



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 10:23 AM EDT

PDB ID : 6EX6  
Title : The GH127, Beta-arabinofuranosidase, BT3674  
Authors : Munoz-Munoz, J.; Gilbert, H.J.  
Deposited on : 2017-11-07  
Resolution : 2.16 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

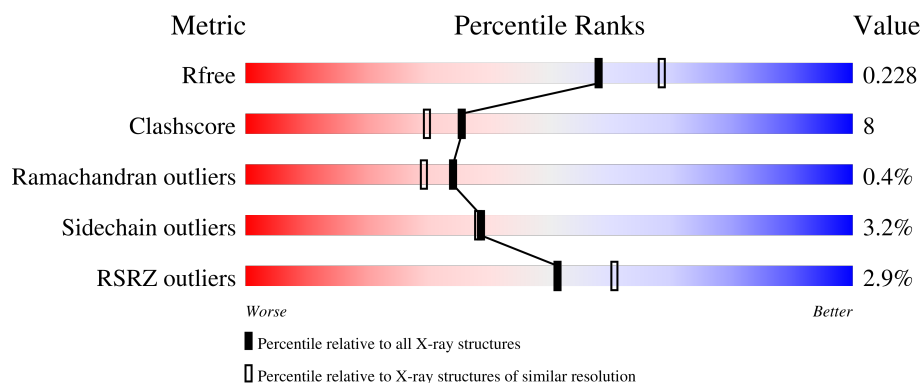
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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	648	
1	B	648	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10524 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 Six-hairpin glycosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	633	Total	C	N	O	S	0	1	0
			4886	3125	821	921	19			
1	A	634	Total	C	N	O	S	0	0	0
			4909	3138	823	929	19			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

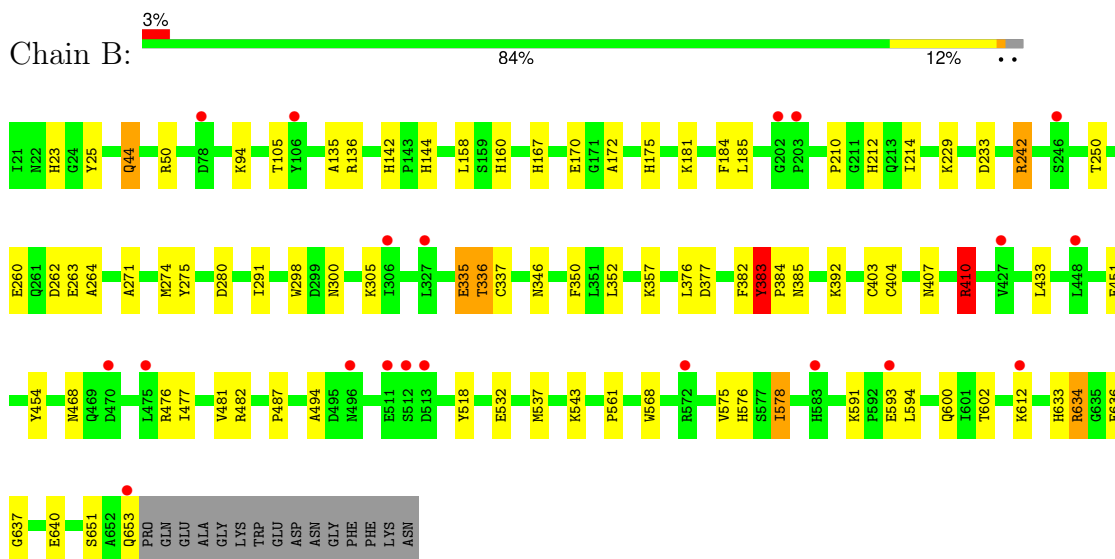
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	365	Total	O	0	0
			365	365		
3	A	362	Total	O	0	0
			362	362		

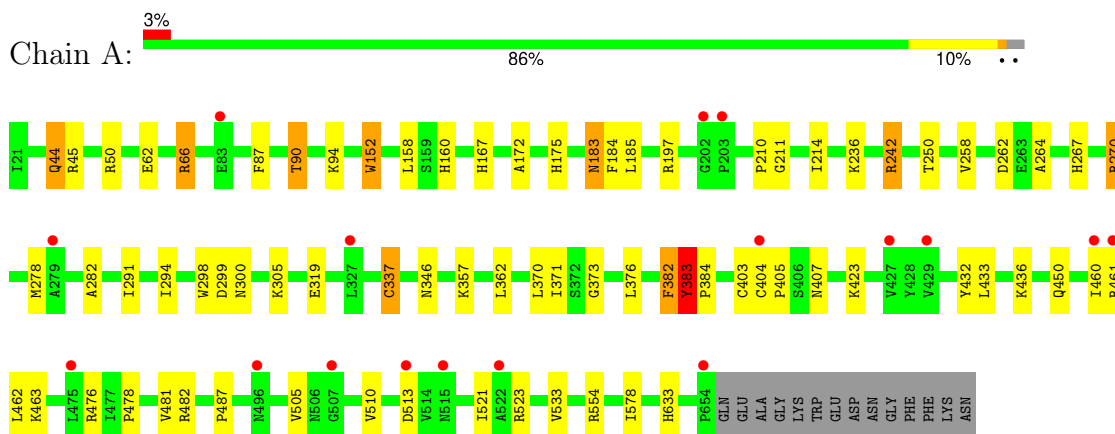
### 3 Residue-property plots [i](#)

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: Six-hairpin glycosidase



- Molecule 1: Six-hairpin glycosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.82Å 136.82Å 135.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.75 – 2.16 19.75 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.75-2.16) 99.9 (19.75-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.176 , 0.221 0.188 , 0.228	Depositor DCC
$R_{free}$ test set	3944 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: ZN

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	0.92	0/5042	0.91	13/6886 (0.2%)
1	B	0.97	1/5020 (0.0%)	0.93	12/6858 (0.2%)
All	All	0.95	1/10062 (0.0%)	0.92	25/13744 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	GLU	CD-OE2	8.61	1.35	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	B	476	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	B	242	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	A	197	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	A	476	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	242	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	476	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	476	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	270	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	A	554	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	B	410	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	554	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	262	ASP	CB-CG-OD1	7.06	124.66	118.30
1	B	262	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	197	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	B	280	ASP	CB-CG-OD1	6.63	124.26	118.30
1	A	242	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	66	ARG	NE-CZ-NH1	6.54	123.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	66	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	136	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	523	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	335	GLU	CG-CD-OE1	-5.15	108.01	118.30
1	B	335	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	B	410	ARG	NE-CZ-NH1	5.13	122.86	120.30

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	4909	0	4605	91	0
1	B	4886	0	4571	63	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	362	0	0	21	0
3	B	365	0	0	27	0
All	All	10524	0	9176	154	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 (154) 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:460:ILE:CG1	1:A:533:VAL:HB	1.38	1.50
1:A:460:ILE:HD11	1:A:533:VAL:CG2	1.73	1.18
1:A:461:ARG:NH1	1:A:463:LYS:HE2	1.59	1.17
1:A:460:ILE:CD1	1:A:533:VAL:HG23	1.76	1.16
1:A:460:ILE:CG1	1:A:533:VAL:CB	2.26	1.14
1:A:460:ILE:HG13	1:A:533:VAL:HB	1.22	1.13
1:A:460:ILE:HG12	1:A:533:VAL:HB	1.14	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ARG:NE	3:A:802:HOH:O	1.60	1.04
1:A:461:ARG:HH12	1:A:463:LYS:HE2	1.19	0.99
1:A:460:ILE:HD11	1:A:533:VAL:HG23	0.99	0.98
1:A:270:ARG:NH2	3:A:802:HOH:O	1.97	0.95
1:A:383:TYR:HB3	1:A:384:PRO:HD3	1.50	0.93
1:B:383:TYR:HB3	1:B:384:PRO:HD3	1.51	0.93
1:A:183:ASN:H	1:A:183:ASN:HD22	1.15	0.91
1:B:336:THR:HG22	1:B:385:ASN:HD21	1.36	0.90
1:A:436:LYS:CD	1:A:436:LYS:NZ	2.34	0.90
1:A:460:ILE:CD1	1:A:533:VAL:CG2	2.44	0.89
1:A:383:TYR:HB3	1:A:384:PRO:CD	2.03	0.88
1:A:460:ILE:HG12	1:A:533:VAL:CB	1.95	0.88
1:A:211:GLY:O	1:A:270:ARG:NH1	2.08	0.86
1:B:454:TYR:CE2	3:B:959:HOH:O	2.28	0.85
1:B:537:MET:HE2	3:B:959:HOH:O	1.77	0.85
1:A:460:ILE:HG13	1:A:533:VAL:CB	2.03	0.83
1:B:274:MET:HB3	3:B:803:HOH:O	1.78	0.82
1:B:454:TYR:CZ	3:B:959:HOH:O	2.32	0.81
1:B:376:LEU:H	1:B:633:HIS:HE1	1.27	0.79
1:A:236:LYS:HE2	3:A:854:HOH:O	1.82	0.79
1:A:383:TYR:CB	1:A:384:PRO:HD3	2.13	0.79
1:A:460:ILE:HD11	1:A:533:VAL:CB	2.12	0.78
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.14	0.78
1:A:460:ILE:CD1	1:A:533:VAL:CB	2.61	0.77
1:A:460:ILE:HD13	1:A:462:LEU:HD12	1.68	0.76
1:A:461:ARG:HH12	1:A:463:LYS:CE	1.97	0.76
1:A:270:ARG:CZ	3:A:802:HOH:O	2.01	0.75
1:B:233:ASP:OD2	3:B:802:HOH:O	2.03	0.75
1:A:383:TYR:HA	1:A:404:CYS:SG	2.27	0.74
1:A:460:ILE:HD11	1:A:533:VAL:N	2.04	0.73
1:A:404:CYS:HB2	1:A:405:PRO:HD3	1.71	0.73
1:B:634:ARG:HD3	3:B:867:HOH:O	1.90	0.72
1:A:460:ILE:CD1	1:A:533:VAL:N	2.54	0.71
1:A:460:ILE:HD13	1:A:462:LEU:CD1	2.21	0.71
1:B:594:LEU:HD11	3:B:801:HOH:O	1.90	0.70
1:B:229:LYS:O	3:B:802:HOH:O	2.11	0.68
1:A:210:PRO:O	1:A:242:ARG:NH2	2.25	0.68
1:B:23:HIS:HD2	1:B:25:TYR:H	1.41	0.68
1:A:298:TRP:HE1	1:A:346:ASN:HD21	1.42	0.67
1:A:94:LYS:HD3	1:A:167:HIS:CE1	2.29	0.67
1:B:275:TYR:CE1	3:B:803:HOH:O	2.47	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG13	1:A:278:MET:CE	2.25	0.67
1:A:432:TYR:HA	1:A:450:GLN:HE22	1.60	0.66
1:B:271:ALA:O	3:B:803:HOH:O	2.14	0.65
1:B:175:HIS:HD2	3:B:916:HOH:O	1.78	0.65
1:A:371:ILE:HG21	3:A:1082:HOH:O	1.97	0.65
1:B:298:TRP:HE1	1:B:346:ASN:HD21	1.43	0.65
1:B:383:TYR:CB	1:B:384:PRO:HD3	2.26	0.64
1:A:376:LEU:H	1:A:633:HIS:HE1	1.45	0.64
1:B:336:THR:HG22	1:B:385:ASN:ND2	2.10	0.64
1:B:561:PRO:HD3	3:B:959:HOH:O	1.97	0.64
1:B:578:ILE:HD13	3:B:1030:HOH:O	1.98	0.64
1:B:229:LYS:C	3:B:802:HOH:O	2.36	0.63
1:B:44:GLN:HG3	3:B:894:HOH:O	1.98	0.63
1:A:461:ARG:CZ	1:A:463:LYS:HE2	2.25	0.62
1:A:300:ASN:HD21	1:A:305:LYS:HE3	1.64	0.62
1:A:460:ILE:CD1	1:A:533:VAL:H	2.13	0.62
1:A:183:ASN:HD22	1:A:183:ASN:N	1.91	0.61
1:A:45:ARG:NH2	1:A:371:ILE:CG2	2.64	0.61
1:A:423:LYS:NZ	3:A:804:HOH:O	2.29	0.61
1:A:299:ASP:HB3	3:A:1098:HOH:O	2.00	0.60
1:B:407:ASN:OD1	1:B:410:ARG:HD3	2.01	0.60
1:A:87:PHE:O	1:A:90:THR:HB	2.01	0.59
1:B:335:GLU:CG	1:B:404:CYS:SG	2.90	0.59
1:B:263:GLU:OE1	3:B:804:HOH:O	2.17	0.58
1:B:591:LYS:HG3	1:B:600:GLN:HG2	1.85	0.58
1:B:653:GLN:C	3:B:998:HOH:O	2.41	0.58
1:B:392:LYS:HA	1:B:636:GLU:OE1	2.04	0.58
1:B:275:TYR:CD1	3:B:803:HOH:O	2.58	0.57
1:B:376:LEU:H	1:B:633:HIS:CE1	2.17	0.56
1:A:50:ARG:HD2	3:A:1016:HOH:O	2.05	0.56
1:A:337:CYS:SG	1:A:407:ASN:ND2	2.75	0.56
1:A:460:ILE:CG1	1:A:533:VAL:CG2	2.79	0.55
1:B:260:GLU:HG2	3:A:1103:HOH:O	2.08	0.54
1:A:90:THR:CG2	3:A:949:HOH:O	2.55	0.54
1:A:45:ARG:CZ	1:A:371:ILE:HG23	2.37	0.54
1:A:460:ILE:C	1:A:460:ILE:HD12	2.29	0.53
1:B:300:ASN:HD21	1:B:305:LYS:HE3	1.72	0.53
1:A:383:TYR:CB	1:A:384:PRO:CD	2.75	0.53
1:B:210:PRO:O	1:B:242:ARG:NH2	2.31	0.53
1:A:371:ILE:HB	3:A:1082:HOH:O	2.08	0.52
1:A:175:HIS:HD2	3:A:872:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:VAL:HG23	1:A:510:VAL:HG21	1.91	0.52
1:A:371:ILE:CG2	3:A:1082:HOH:O	2.53	0.52
1:A:44:GLN:HG3	3:A:907:HOH:O	2.08	0.52
1:A:371:ILE:CB	3:A:1082:HOH:O	2.57	0.52
1:A:294:ILE:HG21	3:A:1137:HOH:O	2.10	0.51
1:B:537:MET:CE	3:B:959:HOH:O	2.45	0.51
1:B:170:GLU:OE1	1:B:410:ARG:NH2	2.42	0.51
1:B:105:THR:HG21	3:B:873:HOH:O	2.10	0.51
1:B:142:HIS:HE1	3:B:1122:HOH:O	1.94	0.51
1:A:258:VAL:HG13	1:A:278:MET:HE1	1.92	0.51
1:A:460:ILE:HG13	1:A:533:VAL:CA	2.41	0.51
1:A:294:ILE:CB	3:A:1137:HOH:O	2.58	0.50
1:B:94:LYS:HD3	1:B:167:HIS:CE1	2.46	0.50
1:A:264:ALA:H	1:A:300:ASN:HD22	1.58	0.50
1:A:403:CYS:O	1:A:407:ASN:HB2	2.11	0.50
1:B:175:HIS:HE1	3:B:860:HOH:O	1.94	0.50
1:B:477:ILE:HG22	1:B:482:ARG:HD2	1.92	0.50
1:A:383:TYR:CG	1:A:384:PRO:HD3	2.47	0.50
1:A:172:ALA:HB1	1:A:185:LEU:HA	1.92	0.50
1:B:23:HIS:HD2	1:B:25:TYR:N	2.08	0.49
1:A:362:LEU:C	1:A:362:LEU:HD23	2.33	0.49
1:A:460:ILE:HG12	1:A:533:VAL:CG2	2.40	0.49
1:B:403:CYS:O	1:B:407:ASN:HB2	2.13	0.48
1:B:383:TYR:CB	1:B:384:PRO:CD	2.89	0.48
1:B:158:LEU:O	1:B:160:HIS:HD2	1.96	0.48
1:A:45:ARG:CZ	1:A:371:ILE:CG2	2.91	0.48
1:A:90:THR:HG21	3:A:949:HOH:O	2.14	0.47
1:A:258:VAL:HG13	1:A:278:MET:SD	2.55	0.47
1:B:336:THR:CG2	1:B:382:PHE:O	2.63	0.47
1:A:267:HIS:HE1	1:A:319:GLU:OE1	1.97	0.47
1:A:460:ILE:HD12	1:A:533:VAL:H	1.80	0.47
1:B:264:ALA:H	1:B:300:ASN:HD22	1.63	0.46
1:B:291:ILE:HD12	1:B:352:LEU:HD13	1.97	0.46
1:B:335:GLU:HG2	1:B:404:CYS:SG	2.54	0.46
1:B:350:PHE:HE1	1:B:518:TYR:HH	1.63	0.46
1:B:233:ASP:CG	3:B:802:HOH:O	2.49	0.45
1:B:274:MET:HE2	3:B:803:HOH:O	2.16	0.45
1:A:158:LEU:O	1:A:160:HIS:HD2	2.00	0.45
1:A:376:LEU:H	1:A:633:HIS:CE1	2.31	0.45
1:A:423:LYS:HG3	3:A:1077:HOH:O	2.17	0.44
1:A:578:ILE:HB	3:A:946:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:C	1:A:370:LEU:HD23	2.38	0.44
1:A:183:ASN:H	1:A:183:ASN:ND2	1.96	0.44
1:A:373:GLY:HA2	1:A:382:PHE:HB2	1.99	0.43
1:B:494:ALA:HB2	1:B:543:LYS:HB2	2.01	0.43
1:B:576:HIS:CD2	1:B:640:GLU:HG2	2.54	0.43
1:A:460:ILE:HD11	1:A:533:VAL:CA	2.48	0.43
1:A:461:ARG:NH1	1:A:463:LYS:CE	2.53	0.42
1:B:477:ILE:CG2	1:B:482:ARG:HD2	2.50	0.42
1:A:478:PRO:O	1:A:482:ARG:HG3	2.20	0.42
1:A:183:ASN:N	1:A:183:ASN:ND2	2.62	0.42
1:A:357:LYS:HB2	1:A:487:PRO:HG3	2.02	0.41
1:B:568:TRP:CD1	1:B:637:GLY:HA3	2.55	0.41
1:B:212:HIS:HE1	3:B:1125:HOH:O	2.03	0.41
1:B:135:ALA:HB1	1:B:144:HIS:HB2	2.01	0.41
1:A:505:VAL:HG21	1:A:521:ILE:HG21	2.02	0.41
1:B:451:GLU:CG	3:B:1126:HOH:O	2.68	0.41
1:A:298:TRP:HE1	1:A:346:ASN:ND2	2.15	0.41
1:A:423:LYS:HA	3:A:1077:HOH:O	2.20	0.41
1:B:181:LYS:HA	3:B:809:HOH:O	2.21	0.41
1:A:282:ALA:CB	1:A:291:ILE:HD11	2.51	0.41
1:B:172:ALA:HB1	1:B:185:LEU:HA	2.02	0.40
1:B:357:LYS:HB2	1:B:487:PRO:HG3	2.04	0.40
1:B:335:GLU:HG2	1:B:337:CYS:H	1.86	0.40
1:A:267:HIS:HD2	1:A:270:ARG:H	1.68	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	632/648 (98%)	611 (97%)	18 (3%)	3 (0%)	29 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	632/648 (98%)	614 (97%)	16 (2%)	2 (0%)	41	37
All	All	1264/1296 (98%)	1225 (97%)	34 (3%)	5 (0%)	34	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	ILE
1	A	214	ILE
1	B	383	TYR
1	A	383	TYR
1	A	152	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	501/546 (92%)	487 (97%)	14 (3%)	43	44
1	B	496/546 (91%)	478 (96%)	18 (4%)	35	33
All	All	997/1092 (91%)	965 (97%)	32 (3%)	39	38

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	44	GLN
1	B	50	ARG
1	B	184	PHE
1	B	250	THR
1	B	336	THR
1	B	383	TYR
1	B	410	ARG
1	B	433	LEU
1	B	468	ASN
1	B	481	VAL
1	B	532	GLU

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Mol	Chain	Res	Type
1	B	575	VAL
1	B	578	ILE
1	B	593	GLU
1	B	602	THR
1	B	612	LYS
1	B	634	ARG
1	B	651	SER
1	A	44	GLN
1	A	62	GLU
1	A	66	ARG
1	A	90	THR
1	A	152	TRP
1	A	183	ASN
1	A	184	PHE
1	A	250	THR
1	A	337	CYS
1	A	382	PHE
1	A	383	TYR
1	A	433	LEU
1	A	481	VAL
1	A	513	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	HIS
1	B	160	HIS
1	B	175	HIS
1	B	212	HIS
1	B	300	ASN
1	B	315	HIS
1	B	346	ASN
1	B	430	ASN
1	B	435	ASN
1	B	552	HIS
1	B	576	HIS
1	B	633	HIS
1	A	104	GLN
1	A	160	HIS
1	A	175	HIS
1	A	183	ASN
1	A	212	HIS

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Mol	Chain	Res	Type
1	A	267	HIS
1	A	300	ASN
1	A	346	ASN
1	A	385	ASN
1	A	435	ASN
1	A	450	GLN
1	A	633	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 monosaccharides 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

### 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, 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	634/648 (97%)	0.03	17 (2%) 54 63	24, 34, 56, 87	0
1	B	633/648 (97%)	-0.07	20 (3%) 47 56	22, 33, 50, 81	0
All	All	1267/1296 (97%)	-0.02	37 (2%) 51 61	22, 34, 52, 87	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	ILE	6.0
1	B	511	GLU	4.2
1	B	572	ARG	4.1
1	B	612	LYS	3.8
1	A	513	ASP	3.8
1	A	427	VAL	3.4
1	B	496	ASN	3.3
1	A	654	PRO	3.2
1	A	461	ARG	3.2
1	A	429	VAL	3.1
1	A	496	ASN	3.1
1	B	106	TYR	2.9
1	B	653	GLN	2.9
1	A	507	GLY	2.8
1	A	475	LEU	2.7
1	B	427	VAL	2.7
1	A	202	GLY	2.5
1	A	203	PRO	2.4
1	B	246	SER	2.4
1	B	327	LEU	2.3
1	B	202	GLY	2.3
1	A	404	CYS	2.3
1	B	583	HIS	2.2
1	B	448	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	593	GLU	2.2
1	B	78	ASP	2.1
1	B	512	SER	2.1
1	A	327	LEU	2.1
1	A	279	ALA	2.1
1	B	513	ASP	2.1
1	A	515	ASN	2.0
1	B	475	LEU	2.0
1	B	470	ASP	2.0
1	B	203	PRO	2.0
1	B	306	ILE	2.0
1	A	522	ALA	2.0
1	A	83	GLU	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 monosaccharides 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	ZN	B	701	1/1	0.93	0.10	31,31,31,31	0
2	ZN	A	701	1/1	0.96	0.07	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.