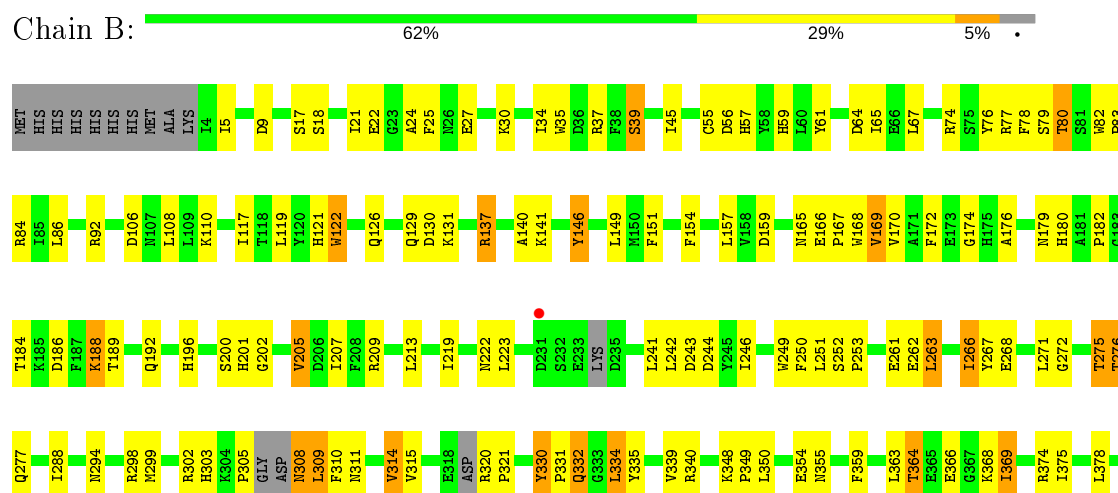
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	76	Total 76	O 76	0	0



- Molecule 1: Glycoside hydrolase family 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.50 Å 99.58 Å 109.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 3.00 43.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (24.89-3.00) 97.8 (43.39-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.70 (at 3.01 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.191 , 0.266 0.194 , 0.267	Depositor DCC
$R_{free}$ test set	998 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NI

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	0.44	0/3727	0.61	0/5062
1	B	0.44	0/3669	0.61	0/4981
All	All	0.44	0/7396	0.61	0/10043

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	ASP	Peptide
1	B	447	GLN	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	3621	0	3399	118	0
1	B	3565	0	3343	104	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	51	0	0	2	0
3	B	76	0	0	6	0
All	All	7315	0	6742	221	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 16.

All (221) 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:B:310:PHE:H	1:B:311:ASN:HA	1.13	1.14
1:A:306:GLY:HA3	1:A:311:ASN:ND2	1.63	1.13
1:A:310:PHE:H	1:A:311:ASN:HA	1.05	1.10
1:A:305:PRO:HA	1:A:311:ASN:HD21	0.99	1.09
1:A:306:GLY:HA3	1:A:311:ASN:HD21	1.13	1.02
1:A:305:PRO:HA	1:A:311:ASN:ND2	1.78	0.97
1:A:18:SER:H	1:A:79:SER:HB3	1.30	0.96
1:A:310:PHE:N	1:A:311:ASN:HA	1.78	0.93
1:B:18:SER:H	1:B:79:SER:HB3	1.37	0.88
1:A:310:PHE:H	1:A:311:ASN:CA	1.87	0.87
1:A:364:THR:HG22	1:A:368:LYS:H	1.41	0.86
1:B:310:PHE:N	1:B:311:ASN:HA	1.88	0.83
1:A:330:TYR:CE2	1:A:332:GLN:HG2	2.18	0.79
1:B:364:THR:HG22	1:B:368:LYS:H	1.49	0.78
1:B:330:TYR:CE2	1:B:332:GLN:HG2	2.19	0.78
1:A:330:TYR:HE2	1:A:332:GLN:HG2	1.46	0.77
1:B:330:TYR:HE2	1:B:332:GLN:HG2	1.47	0.77
1:A:448:VAL:HG12	1:A:449:GLU:H	1.49	0.77
1:A:234:LYS:HG3	1:A:303:HIS:CD2	2.21	0.76
1:B:364:THR:HG23	1:B:366:GLU:H	1.52	0.74
1:B:25:PHE:HA	1:B:30:LYS:HE3	1.70	0.73
1:A:151:PHE:HB3	1:A:213:LEU:HD11	1.69	0.73
1:A:22:GLU:HA	1:A:57:HIS:HB3	1.73	0.71
1:B:151:PHE:HB3	1:B:213:LEU:HD11	1.70	0.71
1:B:159:ASP:HB2	3:B:494:HOH:O	1.90	0.71
1:A:309:LEU:H	1:A:309:LEU:HD23	1.58	0.69
1:B:55:CYS:O	1:B:430:ARG:NH2	2.26	0.69
1:B:439:TYR:O	1:B:443:ILE:HG13	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:CD	1:A:261:GLU:H	1.96	0.68
1:B:309:LEU:HD23	1:B:309:LEU:H	1.58	0.68
1:A:174:GLY:O	1:A:182:PRO:HD2	1.93	0.68
1:B:261:GLU:CD	1:B:261:GLU:H	1.96	0.68
1:A:25:PHE:HA	1:A:30:LYS:HE3	1.75	0.67
1:A:364:THR:HG23	1:A:366:GLU:H	1.59	0.67
1:B:375:ILE:HD13	1:B:435:SER:HA	1.77	0.67
1:A:55:CYS:O	1:A:430:ARG:NH2	2.28	0.67
1:B:330:TYR:HE2	1:B:332:GLN:CG	2.08	0.67
1:A:330:TYR:HE2	1:A:332:GLN:CG	2.07	0.66
1:A:439:TYR:O	1:A:443:ILE:HG13	1.96	0.66
1:B:22:GLU:HA	1:B:57:HIS:HB3	1.78	0.66
1:A:375:ILE:HD13	1:A:435:SER:HA	1.80	0.63
1:B:303:HIS:CE1	1:B:305:PRO:HD3	2.34	0.62
1:B:243:ASP:OD2	3:B:509:HOH:O	2.16	0.61
1:A:310:PHE:N	1:A:311:ASN:CA	2.49	0.61
1:A:303:HIS:CE1	1:A:305:PRO:HD3	2.35	0.61
1:A:61:TYR:O	1:A:65:ILE:HG12	2.01	0.61
1:B:302:ARG:HG3	3:B:508:HOH:O	2.00	0.60
1:A:9:ASP:HA	1:A:74:ARG:NH2	2.17	0.60
1:B:174:GLY:O	1:B:182:PRO:HD2	2.02	0.59
1:B:186:ASP:OD1	1:B:189:THR:HG23	2.01	0.59
1:A:9:ASP:HA	1:A:74:ARG:HH22	1.67	0.59
1:B:9:ASP:HA	1:B:74:ARG:NH2	2.17	0.59
1:A:154:PHE:HA	1:A:157:LEU:HD12	1.85	0.59
1:A:86:LEU:HD12	1:A:146:TYR:HB2	1.83	0.58
1:B:61:TYR:O	1:B:65:ILE:HG12	2.04	0.58
1:B:188:LYS:HE2	1:B:272:GLY:H	1.69	0.58
1:B:9:ASP:HA	1:B:74:ARG:HH22	1.68	0.58
1:B:375:ILE:CD1	1:B:435:SER:HA	2.34	0.58
1:A:186:ASP:OD1	1:A:189:THR:HG23	2.04	0.58
1:B:154:PHE:HA	1:B:157:LEU:HD12	1.86	0.57
1:B:294:ASN:CG	1:B:354:GLU:HB2	2.25	0.57
1:B:86:LEU:HD12	1:B:146:TYR:HB2	1.85	0.57
1:B:166:GLU:HB3	1:B:169:VAL:HG13	1.86	0.56
1:A:234:LYS:O	1:A:303:HIS:HB2	2.06	0.56
1:A:305:PRO:HB3	1:A:311:ASN:OD1	2.05	0.56
1:B:35:TRP:O	1:B:39:SER:HB2	2.06	0.56
1:A:188:LYS:HE2	1:A:272:GLY:H	1.72	0.55
1:B:34:ILE:HG22	1:B:126:GLN:NE2	2.22	0.55
1:A:309:LEU:HD23	1:A:309:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:HB3	1:A:169:VAL:HG13	1.88	0.55
1:B:369:ILE:HG23	1:B:433:LYS:HA	1.89	0.54
1:A:335:TYR:CE1	1:A:387:LYS:HG2	2.43	0.54
1:A:375:ILE:CD1	1:A:435:SER:HA	2.37	0.54
1:B:276:THR:OG1	1:B:277:GLN:N	2.41	0.53
1:A:35:TRP:O	1:A:39:SER:HB2	2.09	0.53
1:A:369:ILE:HG12	1:A:433:LYS:HG2	1.91	0.53
1:A:34:ILE:HG22	1:A:126:GLN:NE2	2.23	0.53
1:B:309:LEU:HD23	1:B:309:LEU:N	2.23	0.53
1:B:262:GLU:O	1:B:266:ILE:HG23	2.08	0.53
1:A:173:GLU:HG3	3:A:459:HOH:O	2.09	0.53
1:A:335:TYR:CE1	1:A:387:LYS:HE2	2.44	0.53
1:B:45:ILE:HB	3:B:469:HOH:O	2.08	0.53
1:A:179:ASN:O	1:A:180:HIS:HD2	1.92	0.53
1:B:335:TYR:CE1	1:B:387:LYS:HG2	2.44	0.52
1:A:276:THR:OG1	1:A:277:GLN:N	2.42	0.52
1:A:369:ILE:HG23	1:A:433:LYS:HA	1.90	0.52
1:A:65:ILE:HD12	1:A:108:LEU:HD23	1.92	0.52
1:B:168:TRP:CD1	1:B:246:ILE:HA	2.46	0.51
1:B:76:TYR:CE2	1:B:78:PHE:HB3	2.46	0.51
1:B:369:ILE:O	1:B:369:ILE:HG13	2.11	0.50
1:B:335:TYR:O	1:B:339:VAL:HG13	2.10	0.50
1:A:262:GLU:O	1:A:266:ILE:HG23	2.10	0.50
1:A:294:ASN:CG	1:A:354:GLU:HB2	2.32	0.49
1:B:364:THR:HB	1:B:368:LYS:O	2.12	0.49
1:A:114:ARG:NH2	1:A:160:LEU:HD21	2.27	0.49
1:B:335:TYR:CE1	1:B:387:LYS:HE2	2.46	0.49
1:A:359:PHE:CE1	1:A:374:ARG:HA	2.48	0.49
1:B:348:LYS:HE2	3:B:507:HOH:O	2.13	0.49
1:B:179:ASN:O	1:B:180:HIS:HD2	1.94	0.49
1:A:405:ASP:OD2	1:A:421:TYR:HA	2.13	0.49
1:B:82:TRP:HB3	1:B:83:PRO:HD3	1.94	0.49
1:B:335:TYR:CZ	1:B:387:LYS:HE2	2.48	0.48
1:A:331:PRO:O	1:A:384:GLN:HG3	2.13	0.48
1:B:121:HIS:O	1:B:122:TRP:HB2	2.14	0.48
1:B:310:PHE:N	1:B:311:ASN:CA	2.64	0.48
1:A:311:ASN:O	1:A:311:ASN:ND2	2.46	0.48
1:B:201:HIS:O	1:B:205:VAL:HG12	2.13	0.48
1:B:263:LEU:HD22	1:B:267:TYR:CZ	2.48	0.48
1:B:393:VAL:HG13	1:B:394:PRO:HD2	1.96	0.48
1:A:129:GLN:O	1:A:131:LYS:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HD2	1:A:84:ARG:HB2	1.95	0.48
1:B:192:GLN:OE1	1:B:275:THR:HG23	2.14	0.48
1:A:335:TYR:O	1:A:339:VAL:HG13	2.14	0.47
1:B:349:PRO:O	1:B:350:LEU:HD23	2.14	0.47
1:B:308:ASN:HD22	1:B:309:LEU:N	2.12	0.47
1:A:334:LEU:HD22	1:A:334:LEU:O	2.14	0.47
1:A:369:ILE:HG13	1:A:369:ILE:O	2.13	0.47
1:A:440:ARG:HD3	1:A:444:GLU:OE2	2.15	0.47
1:A:252:SER:HB3	1:A:253:PRO:HD3	1.97	0.47
1:B:79:SER:OG	1:B:121:HIS:HB2	2.14	0.47
1:B:76:TYR:CZ	1:B:78:PHE:HB3	2.49	0.47
1:B:302:ARG:NH2	1:B:315:VAL:HG13	2.30	0.47
1:A:168:TRP:CD1	1:A:246:ILE:HA	2.50	0.47
1:A:364:THR:HB	1:A:368:LYS:O	2.15	0.47
1:A:448:VAL:HG12	1:A:449:GLU:N	2.25	0.47
1:B:25:PHE:CA	1:B:30:LYS:HE3	2.43	0.47
1:B:78:PHE:CZ	1:B:117:ILE:HG12	2.50	0.47
1:A:335:TYR:CZ	1:A:387:LYS:HE2	2.50	0.47
1:A:370:HIS:HA	1:A:434:ASP:OD2	2.15	0.47
1:A:79:SER:OG	1:A:121:HIS:HB2	2.14	0.46
1:A:263:LEU:HD21	1:A:310:PHE:CE1	2.50	0.46
1:B:359:PHE:CE1	1:B:374:ARG:HA	2.50	0.46
1:B:252:SER:HB3	1:B:253:PRO:HD3	1.96	0.46
1:B:25:PHE:O	1:B:30:LYS:HE3	2.14	0.46
1:B:331:PRO:O	1:B:384:GLN:HG3	2.15	0.46
1:A:308:ASN:HD22	1:A:309:LEU:N	2.13	0.46
1:A:65:ILE:HD12	1:A:108:LEU:CD2	2.45	0.46
1:B:405:ASP:OD2	1:B:421:TYR:HA	2.15	0.46
1:B:440:ARG:HD3	1:B:444:GLU:OE2	2.16	0.46
1:B:369:ILE:HG12	1:B:433:LYS:HG2	1.98	0.46
1:A:182:PRO:HG2	1:A:184:THR:HG23	1.97	0.46
1:B:263:LEU:HD21	1:B:310:PHE:CE1	2.50	0.46
1:B:77:ARG:NH2	1:B:354:GLU:HG3	2.31	0.46
1:A:132:GLY:HA3	1:B:130:ASP:O	2.15	0.46
1:A:359:PHE:HE1	1:A:374:ARG:HA	1.81	0.46
1:A:263:LEU:HD22	1:A:267:TYR:CZ	2.50	0.46
1:B:166:GLU:HG2	1:B:222:ASN:HB3	1.98	0.46
1:A:167:PRO:HB2	1:A:250:PHE:CE1	2.51	0.45
1:B:355:ASN:ND2	1:B:398:TYR:OH	2.49	0.45
1:A:76:TYR:CE2	1:A:78:PHE:HB3	2.52	0.45
1:A:169:VAL:O	1:A:170:VAL:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PHE:O	1:A:176:ALA:HB3	2.17	0.45
1:B:167:PRO:HB2	1:B:250:PHE:CE1	2.51	0.45
1:A:241:LEU:HA	1:A:241:LEU:HD12	1.57	0.45
1:A:159:ASP:O	1:A:215:GLY:HA3	2.16	0.45
1:A:349:PRO:O	1:A:350:LEU:HD23	2.17	0.45
1:B:65:ILE:HD12	1:B:108:LEU:HD23	1.99	0.45
1:B:129:GLN:O	1:B:131:LYS:O	2.35	0.44
1:B:121:HIS:NE2	1:B:165:ASN:ND2	2.65	0.44
1:A:355:ASN:ND2	1:A:398:TYR:OH	2.50	0.44
1:B:244:ASP:O	1:B:249:TRP:HB2	2.16	0.44
1:B:169:VAL:O	1:B:170:VAL:C	2.56	0.44
1:A:121:HIS:O	1:A:122:TRP:HB2	2.17	0.44
1:B:64:ASP:OD1	1:B:430:ARG:NH1	2.50	0.44
1:A:192:GLN:OE1	1:A:275:THR:HG23	2.18	0.44
1:A:243:ASP:OD2	1:A:340:ARG:NH2	2.49	0.44
1:A:281:MET:HB3	1:A:281:MET:HE2	1.81	0.44
1:A:76:TYR:CZ	1:A:78:PHE:HB3	2.52	0.44
1:A:80:THR:CG2	1:A:146:TYR:OH	2.66	0.44
1:A:77:ARG:NH2	1:A:354:GLU:HG3	2.32	0.44
1:A:401:TRP:HA	1:A:402:SER:HA	1.73	0.44
1:B:65:ILE:HD12	1:B:108:LEU:CD2	2.48	0.44
1:B:159:ASP:N	3:B:494:HOH:O	2.50	0.44
1:A:393:VAL:HG13	1:A:394:PRO:HD2	2.00	0.44
1:B:334:LEU:HD22	1:B:334:LEU:O	2.17	0.44
1:A:325:MET:SD	1:A:415:LYS:HG2	2.58	0.43
1:B:137:ARG:HG3	1:B:196:HIS:NE2	2.33	0.43
1:B:21:ILE:HG13	1:B:22:GLU:N	2.32	0.43
1:A:21:ILE:HG13	1:A:22:GLU:N	2.33	0.43
1:A:288:ILE:HG23	3:A:488:HOH:O	2.18	0.43
1:A:78:PHE:CZ	1:A:117:ILE:HG12	2.53	0.43
1:A:149:LEU:O	1:A:149:LEU:HD22	2.19	0.43
1:A:201:HIS:O	1:A:205:VAL:HG12	2.18	0.43
1:B:30:LYS:HD2	1:B:84:ARG:HB2	2.00	0.43
1:A:244:ASP:O	1:A:249:TRP:HB2	2.19	0.43
1:B:24:ALA:HB1	1:B:27:GLU:HB3	2.01	0.43
1:A:363:LEU:HD11	1:A:431:PHE:CE2	2.54	0.42
1:B:119:LEU:HA	1:B:119:LEU:HD23	1.82	0.42
1:B:80:THR:CG2	1:B:146:TYR:OH	2.67	0.42
1:A:124:LEU:HD12	1:A:125:PRO:HD2	2.00	0.42
1:A:234:LYS:HG3	1:A:303:HIS:CG	2.54	0.42
1:B:140:ALA:CB	1:B:200:SER:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LEU:O	1:B:395:LEU:HD12	2.18	0.42
1:B:188:LYS:HE2	1:B:272:GLY:N	2.35	0.42
1:B:330:TYR:CE2	1:B:332:GLN:CG	2.92	0.42
1:B:202:GLY:HA2	1:B:205:VAL:CG1	2.50	0.42
1:A:37:ARG:HG3	1:A:126:GLN:NE2	2.34	0.42
1:A:250:PHE:C	1:A:253:PRO:HD2	2.41	0.42
1:B:172:PHE:O	1:B:176:ALA:HB3	2.19	0.41
1:B:223:LEU:HD11	1:B:251:LEU:HD11	2.02	0.41
1:A:242:LEU:HA	1:A:242:LEU:HD23	1.80	0.41
1:A:223:LEU:HD11	1:A:251:LEU:HD11	2.01	0.41
1:A:5:ILE:HG13	1:A:5:ILE:O	2.21	0.41
1:A:64:ASP:OD1	1:A:430:ARG:NH1	2.53	0.41
1:B:268:GLU:O	1:B:271:LEU:O	2.38	0.41
1:A:302:ARG:NH2	1:A:315:VAL:HG13	2.36	0.41
1:B:205:VAL:O	1:B:209:ARG:HG2	2.21	0.41
1:A:227:TYR:HA	1:A:228:PRO:HD3	1.81	0.41
1:A:299:MET:HE2	1:A:314:VAL:CG1	2.51	0.41
1:A:188:LYS:HE2	1:A:272:GLY:N	2.36	0.41
1:A:389:LEU:HD13	1:A:395:LEU:HB3	2.03	0.41
1:B:188:LYS:CE	1:B:272:GLY:H	2.32	0.41
1:B:320:ARG:HA	1:B:321:PRO:HD3	1.92	0.40
1:A:82:TRP:HB3	1:A:83:PRO:HD3	2.03	0.40
1:B:56:ASP:OD1	1:B:59:HIS:ND1	2.50	0.40
1:A:17:SER:HB3	1:A:20:GLN:OE1	2.21	0.40
1:B:243:ASP:OD2	1:B:340:ARG:NH2	2.53	0.40
1:A:255:PHE:CD1	1:A:346:THR:HB	2.56	0.40
1:A:188:LYS:CE	1:A:272:GLY:H	2.34	0.40
1:A:306:GLY:CA	1:A:311:ASN:ND2	2.56	0.40
1:B:299:MET:HE2	1:B:314:VAL:CG1	2.51	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	444/458 (97%)	402 (90%)	41 (9%)	1 (0%)	47	82
1	B	433/458 (94%)	394 (91%)	37 (8%)	2 (0%)	29	68
All	All	877/916 (96%)	796 (91%)	78 (9%)	3 (0%)	41	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	VAL
1	B	447	GLN
1	B	122	TRP

### 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	369/391 (94%)	327 (89%)	42 (11%)	5	24
1	B	363/391 (93%)	320 (88%)	43 (12%)	5	22
All	All	732/782 (94%)	647 (88%)	85 (12%)	5	23

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	37	ARG
1	A	39	SER
1	A	67	LEU
1	A	80	THR
1	A	92	ARG
1	A	106	ASP
1	A	137	ARG
1	A	141	LYS
1	A	146	TYR
1	A	149	LEU
1	A	169	VAL
1	A	184	THR

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Mol	Chain	Res	Type
1	A	188	LYS
1	A	199	LEU
1	A	205	VAL
1	A	207	ILE
1	A	219	ILE
1	A	241	LEU
1	A	242	LEU
1	A	263	LEU
1	A	266	ILE
1	A	275	THR
1	A	276	THR
1	A	298	ARG
1	A	307	ASP
1	A	308	ASN
1	A	309	LEU
1	A	311	ASN
1	A	314	VAL
1	A	330	TYR
1	A	332	GLN
1	A	334	LEU
1	A	363	LEU
1	A	364	THR
1	A	369	ILE
1	A	398	TYR
1	A	403	LEU
1	A	429	ARG
1	A	430	ARG
1	A	440	ARG
1	A	447	GLN
1	B	5	ILE
1	B	17	SER
1	B	37	ARG
1	B	39	SER
1	B	67	LEU
1	B	80	THR
1	B	92	ARG
1	B	106	ASP
1	B	110	LYS
1	B	137	ARG
1	B	141	LYS
1	B	146	TYR
1	B	149	LEU

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Mol	Chain	Res	Type
1	B	169	VAL
1	B	184	THR
1	B	188	LYS
1	B	205	VAL
1	B	207	ILE
1	B	219	ILE
1	B	241	LEU
1	B	242	LEU
1	B	263	LEU
1	B	266	ILE
1	B	275	THR
1	B	276	THR
1	B	288	ILE
1	B	298	ARG
1	B	308	ASN
1	B	309	LEU
1	B	314	VAL
1	B	330	TYR
1	B	332	GLN
1	B	334	LEU
1	B	363	LEU
1	B	364	THR
1	B	369	ILE
1	B	378	LEU
1	B	398	TYR
1	B	403	LEU
1	B	429	ARG
1	B	430	ARG
1	B	440	ARG
1	B	448	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	126	GLN
1	A	264	HIS
1	A	303	HIS
1	A	308	ASN
1	A	311	ASN
1	A	355	ASN
1	A	370	HIS

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Mol	Chain	Res	Type
1	B	107	ASN
1	B	126	GLN
1	B	180	HIS
1	B	264	HIS
1	B	308	ASN
1	B	355	ASN
1	B	370	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](#)

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 [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	448/458 (97%)	-0.43	4 (0%)	84 63	6, 19, 55, 75	0
1	B	441/458 (96%)	-0.33	1 (0%)	95 87	5, 19, 51, 77	0
All	All	889/916 (97%)	-0.38	5 (0%)	89 72	5, 19, 53, 77	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	3.5
1	B	231	ASP	2.6
1	A	238	ALA	2.2
1	A	47	ASN	2.0
1	A	230	GLY	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	NI	B	500	1/1	0.96	0.11	59,59,59,59	0
2	NI	A	500	1/1	0.97	0.08	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.