



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:33 PM UTC

PDB ID : 9HYQ / pdb_00009hyq
Title : BT984 a GH139 rhamnogalacturonan II exo- α -1,2-(2-Omethyl)-fucosidase
Authors : Cartmell, A.
Deposited on : 2025-01-10
Resolution : 2.70 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
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

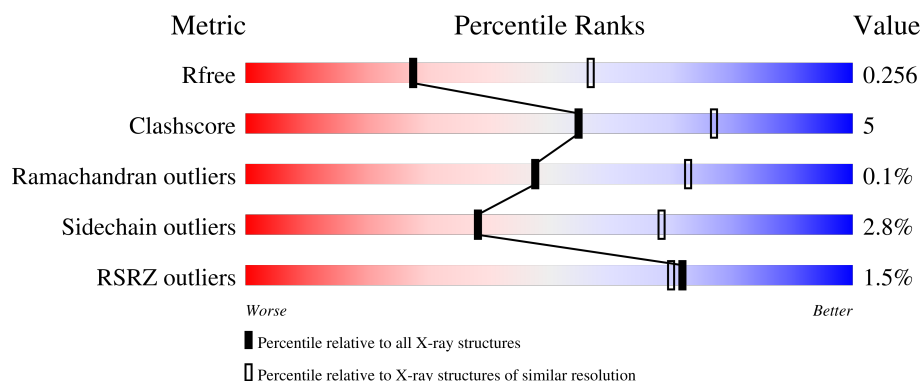
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	802	78% 14% 7%
1	B	802	2% 79% 14% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12181 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 DUF5703 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	0	0	0
			6084	3902	1037	1116	29			
1	B	746	Total	C	N	O	S	0	0	0
			6085	3902	1039	1115	29			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q8A933
A	3	GLY	-	expression tag	UNP Q8A933
A	4	SER	-	expression tag	UNP Q8A933
A	5	SER	-	expression tag	UNP Q8A933
A	6	HIS	-	expression tag	UNP Q8A933
A	7	HIS	-	expression tag	UNP Q8A933
A	8	HIS	-	expression tag	UNP Q8A933
A	9	HIS	-	expression tag	UNP Q8A933
A	10	HIS	-	expression tag	UNP Q8A933
A	11	HIS	-	expression tag	UNP Q8A933
A	12	SER	-	expression tag	UNP Q8A933
A	13	SER	-	expression tag	UNP Q8A933
A	14	GLY	-	expression tag	UNP Q8A933
A	15	PRO	-	expression tag	UNP Q8A933
A	16	GLN	-	expression tag	UNP Q8A933
A	17	GLN	-	expression tag	UNP Q8A933
A	18	GLY	-	expression tag	UNP Q8A933
A	19	LEU	-	expression tag	UNP Q8A933
A	20	ARG	-	expression tag	UNP Q8A933
B	2	MET	-	initiating methionine	UNP Q8A933
B	3	GLY	-	expression tag	UNP Q8A933
B	4	SER	-	expression tag	UNP Q8A933
B	5	SER	-	expression tag	UNP Q8A933
B	6	HIS	-	expression tag	UNP Q8A933
B	7	HIS	-	expression tag	UNP Q8A933

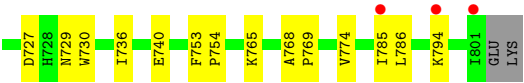
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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	HIS	-	expression tag	UNP Q8A933
B	9	HIS	-	expression tag	UNP Q8A933
B	10	HIS	-	expression tag	UNP Q8A933
B	11	HIS	-	expression tag	UNP Q8A933
B	12	SER	-	expression tag	UNP Q8A933
B	13	SER	-	expression tag	UNP Q8A933
B	14	GLY	-	expression tag	UNP Q8A933
B	15	PRO	-	expression tag	UNP Q8A933
B	16	GLN	-	expression tag	UNP Q8A933
B	17	GLN	-	expression tag	UNP Q8A933
B	18	GLY	-	expression tag	UNP Q8A933
B	19	LEU	-	expression tag	UNP Q8A933
B	20	ARG	-	expression tag	UNP Q8A933

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	5	Total O 5 5	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.20Å 138.32Å 195.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.48 – 2.70 47.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.48-2.70) 98.6 (47.48-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.218 , 0.256 0.222 , 0.256	Depositor DCC
R_{free} test set	3736 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.856	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12181	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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	0.52	0/6261	1.04	8/8490 (0.1%)
1	B	0.51	0/6261	1.02	6/8489 (0.1%)
All	All	0.52	0/12522	1.03	14/16979 (0.1%)

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	5
1	B	0	3
All	All	0	8

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	22	HIS	CA-CB-CG	9.01	122.81	113.80
1	A	22	HIS	CA-CB-CG	8.26	122.06	113.80
1	B	696	THR	CA-CB-OG1	-6.60	99.70	109.60
1	A	482	ASP	CA-CB-CG	6.25	118.86	112.60
1	A	681	THR	CA-CB-OG1	-6.04	100.54	109.60
1	B	547	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	496	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	67	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	58	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	632	LYS	N-CA-C	-5.20	105.69	111.36
1	B	561	GLU	CB-CA-C	-5.19	101.43	110.09
1	A	173	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	67	ASP	CA-CB-CG	5.17	117.78	112.60
1	B	632	LYS	N-CA-C	-5.07	105.83	111.36

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Sidechain
1	A	319	ARG	Sidechain
1	A	363	ARG	Sidechain
1	A	535	ARG	Sidechain
1	A	652	ARG	Sidechain
1	B	250	ARG	Sidechain
1	B	363	ARG	Sidechain
1	B	636	ARG	Sidechain

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	6084	0	5871	60	1
1	B	6085	0	5876	54	1
2	A	7	0	0	0	0
2	B	5	0	0	1	0
All	All	12181	0	11747	114	1

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 5.

All (114) 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:609:VAL:O	1:B:610:LYS:HG3	1.82	0.79
1:A:417:TYR:C	1:A:419:PRO:HD2	2.18	0.69
1:B:417:TYR:C	1:B:419:PRO:HD2	2.18	0.68
1:B:118:ASP:OD2	1:B:121:HIS:ND1	2.21	0.67
1:A:118:ASP:OD2	1:A:121:HIS:ND1	2.20	0.66
1:A:777:THR:HB	1:A:785:ILE:HG22	1.77	0.66
1:A:428:MET:O	1:A:431:SER:OG	2.16	0.63
1:B:560:CYS:SG	1:B:643:PRO:HB3	2.42	0.58
1:B:411:GLN:HB3	2:B:902:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:VAL:HG12	1:B:586:VAL:O	2.04	0.57
1:A:48:ASN:O	1:A:58:PHE:HA	2.05	0.57
1:A:586:VAL:HG12	1:A:586:VAL:O	2.06	0.56
1:B:48:ASN:O	1:B:58:PHE:HA	2.05	0.56
1:A:727:ASP:OD1	1:A:729:ASN:ND2	2.39	0.56
1:B:86:PRO:O	1:B:90:ALA:HB2	2.04	0.56
1:A:777:THR:CB	1:A:785:ILE:HG22	2.37	0.55
1:B:517:THR:N	1:B:518:PRO:CD	2.70	0.54
1:B:683:TRP:HB3	1:B:729:ASN:OD1	2.06	0.54
1:A:324:THR:O	1:A:325:ILE:HG23	2.06	0.54
1:A:517:THR:N	1:A:518:PRO:CD	2.70	0.54
1:B:649:PHE:CG	1:B:650:PRO:HA	2.43	0.53
1:B:370:ALA:HB2	1:B:428:MET:SD	2.48	0.53
1:A:370:ALA:HB2	1:A:428:MET:SD	2.50	0.52
1:A:236:TYR:CZ	1:A:238:GLY:HA2	2.45	0.52
1:A:108:ALA:O	1:A:109:GLU:C	2.52	0.52
1:A:649:PHE:CG	1:A:650:PRO:HA	2.45	0.51
1:B:43:GLY:O	1:B:370:ALA:O	2.27	0.51
1:A:43:GLY:O	1:A:370:ALA:O	2.28	0.51
1:A:65:THR:HB	1:A:225:PHE:CE2	2.46	0.51
1:A:177:LEU:HD21	1:A:236:TYR:CG	2.46	0.51
1:B:209:MET:HE1	1:B:446:ARG:HA	1.92	0.50
1:B:236:TYR:CZ	1:B:238:GLY:HA2	2.47	0.50
1:B:727:ASP:CG	1:B:730:TRP:HB2	2.37	0.50
1:A:429:MET:N	1:A:430:PRO:CD	2.75	0.50
1:A:386:ASP:OD1	1:A:398:PRO:HG3	2.12	0.49
1:A:753:PHE:N	1:A:754:PRO:CD	2.75	0.49
1:B:753:PHE:N	1:B:754:PRO:CD	2.75	0.49
1:A:736:ILE:O	1:A:740:GLU:HG2	2.12	0.49
1:B:736:ILE:O	1:B:740:GLU:HG2	2.12	0.49
1:B:515:ASP:OD1	1:B:517:THR:HG23	2.13	0.49
1:B:378:PHE:HB2	1:B:729:ASN:HD22	1.78	0.48
1:B:402:LYS:O	1:B:403:TRP:HB2	2.12	0.48
1:B:111:THR:OG1	1:B:130:ASN:ND2	2.45	0.48
1:A:425:ASP:HB3	1:A:428:MET:HE2	1.95	0.48
1:A:485:LEU:HD11	1:A:493:TYR:OH	2.13	0.48
1:B:493:TYR:CZ	1:B:556:PRO:HG2	2.49	0.48
1:B:429:MET:N	1:B:430:PRO:CD	2.77	0.48
1:A:65:THR:HB	1:A:225:PHE:CD2	2.48	0.47
1:A:776:ALA:HA	1:A:785:ILE:HG23	1.96	0.47
1:B:646:TYR:N	1:B:647:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ASN:OD1	1:A:590:GLU:N	2.48	0.47
1:B:586:VAL:O	1:B:586:VAL:CG1	2.62	0.47
1:A:646:TYR:N	1:A:647:PRO:CD	2.78	0.47
1:A:150:ILE:HG23	1:A:154:GLU:HB3	1.97	0.46
1:B:589:ASN:OD1	1:B:590:GLU:N	2.48	0.46
1:B:649:PHE:CD1	1:B:650:PRO:HA	2.50	0.46
1:A:493:TYR:CZ	1:A:556:PRO:HG2	2.50	0.46
1:B:150:ILE:HG23	1:B:154:GLU:HB3	1.97	0.46
1:A:711:PRO:HG2	1:A:712:HIS:CD2	2.51	0.46
1:A:586:VAL:O	1:A:586:VAL:CG1	2.63	0.46
1:A:418:TRP:CD2	1:A:504:MET:HE2	2.51	0.45
1:A:765:LYS:HA	1:A:774:VAL:O	2.16	0.45
1:B:696:THR:O	1:B:697:GLU:C	2.59	0.45
1:B:711:PRO:HG2	1:B:712:HIS:CD2	2.52	0.45
1:A:485:LEU:HD11	1:A:493:TYR:CZ	2.51	0.45
1:A:292:ALA:HA	1:A:296:LYS:O	2.17	0.44
1:A:149:LEU:HD12	1:A:169:MET:HB3	1.99	0.44
1:B:418:TRP:N	1:B:419:PRO:CD	2.81	0.44
1:A:111:THR:HG23	1:A:130:ASN:OD1	2.18	0.44
1:B:162:TRP:C	1:B:164:PRO:HD3	2.42	0.44
1:B:425:ASP:HB3	1:B:428:MET:HE2	1.99	0.44
1:B:116:TRP:CZ2	1:B:125:HIS:CD2	3.07	0.43
1:B:418:TRP:CD2	1:B:504:MET:HE2	2.53	0.43
1:A:84:PRO:HD2	1:A:134:LEU:HD22	1.99	0.43
1:A:765:LYS:HE3	1:A:773:THR:HG23	1.99	0.43
1:A:768:ALA:HB1	1:A:769:PRO:CD	2.49	0.43
1:A:145:TYR:CE1	1:A:146:GLN:HG2	2.53	0.43
1:A:727:ASP:CG	1:A:730:TRP:HB2	2.43	0.43
1:A:65:THR:HG21	1:A:75:GLN:NE2	2.33	0.43
1:B:785:ILE:CG2	1:B:786:LEU:N	2.82	0.43
1:A:418:TRP:N	1:A:419:PRO:CD	2.82	0.43
1:A:696:THR:C	1:A:698:GLU:H	2.27	0.43
1:B:95:GLN:HG3	1:B:106:ILE:HG12	2.00	0.43
1:B:74:LYS:HE2	1:B:384:THR:OG1	2.18	0.42
1:B:116:TRP:CH2	1:B:125:HIS:CD2	3.07	0.42
1:A:116:TRP:CH2	1:A:125:HIS:CD2	3.08	0.42
1:A:800:MET:HE3	1:A:800:MET:HB3	1.90	0.42
1:B:765:LYS:HA	1:B:774:VAL:O	2.19	0.42
1:B:163:ALA:N	1:B:164:PRO:HD3	2.35	0.42
1:A:511:TYR:HA	1:A:769:PRO:HA	2.02	0.42
1:A:562:THR:OG1	1:A:641:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LYS:O	1:A:403:TRP:HB2	2.20	0.41
1:B:65:THR:HG21	1:B:75:GLN:NE2	2.34	0.41
1:B:108:ALA:O	1:B:109:GLU:C	2.63	0.41
1:B:74:LYS:HE3	1:B:384:THR:O	2.20	0.41
1:B:562:THR:OG1	1:B:641:GLU:HB2	2.20	0.41
1:A:418:TRP:CZ3	1:A:504:MET:HG2	2.56	0.41
1:A:40:CYS:HB2	1:A:104:VAL:CG2	2.50	0.41
1:A:137:GLU:HA	1:A:254:PHE:O	2.20	0.41
1:A:233:ASN:O	1:A:256:SER:HA	2.21	0.41
1:B:40:CYS:HB2	1:B:104:VAL:CG2	2.51	0.41
1:B:119:VAL:HG23	1:B:309:THR:HG23	2.02	0.41
1:A:756:TRP:HA	1:A:757:PRO:HD3	1.95	0.41
1:A:473:TYR:OH	1:A:483:LYS:HE3	2.20	0.41
1:B:218:ASN:OD1	1:B:218:ASN:C	2.64	0.41
1:A:386:ASP:HA	1:A:387:PRO:HD3	1.91	0.40
1:B:44:ASP:CG	1:B:62:ARG:HE	2.28	0.40
1:B:517:THR:N	1:B:518:PRO:HD3	2.36	0.40
1:B:768:ALA:HB1	1:B:769:PRO:CD	2.51	0.40
1:B:567:ASN:HD22	1:B:632:LYS:HB3	1.85	0.40
1:A:95:GLN:HG3	1:A:106:ILE:HG12	2.02	0.40
1:A:372:GLY:O	1:A:431:SER:HB3	2.20	0.40
1:B:137:GLU:HA	1:B:254:PHE:O	2.22	0.40
1:A:119:VAL:HG23	1:A:309:THR:HG23	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ARG:NH2	1:B:487:TYR:OH[1_455]	2.19	0.01

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	738/802 (92%)	696 (94%)	41 (6%)	1 (0%)	48	73
1	B	738/802 (92%)	696 (94%)	42 (6%)	0	100	100
All	All	1476/1604 (92%)	1392 (94%)	83 (6%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU

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	648/698 (93%)	627 (97%)	21 (3%)	34	64
1	B	648/698 (93%)	633 (98%)	15 (2%)	44	73
All	All	1296/1396 (93%)	1260 (97%)	36 (3%)	38	68

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	35	SER
1	A	68	GLU
1	A	94	ARG
1	A	132	ARG
1	A	177	LEU
1	A	184	ASP
1	A	204	VAL
1	A	239	THR
1	A	240	SER
1	A	300	LYS
1	A	349	LYS
1	A	431	SER
1	A	438	ARG
1	A	483	LYS

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Mol	Chain	Res	Type
1	A	543	ARG
1	A	627	THR
1	A	675	LEU
1	A	729	ASN
1	A	773	THR
1	A	786	LEU
1	B	35	SER
1	B	68	GLU
1	B	83	SER
1	B	129	ILE
1	B	132	ARG
1	B	204	VAL
1	B	239	THR
1	B	377	LYS
1	B	388	CYS
1	B	483	LYS
1	B	485	LEU
1	B	597	GLU
1	B	627	THR
1	B	685	GLN
1	B	794	LYS

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

Mol	Chain	Res	Type
1	A	24	ASN
1	A	72	GLN
1	A	112	GLN
1	A	279	GLN
1	A	304	GLN
1	A	314	ASN
1	A	746	ASN
1	A	749	GLN
1	A	771	ASN
1	B	75	GLN
1	B	279	GLN
1	B	358	ASN
1	B	448	HIS
1	B	749	GLN
1	B	771	ASN

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 oligosaccharides 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 [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, 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	746/802 (93%)	-0.11	9 (1%) 76 75	42, 69, 100, 154	0
1	B	746/802 (93%)	0.09	14 (1%) 66 63	49, 79, 112, 158	0
All	All	1492/1604 (93%)	-0.01	23 (1%) 72 70	42, 73, 109, 158	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	ALA	4.2
1	B	486	GLU	4.1
1	B	801	ILE	4.1
1	B	785	ILE	3.6
1	A	91	LYS	3.4
1	B	543	ARG	3.3
1	A	22	HIS	3.1
1	B	623	ALA	3.0
1	B	22	HIS	2.9
1	B	610	LYS	2.9
1	B	411	GLN	2.6
1	B	345	LYS	2.6
1	A	610	LYS	2.5
1	B	794	LYS	2.4
1	B	23	ALA	2.4
1	A	178	GLU	2.3
1	A	758	LYS	2.3
1	B	257	LEU	2.3
1	B	174	PHE	2.3
1	A	253	GLY	2.2
1	A	277	VAL	2.1
1	B	348	ALA	2.0
1	A	624	TRP	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.