Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:01 am BST

PDB ID	:	1UT9
Title	:	Structural Basis for the Exocellulase Activity of the Cellobiohydrolase CbhA from C. thermocellum
Authors	:	Schubot, F.D.; Kataeva, I.A.; Chang, J.; Shah, A.K.; Ljungdahl, L.G.; Rose, J.P.; Wang, B.C.
Deposited on	:	2003-12-04
Resolution	:	2.10 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:

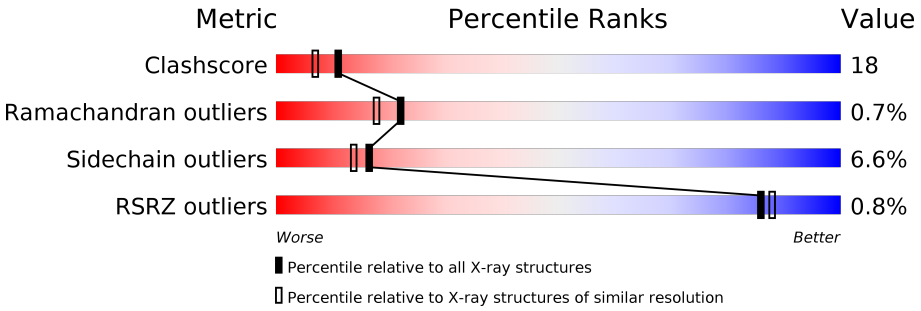
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	609	% 76% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5669 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 CELLULOSE 1,4-BETA-CELLOBIOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	605	4809	3070	803	916	20	37	0	0

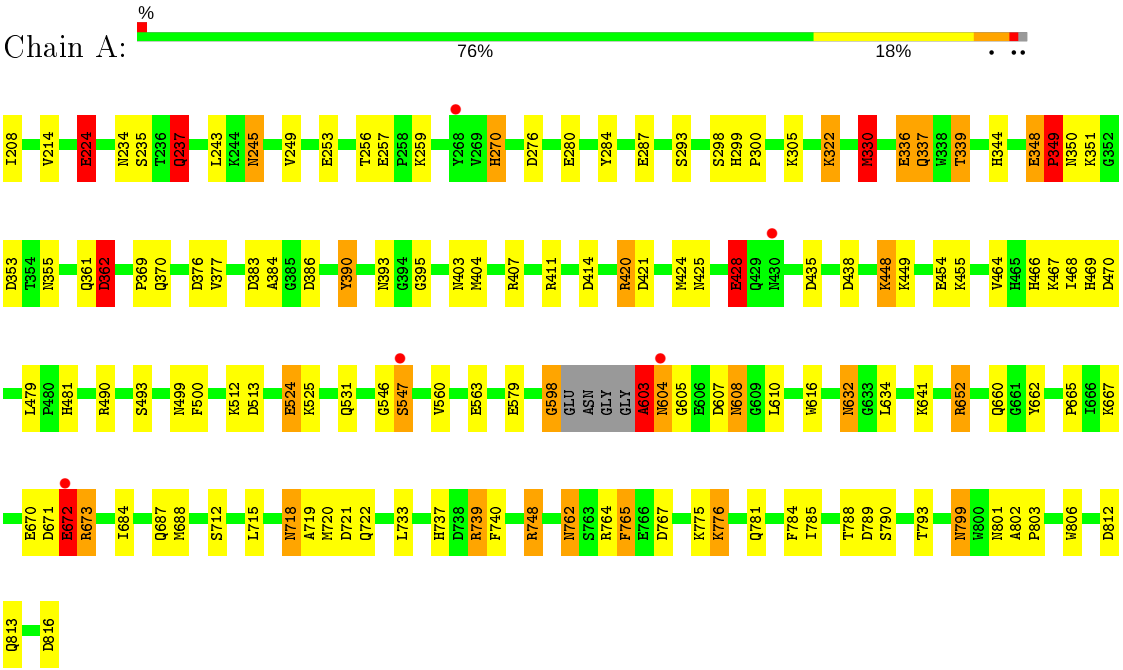
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	860	860	860	27	0

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: CELLULOSE 1,4-BETA-CELLOBIOSIDASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.55Å 75.76Å 137.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.01 – 2.10 24.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (69.01-2.10) 93.9 (24.84-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.147 , 0.186 0.154 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 80.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5669	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.48	21/4964 (0.4%)	1.54	49/6773 (0.7%)

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	6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	603	ALA	CA-CB	51.06	2.59	1.52
1	A	765	PHE	CE2-CZ	34.91	2.03	1.37
1	A	603	ALA	N-CA	32.15	2.10	1.46
1	A	776	LYS	CD-CE	30.93	2.28	1.51
1	A	598	GLY	CA-C	27.30	1.95	1.51
1	A	336	GLU	CD-OE2	26.93	1.55	1.25
1	A	765	PHE	CD2-CE2	-26.58	0.86	1.39
1	A	672	GLU	CB-CG	21.88	1.93	1.52
1	A	775	LYS	CD-CE	20.47	2.02	1.51
1	A	224	GLU	CD-OE2	13.76	1.40	1.25
1	A	428	GLU	CD-OE1	-12.73	1.11	1.25
1	A	652	ARG	CD-NE	-12.25	1.25	1.46
1	A	237	GLN	CG-CD	11.09	1.76	1.51
1	A	330	MET	SD-CE	-10.31	1.20	1.77
1	A	362	ASP	CG-OD1	9.60	1.47	1.25
1	A	336	GLU	CG-CD	-9.36	1.38	1.51
1	A	524	GLU	CD-OE1	-9.07	1.15	1.25
1	A	652	ARG	CZ-NH2	-7.22	1.23	1.33
1	A	424	MET	SD-CE	-6.36	1.42	1.77
1	A	672	GLU	CG-CD	5.24	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	LYS	CD-CE	5.09	1.64	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	652	ARG	NE-CZ-NH2	59.45	150.02	120.30
1	A	603	ALA	N-CA-CB	-34.89	61.25	110.10
1	A	420	ARG	NE-CZ-NH2	34.41	137.50	120.30
1	A	652	ARG	NH1-CZ-NH2	-32.26	83.92	119.40
1	A	224	GLU	OE1-CD-OE2	-30.59	86.59	123.30
1	A	348	GLU	C-N-CD	-26.37	62.59	120.60
1	A	362	ASP	CB-CG-OD1	-23.46	97.19	118.30
1	A	765	PHE	CG-CD2-CE2	22.78	145.85	120.80
1	A	603	ALA	CB-CA-C	-18.02	83.08	110.10
1	A	672	GLU	CG-CD-OE2	-17.41	83.48	118.30
1	A	420	ARG	NH1-CZ-NH2	-16.32	101.45	119.40
1	A	237	GLN	CG-CD-OE1	-13.79	94.02	121.60
1	A	652	ARG	CD-NE-CZ	12.39	140.95	123.60
1	A	765	PHE	CZ-CE2-CD2	-12.25	105.41	120.10
1	A	776	LYS	CG-CD-CE	-11.76	76.62	111.90
1	A	672	GLU	OE1-CD-OE2	10.57	135.99	123.30
1	A	362	ASP	OD1-CG-OD2	-10.29	103.74	123.30
1	A	349	PRO	CA-N-CD	-9.64	98.00	111.50
1	A	775	LYS	CG-CD-CE	-9.39	83.72	111.90
1	A	237	GLN	CG-CD-NE2	8.82	137.86	116.70
1	A	348	GLU	C-N-CA	8.53	157.84	122.00
1	A	524	GLU	OE1-CD-OE2	-8.32	113.31	123.30
1	A	336	GLU	CB-CG-CD	7.97	135.71	114.20
1	A	455	LYS	CG-CD-CE	7.92	135.66	111.90
1	A	330	MET	CG-SD-CE	7.52	112.23	100.20
1	A	598	GLY	CA-C-O	-7.46	107.17	120.60
1	A	652	ARG	CG-CD-NE	7.40	127.34	111.80
1	A	598	GLY	C-N-CA	6.94	139.05	121.70
1	A	598	GLY	N-CA-C	-6.62	96.55	113.10
1	A	428	GLU	CG-CD-OE1	-6.30	105.69	118.30
1	A	414	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	424	MET	CG-SD-CE	6.14	110.03	100.20
1	A	672	GLU	CG-CD-OE1	6.12	130.55	118.30
1	A	455	LYS	CD-CE-NZ	6.01	125.53	111.70
1	A	349	PRO	N-CD-CG	6.01	112.21	103.20
1	A	765	PHE	CE1-CZ-CE2	-5.92	109.35	120.00
1	A	421	ASP	CB-CG-OD2	5.90	123.61	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	435	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	598	GLY	CA-C-N	5.64	129.62	117.20
1	A	276	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	767	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	513	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	428	GLU	OE1-CD-OE2	5.48	129.88	123.30
1	A	353	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	386	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	789	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	812	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	376	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	671	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	GLU	Sidechain
1	A	237	GLN	Sidechain
1	A	362	ASP	Sidechain
1	A	428	GLU	Sidechain
1	A	524	GLU	Sidechain
1	A	672	GLU	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	4809	0	4511	167	0
2	A	860	0	0	96	6
All	All	5669	0	4511	167	6

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 18.

All (167) 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:330:MET:CG	2:A:2229:HOH:O	1.66	1.33
1:A:428:GLU:HG2	2:A:2422:HOH:O	1.18	1.33
1:A:608:ASN:HB2	2:A:2670:HOH:O	1.30	1.32
1:A:355:ASN:HB3	2:A:2285:HOH:O	1.16	1.32
1:A:330:MET:CB	2:A:2229:HOH:O	1.75	1.29
1:A:748:ARG:HD3	2:A:2801:HOH:O	1.33	1.27
1:A:351:LYS:HE2	2:A:2277:HOH:O	1.12	1.24
1:A:776:LYS:CD	2:A:2824:HOH:O	1.87	1.22
1:A:598:GLY:HA3	2:A:2654:HOH:O	1.39	1.21
1:A:428:GLU:CG	2:A:2422:HOH:O	1.72	1.21
1:A:673:ARG:N	2:A:2735:HOH:O	1.59	1.19
1:A:330:MET:SD	2:A:2210:HOH:O	2.00	1.16
1:A:448:LYS:HE3	2:A:2464:HOH:O	1.16	1.15
1:A:234:ASN:HB2	2:A:2037:HOH:O	0.99	1.15
1:A:667:LYS:HD2	2:A:2727:HOH:O	1.44	1.15
1:A:208:ILE:N	2:A:2002:HOH:O	1.80	1.12
1:A:816:ASP:CA	2:A:2860:HOH:O	1.98	1.09
1:A:351:LYS:CE	2:A:2277:HOH:O	1.64	1.09
1:A:672:GLU:HA	2:A:2735:HOH:O	1.52	1.09
1:A:428:GLU:OE2	2:A:2422:HOH:O	1.71	1.06
1:A:816:ASP:C	2:A:2860:HOH:O	1.95	1.05
1:A:765:PHE:CD2	1:A:765:PHE:CZ	2.41	1.04
1:A:608:ASN:CB	2:A:2670:HOH:O	1.86	1.03
1:A:448:LYS:HB3	2:A:2464:HOH:O	0.98	1.02
1:A:608:ASN:ND2	2:A:2670:HOH:O	1.77	1.01
1:A:672:GLU:CB	2:A:2734:HOH:O	2.09	0.99
1:A:330:MET:HB2	2:A:2229:HOH:O	1.41	0.98
1:A:748:ARG:NH2	2:A:2804:HOH:O	1.96	0.97
1:A:652:ARG:HG2	2:A:2712:HOH:O	1.64	0.96
1:A:330:MET:SD	2:A:2229:HOH:O	2.02	0.95
1:A:448:LYS:CD	2:A:2464:HOH:O	1.83	0.95
1:A:546:GLY:C	2:A:2593:HOH:O	2.03	0.95
1:A:330:MET:CG	2:A:2210:HOH:O	2.12	0.93
1:A:257:GLU:HB3	2:A:2062:HOH:O	0.75	0.93
1:A:454:GLU:CG	2:A:2478:HOH:O	2.19	0.89
1:A:547:SER:N	2:A:2593:HOH:O	2.06	0.89
1:A:336:GLU:HG3	2:A:2209:HOH:O	1.73	0.88
1:A:336:GLU:CG	2:A:2238:HOH:O	2.22	0.87
1:A:337:GLN:HE21	1:A:337:GLN:H	1.18	0.87
1:A:361:GLN:O	2:A:2303:HOH:O	1.85	0.86
1:A:672:GLU:HB3	2:A:2734:HOH:O	1.73	0.85
1:A:234:ASN:CB	2:A:2037:HOH:O	1.73	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:GLU:O	1:A:673:ARG:HB2	1.80	0.81
1:A:253:GLU:OE1	2:A:2058:HOH:O	1.99	0.80
1:A:684:ILE:HG22	1:A:688:MET:HE2	1.64	0.80
1:A:395:GLY:HA3	1:A:499:ASN:HD22	1.46	0.79
1:A:339:THR:HG22	2:A:2256:HOH:O	1.83	0.78
1:A:672:GLU:O	2:A:2733:HOH:O	2.01	0.78
1:A:816:ASP:O	2:A:2858:HOH:O	2.00	0.77
1:A:336:GLU:HG2	2:A:2238:HOH:O	1.82	0.77
1:A:718:ASN:HD22	1:A:720:MET:H	1.32	0.74
1:A:448:LYS:CG	2:A:2464:HOH:O	1.94	0.73
1:A:336:GLU:HG3	2:A:2238:HOH:O	1.85	0.73
1:A:684:ILE:HG22	1:A:688:MET:CE	2.18	0.73
1:A:739:ARG:NH2	2:A:2788:HOH:O	2.22	0.73
1:A:737:HIS:HE1	2:A:2787:HOH:O	1.72	0.72
1:A:355:ASN:CB	2:A:2285:HOH:O	1.94	0.72
1:A:748:ARG:NE	2:A:2804:HOH:O	2.21	0.72
1:A:579:GLU:OE1	2:A:2635:HOH:O	2.07	0.72
1:A:235:SER:OG	2:A:2042:HOH:O	2.08	0.71
1:A:454:GLU:HG3	2:A:2478:HOH:O	1.86	0.71
1:A:748:ARG:CZ	2:A:2804:HOH:O	2.35	0.71
1:A:579:GLU:CD	2:A:2635:HOH:O	2.29	0.70
1:A:428:GLU:HG3	1:A:438:ASP:HB3	1.74	0.70
1:A:403:ASN:HD22	1:A:806:TRP:HE1	1.38	0.70
1:A:719:ALA:H	1:A:781:GLN:HE21	1.41	0.69
1:A:245:ASN:HD22	1:A:245:ASN:C	1.96	0.68
1:A:816:ASP:HA	2:A:2860:HOH:O	1.74	0.68
1:A:259:LYS:O	2:A:2067:HOH:O	1.80	0.68
1:A:237:GLN:CD	1:A:237:GLN:CB	2.62	0.68
1:A:299:HIS:HE1	1:A:721:ASP:OD1	1.77	0.67
1:A:407:ARG:HH22	1:A:813:GLN:HE22	1.43	0.67
1:A:739:ARG:NH1	2:A:2786:HOH:O	1.86	0.67
1:A:632:ASN:HD22	1:A:634:LEU:H	1.42	0.66
1:A:224:GLU:HG3	2:A:2024:HOH:O	1.95	0.66
1:A:393:ASN:HD21	1:A:799:ASN:CG	1.98	0.66
1:A:547:SER:CA	2:A:2593:HOH:O	2.43	0.66
1:A:563:GLU:OE2	2:A:2620:HOH:O	2.14	0.65
1:A:287:GLU:HG2	2:A:2116:HOH:O	1.95	0.65
1:A:404:MET:HB3	1:A:806:TRP:CD1	2.31	0.65
1:A:785:ILE:HD12	2:A:2831:HOH:O	1.97	0.65
1:A:718:ASN:HD21	1:A:722:GLN:H	1.45	0.65
1:A:256:THR:OG1	1:A:270:HIS:HD2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLN:HE22	1:A:369:PRO:HA	1.61	0.64
1:A:816:ASP:CB	2:A:2860:HOH:O	2.38	0.64
1:A:287:GLU:CG	2:A:2116:HOH:O	2.45	0.64
1:A:339:THR:CG2	2:A:2256:HOH:O	2.44	0.64
1:A:531:GLN:NE2	2:A:2570:HOH:O	2.31	0.63
1:A:785:ILE:H	1:A:793:THR:HG21	1.64	0.63
1:A:672:GLU:CA	2:A:2735:HOH:O	2.08	0.62
1:A:765:PHE:CD1	2:A:2815:HOH:O	2.51	0.62
1:A:672:GLU:O	1:A:673:ARG:CB	2.48	0.61
1:A:467:LYS:NZ	1:A:469:HIS:HE1	1.98	0.61
1:A:355:ASN:CG	2:A:2285:HOH:O	2.29	0.60
1:A:762:ASN:C	1:A:762:ASN:HD22	2.05	0.59
1:A:336:GLU:HB2	2:A:2209:HOH:O	2.02	0.59
1:A:299:HIS:HD2	2:A:2110:HOH:O	1.86	0.58
1:A:336:GLU:CB	2:A:2209:HOH:O	2.52	0.58
1:A:604:ASN:HD22	1:A:605:GLY:H	1.52	0.57
1:A:762:ASN:ND2	1:A:764:ARG:H	2.03	0.57
1:A:287:GLU:CD	2:A:2116:HOH:O	2.43	0.56
1:A:479:LEU:HD22	1:A:740:PHE:CD1	2.40	0.56
1:A:790:SER:OG	1:A:793:THR:HB	2.05	0.56
1:A:469:HIS:HD2	1:A:470:ASP:O	1.89	0.56
1:A:684:ILE:CG2	1:A:688:MET:HE2	2.35	0.56
1:A:420:ARG:HD3	2:A:2403:HOH:O	2.06	0.56
1:A:344:HIS:H	1:A:350:ASN:ND2	2.04	0.55
1:A:604:ASN:HD22	1:A:605:GLY:N	2.05	0.55
1:A:428:GLU:CD	2:A:2422:HOH:O	1.92	0.54
1:A:607:ASP:HA	1:A:610:LEU:HD22	1.88	0.54
1:A:407:ARG:HH22	1:A:813:GLN:NE2	2.04	0.54
1:A:467:LYS:HZ1	1:A:469:HIS:HE1	1.54	0.53
1:A:284:TYR:O	1:A:300:PRO:HA	2.08	0.53
1:A:762:ASN:HD21	1:A:764:ARG:HB2	1.73	0.53
1:A:448:LYS:CE	2:A:2464:HOH:O	1.70	0.52
1:A:438:ASP:OD2	2:A:2446:HOH:O	2.18	0.52
1:A:525:LYS:HE3	2:A:2565:HOH:O	2.09	0.51
1:A:337:GLN:H	1:A:337:GLN:NE2	1.99	0.51
1:A:448:LYS:CB	2:A:2464:HOH:O	1.65	0.50
1:A:403:ASN:ND2	1:A:806:TRP:HE1	2.08	0.49
1:A:563:GLU:CD	2:A:2620:HOH:O	2.49	0.49
1:A:454:GLU:HG2	2:A:2478:HOH:O	1.97	0.49
1:A:361:GLN:NE2	1:A:370:GLN:H	2.11	0.49
1:A:336:GLU:CG	2:A:2209:HOH:O	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ASN:ND2	1:A:634:LEU:H	2.10	0.49
1:A:718:ASN:ND2	1:A:720:MET:H	2.07	0.48
1:A:466:HIS:HD2	1:A:493:SER:OG	1.95	0.48
1:A:280:GLU:OE1	2:A:2101:HOH:O	2.20	0.47
1:A:411:ARG:NE	2:A:2384:HOH:O	1.76	0.47
1:A:718:ASN:HD22	1:A:720:MET:N	2.07	0.47
1:A:762:ASN:ND2	1:A:762:ASN:C	2.67	0.47
1:A:467:LYS:NZ	1:A:469:HIS:CE1	2.82	0.47
1:A:560:VAL:HA	1:A:563:GLU:OE1	2.14	0.47
1:A:322:LYS:HD2	1:A:322:LYS:HA	1.76	0.47
1:A:784:PHE:HA	1:A:793:THR:CG2	2.45	0.46
1:A:547:SER:HB3	2:A:2592:HOH:O	2.16	0.46
1:A:737:HIS:HD2	1:A:788:THR:O	1.98	0.46
1:A:467:LYS:HE3	1:A:490:ARG:HG3	1.98	0.46
1:A:784:PHE:HA	1:A:793:THR:HG21	1.98	0.45
1:A:361:GLN:NE2	1:A:369:PRO:HA	2.28	0.45
1:A:546:GLY:O	2:A:2593:HOH:O	2.21	0.45
1:A:667:LYS:CD	2:A:2727:HOH:O	2.26	0.44
1:A:330:MET:HG3	2:A:2210:HOH:O	1.98	0.44
1:A:336:GLU:O	1:A:339:THR:HB	2.18	0.44
1:A:802:ALA:N	1:A:803:PRO:HD2	2.34	0.43
1:A:799:ASN:H	1:A:799:ASN:HD22	1.65	0.43
1:A:684:ILE:HA	1:A:687:GLN:HE21	1.83	0.43
1:A:665:PRO:HG2	1:A:687:GLN:NE2	2.34	0.43
1:A:466:HIS:CD2	1:A:493:SER:OG	2.71	0.43
1:A:237:GLN:NE2	2:A:2046:HOH:O	2.51	0.43
1:A:393:ASN:HD22	1:A:616:TRP:HB3	1.84	0.43
1:A:816:ASP:C	2:A:2859:HOH:O	2.57	0.43
1:A:350:ASN:HD21	1:A:481:HIS:HA	1.84	0.42
1:A:214:VAL:HB	1:A:298:SER:HB3	2.01	0.42
1:A:383:ASP:HB2	1:A:390:TYR:CD1	2.54	0.42
1:A:208:ILE:HA	2:A:2002:HOH:O	2.16	0.42
1:A:299:HIS:CE1	1:A:721:ASP:OD1	2.66	0.42
1:A:464:VAL:HG21	1:A:500:PHE:CG	2.55	0.42
1:A:245:ASN:ND2	1:A:245:ASN:C	2.68	0.41
1:A:337:GLN:HE21	1:A:337:GLN:N	1.99	0.41
1:A:377:VAL:HA	1:A:449:LYS:HD2	2.03	0.41
1:A:670:GLU:OE2	2:A:2731:HOH:O	2.21	0.41
1:A:662:TYR:CD2	1:A:718:ASN:HA	2.55	0.41
1:A:603:ALA:C	2:A:2656:HOH:O	2.25	0.41
1:A:390:TYR:CD1	1:A:390:TYR:N	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASN:ND2	1:A:249:VAL:H	2.19	0.41
1:A:208:ILE:CA	2:A:2002:HOH:O	2.47	0.40

All (6) 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)
2:A:2105:HOH:O	2:A:2120:HOH:O[4_566]	1.86	0.34
2:A:2008:HOH:O	2:A:2120:HOH:O[4_566]	1.94	0.26
2:A:2576:HOH:O	2:A:2680:HOH:O[3_645]	1.98	0.22
2:A:2111:HOH:O	2:A:2710:HOH:O[4_566]	2.05	0.15
2:A:2003:HOH:O	2:A:2449:HOH:O[4_566]	2.11	0.09
2:A:2003:HOH:O	2:A:2448:HOH:O[4_566]	2.19	0.01

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	603/609 (99%)	584 (97%)	15 (2%)	4 (1%)	22 18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	PRO
1	A	603	ALA
1	A	673	ARG
1	A	384	ALA

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	A	498/503 (99%)	465 (93%)	33 (7%)	16 14

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	LEU
1	A	245	ASN
1	A	270	HIS
1	A	293	SER
1	A	322	LYS
1	A	330	MET
1	A	337	GLN
1	A	339	THR
1	A	348	GLU
1	A	349	PRO
1	A	362	ASP
1	A	390	TYR
1	A	425	ASN
1	A	428	GLU
1	A	448	LYS
1	A	468	ILE
1	A	512	LYS
1	A	547	SER
1	A	604	ASN
1	A	608	ASN
1	A	632	ASN
1	A	641	LYS
1	A	660	GLN
1	A	672	GLU
1	A	712	SER
1	A	715	LEU
1	A	718	ASN
1	A	733	LEU
1	A	739	ARG
1	A	748	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	762	ASN
1	A	799	ASN
1	A	801	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	270	HIS
1	A	299	HIS
1	A	310	GLN
1	A	337	GLN
1	A	350	ASN
1	A	361	GLN
1	A	393	ASN
1	A	403	ASN
1	A	425	ASN
1	A	429	GLN
1	A	451	GLN
1	A	466	HIS
1	A	469	HIS
1	A	499	ASN
1	A	604	ASN
1	A	632	ASN
1	A	660	GLN
1	A	687	GLN
1	A	718	ASN
1	A	722	GLN
1	A	737	HIS
1	A	762	ASN
1	A	781	GLN
1	A	799	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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^{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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	605/609 (99%)	-0.58	5 (0%)	86	88	12, 16, 24, 30	20 (3%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	672	GLU	2.6
1	A	268	TYR	2.4
1	A	430	ASN	2.2
1	A	547	SER	2.1
1	A	604	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.