



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:23 PM UTC

PDB ID : 1MPT / pdb_00001mpt
Title : CRYSTAL STRUCTURE OF A NEW ALKALINE SERINE PROTEASE (M-PROTEASE) FROM BACILLUS SP. KSM-K16
Authors : Yamane, T.; Kani, T.; Hatanaka, T.; Suzuki, A.; Ashida, T.; Kobayashi, T.; Ito, S.; Yamashita, O.
Deposited on : 1994-04-13
Resolution : 2.40 Å(reported)

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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

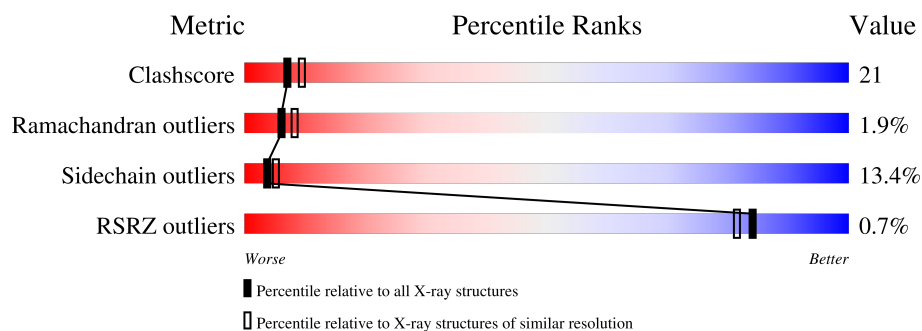
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	269	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1928 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 M-PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			1882	1152	348	379	3			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

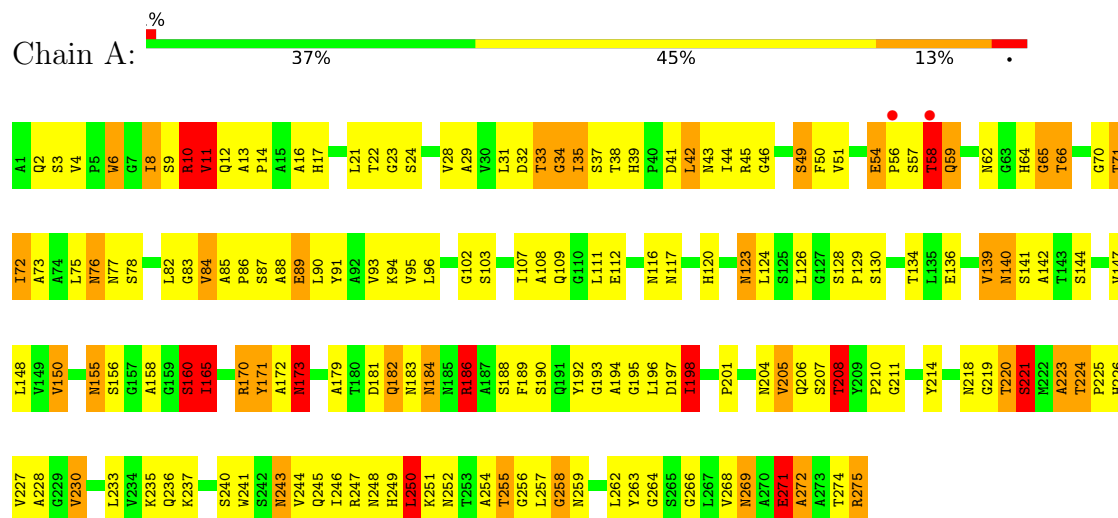
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		

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: M-PROTEASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.82Å 57.79Å 54.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.40 7.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.40) 82.9 (7.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.41Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.189 , (Not available) 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	1928	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	2.26	60/1915 (3.1%)	2.55	124/2613 (4.7%)

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	2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	SER	C-N	20.16	1.63	1.33
1	A	35	ILE	C-N	16.33	1.54	1.33
1	A	54	GLU	N-CA	11.42	1.53	1.46
1	A	85	ALA	CA-CB	8.52	1.62	1.53
1	A	32	ASP	C-O	-7.84	1.18	1.24
1	A	211	GLY	C-N	7.79	1.43	1.33
1	A	140	ASN	C-N	-7.14	1.24	1.33
1	A	10	ARG	C-N	-7.03	1.26	1.34
1	A	120	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	102	GLY	C-O	6.82	1.29	1.24
1	A	210	PRO	C-O	6.74	1.31	1.23
1	A	29	ALA	C-N	-6.65	1.24	1.33
1	A	256	GLY	CA-C	6.65	1.61	1.52
1	A	51	VAL	N-CA	6.61	1.52	1.46
1	A	256	GLY	N-CA	6.49	1.53	1.45
1	A	102	GLY	C-N	-6.46	1.25	1.33
1	A	76	ASN	CA-CB	-6.46	1.44	1.52
1	A	83	GLY	N-CA	6.38	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLN	N-CA	6.05	1.54	1.46
1	A	117	ASN	N-CA	6.04	1.54	1.46
1	A	76	ASN	CA-C	6.00	1.60	1.52
1	A	86	PRO	C-N	-5.99	1.26	1.33
1	A	249	HIS	ND1-CE1	5.98	1.38	1.32
1	A	186	ARG	N-CA	5.98	1.53	1.46
1	A	82	LEU	CA-C	5.97	1.59	1.52
1	A	66	THR	CA-C	5.97	1.60	1.52
1	A	165	ILE	N-CA	5.95	1.52	1.46
1	A	42	LEU	N-CA	5.93	1.53	1.45
1	A	65	GLY	C-O	5.81	1.30	1.23
1	A	269	ASN	C-O	5.77	1.30	1.23
1	A	223	ALA	C-O	5.74	1.30	1.24
1	A	139	VAL	N-CA	5.69	1.53	1.46
1	A	88	ALA	N-CA	5.68	1.53	1.46
1	A	78	SER	C-N	5.62	1.40	1.33
1	A	240	SER	C-O	-5.62	1.16	1.24
1	A	247	ARG	CA-C	5.61	1.60	1.52
1	A	39	HIS	CG-CD2	5.56	1.42	1.35
1	A	259	ASN	C-N	5.54	1.41	1.33
1	A	224	THR	N-CA	5.50	1.51	1.46
1	A	103	SER	N-CA	5.47	1.52	1.46
1	A	208	THR	CA-CB	5.42	1.62	1.53
1	A	184	ASN	C-O	5.29	1.30	1.24
1	A	156	SER	N-CA	5.28	1.53	1.46
1	A	227	VAL	C-O	5.27	1.30	1.24
1	A	11	VAL	C-O	-5.26	1.16	1.24
1	A	134	THR	CA-CB	5.24	1.61	1.53
1	A	263	TYR	CA-CB	5.21	1.62	1.54
1	A	120	HIS	CG-ND1	-5.21	1.32	1.38
1	A	252	ASN	C-O	5.16	1.30	1.24
1	A	251	LYS	N-CA	5.15	1.52	1.46
1	A	189	PHE	N-CA	5.13	1.52	1.46
1	A	103	SER	C-N	-5.11	1.27	1.34
1	A	41	ASP	CA-C	5.10	1.60	1.52
1	A	171	TYR	C-O	5.08	1.29	1.23
1	A	183	ASN	C-N	-5.08	1.26	1.33
1	A	224	THR	C-O	5.06	1.29	1.24
1	A	255	THR	CA-CB	5.05	1.60	1.53
1	A	255	THR	C-N	-5.02	1.29	1.33
1	A	134	THR	CB-OG1	5.02	1.51	1.43
1	A	141	SER	C-O	5.01	1.29	1.24

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ILE	O-C-N	-25.09	98.69	123.03
1	A	170	ARG	CD-NE-CZ	14.88	145.23	124.40
1	A	73	ALA	N-CA-C	13.54	126.39	110.41
1	A	160	SER	O-C-N	-12.28	107.48	122.96
1	A	257	LEU	N-CA-C	-12.02	86.99	108.02
1	A	34	GLY	CA-C-O	-11.09	112.26	122.13
1	A	73	ALA	CA-C-O	-10.28	111.77	121.02
1	A	271	GLU	CA-C-O	-10.13	110.52	121.56
1	A	271	GLU	N-CA-C	-9.64	96.90	110.50
1	A	139	VAL	N-CA-C	-9.55	100.88	110.62
1	A	208	THR	N-CA-CB	-8.77	97.15	110.04
1	A	73	ALA	N-CA-CB	-8.76	101.28	111.79
1	A	35	ILE	N-CA-CB	8.63	123.14	112.10
1	A	259	ASN	OD1-CG-ND2	-8.32	114.28	122.60
1	A	59	GLN	CA-C-O	7.92	129.39	120.84
1	A	243	ASN	O-C-N	7.89	130.29	122.09
1	A	173	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	A	172	ALA	CA-C-O	7.58	128.66	120.10
1	A	141	SER	O-C-N	7.49	129.78	122.07
1	A	243	ASN	CA-C-O	-7.45	112.92	120.90
1	A	170	ARG	NE-CZ-NH1	7.33	128.83	121.50
1	A	195	GLY	O-C-N	7.29	130.85	122.33
1	A	271	GLU	CA-CB-CG	7.27	128.65	114.10
1	A	130	SER	N-CA-C	7.22	119.17	110.07
1	A	236	GLN	OE1-CD-NE2	-7.13	115.47	122.60
1	A	214	TYR	CA-C-O	-7.10	113.38	121.40
1	A	41	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	155	ASN	N-CA-C	6.96	121.08	112.59
1	A	142	ALA	CB-CA-C	6.92	122.45	110.68
1	A	116	ASN	CA-CB-CG	-6.90	105.70	112.60
1	A	43	ASN	N-CA-CB	6.89	121.32	110.84
1	A	218	ASN	CA-CB-CG	6.89	119.49	112.60
1	A	58	THR	CA-C-N	-6.82	113.37	122.85
1	A	58	THR	C-N-CA	-6.82	113.37	122.85
1	A	188	SER	N-CA-CB	6.77	120.22	110.06
1	A	205	VAL	CB-CA-C	6.75	120.22	110.98
1	A	84	VAL	O-C-N	6.73	128.50	121.91
1	A	141	SER	CA-C-O	-6.71	113.78	120.82
1	A	2	GLN	OE1-CD-NE2	6.67	129.27	122.60
1	A	275	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	A	11	VAL	CA-C-N	6.65	131.57	122.07
1	A	11	VAL	C-N-CA	6.65	131.57	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	GLN	CB-CA-C	6.61	122.42	111.31
1	A	244	VAL	CA-C-N	6.58	129.39	120.44
1	A	244	VAL	C-N-CA	6.58	129.39	120.44
1	A	62	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	A	173	ASN	CA-CB-CG	6.54	119.14	112.60
1	A	160	SER	N-CA-CB	6.53	122.20	111.62
1	A	2	GLN	CA-C-N	-6.51	112.59	122.81
1	A	2	GLN	C-N-CA	-6.51	112.59	122.81
1	A	39	HIS	CA-CB-CG	6.51	120.31	113.80
1	A	207	SER	CA-C-O	6.50	128.26	121.31
1	A	263	TYR	N-CA-C	6.49	122.16	113.72
1	A	186	ARG	CB-CA-C	6.46	120.69	109.65
1	A	183	ASN	CA-C-O	-6.45	112.05	119.14
1	A	165	ILE	CB-CA-C	6.43	120.99	110.69
1	A	250	LEU	CB-CA-C	6.36	120.87	110.88
1	A	51	VAL	O-C-N	6.36	126.42	121.46
1	A	198	ILE	N-CA-CB	-6.30	100.83	111.23
1	A	43	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	103	SER	CA-C-O	-6.28	112.81	120.54
1	A	9	SER	N-CA-C	-6.21	104.44	111.14
1	A	71	THR	O-C-N	6.13	128.62	122.12
1	A	109	GLN	CB-CG-CD	-6.04	102.33	112.60
1	A	220	THR	N-CA-C	-6.01	105.05	112.38
1	A	77	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	193	GLY	CA-C-N	5.99	129.89	121.02
1	A	193	GLY	C-N-CA	5.99	129.89	121.02
1	A	264	GLY	N-CA-C	-5.97	101.11	111.50
1	A	186	ARG	NE-CZ-NH2	-5.95	113.84	119.20
1	A	275	ARG	CA-CB-CG	5.95	126.00	114.10
1	A	150	VAL	CA-C-O	-5.94	114.22	120.39
1	A	140	ASN	CA-C-O	-5.91	114.61	120.70
1	A	248	ASN	CA-CB-CG	-5.89	106.71	112.60
1	A	255	THR	CA-CB-OG1	-5.88	100.78	109.60
1	A	66	THR	O-C-N	5.87	128.34	122.12
1	A	197	ASP	CA-C-O	-5.85	112.87	120.00
1	A	123	ASN	CA-C-O	-5.84	114.11	120.36
1	A	6	TRP	CA-C-O	-5.84	114.32	120.63
1	A	170	ARG	CA-CB-CG	5.79	125.68	114.10
1	A	269	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	58	THR	CA-CB-OG1	-5.71	101.03	109.60
1	A	4	VAL	O-C-N	5.67	127.56	121.10
1	A	228	ALA	N-CA-C	-5.65	105.12	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LEU	O-C-N	5.65	129.90	122.33
1	A	12	GLN	N-CA-C	5.61	119.17	111.54
1	A	95	VAL	CB-CA-C	5.61	116.15	110.65
1	A	165	ILE	N-CA-CB	-5.59	101.58	111.93
1	A	233	LEU	N-CA-CB	-5.54	101.95	110.16
1	A	230	VAL	N-CA-C	-5.54	105.10	110.42
1	A	179	ALA	N-CA-C	5.52	118.47	109.59
1	A	117	ASN	CB-CA-C	5.51	119.49	110.17
1	A	160	SER	N-CA-C	-5.50	100.94	109.14
1	A	35	ILE	CA-CB-CG1	5.50	119.75	110.40
1	A	50	PHE	CA-CB-CG	-5.48	108.32	113.80
1	A	77	ASN	CA-C-O	-5.43	115.29	120.56
1	A	250	LEU	N-CA-C	-5.42	105.27	111.07
1	A	11	VAL	CA-CB-CG1	5.41	119.59	110.40
1	A	233	LEU	CA-C-N	5.38	127.34	120.56
1	A	233	LEU	C-N-CA	5.38	127.34	120.56
1	A	17	HIS	N-CA-CB	5.37	118.01	110.12
1	A	33	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	51	VAL	CB-CA-C	5.35	116.93	110.78
1	A	194	ALA	N-CA-C	5.35	117.93	109.96
1	A	221	SER	N-CA-C	-5.34	105.57	111.71
1	A	23	GLY	N-CA-C	-5.30	107.90	115.64
1	A	204	ASN	CA-C-O	-5.29	115.47	121.65
1	A	10	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	247	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	A	93	VAL	O-C-N	5.24	129.95	122.62
1	A	64	HIS	CA-CB-CG	5.23	119.03	113.80
1	A	49	SER	O-C-N	5.22	130.01	123.23
1	A	16	ALA	N-CA-C	-5.22	105.49	111.07
1	A	258	GLY	N-CA-C	5.21	125.54	113.18
1	A	221	SER	CA-CB-OG	5.19	121.49	111.10
1	A	8	ILE	CB-CA-C	5.16	120.62	112.26
1	A	155	ASN	CB-CG-ND2	5.13	124.10	116.40
1	A	38	THR	N-CA-CB	-5.09	102.14	109.83
1	A	17	HIS	CG-CD2-NE2	5.07	112.27	107.20
1	A	66	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	77	ASN	CB-CG-ND2	5.07	124.00	116.40
1	A	89	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	275	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	254	ALA	CA-C-O	-5.00	116.11	121.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	SER	Mainchain
1	A	186	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	1882	0	1841	78	0
2	A	2	0	0	0	0
3	A	44	0	0	0	0
All	All	1928	0	1841	78	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 21.

All (78) 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:182:GLN:HE21	1:A:182:GLN:H	1.13	0.94
1:A:57:SER:O	1:A:59:GLN:N	2.00	0.94
1:A:28:VAL:HG11	1:A:72:ILE:HD13	1.49	0.94
1:A:35:ILE:O	1:A:58:THR:O	1.91	0.88
1:A:37:SER:HA	1:A:58:THR:O	1.73	0.87
1:A:66:THR:O	1:A:208:THR:HG22	1.75	0.86
1:A:140:ASN:OD1	1:A:173:ASN:ND2	2.10	0.84
1:A:155:ASN:HD21	1:A:220:THR:H	1.27	0.83
1:A:35:ILE:O	1:A:58:THR:HG23	1.80	0.81
1:A:271:GLU:O	1:A:272:ALA:HB3	1.82	0.80
1:A:22:THR:HG23	1:A:87:SER:HB2	1.64	0.78
1:A:108:ALA:O	1:A:112:GLU:HG2	1.83	0.77
1:A:57:SER:C	1:A:59:GLN:H	1.91	0.77
1:A:58:THR:HG22	1:A:59:GLN:OE1	1.85	0.75
1:A:57:SER:C	1:A:59:GLN:N	2.44	0.73
1:A:230:VAL:HG12	1:A:250:LEU:HD11	1.70	0.72
1:A:155:ASN:HD22	1:A:220:THR:HG23	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:GLU:C	1:A:56:PRO:N	2.55	0.65
1:A:35:ILE:HG22	1:A:44:ILE:HD11	1.79	0.65
1:A:66:THR:HG22	1:A:208:THR:HG23	1.80	0.63
1:A:155:ASN:ND2	1:A:220:THR:H	1.96	0.62
1:A:56:PRO:O	1:A:94:LYS:HD3	2.00	0.62
1:A:28:VAL:HG11	1:A:72:ILE:CD1	2.26	0.60
1:A:37:SER:CA	1:A:58:THR:O	2.46	0.60
1:A:49:SER:HA	1:A:94:LYS:HB3	1.84	0.60
1:A:66:THR:O	1:A:208:THR:CG2	2.49	0.59
1:A:182:GLN:H	1:A:182:GLN:NE2	1.95	0.58
1:A:155:ASN:ND2	1:A:220:THR:HG23	2.18	0.57
1:A:35:ILE:C	1:A:58:THR:O	2.47	0.57
1:A:235:LYS:HG2	1:A:246:ILE:HD11	1.87	0.56
1:A:57:SER:OG	1:A:58:THR:N	2.39	0.55
1:A:271:GLU:O	1:A:272:ALA:CB	2.45	0.55
1:A:165:ILE:CD1	1:A:196:LEU:HB2	2.38	0.53
1:A:46:GLY:O	1:A:91:TYR:HA	2.08	0.53
1:A:198:ILE:HG13	1:A:266:GLY:O	2.08	0.53
1:A:237:LYS:NZ	1:A:274:THR:O	2.34	0.53
1:A:22:THR:HG23	1:A:87:SER:CB	2.38	0.52
1:A:186:ARG:NH2	1:A:190:SER:O	2.28	0.51
1:A:13:ALA:HB3	1:A:14:PRO:HD3	1.92	0.51
1:A:34:GLY:O	1:A:65:GLY:HA3	2.10	0.51
1:A:192:TYR:HA	1:A:196:LEU:HD22	1.93	0.51
1:A:35:ILE:O	1:A:58:THR:CG2	2.57	0.49
1:A:123:ASN:OD1	1:A:224:THR:HG22	2.12	0.49
1:A:6:TRP:CH2	1:A:201:PRO:HB3	2.48	0.49
1:A:45:ARG:HG3	1:A:89:GLU:HB3	1.95	0.48
1:A:136:GLU:HB3	1:A:171:TYR:CE2	2.48	0.48
1:A:35:ILE:CG2	1:A:44:ILE:HD11	2.42	0.48
1:A:22:THR:CG2	1:A:24:SER:HB2	2.44	0.48
1:A:57:SER:O	1:A:58:THR:C	2.56	0.47
1:A:70:GLY:HA3	1:A:208:THR:HB	1.96	0.47
1:A:136:GLU:HB3	1:A:171:TYR:CZ	2.49	0.47
1:A:237:LYS:NZ	1:A:275:ARG:C	2.72	0.47
1:A:13:ALA:N	1:A:14:PRO:CD	2.78	0.47
1:A:139:VAL:HG12	1:A:173:ASN:HB2	1.96	0.47
1:A:107:ILE:HD12	1:A:126:LEU:HD22	1.97	0.47
1:A:11:VAL:HG22	1:A:268:VAL:HG13	1.96	0.46
1:A:223:ALA:O	1:A:226:HIS:HB2	2.15	0.46
1:A:33:THR:HA	1:A:96:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASN:C	1:A:76:ASN:HD22	2.24	0.45
1:A:226:HIS:O	1:A:230:VAL:HG23	2.16	0.45
1:A:13:ALA:N	1:A:14:PRO:HD2	2.31	0.45
1:A:219:GLY:C	1:A:221:SER:N	2.74	0.45
1:A:165:ILE:HD11	1:A:196:LEU:HB2	1.98	0.45
1:A:44:ILE:HG21	1:A:58:THR:OG1	2.17	0.45
1:A:71:THR:O	1:A:84:VAL:HG23	2.18	0.44
1:A:128:SER:HA	1:A:129:PRO:HD3	1.86	0.43
1:A:269:ASN:OD1	1:A:271:GLU:O	2.37	0.43
1:A:224:THR:N	1:A:225:PRO:HD2	2.34	0.43
1:A:107:ILE:HD12	1:A:126:LEU:CD2	2.48	0.43
1:A:158:ALA:C	1:A:160:SER:H	2.26	0.43
1:A:31:LEU:N	1:A:31:LEU:HD12	2.34	0.42
1:A:10:ARG:HD3	1:A:10:ARG:HA	1.85	0.42
1:A:181:ASP:OD1	1:A:181:ASP:C	2.63	0.41
1:A:255:THR:O	1:A:266:GLY:HA3	2.20	0.41
1:A:150:VAL:HG12	1:A:224:THR:HG23	2.03	0.41
1:A:275:ARG:HE	1:A:275:ARG:HB2	1.20	0.41
1:A:241:TRP:HA	1:A:245:GLN:OE1	2.22	0.40
1:A:237:LYS:HZ1	1:A:275:ARG:C	2.30	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	265/269 (98%)	249 (94%)	11 (4%)	5 (2%)	6 8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	THR

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	258	GLY
1	A	272	ALA
1	A	198	ILE

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	194/194 (100%)	168 (87%)	26 (13%)	4 5

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	8	ILE
1	A	10	ARG
1	A	11	VAL
1	A	21	LEU
1	A	42	LEU
1	A	72	ILE
1	A	75	LEU
1	A	90	LEU
1	A	111	LEU
1	A	124	LEU
1	A	144	SER
1	A	147	VAL
1	A	148	LEU
1	A	160	SER
1	A	165	ILE
1	A	170	ARG
1	A	173	ASN
1	A	182	GLN
1	A	205	VAL
1	A	206	GLN
1	A	208	THR

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Mol	Chain	Res	Type
1	A	221	SER
1	A	243	ASN
1	A	250	LEU
1	A	271	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	76	ASN
1	A	155	ASN
1	A	182	GLN
1	A	184	ASN
1	A	185	ASN
1	A	204	ASN
1	A	238	ASN
1	A	249	HIS
1	A	261	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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	54:GLU	C	56:PRO	N	2.55
1	A	160:SER	C	165:ILE	N	1.63

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	269/269 (100%)	-0.44	2 (0%) 84 81	3, 8, 16, 27	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	THR	5.1
1	A	56	PRO	2.9

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	276	1/1	0.94	0.03	10,10,10,10	0
2	CA	A	277	1/1	0.95	0.11	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.