



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:43 AM UTC

PDB ID : 1CTN / pdb_00001ctn
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 ⓘ 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

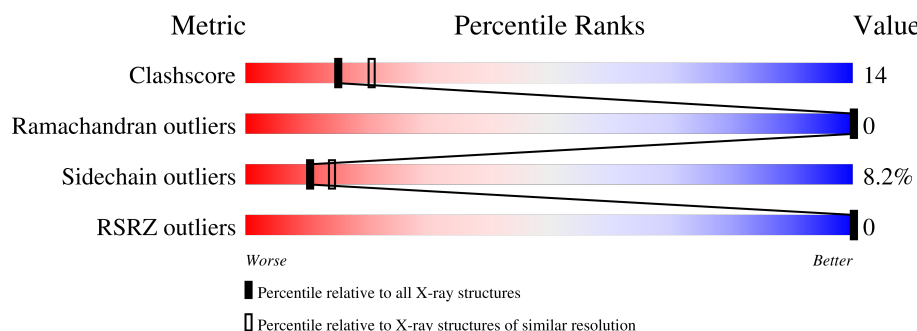
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	540	

2 Entry composition

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
1	A	538	Total	C	N	O	S	0	0	0
			4122	2623	694	791	14			

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.

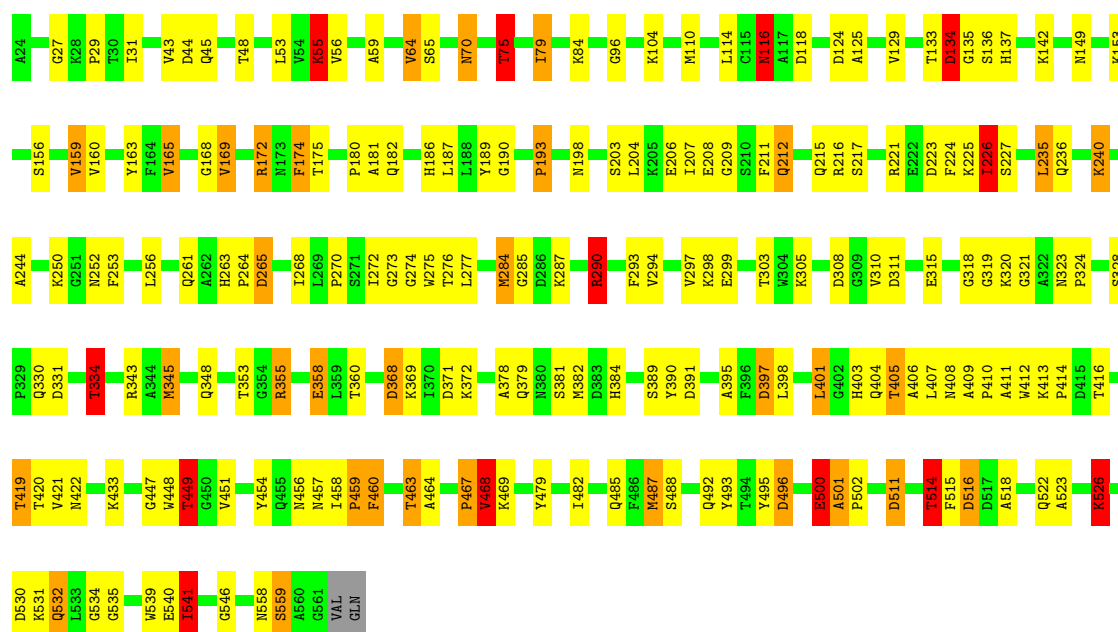
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	332	Total	O	0	0
			332	332		

3 Residue-property plots

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

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 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 96.2 (10.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.27 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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 [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	1.19	6/4223 (0.1%)	2.16	162/5731 (2.8%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	TYR	C-N	-8.90	1.29	1.33
1	A	134	ASP	CA-CB	8.25	1.66	1.53
1	A	172	ARG	NE-CZ	-6.31	1.26	1.33
1	A	274	GLY	N-CA	5.77	1.52	1.45
1	A	449	THR	CA-C	5.17	1.59	1.52
1	A	225	LYS	C-N	-5.02	1.28	1.33

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	CD-NE-CZ	21.41	154.38	124.40
1	A	133	THR	CA-C-N	14.91	141.46	120.29
1	A	133	THR	C-N-CA	14.91	141.46	120.29
1	A	449	THR	N-CA-CB	11.78	128.26	110.70
1	A	290	ARG	CD-NE-CZ	11.69	140.77	124.40
1	A	165	VAL	N-CA-CB	-11.01	96.28	111.25
1	A	226	ILE	CA-CB-CG2	9.83	127.21	110.50
1	A	75	THR	N-CA-CB	-9.16	97.25	110.81
1	A	221	ARG	CD-NE-CZ	9.00	137.00	124.40
1	A	272	ILE	CA-C-N	-8.83	113.53	122.63
1	A	272	ILE	C-N-CA	-8.83	113.53	122.63
1	A	408	ASN	CA-CB-CG	8.56	121.16	112.60
1	A	397	ASP	CA-CB-CG	-8.51	104.09	112.60
1	A	468	VAL	O-C-N	8.38	130.02	122.65
1	A	330	GLN	CA-CB-CG	8.32	130.73	114.10
1	A	134	ASP	CB-CA-C	-8.26	96.80	110.85
1	A	134	ASP	N-CA-CB	-8.26	97.94	110.16
1	A	514	THR	CB-CA-C	-8.23	96.16	109.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	VAL	CB-CA-C	8.05	122.82	110.83
1	A	240	LYS	CA-CB-CG	8.03	130.15	114.10
1	A	514	THR	N-CA-CB	8.02	123.50	110.43
1	A	45	GLN	OE1-CD-NE2	-7.71	114.89	122.60
1	A	70	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	A	124	ASP	N-CA-C	-7.55	100.57	110.53
1	A	539	TRP	CA-C-O	-7.53	112.26	120.24
1	A	315	GLU	CA-C-N	7.51	135.21	121.70
1	A	315	GLU	C-N-CA	7.51	135.21	121.70
1	A	516	ASP	CA-CB-CG	7.49	120.09	112.60
1	A	511	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	240	LYS	N-CA-CB	7.42	120.98	109.48
1	A	530	ASP	CA-CB-CG	7.37	119.97	112.60
1	A	285	GLY	N-CA-C	-7.31	103.58	113.37
1	A	559	SER	O-C-N	7.29	131.61	123.01
1	A	485	GLN	N-CA-C	7.26	123.67	114.31
1	A	348	GLN	CA-C-N	7.04	129.72	120.28
1	A	348	GLN	C-N-CA	7.04	129.72	120.28
1	A	468	VAL	CB-CA-C	-7.04	102.19	111.13
1	A	225	LYS	CA-C-N	7.03	130.13	120.35
1	A	225	LYS	C-N-CA	7.03	130.13	120.35
1	A	75	THR	CB-CA-C	6.97	121.56	109.15
1	A	541	ILE	CB-CA-C	-6.97	101.36	112.16
1	A	449	THR	CB-CA-C	-6.91	98.06	110.36
1	A	212	GLN	CB-CG-CD	6.90	124.32	112.60
1	A	406	ALA	CA-C-O	6.89	128.86	121.55
1	A	460	PHE	CA-CB-CG	6.87	120.67	113.80
1	A	163	TYR	O-C-N	6.87	131.23	123.19
1	A	70	ASN	N-CA-CB	-6.77	100.34	110.90
1	A	358	GLU	CA-CB-CG	6.75	127.60	114.10
1	A	321	GLY	CA-C-O	-6.72	114.40	121.53
1	A	70	ASN	N-CA-C	6.70	119.39	107.80
1	A	541	ILE	N-CA-CB	6.69	122.10	110.65
1	A	180	PRO	CA-C-N	6.67	130.11	120.38
1	A	180	PRO	C-N-CA	6.67	130.11	120.38
1	A	401	LEU	CB-CA-C	6.61	120.67	109.50
1	A	411	ALA	CA-C-N	6.44	133.94	121.18
1	A	411	ALA	C-N-CA	6.44	133.94	121.18
1	A	190	GLY	O-C-N	-6.39	119.33	123.35
1	A	198	ASN	CA-CB-CG	6.33	118.93	112.60
1	A	294	VAL	CA-C-N	6.24	126.86	120.00
1	A	294	VAL	C-N-CA	6.24	126.86	120.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	PHE	CA-C-N	6.22	126.84	119.94
1	A	253	PHE	C-N-CA	6.22	126.84	119.94
1	A	172	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	A	559	SER	N-CA-CB	6.20	119.42	110.06
1	A	134	ASP	CA-C-O	6.20	126.99	120.42
1	A	240	LYS	CB-CA-C	-6.16	100.61	109.84
1	A	168	GLY	CA-C-O	6.10	126.94	119.01
1	A	252	ASN	CA-C-O	-6.05	114.47	120.70
1	A	331	ASP	CA-C-N	6.02	126.67	119.98
1	A	331	ASP	C-N-CA	6.02	126.67	119.98
1	A	501	ALA	O-C-N	6.02	126.54	121.84
1	A	174	PHE	CB-CA-C	5.99	120.39	110.74
1	A	217	SER	CA-CB-OG	-5.97	99.15	111.10
1	A	135	GLY	N-CA-C	-5.97	106.48	115.32
1	A	209	GLY	CA-C-N	5.96	128.19	120.44
1	A	209	GLY	C-N-CA	5.96	128.19	120.44
1	A	182	GLN	OE1-CD-NE2	5.93	128.53	122.60
1	A	163	TYR	CB-CA-C	-5.92	99.53	109.48
1	A	303	THR	CA-CB-OG1	-5.88	100.78	109.60
1	A	492	GLN	CA-C-O	-5.87	114.88	121.81
1	A	208	GLU	CB-CA-C	-5.87	100.74	109.90
1	A	303	THR	CA-C-O	-5.87	114.28	120.55
1	A	181	ALA	N-CA-C	5.83	119.21	111.75
1	A	492	GLN	N-CA-C	-5.83	102.68	110.55
1	A	116	ASN	N-CA-CB	5.78	120.87	111.21
1	A	256	LEU	CA-C-N	5.78	128.03	120.28
1	A	256	LEU	C-N-CA	5.78	128.03	120.28
1	A	541	ILE	N-CA-C	5.78	118.28	111.05
1	A	224	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	303	THR	O-C-N	5.72	129.09	122.17
1	A	284	MET	CA-CB-CG	-5.72	102.66	114.10
1	A	165	VAL	CA-C-O	5.72	126.54	120.48
1	A	252	ASN	O-C-N	5.71	128.26	122.09
1	A	160	VAL	CA-C-O	-5.71	114.72	120.31
1	A	391	ASP	CA-C-N	5.69	127.90	120.28
1	A	391	ASP	C-N-CA	5.69	127.90	120.28
1	A	55	LYS	CA-C-O	-5.69	114.19	120.33
1	A	526	LYS	N-CA-CB	5.68	118.57	110.16
1	A	264	PRO	CA-C-N	5.65	131.60	121.66
1	A	264	PRO	C-N-CA	5.65	131.60	121.66
1	A	223	ASP	CA-CB-CG	-5.63	106.97	112.60
1	A	159	VAL	CA-CB-CG1	5.59	119.91	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	LEU	CB-CA-C	5.56	119.89	109.71
1	A	261	GLN	CA-C-N	5.56	128.76	120.31
1	A	261	GLN	C-N-CA	5.56	128.76	120.31
1	A	299	GLU	CA-CB-CG	5.55	125.20	114.10
1	A	496	ASP	CA-C-O	-5.54	114.34	120.60
1	A	368	ASP	CA-C-O	-5.53	114.69	120.55
1	A	27	GLY	N-CA-C	-5.53	103.94	112.85
1	A	308	ASP	N-CA-C	5.53	119.34	112.59
1	A	125	ALA	CA-C-N	5.53	130.79	122.99
1	A	125	ALA	C-N-CA	5.53	130.79	122.99
1	A	534	GLY	N-CA-C	5.52	122.14	113.86
1	A	217	SER	O-C-N	-5.49	116.30	122.12
1	A	236	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	A	488	SER	O-C-N	5.48	128.77	123.29
1	A	514	THR	OG1-CB-CG2	5.42	120.15	109.30
1	A	449	THR	N-CA-C	-5.41	102.19	110.14
1	A	540	GLU	CA-C-O	-5.39	111.64	120.80
1	A	398	LEU	O-C-N	5.38	129.47	122.42
1	A	75	THR	OG1-CB-CG2	5.35	120.00	109.30
1	A	345	MET	CA-CB-CG	5.33	124.77	114.10
1	A	526	LYS	CA-CB-CG	5.33	124.75	114.10
1	A	265	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	321	GLY	N-CA-C	-5.29	104.93	112.55
1	A	59	ALA	N-CA-CB	-5.28	102.85	111.66
1	A	459	PRO	CA-C-N	5.27	131.61	121.18
1	A	459	PRO	C-N-CA	5.27	131.61	121.18
1	A	216	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	A	268	ILE	CA-C-O	-5.26	114.51	120.66
1	A	526	LYS	CB-CA-C	-5.26	101.91	110.85
1	A	55	LYS	CB-CA-C	-5.25	102.69	110.62
1	A	75	THR	CA-CB-CG2	5.24	119.41	110.50
1	A	153	LYS	N-CA-C	-5.23	101.18	109.76
1	A	45	GLN	CB-CG-CD	5.20	121.43	112.60
1	A	270	PRO	CA-C-O	-5.20	115.07	121.31
1	A	56	VAL	CB-CA-C	5.19	117.24	110.96
1	A	298	LYS	N-CA-C	-5.19	105.52	111.07
1	A	235	LEU	N-CA-CB	-5.18	104.14	110.98
1	A	515	PHE	CA-C-O	-5.17	115.78	121.31
1	A	263	HIS	CA-C-N	5.17	124.83	119.56
1	A	263	HIS	C-N-CA	5.17	124.83	119.56
1	A	165	VAL	O-C-N	-5.17	117.76	123.18
1	A	189	TYR	CA-C-O	-5.16	114.94	120.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	ILE	CA-C-O	-5.13	115.08	120.57
1	A	48	THR	CA-CB-CG2	5.12	119.21	110.50
1	A	275	TRP	N-CA-C	5.12	116.55	111.07
1	A	45	GLN	N-CA-C	5.09	119.34	113.18
1	A	318	GLY	O-C-N	-5.09	116.89	122.65
1	A	535	GLY	CA-C-O	-5.08	116.48	121.05
1	A	463	THR	O-C-N	5.06	129.14	123.27
1	A	500	GLU	CA-CB-CG	-5.05	104.00	114.10
1	A	360	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	305	LYS	CA-C-O	-5.03	112.51	119.05
1	A	334	THR	CB-CA-C	5.03	119.14	110.79
1	A	469	LYS	N-CA-C	-5.03	102.20	109.59
1	A	64	VAL	CB-CA-C	-5.02	101.72	110.71
1	A	226	ILE	N-CA-CB	-5.01	100.08	110.64
1	A	84	LYS	CB-CA-C	5.00	118.38	109.72
1	A	311	ASP	CB-CA-C	5.00	118.38	109.72
1	A	168	GLY	CA-C-N	5.00	128.84	120.64
1	A	168	GLY	C-N-CA	5.00	128.84	120.64

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	4122	0	3996	110	0
2	A	332	0	0	30	0
All	All	4454	0	3996	110	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 14.

All (110) 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
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:487:MET:HE1	1:A:493:TYR:CD2	2.11	0.85
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:116:ASN:HD22	1:A:116:ASN:C	2.00	0.70
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:487:MET:HE1	1:A:493:TYR:HD2	1.57	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:75:THR:HG23	2:A:755:HOH:O	2.07	0.55
1:A:447:GLY:C	1:A:468:VAL:HG22	2.33	0.54
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:390:TYR:CB	1:A:405:THR:HG23	2.43	0.49
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:412:TRP:H	1:A:412:TRP:CD1	2.31	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: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:378:ALA:HB1	1:A:382:MET:HE2	1.98	0.45
1:A:531:LYS:O	1:A:532:GLN:CB	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:487:MET:HE2	1:A:487:MET:HB3	1.77	0.43
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:186:HIS:HE2	1:A:358:GLU:CD	2.27	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:493:TYR:CD1	1:A:493:TYR:C	2.99	0.41
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

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	536/540 (99%)	523 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	428/430 (100%)	393 (92%)	35 (8%)	10	14

All (35) 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	79	ILE
1	A	104	LYS
1	A	116	ASN
1	A	134	ASP
1	A	142	LYS
1	A	159	VAL
1	A	165	VAL
1	A	169	VAL
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	369	LYS
1	A	401	LEU
1	A	405	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	419	THR
1	A	449	THR
1	A	467	PRO
1	A	468	VAL
1	A	487	MET
1	A	500	GLU
1	A	514	THR
1	A	516	ASP
1	A	526	LYS
1	A	532	GLN
1	A	541	ILE
1	A	559	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	116	ASN
1	A	173	ASN
1	A	198	ASN
1	A	201	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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 [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%)	-0.95	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 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.