Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:03 PM EDT

PDB ID	:	1CTN
Title	:	CRYSTAL STRUCTURE OF A BACTERIAL CHITINASE AT 2.3 ANGSTROMS RESOLUTION
Authors	:	Perrakis, A.; Tews, I.; Dauter, Z.; Wilson, K.S.; Vorgias, C.E.
Deposited on	:	1994-10-10
Resolution	:	2.30 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:

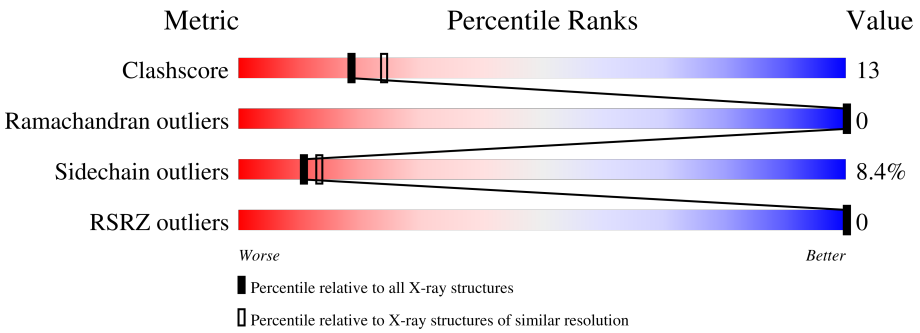
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	A	540	71% 22% 5% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4454 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 CHITINASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	538	4122	2623	694	791	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	THR	ALA	CONFLICT	UNP P07254
A	226	ILE	VAL	CONFLICT	UNP P07254
A	351	THR	ALA	CONFLICT	UNP P07254
A	395	ALA	PRO	CONFLICT	UNP P07254
A	437	ILE	VAL	CONFLICT	UNP P07254
A	473	GLU	LYS	CONFLICT	UNP P07254

- Molecule 2 is water.

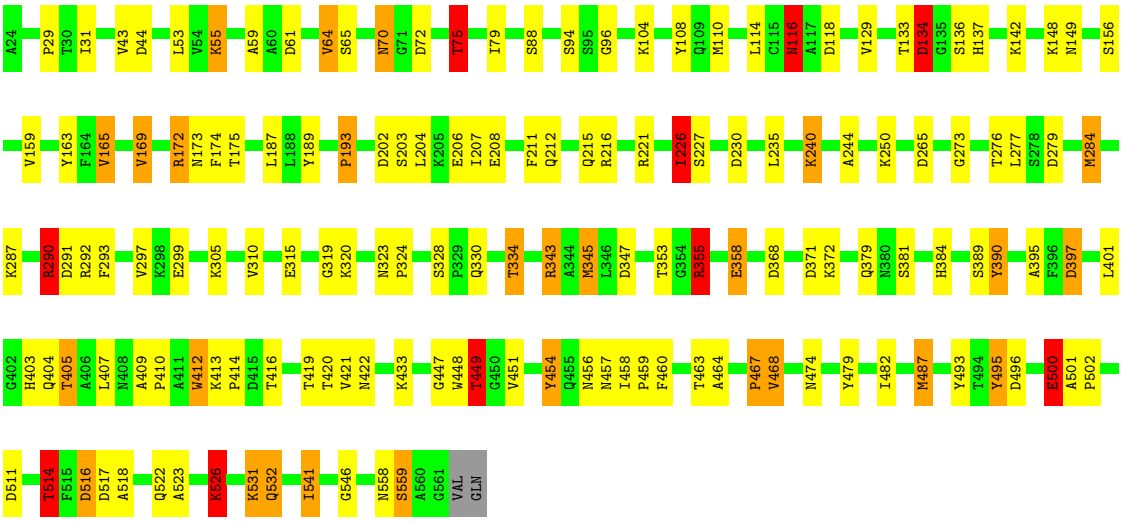
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	332	332	332	0	0

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: CHITINASE A

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	203.10Å 133.90Å 59.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 19.87 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 97.1 (19.87-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.53 (at 2.26Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.162 , (Not available) 0.151 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 71.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4454	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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 (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	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.93	3/4223 (0.1%)	1.70	72/5731 (1.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ASP	CA-CB	5.66	1.66	1.53
1	A	172	ARG	NE-CZ	-5.34	1.26	1.33
1	A	500	GLU	CB-CG	5.00	1.61	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	ARG	CD-NE-CZ	21.99	154.38	123.60
1	A	290	ARG	CD-NE-CZ	12.27	140.77	123.60
1	A	279	ASP	CB-CG-OD1	10.20	127.48	118.30
1	A	172	ARG	NE-CZ-NH1	-9.99	115.30	120.30
1	A	221	ARG	CD-NE-CZ	9.57	137.00	123.60
1	A	449	THR	N-CA-CB	9.45	128.26	110.30
1	A	72	ASP	CB-CG-OD1	9.37	126.73	118.30
1	A	202	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	A	221	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	226	ILE	CA-CB-CG2	8.16	127.21	110.90
1	A	216	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	208	GLU	OE1-CD-OE2	7.91	132.79	123.30
1	A	133	THR	C-N-CA	7.90	141.46	121.70
1	A	330	GLN	CA-CB-CG	7.88	130.73	113.40
1	A	291	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	240	LYS	CA-CB-CG	7.61	130.15	113.40
1	A	517	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	A	134	ASP	N-CA-CB	-7.03	97.94	110.60
1	A	454	TYR	CB-CG-CD1	-7.01	116.80	121.00
1	A	343	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	514	THR	N-CA-CB	6.95	123.50	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	165	VAL	N-CA-CB	-6.92	96.28	111.50
1	A	75	THR	N-CA-CB	-6.87	97.25	110.30
1	A	134	ASP	CB-CA-C	-6.80	96.80	110.40
1	A	345	MET	CA-CB-CG	6.75	124.77	113.30
1	A	165	VAL	CG1-CB-CG2	6.70	121.61	110.90
1	A	358	GLU	CA-CB-CG	6.46	127.60	113.40
1	A	500	GLU	OE1-CD-OE2	6.43	131.01	123.30
1	A	134	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	516	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	347	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	345	MET	CG-SD-CE	-6.29	90.14	100.20
1	A	284	MET	CA-CB-CG	-6.26	102.66	113.30
1	A	61	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	A	165	VAL	CB-CA-C	6.01	122.82	111.40
1	A	159	VAL	CA-CB-CG1	6.00	119.91	110.90
1	A	559	SER	N-CA-CB	5.95	119.42	110.50
1	A	240	LYS	N-CA-CB	5.77	120.98	110.60
1	A	108	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	514	THR	CB-CA-C	-5.72	96.16	111.60
1	A	116	ASN	N-CA-CB	5.71	120.87	110.60
1	A	70	ASN	N-CA-CB	-5.70	100.34	110.60
1	A	292	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	559	SER	O-C-N	5.57	131.61	122.70
1	A	343	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	401	LEU	CB-CA-C	5.51	120.67	110.20
1	A	517	ASP	CB-CA-C	5.46	121.32	110.40
1	A	355	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	517	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	163	TYR	CB-CA-C	-5.43	99.53	110.40
1	A	290	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	495	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	315	GLU	C-N-CA	5.40	135.21	121.70
1	A	299	GLU	CA-CB-CG	5.37	125.20	113.40
1	A	358	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	A	163	TYR	O-C-N	5.33	131.23	122.70
1	A	358	GLU	CG-CD-OE2	5.29	128.89	118.30
1	A	299	GLU	CG-CD-OE1	5.27	128.83	118.30
1	A	134	ASP	OD1-CG-OD2	-5.25	113.32	123.30
1	A	397	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	59	ALA	N-CA-CB	-5.18	102.85	110.10
1	A	526	LYS	CA-CB-CG	5.16	124.75	113.40
1	A	291	ASP	CB-CG-OD1	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	541	ILE	CB-CA-C	-5.12	101.36	111.60
1	A	390	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	187	LEU	CB-CA-C	5.10	119.89	110.20
1	A	64	VAL	CB-CA-C	-5.09	101.72	111.40
1	A	202	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	189	TYR	CB-CG-CD2	5.02	124.01	121.00
1	A	449	THR	CB-CA-C	-5.01	98.06	111.60
1	A	75	THR	CA-CB-CG2	5.00	119.41	112.40

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	A	4122	0	3995	107	0
2	A	332	0	0	31	0
All	All	4454	0	3995	107	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 13.

All (107) 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:53:LEU:HD22	2:A:788:HOH:O	1.48	1.14
1:A:53:LEU:HB2	2:A:788:HOH:O	1.55	1.07
1:A:53:LEU:CB	2:A:788:HOH:O	2.00	1.06
1:A:207:ILE:HD11	1:A:276:THR:HG21	1.34	1.05
1:A:53:LEU:CG	2:A:788:HOH:O	2.06	1.01
1:A:110:MET:CG	2:A:735:HOH:O	2.09	0.99
1:A:379:GLN:HE22	1:A:433:LYS:H	1.13	0.95
1:A:265:ASP:HB2	2:A:713:HOH:O	1.70	0.92
1:A:44:ASP:HB2	1:A:55:LYS:HE2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:MET:SD	2:A:735:HOH:O	2.29	0.90
1:A:110:MET:HG2	2:A:735:HOH:O	1.68	0.89
1:A:404:GLN:H	1:A:514:THR:HG21	1.40	0.86
1:A:412:TRP:HZ3	2:A:719:HOH:O	1.59	0.83
1:A:53:LEU:HD13	2:A:788:HOH:O	1.80	0.81
1:A:514:THR:CG2	2:A:637:HOH:O	2.29	0.80
1:A:384:HIS:HD2	2:A:632:HOH:O	1.65	0.79
1:A:419:THR:HG22	1:A:422:ASN:H	1.49	0.78
1:A:514:THR:HG23	2:A:637:HOH:O	1.86	0.76
1:A:134:ASP:HB3	1:A:136:SER:H	1.53	0.73
1:A:334:THR:HG22	2:A:613:HOH:O	1.89	0.73
1:A:403:HIS:HA	1:A:514:THR:HG21	1.71	0.72
1:A:358:GLU:OE2	1:A:384:HIS:HE1	1.73	0.71
1:A:404:GLN:N	1:A:514:THR:HG21	2.06	0.71
1:A:334:THR:HG21	2:A:621:HOH:O	1.92	0.70
1:A:449:THR:HG23	1:A:511:ASP:OD1	1.94	0.68
1:A:523:ALA:HA	1:A:526:LYS:HE2	1.77	0.67
1:A:416:THR:O	2:A:732:HOH:O	2.11	0.66
1:A:203:SER:O	1:A:206:GLU:HG2	1.95	0.66
1:A:116:ASN:HD22	1:A:116:ASN:C	2.00	0.65
1:A:454:TYR:HB2	1:A:458:ILE:O	1.97	0.65
1:A:390:TYR:HB3	1:A:405:THR:HG23	1.79	0.65
1:A:226:ILE:HD11	1:A:293:PHE:HE1	1.62	0.65
1:A:379:GLN:NE2	1:A:433:LYS:H	1.91	0.64
1:A:53:LEU:CD2	2:A:788:HOH:O	2.06	0.62
1:A:390:TYR:HA	1:A:405:THR:HG23	1.82	0.62
1:A:75:THR:CG2	2:A:755:HOH:O	2.48	0.61
1:A:487:MET:HE3	1:A:493:TYR:HD2	1.67	0.60
1:A:371:ASP:OD1	2:A:751:HOH:O	2.17	0.59
1:A:514:THR:HG22	2:A:637:HOH:O	1.96	0.59
1:A:226:ILE:CD1	1:A:293:PHE:HE1	2.15	0.58
1:A:129:VAL:HG13	1:A:137:HIS:HB2	1.86	0.57
1:A:413:LYS:N	1:A:414:PRO:HD3	2.19	0.57
1:A:226:ILE:CD1	1:A:293:PHE:CE1	2.87	0.57
1:A:403:HIS:HA	1:A:514:THR:CG2	2.34	0.57
1:A:319:GLY:O	1:A:320:LYS:HB2	2.05	0.56
1:A:389:SER:O	1:A:405:THR:HG22	2.05	0.56
1:A:172:ARG:NH2	2:A:716:HOH:O	2.32	0.56
1:A:174:PHE:CE1	1:A:541:ILE:HD13	2.42	0.55
1:A:353:THR:OG1	1:A:355:ARG:HG3	2.07	0.55
1:A:407:LEU:O	1:A:419:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:HG23	2:A:755:HOH:O	2.07	0.55
1:A:334:THR:CG2	2:A:621:HOH:O	2.53	0.54
1:A:395:ALA:HB1	1:A:467:PRO:HB3	1.88	0.54
1:A:397:ASP:HB3	2:A:666:HOH:O	2.08	0.53
1:A:156:SER:H	1:A:558:ASN:ND2	2.07	0.53
1:A:53:LEU:HD21	1:A:235:LEU:HD12	1.91	0.53
1:A:447:GLY:CA	1:A:468:VAL:HG22	2.39	0.53
1:A:284:MET:HB3	1:A:290:ARG:HG3	1.91	0.53
1:A:412:TRP:CZ3	2:A:719:HOH:O	2.44	0.53
1:A:297:VAL:CG1	1:A:310:VAL:HG11	2.39	0.53
1:A:404:GLN:HG2	1:A:514:THR:HB	1.92	0.52
1:A:53:LEU:CD1	2:A:788:HOH:O	2.30	0.50
1:A:29:PRO:HG3	1:A:114:LEU:HG	1.93	0.50
1:A:64:VAL:HG21	1:A:79:ILE:HD12	1.94	0.50
1:A:211:PHE:O	1:A:215:GLN:HG2	2.12	0.49
1:A:305:LYS:NZ	2:A:880:HOH:O	2.46	0.49
1:A:390:TYR:CB	1:A:405:THR:HG23	2.43	0.49
1:A:447:GLY:C	1:A:468:VAL:HG22	2.33	0.48
1:A:419:THR:CG2	1:A:421:VAL:HG22	2.43	0.48
1:A:456:ASN:O	1:A:457:ASN:HB2	2.13	0.48
1:A:273:GLY:O	1:A:277:LEU:HB2	2.14	0.48
1:A:244:ALA:O	1:A:250:LYS:HE3	2.14	0.47
1:A:64:VAL:CG2	1:A:79:ILE:HD12	2.44	0.47
1:A:169:VAL:HG22	1:A:175:THR:HG22	1.97	0.47
1:A:487:MET:HE3	1:A:493:TYR:CD2	2.47	0.47
1:A:404:GLN:CG	1:A:514:THR:HB	2.45	0.47
1:A:403:HIS:HE1	1:A:496:ASP:OD2	1.98	0.46
1:A:419:THR:HG21	2:A:714:HOH:O	2.16	0.46
1:A:43:VAL:HA	1:A:53:LEU:O	2.16	0.46
1:A:358:GLU:OE2	1:A:384:HIS:CE1	2.62	0.46
1:A:116:ASN:ND2	1:A:118:ASP:H	2.15	0.45
1:A:531:LYS:O	1:A:532:GLN:CB	2.64	0.45
1:A:495:TYR:OH	1:A:500:GLU:HG2	2.16	0.45
1:A:407:LEU:HA	1:A:420:THR:HB	1.99	0.44
1:A:518:ALA:O	1:A:522:GLN:HG2	2.17	0.44
1:A:65:SER:HA	1:A:96:GLY:O	2.17	0.44
1:A:343:ARG:HD2	1:A:381:SER:O	2.18	0.44
1:A:297:VAL:HG11	1:A:310:VAL:HG11	2.00	0.44
1:A:448:TRP:HB3	1:A:464:ALA:HB1	2.00	0.43
1:A:149:ASN:ND2	1:A:546:GLY:HA2	2.33	0.43
1:A:390:TYR:CA	1:A:405:THR:HG23	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:HD3	1:A:290:ARG:NH2	2.33	0.43
1:A:368:ASP:O	1:A:372:LYS:HE3	2.19	0.43
1:A:409:ALA:O	2:A:697:HOH:O	2.21	0.42
1:A:487:MET:HA	1:A:487:MET:HE2	2.01	0.42
1:A:412:TRP:CH2	1:A:460:PHE:CB	3.02	0.42
1:A:31:ILE:HD13	2:A:735:HOH:O	2.20	0.42
1:A:193:PRO:HD2	1:A:227:SER:O	2.20	0.41
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.90	0.41
1:A:323:ASN:HA	1:A:324:PRO:HD2	1.88	0.41
1:A:389:SER:O	1:A:405:THR:CG2	2.68	0.41
1:A:495:TYR:OH	1:A:500:GLU:CG	2.69	0.41
1:A:454:TYR:CG	1:A:459:PRO:HA	2.56	0.41
1:A:479:TYR:HA	1:A:482:ILE:HD12	2.03	0.41
1:A:501:ALA:HA	1:A:502:PRO:HD3	1.95	0.41
1:A:451:VAL:HA	1:A:463:THR:O	2.21	0.41
1:A:410:PRO:HD3	2:A:634:HOH:O	2.21	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	536/540 (99%)	523 (98%)	13 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	428/430 (100%)	392 (92%)	36 (8%)	11 13

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

Mol	Chain	Res	Type
1	A	55	LYS
1	A	70	ASN
1	A	75	THR
1	A	88	SER
1	A	94	SER
1	A	104	LYS
1	A	116	ASN
1	A	134	ASP
1	A	142	LYS
1	A	148	LYS
1	A	165	VAL
1	A	169	VAL
1	A	173	ASN
1	A	193	PRO
1	A	212	GLN
1	A	226	ILE
1	A	240	LYS
1	A	290	ARG
1	A	328	SER
1	A	334	THR
1	A	345	MET
1	A	355	ARG
1	A	405	THR
1	A	412	TRP
1	A	449	THR
1	A	467	PRO
1	A	468	VAL
1	A	474	ASN
1	A	487	MET
1	A	500	GLU
1	A	514	THR
1	A	516	ASP
1	A	526	LYS
1	A	531	LYS
1	A	532	GLN

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Mol	Chain	Res	Type
1	A	559	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	111	GLN
1	A	116	ASN
1	A	173	ASN
1	A	263	HIS
1	A	348	GLN
1	A	379	GLN
1	A	384	HIS
1	A	403	HIS
1	A	474	ASN
1	A	558	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, 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	538/540 (99%)	-0.94	0 100 100	7, 21, 45, 69	0

There are no RSRZ outliers to report.

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.