

Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2024 – 06:08 PM JST

PDB ID	:	8IDZ
Title	:	Beta-glucosidase BglPcC1
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Deposited on	:	2023-02-14
Resolution	:	4.00 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 4.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	$1087 \ (4.30-3.70)$
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	$1028 \ (4.34-3.66)$

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 <=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	А	761	% 7 5%	17%	• 7%
1	В	761	% 67%	24%	• 7%



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2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10937 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 Beta-glucosidase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	710	Total 5473	C 3470	N 932	O 1042	S 29	0	0	0
1	В	709	Total 5464	C 3465	N 930	O 1040	S 29	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP A0A413BNF4
В	1	MET	-	initiating methionine	UNP A0A413BNF4



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: Beta-glucosidase



MT17 T612 D518 K345 Y724 W615 L521 L362 Y724 P620 L521 L362 W530 W530 L525 L362 Y724 P636 L521 L362 Y741 W631 L525 L362 Y741 W630 L526 L362 Y741 D640 L549 L386 Y741 D640 M550 L448 V741 D640 M550 L448 V741 D640 M550 L448 V741 D643 M550 L448 V741 M550 L448 L446 V741 W550 L446 L446 V741 W550 L736 L466 V743 W550 L446 L446 V744 W550 L746 L446 V663 W550 L546 L446 V663 W550 L446 L446



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	182.61Å 133.84Å 69.84Å	Depositor
a, b, c, α , β , γ	90.00° 102.62° 90.00°	Depositor
Bosolution(A)	37.45 - 4.00	Depositor
Resolution (A)	43.28 - 4.00	EDS
% Data completeness	72.7 (37.45-4.00)	Depositor
(in resolution range)	72.7 (43.28 - 4.00)	EDS
R_{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.21 (at 4.00 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.250 , 0.302	Depositor
II, II, <i>free</i>	0.251 , 0.299	DCC
R_{free} test set	491 reflections $(4.83%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	105.6	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.30 , 53.6	EDS
L-test for $twinning^2$	$ < L >=0.45, < L^2>=0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10937	wwPDB-VP
Average B, all atoms $(Å^2)$	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 14.93% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.26	0/5575	0.48	0/7551	
1	В	0.27	0/5566	0.48	0/7539	
All	All	0.27	0/11141	0.48	0/15090	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	А	5473	0	5506	89	0
1	В	5464	0	5498	131	0
All	All	10937	0	11004	220	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 (220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-1 Atom-2		Clash overlap (Å)
1:A:132:ALA:HB2	1:A:176:LYS:HB2	1.60	0.83
1:B:120:VAL:HG13	1:B:125:VAL:HB	1.61	0.82



Interstomic Clash							
Atom-1	Atom-2	distance (Å)	overlap (Å)				
1:B:635:PRO:HG3	1:B:738:LEU:HB3	1.61	0.81				
1:B:468:ARG:NH2	1:B:505:CYS:SG	2.55	0.79				
1:A:143:ARG:NH1	1:A:464:GLU:OE2	2.17	0.78				
1:B:132:ALA:HB2	1:B:176:LYS:HB3	1.69	0.74				
1:B:505:CYS:HB3	1:B:525:LEU:HD11	1.68	0.73				
1:B:286:LYS:O	1:B:290:ASN:ND2	2.22	0.73				
1:B:225:LEU:HG	1:B:230:MET:HA	1.70	0.73				
1:B:367:SER:HB3	1:B:388:LEU:HD23	1.71	0.72				
1:B:469:LYS:HB2	1:B:472:ASP:HB3	1.72	0.71				
1:B:267:GLU:HG2	1:B:297:ILE:HD13	1.73	0.71				
1:B:647:VAL:N	1:B:700:ILE:O	2.25	0.70				
1:B:224:ASN:O	1:B:231:SER:OG	2.09	0.69				
1:A:127:VAL:HG22	1:A:172:GLY:HA3	1.75	0.69				
1:A:127:VAL:HG21	1:A:308:TYR:HE1	1.60	0.67				
1:B:654:ALA:HA	1:B:693:GLY:H	1.60	0.67				
1:A:202:ILE:HD11	1:A:603:VAL:HG23	1.77	0.67				
1:A:267:GLU:HG2	1:A:297:ILE:HD13	1.76	0.67				
1:B:127:VAL:HG22	1:B:172:GLY:HA3	1.77	0.65				
1:B:180:LEU:O	1:B:224:ASN:ND2	2.29	0.65				
1:B:186:ASN:HD22	1:B:594:VAL:HG12	1.62	0.64				
1:B:635:PRO:O	1:B:740:THR:OG1	2.12	0.64				
1:B:687:THR:HG22	1:B:698:VAL:HG11	1.80	0.64				
1:B:86:ASP:OD1	1:B:86:ASP:N	2.30	0.63				
1:B:178:PHE:HB3	1:B:221:THR:HA	1.80	0.63				
1:B:178:PHE:HA	1:B:207:PHE:CE2	2.34	0.62				
1:B:127:VAL:HG21	1:B:308:TYR:HE1	1.64	0.62				
1:B:147:TYR:HH	1:B:181:ASN:HD22	1.47	0.62				
1:B:366:THR:HG21	1:B:459:GLY:HA3	1.81	0.61				
1:B:507:VAL:HG12	1:B:552:TRP:CE2	2.36	0.60				
1:A:690:LEU:HD22	1:A:694:GLU:HB3	1.83	0.60				
1:A:651:VAL:HG11	1:A:661:GLU:HG2	1.84	0.60				
1:A:628:THR:OG1	1:A:653:ASN:OD1	2.21	0.59				
1:B:362:LEU:HD21	1:B:388:LEU:HG	1.84	0.59				
1:A:502:LEU:HD21	1:A:513:TRP:HH2	1.67	0.58				
1:A:286:LYS:O	1:A:290:ASN:ND2	2.36	0.58				
1:B:69:VAL:HG12	1:B:127:VAL:HB	1.85	0.58				
1:A:69:VAL:HG12	1:A:127:VAL:HB	1.85	0.57				
1:B:140:LEU:HD11	1:B:470:ILE:HG12	1.85	0.57				
1:B:631:LYS:O	1:B:652:LYS:N	2.35	0.57				
1:B:651:VAL:HG21	1:B:687:THR:HG21	1.85	0.57				
1:A:665:VAL:HG22	1:A:728:VAL:HG22	1.87	0.56				



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:345:LYS:HE2	1:B:347:ASN:HB2	1.86	0.56
1:B:180:LEU:HD22	1:B:192:VAL:HG11	1.88	0.56
1:A:667:VAL:HG22	1:A:726:VAL:HG13	1.88	0.56
1:A:499:VAL:HG22	1:A:519:ALA:HB3	1.86	0.56
1:A:691:GLN:HG3	1:A:692:PRO:HD2	1.87	0.56
1:A:78:ILE:O	1:A:381:ASN:ND2	2.39	0.55
1:A:727:MET:HG2	1:A:737:PRO:HG2	1.87	0.55
1:B:224:ASN:OD1	1:B:224:ASN:N	2.36	0.55
1:B:80:PRO:HA	1:B:89:PHE:O	2.06	0.55
1:B:646:LYS:HE3	1:B:699:THR:HG21	1.88	0.55
1:B:133:THR:HG22	1:B:175:LEU:HD11	1.88	0.55
1:B:557:ASN:OD1	1:B:562:LYS:NZ	2.34	0.55
1:A:81:LYS:HB2	1:A:88:THR:HA	1.89	0.55
1:A:368:TYR:HD2	1:A:389:LEU:HD22	1.72	0.55
1:B:175:LEU:O	1:B:220:MET:HB3	2.07	0.54
1:A:256:TRP:HB3	1:A:275:PRO:HD3	1.89	0.54
1:A:145:PHE:CE2	1:A:146:GLU:HG3	2.42	0.54
1:B:341:MET:SD	1:B:537:ILE:HG13	2.48	0.54
1:A:547:ARG:HD3	1:A:624:GLY:HA3	1.88	0.54
1:B:468:ARG:HH22	1:B:505:CYS:C	2.11	0.54
1:A:92:THR:OG1	1:A:119:GLU:OE2	2.23	0.54
1:A:185:THR:OG1	1:A:566:PRO:HG3	2.08	0.54
1:B:127:VAL:HG21	1:B:308:TYR:CE1	2.43	0.54
1:B:70:ALA:O	1:B:129:LEU:HG	2.08	0.53
1:B:220:MET:HA	1:B:253:MET:O	2.08	0.53
1:A:175:LEU:HD21	1:A:219:VAL:HG22	1.90	0.53
1:A:507:VAL:HG11	1:A:553:PRO:HD2	1.90	0.53
1:B:187:ARG:HD2	1:B:465:PHE:CE1	2.44	0.53
1:B:49:VAL:HG22	1:B:82:ARG:HH22	1.72	0.53
1:A:551:THR:HG23	1:A:620:PRO:HA	1.90	0.53
1:A:257:PHE:HD1	1:A:277:LYS:HD3	1.73	0.52
1:A:497:LYS:HD2	1:A:518:ASP:OD2	2.10	0.52
1:B:187:ARG:HA	1:B:190:ASN:HB2	1.92	0.52
1:B:461:SER:HA	1:B:505:CYS:SG	2.51	0.51
1:A:729:ALA:HB2	1:A:737:PRO:HB3	1.92	0.51
1:A:57:ASN:N	1:A:57:ASN:OD1	2.43	0.51
1:A:609:TYR:CE1	1:A:613:LYS:HG3	2.46	0.51
1:A:504:VAL:HG11	1:A:508:ILE:HD13	1.92	0.51
1:A:710:PHE:HA	1:A:717:TRP:HA	1.93	0.51
1:B:207:PHE:O	1:B:211:ILE:HG12	2.10	0.51
1:A:644:ASN:OD1	1:A:644:ASN:N	2.34	0.50



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Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:184:GLU:HB2	1:B:467:ASP:OD1	2.11	0.50	
1:B:551:THR:HG23	1:B:620:PRO:HA	1.93	0.50	
1:B:12:GLN:NE2	1:B:16:ASN:OD1	2.44	0.50	
1:B:710:PHE:HD1	1:B:717:TRP:CD1	2.28	0.50	
1:B:78:ILE:O	1:B:381:ASN:ND2	2.44	0.50	
1:A:77:ARG:NH1	1:A:377:SER:HA	2.27	0.50	
1:B:258:GLY:O	1:B:265:GLN:NE2	2.42	0.50	
1:B:347:ASN:HB3	1:B:518:ASP:OD1	2.11	0.50	
1:B:467:ASP:HB3	1:B:568:PRO:HG3	1.92	0.50	
1:B:6:LEU:HB2	1:B:64:ILE:HG12	1.93	0.50	
1:B:57:ASN:OD1	1:B:57:ASN:N	2.41	0.50	
1:A:163:VAL:HG13	1:A:173:THR:OG1	2.12	0.50	
1:B:664:GLN:NE2	1:B:730:LYS:O	2.44	0.50	
1:B:76:LEU:HD22	1:B:120:VAL:HA	1.94	0.49	
1:B:256:TRP:HB3	1:B:275:PRO:HD3	1.95	0.49	
1:A:342:VAL:HG13	1:A:522:LEU:HB3	1.94	0.49	
1:A:637:VAL:HG21	1:A:645:ILE:HG23	1.95	0.49	
1:B:103:THR:HG22	1:B:340:GLY:HA2	1.95	0.49	
1:B:342:VAL:HG13	1:B:522:LEU:HD23	1.95	0.49	
1:B:69:VAL:HA	1:B:127:VAL:O	2.12	0.48	
1:B:665:VAL:HG11	1:B:702:ILE:HD11	1.95	0.48	
1:A:175:LEU:HD13	1:A:175:LEU:H	1.78	0.48	
1:B:682:ARG:NH1	1:B:706:ASN:O	2.46	0.48	
1:A:637:VAL:HB	1:A:647:VAL:HA	1.96	0.48	
1:A:670:PRO:HD2	1:A:724:TYR:CZ	2.48	0.48	
1:B:65:PRO:HG3	1:B:315:PHE:HA	1.96	0.48	
1:A:123:TYR:OH	1:A:324:PRO:HG3	2.14	0.48	
1:A:325:ASP:O	1:A:327:LYS:N	2.47	0.48	
1:B:50:GLN:HB2	1:B:82:ARG:NE	2.29	0.48	
1:B:179:ALA:O	1:B:222:SER:OG	2.31	0.48	
1:B:637:VAL:HG23	1:B:647:VAL:HA	1.95	0.48	
1:A:451:ASN:O	1:A:496:LYS:NZ	2.40	0.48	
1:A:226:ILE:O	1:A:234:ARG:NH1	2.47	0.47	
1:B:507:VAL:HG11	1:B:550:MET:HG3	1.95	0.47	
1:A:366:THR:HG21	1:A:459:GLY:HA3	1.96	0.47	
1:B:180:LEU:HD11	1:B:199:PHE:CE1	2.49	0.47	
1:B:639:LYS:HB3	1:B:639:LYS:HE3	1.50	0.47	
1:B:468:ARG:HB3	1:B:473:SER:HB2	1.97	0.47	
1:B:604:TYR:O	1:B:609:TYR:HB2	2.15	0.47	
1:A:230:MET:O	1:A:234:ARG:HB2	2.15	0.47	
1:B:548:LEU:HD13	1:B:552:TRP:CD1	2.50	0.47	



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Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:229:THR:HB	1:B:234:ARG:HH11	1.81	0.46	
1:B:238:ILE:O	1:B:242:LEU:HB3	2.15	0.46	
1:B:50:GLN:HB2	1:B:82:ARG:HE	1.81	0.46	
1:B:128:LEU:O	1:B:173:THR:HA	2.14	0.46	
1:B:609:TYR:CE2	1:B:615:VAL:HG21	2.51	0.46	
1:B:29:GLY:O	1:B:276:GLY:HA3	2.16	0.46	
1:B:341:MET:SD	1:B:521:LEU:HD21	2.56	0.46	
1:A:76:LEU:HD11	1:A:125:VAL:HG21	1.98	0.46	
1:B:66:ALA:O	1:B:314:ARG:HG2	2.15	0.46	
1:B:499:VAL:HG22	1:B:519:ALA:HB3	1.96	0.46	
1:B:507:VAL:HG13	1:B:550:MET:SD	2.56	0.46	
1:A:604:TYR:HA	1:A:608:ARG:HB2	1.97	0.46	
1:B:201:GLU:OE2	1:B:710:PHE:N	2.49	0.46	
1:B:666:TYR:CD2	1:B:679:LYS:HD3	2.51	0.45	
1:B:121:LYS:HD2	1:B:169:ASN:HB3	1.97	0.45	
1:A:143:ARG:HD2	1:A:464:GLU:HG3	1.98	0.45	
1:B:674:MET:HB2	1:B:676:LYS:HE3	1.98	0.45	
1:B:120:VAL:HG12	1:B:171:VAL:HG11	1.97	0.45	
1:B:703:PRO:HD2	1:B:706:ASN:ND2	2.31	0.45	
1:A:637:VAL:HG21	1:A:645:ILE:CG2	2.46	0.45	
1:B:460:LYS:NZ	1:B:472:ASP:O	2.31	0.45	
1:A:11:ILE:HD11	1:A:303:ARG:HG3	1.98	0.45	
1:A:448:VAL:HA	1:A:496:LYS:HZ2	1.82	0.45	
1:A:518:ASP:OD1	1:A:518:ASP:N	2.48	0.45	
1:A:665:VAL:HG11	1:A:702:ILE:HD11	1.98	0.45	
1:B:137:ARG:HH22	1:B:564:ASP:HB3	1.82	0.45	
1:B:67:THR:HG21	1:B:312:THR:HG21	1.99	0.44	
1:B:180:LEU:HD13	1:B:192:VAL:HB	1.99	0.44	
1:B:666:TYR:HD2	1:B:679:LYS:HD3	1.82	0.44	
1:A:184:GLU:HB2	1:A:467:ASP:OD1	2.17	0.44	
1:B:138:ASN:ND2	1:B:561:SER:OG	2.47	0.44	
1:A:675:ASP:OD1	1:A:675:ASP:N	2.49	0.44	
1:B:27:VAL:HG23	1:B:28:VAL:HG23	1.99	0.44	
1:B:604:TYR:HE1	1:B:677:PRO:HA	1.82	0.44	
1:B:126:ASP:O	1:B:172:GLY:N	2.50	0.44	
1:B:663:VAL:N	1:B:685:ALA:O	2.50	0.44	
1:B:133:THR:O	1:B:133:THR:OG1	2.34	0.44	
1:A:680:GLU:N	1:A:680:GLU:OE1	2.51	0.44	
1:B:200:ARG:NH2	1:B:245:GLU:OE2	2.39	0.44	
1:A:341:MET:HG2	1:A:523:SER:HA	1.99	0.44	
1:A:439:LEU:HD21	1:A:483:MET:HG3	2.00	0.43	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:474:PHE:CE2	1:A:556:TYR:HB2	2.52	0.43
1:A:717:TRP:CD1	1:A:750:GLU:HB3	2.53	0.43
1:B:166:ILE:HD13	1:B:173:THR:HG21	1.99	0.43
1:B:723:ASN:OD1	1:B:723:ASN:N	2.51	0.43
1:A:286:LYS:HG2	1:A:290:ASN:HD22	1.83	0.43
1:A:324:PRO:HG2	1:A:326:LEU:HG	1.99	0.43
1:B:185:THR:OG1	1:B:566:PRO:HG3	2.18	0.43
1:B:211:ILE:HG13	1:B:246:TRP:HE3	1.83	0.43
1:B:190:ASN:HD22	1:B:224:ASN:HB3	1.83	0.43
1:B:612:THR:HA	1:B:678:ALA:HB2	2.01	0.43
1:A:339:GLU:HG2	1:A:686:LYS:HZ3	1.83	0.43
1:B:145:PHE:CE2	1:B:146:GLU:HG3	2.53	0.43
1:A:178:PHE:HE1	1:A:242:LEU:HD13	1.84	0.43
1:B:80:PRO:HD3	1:B:381:ASN:ND2	2.34	0.43
1:B:477:THR:N	1:B:480:GLU:OE1	2.48	0.43
1:B:640:ASP:OD1	1:B:641:ALA:N	2.51	0.43
1:A:150:GLU:OE2	1:A:607:TYR:HB3	2.19	0.43
1:B:724:TYR:N	1:B:742:ILE:O	2.51	0.42
1:A:467:ASP:OD1	1:A:467:ASP:N	2.52	0.42
1:A:544:PRO:HD2	1:A:627:TYR:CE2	2.54	0.42
1:A:238:ILE:O	1:A:242:LEU:HB3	2.19	0.42
1:B:266:MET:HA	1:B:301:ASN:HD21	1.83	0.42
1:A:69:VAL:HA	1:A:127:VAL:O	2.20	0.42
1:A:324:PRO:O	1:A:325:ASP:HB2	2.20	0.42
1:A:329:HIS:ND1	1:A:329:HIS:N	2.68	0.42
1:B:595:ASP:OD1	1:B:595:ASP:N	2.52	0.42
1:A:81:LYS:HB3	1:A:88:THR:HG22	2.02	0.42
1:B:76:LEU:HD13	1:B:120:VAL:HG22	2.02	0.42
1:B:612:THR:CA	1:B:678:ALA:HB2	2.50	0.41
1:A:178:PHE:CE1	1:A:242:LEU:HD13	2.55	0.41
1:A:468:ARG:HB3	1:A:473:SER:CB	2.50	0.41
1:B:180:LEU:HD12	1:B:226:ILE:HG12	2.01	0.41
1:A:121:LYS:HE2	1:A:318:TYR:CD2	2.56	0.41
1:A:185:THR:HG23	1:A:467:ASP:OD2	2.20	0.41
1:B:104:TRP:NE1	1:B:547:ARG:HB2	2.36	0.41
1:B:668:ALA:HA	1:B:679:LYS:HA	2.03	0.41
1:A:277:LYS:HB2	1:A:277:LYS:HE3	1.85	0.41
1:B:468:ARG:HB3	1:B:473:SER:CB	2.51	0.41
1:B:666:TYR:CE2	1:B:732:ALA:HA	2.55	0.41
1:B:254:THR:HG22	1:B:270:ASN:ND2	2.35	0.41
1:A:178:PHE:HB3	1:A:221:THR:HA	2.02	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:192:VAL:HG13	1:A:599:TYR:CE1	2.56	0.41
1:A:688:LYS:HE2	1:A:690:LEU:HD23	2.03	0.41
1:B:187:ARG:H	1:B:187:ARG:NE	2.19	0.41
1:B:510:THR:HG22	1:B:513:TRP:CZ2	2.55	0.41
1:B:187:ARG:H	1:B:187:ARG:CD	2.34	0.41
1:B:468:ARG:O	1:B:568:PRO:HG2	2.21	0.41
1:B:548:LEU:HD22	1:B:552:TRP:HE1	1.86	0.41
1:A:235:CYS:SG	1:A:236:ASP:N	2.94	0.40
1:A:146:GLU:OE1	1:A:176:LYS:NZ	2.39	0.40
1:A:152:PRO:HA	1:A:206:PRO:HG3	2.04	0.40
1:A:690:LEU:HD23	1:A:690:LEU:HA	1.95	0.40
1:B:203:TYR:CE2	1:B:599:TYR:HE2	2.40	0.40
1:A:81:LYS:HD3	1:A:88:THR:HG22	2.03	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	Perce	ntiles
1	А	700/761~(92%)	655~(94%)	41 (6%)	4 (1%)	25	63
1	В	699/761~(92%)	658 (94%)	38~(5%)	3~(0%)	34	71
All	All	1399/1522~(92%)	1313 (94%)	79(6%)	7 (0%)	29	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	326	LEU
1	А	605	VAL
1	В	131	PRO
1	В	635	PRO
1	В	324	PRO



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
1	А	324	PRO
1	А	131	PRO

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	А	598/637~(94%)	578~(97%)	20 (3%)	38 62
1	В	597/637~(94%)	574 (96%)	23~(4%)	32 58
All	All	1195/1274~(94%)	1152 (96%)	43 (4%)	35 61

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	57	ASN
1	А	85	THR
1	А	86	ASP
1	А	93	HIS
1	А	175	LEU
1	А	235	CYS
1	А	325	ASP
1	А	329	HIS
1	А	344	LEU
1	А	417	ASN
1	А	433	PHE
1	А	518	ASP
1	А	603	VAL
1	А	605	VAL
1	А	634	LYS
1	А	637	VAL
1	А	644	ASN
1	А	691	GLN
1	A	718	GLN
1	A	749	THR
1	В	57	ASN



Mol	Chain	Res	Type
1	В	61	ARG
1	В	67	THR
1	В	71	ASP
1	В	86	ASP
1	В	125	VAL
1	В	171	VAL
1	В	173	THR
1	В	174	SER
1	В	175	LEU
1	В	187	ARG
1	В	224	ASN
1	В	321	ASP
1	В	342	VAL
1	В	343	LEU
1	В	367	SER
1	В	433	PHE
1	В	556	TYR
1	В	639	LYS
1	В	648	LEU
1	В	701	ASP
1	В	723	ASN
1	В	744	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	А	181	ASN
1	А	381	ASN
1	В	190	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 monosaccharides 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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	710/761~(93%)	0.01	11 (1%) 73 64	54, 112, 178, 291	0
1	В	709/761~(93%)	0.09	6 (0%) 86 79	63, 124, 185, 281	0
All	All	1419/1522~(93%)	0.05	17 (1%) 79 70	54, 118, 180, 291	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	443	ASN	5.1
1	А	443	ASN	4.6
1	В	31	SER	3.4
1	А	635	PRO	3.4
1	А	415	LYS	3.3
1	А	90	TYR	3.1
1	В	322	ASN	2.8
1	А	633	GLY	2.7
1	А	442	LEU	2.6
1	А	317	GLN	2.4
1	А	593	ASN	2.3
1	А	88	THR	2.3
1	А	433	PHE	2.2
1	В	643	GLY	2.2
1	В	321	ASP	2.1
1	В	640	ASP	2.1
1	А	598	GLU	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

