



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:57 AM UTC

PDB ID : 3H1B / pdb_00003h1b
Title : Crystal structure of EstE5, was soaked by isopropyl alcohol
Authors : Hwang, K.Y.; Nam, K.H.
Deposited on : 2009-04-11
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 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

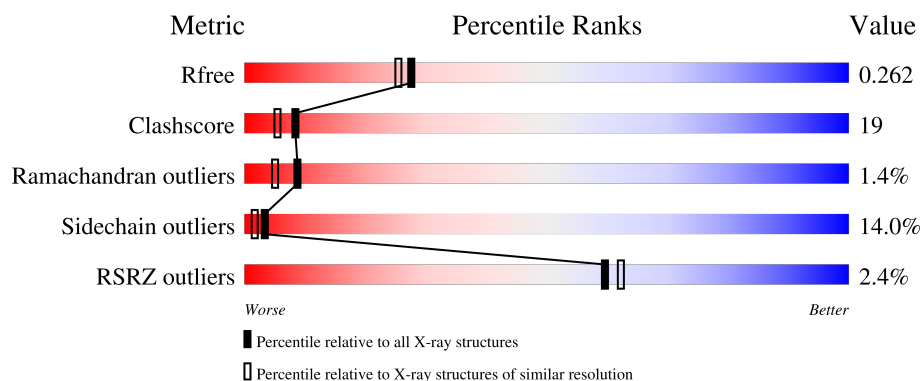
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	322	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2261 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 Esterase/lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2241	1426	393	407	15			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP Q0GMU2
A	-11	ALA	-	expression tag	UNP Q0GMU2
A	-10	SER	-	expression tag	UNP Q0GMU2
A	-9	MET	-	expression tag	UNP Q0GMU2
A	-8	THR	-	expression tag	UNP Q0GMU2
A	-7	GLY	-	expression tag	UNP Q0GMU2
A	-6	GLY	-	expression tag	UNP Q0GMU2
A	-5	GLN	-	expression tag	UNP Q0GMU2
A	-4	GLN	-	expression tag	UNP Q0GMU2
A	-3	MET	-	expression tag	UNP Q0GMU2
A	-2	GLY	-	expression tag	UNP Q0GMU2
A	-1	ARG	-	expression tag	UNP Q0GMU2
A	0	GLY	-	expression tag	UNP Q0GMU2
A	298	LEU	-	expression tag	UNP Q0GMU2
A	299	ALA	-	expression tag	UNP Q0GMU2
A	300	ALA	-	expression tag	UNP Q0GMU2
A	301	ALA	-	expression tag	UNP Q0GMU2
A	302	LEU	-	expression tag	UNP Q0GMU2
A	303	GLU	-	expression tag	UNP Q0GMU2
A	304	HIS	-	expression tag	UNP Q0GMU2
A	305	HIS	-	expression tag	UNP Q0GMU2
A	306	HIS	-	expression tag	UNP Q0GMU2
A	307	HIS	-	expression tag	UNP Q0GMU2
A	308	HIS	-	expression tag	UNP Q0GMU2
A	309	HIS	-	expression tag	UNP Q0GMU2

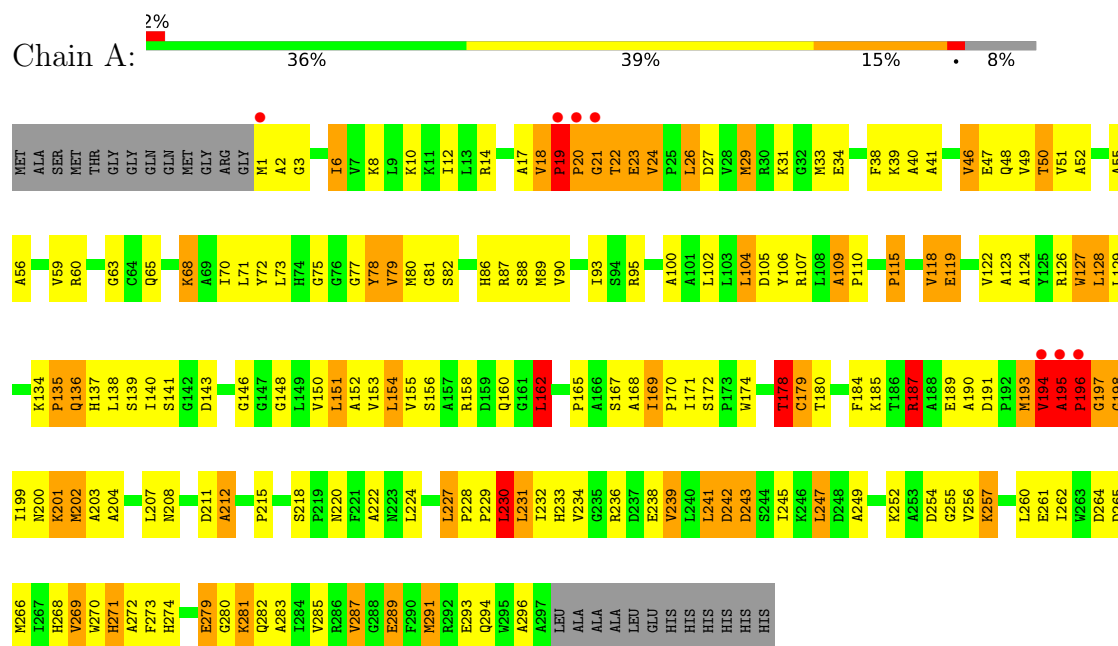
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		

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: Esterase/lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	61.31Å 61.31Å 150.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 2.10 47.49 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.8 (47.49-2.10) 90.8 (47.49-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.239 , 0.295 0.247 , 0.262	Depositor DCC
R_{free} test set	806 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2261	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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	2.38	100/2295 (4.4%)	2.20	103/3116 (3.3%)

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	8

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	SER	C-O	9.94	1.28	1.23
1	A	2	ALA	CA-CB	9.68	1.67	1.53
1	A	287	VAL	CA-CB	9.24	1.64	1.54
1	A	40	ALA	CA-C	9.19	1.64	1.52
1	A	153	VAL	N-CA	9.11	1.57	1.46
1	A	272	ALA	CA-CB	-8.60	1.38	1.53
1	A	208	ASN	CA-C	8.22	1.63	1.53
1	A	249	ALA	CA-C	8.10	1.63	1.52
1	A	283	ALA	CA-CB	-7.95	1.40	1.53
1	A	123	ALA	CA-CB	-7.67	1.41	1.53
1	A	231	LEU	C-O	-7.66	1.14	1.24
1	A	141	SER	CA-C	7.63	1.61	1.52
1	A	190	ALA	N-CA	7.61	1.56	1.46
1	A	46	VAL	CA-CB	-7.45	1.44	1.55
1	A	155	VAL	N-CA	7.25	1.55	1.46
1	A	2	ALA	N-CA	7.13	1.55	1.46
1	A	179	CYS	CA-C	-7.13	1.44	1.53
1	A	273	PHE	C-O	-7.04	1.14	1.24
1	A	79	VAL	CA-CB	7.01	1.63	1.54
1	A	47	GLU	CA-C	-6.96	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	ARG	CA-C	-6.95	1.43	1.52
1	A	289	GLU	C-O	-6.90	1.16	1.24
1	A	50	THR	C-O	6.86	1.32	1.24
1	A	242	ASP	CA-C	6.83	1.61	1.52
1	A	257	LYS	C-O	-6.82	1.16	1.24
1	A	50	THR	CA-C	6.81	1.60	1.52
1	A	107	ARG	N-CA	6.78	1.54	1.46
1	A	22	THR	C-O	-6.75	1.15	1.24
1	A	270	TRP	C-O	-6.74	1.15	1.24
1	A	172	SER	CA-C	6.70	1.58	1.53
1	A	156	SER	C-O	-6.69	1.16	1.24
1	A	155	VAL	CA-C	6.65	1.60	1.52
1	A	115	PRO	N-CA	-6.50	1.36	1.47
1	A	289	GLU	CA-C	-6.49	1.44	1.52
1	A	174	TRP	CA-C	-6.41	1.45	1.53
1	A	245	ILE	N-CA	6.31	1.53	1.46
1	A	152	ALA	CA-C	-6.29	1.44	1.52
1	A	148	GLY	N-CA	-6.28	1.38	1.45
1	A	167	SER	N-CA	6.25	1.53	1.46
1	A	71	LEU	N-CA	-6.20	1.38	1.46
1	A	88	SER	CB-OG	6.17	1.54	1.42
1	A	100	ALA	C-O	-6.12	1.16	1.23
1	A	296	ALA	CA-C	6.05	1.61	1.52
1	A	294	GLN	C-O	-6.04	1.16	1.24
1	A	93	ILE	CA-CB	6.03	1.61	1.54
1	A	80	MET	N-CA	6.00	1.53	1.46
1	A	140	ILE	N-CA	5.96	1.53	1.46
1	A	230	LEU	CG-CD2	-5.92	1.33	1.52
1	A	70	ILE	C-O	-5.87	1.17	1.24
1	A	261	GLU	N-CA	5.85	1.53	1.46
1	A	50	THR	CA-CB	5.84	1.64	1.53
1	A	266	MET	CA-C	-5.84	1.45	1.52
1	A	60	ARG	CD-NE	5.81	1.54	1.46
1	A	23	GLU	C-O	-5.80	1.17	1.24
1	A	52	ALA	CA-CB	5.73	1.62	1.53
1	A	272	ALA	CA-C	-5.71	1.44	1.52
1	A	39	LYS	CA-C	5.71	1.60	1.52
1	A	12	ILE	N-CA	5.70	1.53	1.46
1	A	119	GLU	CA-C	-5.70	1.45	1.52
1	A	187	ARG	N-CA	5.66	1.53	1.46
1	A	256	VAL	CA-C	5.66	1.59	1.52
1	A	75	GLY	N-CA	5.65	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	LEU	N-CA	-5.64	1.39	1.46
1	A	160	GLN	C-O	5.64	1.31	1.24
1	A	202	MET	C-O	-5.63	1.17	1.24
1	A	56	ALA	N-CA	5.62	1.53	1.46
1	A	281	LYS	CG-CD	5.62	1.69	1.52
1	A	89	MET	C-O	-5.55	1.17	1.24
1	A	60	ARG	NE-CZ	5.54	1.39	1.33
1	A	73	LEU	N-CA	5.53	1.54	1.46
1	A	230	LEU	CG-CD1	5.46	1.70	1.52
1	A	17	ALA	N-CA	5.46	1.52	1.46
1	A	232	ILE	CA-CB	5.43	1.61	1.54
1	A	126	ARG	CZ-NH1	5.42	1.40	1.32
1	A	128	LEU	CG-CD1	-5.40	1.34	1.52
1	A	136	GLN	CA-C	-5.38	1.45	1.52
1	A	115	PRO	C-O	-5.35	1.12	1.23
1	A	56	ALA	C-O	-5.32	1.17	1.23
1	A	281	LYS	CE-NZ	5.32	1.65	1.49
1	A	228	PRO	C-N	5.31	1.39	1.33
1	A	228	PRO	CA-C	5.31	1.57	1.52
1	A	51	VAL	CA-C	5.31	1.59	1.52
1	A	60	ARG	CA-C	-5.30	1.46	1.52
1	A	14	ARG	CA-C	5.30	1.59	1.52
1	A	48	GLN	CA-CB	-5.28	1.45	1.53
1	A	115	PRO	CB-CG	-5.25	1.30	1.51
1	A	208	ASN	C-O	5.25	1.30	1.23
1	A	148	GLY	C-O	-5.25	1.17	1.23
1	A	274	HIS	C-N	5.20	1.40	1.34
1	A	231	LEU	CA-C	-5.17	1.46	1.52
1	A	59	VAL	CB-CG2	-5.17	1.35	1.52
1	A	283	ALA	CA-C	-5.16	1.45	1.52
1	A	55	ALA	C-O	-5.13	1.17	1.23
1	A	70	ILE	N-CA	5.12	1.52	1.46
1	A	178	THR	C-O	-5.12	1.17	1.24
1	A	109	ALA	CA-C	5.11	1.59	1.52
1	A	272	ALA	N-CA	-5.07	1.39	1.46
1	A	282	GLN	C-O	5.07	1.30	1.24
1	A	127	TRP	C-O	-5.04	1.18	1.24
1	A	224	LEU	N-CA	-5.03	1.39	1.46

All (103) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	PRO	N-CA-C	17.19	131.67	110.70
1	A	19	PRO	CB-CA-C	-16.88	90.33	110.92
1	A	178	THR	CB-CA-C	-15.12	84.62	110.17
1	A	178	THR	CA-C-N	12.10	140.15	122.36
1	A	178	THR	C-N-CA	12.10	140.15	122.36
1	A	274	HIS	CA-C-N	-11.43	108.01	119.56
1	A	274	HIS	C-N-CA	-11.43	108.01	119.56
1	A	50	THR	CB-CA-C	9.85	127.74	109.71
1	A	153	VAL	N-CA-C	9.41	121.35	110.62
1	A	202	MET	CG-SD-CE	9.34	121.44	100.90
1	A	255	GLY	N-CA-C	-9.18	102.01	114.95
1	A	190	ALA	N-CA-C	9.00	124.04	112.34
1	A	12	ILE	N-CA-C	8.70	118.71	110.53
1	A	18	VAL	N-CA-C	8.65	118.47	108.96
1	A	23	GLU	N-CA-C	-8.47	93.72	108.20
1	A	170	PRO	CB-CA-C	-8.43	101.26	111.46
1	A	68	LYS	CB-CA-C	8.08	123.06	109.48
1	A	63	GLY	CA-C-N	-7.94	110.34	122.09
1	A	63	GLY	C-N-CA	-7.94	110.34	122.09
1	A	265	ASP	N-CA-C	7.86	122.58	113.38
1	A	89	MET	CG-SD-CE	-7.55	84.29	100.90
1	A	162	LEU	CA-C-N	-7.49	112.29	119.85
1	A	162	LEU	C-N-CA	-7.49	112.29	119.85
1	A	254	ASP	N-CA-C	7.48	122.23	113.18
1	A	127	TRP	CB-CA-C	-7.44	98.49	110.84
1	A	47	GLU	CB-CA-C	-7.39	101.47	110.94
1	A	95	ARG	N-CA-C	7.33	119.90	111.11
1	A	127	TRP	N-CA-C	7.33	123.38	111.37
1	A	194	VAL	N-CA-C	7.03	118.94	108.54
1	A	211	ASP	N-CA-C	-6.99	97.83	108.67
1	A	154	LEU	N-CA-C	-6.99	103.28	111.03
1	A	59	VAL	CA-C-N	-6.95	113.20	123.00
1	A	59	VAL	C-N-CA	-6.95	113.20	123.00
1	A	279	GLU	N-CA-C	6.77	119.52	111.33
1	A	270	TRP	N-CA-C	-6.74	104.00	111.82
1	A	272	ALA	N-CA-C	-6.63	105.16	113.18
1	A	245	ILE	N-CA-CB	6.63	118.30	110.55
1	A	134	LYS	CD-CE-NZ	-6.59	90.81	111.90
1	A	78	TYR	CA-C-N	6.45	129.45	121.71
1	A	78	TYR	C-N-CA	6.45	129.45	121.71
1	A	264	ASP	O-C-N	6.41	130.42	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	MET	N-CA-C	-6.22	104.50	111.28
1	A	46	VAL	N-CA-C	-6.18	98.87	108.44
1	A	17	ALA	N-CA-C	6.17	119.41	110.28
1	A	280	GLY	N-CA-C	-6.15	105.34	112.73
1	A	194	VAL	CB-CA-C	6.14	118.27	111.08
1	A	3	GLY	CA-C-N	-6.11	113.39	119.56
1	A	3	GLY	C-N-CA	-6.11	113.39	119.56
1	A	34	GLU	N-CA-C	-6.08	104.73	111.36
1	A	203	ALA	CA-C-N	6.08	130.86	121.19
1	A	203	ALA	C-N-CA	6.08	130.86	121.19
1	A	243	ASP	CA-C-N	6.07	128.69	120.44
1	A	243	ASP	C-N-CA	6.07	128.69	120.44
1	A	73	LEU	N-CA-C	6.04	118.98	107.75
1	A	242	ASP	CB-CA-C	5.89	120.21	110.90
1	A	40	ALA	N-CA-C	5.88	117.88	110.24
1	A	105	ASP	N-CA-C	-5.87	100.77	109.11
1	A	2	ALA	N-CA-C	5.86	119.19	109.46
1	A	18	VAL	CB-CA-C	5.85	116.61	110.88
1	A	196	PRO	CA-C-N	5.79	132.77	121.41
1	A	196	PRO	C-N-CA	5.79	132.77	121.41
1	A	238	GLU	N-CA-C	5.69	117.83	109.24
1	A	141	SER	O-C-N	-5.67	116.70	123.27
1	A	100	ALA	N-CA-C	-5.64	102.13	110.48
1	A	193	MET	N-CA-C	5.63	119.73	111.34
1	A	152	ALA	CA-C-O	-5.61	114.60	120.55
1	A	29	MET	CA-C-N	5.60	127.72	120.44
1	A	29	MET	C-N-CA	5.60	127.72	120.44
1	A	167	SER	N-CA-C	5.60	116.78	108.60
1	A	38	PHE	CA-C-N	5.57	130.11	121.26
1	A	38	PHE	C-N-CA	5.57	130.11	121.26
1	A	90	VAL	N-CA-C	5.56	116.29	110.62
1	A	158	ARG	N-CA-C	5.46	116.91	111.07
1	A	252	LYS	CD-CE-NZ	-5.44	94.50	111.90
1	A	198	GLY	CA-C-N	5.43	129.06	120.47
1	A	198	GLY	C-N-CA	5.43	129.06	120.47
1	A	162	LEU	CB-CA-C	5.42	116.51	108.87
1	A	151	LEU	N-CA-C	-5.41	104.94	112.45
1	A	156	SER	CA-C-O	-5.38	115.14	120.90
1	A	38	PHE	O-C-N	5.33	129.49	122.93
1	A	41	ALA	CA-C-N	-5.33	113.81	122.65
1	A	41	ALA	C-N-CA	-5.33	113.81	122.65
1	A	21	GLY	CA-C-N	-5.32	114.69	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	GLY	C-N-CA	-5.32	114.69	122.19
1	A	189	GLU	CA-C-N	5.31	129.18	120.63
1	A	189	GLU	C-N-CA	5.31	129.18	120.63
1	A	191	ASP	N-CA-C	5.29	121.49	109.81
1	A	195	ALA	CA-C-N	-5.26	113.27	119.84
1	A	195	ALA	C-N-CA	-5.26	113.27	119.84
1	A	207	LEU	N-CA-C	5.25	117.68	111.33
1	A	93	ILE	N-CA-CB	5.24	117.27	110.57
1	A	24	VAL	N-CA-C	-5.22	101.93	107.77
1	A	172	SER	CB-CA-C	5.20	115.60	110.71
1	A	179	CYS	CB-CA-C	-5.20	105.17	111.82
1	A	6	ILE	N-CA-C	-5.19	104.49	111.44
1	A	80	MET	CA-C-O	-5.16	115.92	121.38
1	A	14	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	72	TYR	N-CA-C	5.14	116.91	108.52
1	A	100	ALA	CA-C-O	-5.09	115.62	121.47
1	A	256	VAL	CB-CA-C	5.07	118.54	111.34
1	A	236	ARG	CA-C-N	5.02	131.56	122.27
1	A	236	ARG	C-N-CA	5.02	131.56	122.27
1	A	243	ASP	N-CA-C	5.01	121.48	110.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	THR	Peptide
1	A	179	CYS	Peptide
1	A	19	PRO	Peptide
1	A	195	ALA	Peptide
1	A	196	PRO	Peptide
1	A	197	GLY	Peptide
1	A	20	PRO	Peptide
1	A	21	GLY	Peptide

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	2241	0	2254	86	0
2	A	20	0	0	0	0
All	All	2261	0	2254	86	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 19.

All (86) 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:18:VAL:CG1	1:A:22:THR:HG21	1.77	1.12
1:A:18:VAL:CG1	1:A:22:THR:CG2	2.29	1.11
1:A:195:ALA:H	1:A:196:PRO:HG3	1.17	1.06
1:A:18:VAL:HG13	1:A:22:THR:HG21	1.32	1.05
1:A:195:ALA:N	1:A:196:PRO:HG3	1.84	0.91
1:A:178:THR:O	1:A:180:THR:HG23	1.74	0.86
1:A:18:VAL:HG12	1:A:22:THR:CG2	2.06	0.82
1:A:195:ALA:HB3	1:A:196:PRO:CB	2.11	0.81
1:A:169:ILE:N	1:A:169:ILE:HD12	1.95	0.81
1:A:196:PRO:HB2	1:A:198:GLY:N	1.97	0.78
1:A:195:ALA:HB3	1:A:196:PRO:HB3	1.67	0.76
1:A:168:ALA:HB3	1:A:230:LEU:HD12	1.71	0.73
1:A:233:HIS:HD2	1:A:271:HIS:NE2	1.90	0.69
1:A:26:LEU:HA	1:A:29:MET:HE3	1.76	0.68
1:A:104:LEU:HD13	1:A:106:TYR:HB3	1.74	0.67
1:A:24:VAL:O	1:A:29:MET:HE2	1.94	0.66
1:A:195:ALA:N	1:A:196:PRO:CG	2.58	0.66
1:A:194:VAL:HG12	1:A:196:PRO:HD3	1.78	0.65
1:A:6:ILE:HG13	1:A:10:LYS:HD2	1.80	0.64
1:A:187:ARG:HD3	1:A:241:LEU:HD12	1.79	0.64
1:A:184:PHE:HA	1:A:239:VAL:HG22	1.80	0.63
1:A:18:VAL:HG12	1:A:22:THR:HG22	1.78	0.63
1:A:271:HIS:H	1:A:271:HIS:HD1	1.47	0.63
1:A:178:THR:O	1:A:180:THR:CG2	2.47	0.62
1:A:178:THR:C	1:A:180:THR:HG23	2.25	0.61
1:A:196:PRO:CB	1:A:198:GLY:H	2.13	0.61
1:A:18:VAL:HG11	1:A:22:THR:CG2	2.28	0.58
1:A:195:ALA:N	1:A:196:PRO:CD	2.66	0.58
1:A:77:GLY:O	1:A:78:TYR:HB2	2.04	0.57
1:A:195:ALA:HB3	1:A:196:PRO:CA	2.34	0.57
1:A:268:HIS:O	1:A:269:VAL:C	2.48	0.56
1:A:168:ALA:C	1:A:169:ILE:HD12	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG12	1:A:29:MET:HG3	1.88	0.54
1:A:109:ALA:HB1	1:A:110:PRO:HA	1.90	0.54
1:A:195:ALA:CA	1:A:196:PRO:HG3	2.38	0.54
1:A:27:ASP:O	1:A:31:LYS:HG3	2.09	0.53
1:A:220:ASN:OD1	1:A:247:LEU:HB2	2.09	0.53
1:A:195:ALA:CB	1:A:196:PRO:CA	2.86	0.53
1:A:128:LEU:HD13	1:A:138:LEU:HD22	1.91	0.53
1:A:194:VAL:HG11	1:A:199:ILE:HD12	1.92	0.52
1:A:195:ALA:N	1:A:196:PRO:HD3	2.24	0.52
1:A:199:ILE:HG13	1:A:202:MET:HE2	1.91	0.51
1:A:285:VAL:O	1:A:289:GLU:HG3	2.11	0.51
1:A:154:LEU:HD11	1:A:168:ALA:HB2	1.94	0.50
1:A:196:PRO:CB	1:A:198:GLY:N	2.68	0.50
1:A:195:ALA:HB3	1:A:196:PRO:CG	2.41	0.50
1:A:86:HIS:HE2	1:A:143:ASP:CG	2.19	0.50
1:A:169:ILE:N	1:A:169:ILE:CD1	2.71	0.50
1:A:79:VAL:HA	1:A:109:ALA:O	2.11	0.50
1:A:196:PRO:HD2	1:A:199:ILE:HG22	1.94	0.49
1:A:233:HIS:CD2	1:A:271:HIS:NE2	2.75	0.49
1:A:289:GLU:O	1:A:293:GLU:HG3	2.13	0.48
1:A:195:ALA:CA	1:A:196:PRO:CG	2.92	0.48
1:A:194:VAL:HG12	1:A:196:PRO:CD	2.42	0.48
1:A:143:ASP:HB2	1:A:269:VAL:CG2	2.43	0.48
1:A:124:ALA:O	1:A:127:TRP:HB3	2.14	0.48
1:A:196:PRO:HB2	1:A:199:ILE:H	1.79	0.48
1:A:143:ASP:HA	1:A:171:ILE:O	2.15	0.47
1:A:169:ILE:HG21	1:A:287:VAL:HG13	1.97	0.47
1:A:195:ALA:CB	1:A:196:PRO:HA	2.45	0.46
1:A:146:GLY:O	1:A:150:VAL:HG23	2.16	0.46
1:A:169:ILE:HG13	1:A:231:LEU:HB3	1.97	0.46
1:A:195:ALA:HB3	1:A:196:PRO:HG3	1.98	0.46
1:A:18:VAL:HG11	1:A:22:THR:HG23	1.97	0.45
1:A:115:PRO:O	1:A:119:GLU:HG3	2.17	0.45
1:A:195:ALA:H	1:A:196:PRO:CG	2.06	0.45
1:A:215:PRO:HB3	1:A:222:ALA:HA	1.99	0.44
1:A:118:VAL:O	1:A:122:VAL:HG23	2.17	0.44
1:A:18:VAL:HA	1:A:19:PRO:HD3	1.97	0.44
1:A:162:LEU:HA	1:A:162:LEU:HD12	1.74	0.43
1:A:242:ASP:O	1:A:243:ASP:C	2.61	0.43
1:A:201:LYS:O	1:A:204:ALA:HB3	2.19	0.43
1:A:129:LEU:HD21	1:A:135:PRO:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:CG1	1:A:22:THR:HG23	2.36	0.43
1:A:279:GLU:H	1:A:279:GLU:CD	2.26	0.42
1:A:197:GLY:CA	1:A:200:ASN:HB2	2.49	0.42
1:A:178:THR:HB	1:A:180:THR:HG23	2.01	0.42
1:A:154:LEU:HB3	1:A:227:LEU:HD13	2.02	0.42
1:A:139:SER:OG	1:A:291:MET:HE2	2.19	0.41
1:A:212:ALA:O	1:A:218:SER:OG	2.23	0.41
1:A:287:VAL:O	1:A:291:MET:HG3	2.21	0.41
1:A:68:LYS:HG2	1:A:137:HIS:HB3	2.03	0.41
1:A:234:VAL:HG13	1:A:262:ILE:HG23	2.02	0.41
1:A:195:ALA:CB	1:A:196:PRO:HG3	2.51	0.40
1:A:81:GLY:O	1:A:82:SER:HB3	2.21	0.40
1:A:20:PRO:HA	1:A:22:THR:H	1.86	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	295/322 (92%)	263 (89%)	28 (10%)	4 (1%)	9 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	PRO
1	A	212	ALA
1	A	271	HIS
1	A	269	VAL

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	229/246 (93%)	197 (86%)	32 (14%)	3 2

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	LYS
1	A	23	GLU
1	A	26	LEU
1	A	33	MET
1	A	46	VAL
1	A	49	VAL
1	A	50	THR
1	A	65	GLN
1	A	104	LEU
1	A	118	VAL
1	A	135	PRO
1	A	136	GLN
1	A	151	LEU
1	A	162	LEU
1	A	165	PRO
1	A	169	ILE
1	A	178	THR
1	A	185	LYS
1	A	187	ARG
1	A	193	MET
1	A	194	VAL
1	A	201	LYS
1	A	227	LEU
1	A	229	PRO
1	A	230	LEU
1	A	239	VAL
1	A	241	LEU
1	A	247	LEU
1	A	257	LYS

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Mol	Chain	Res	Type
1	A	260	LEU
1	A	281	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	181	ASN
1	A	200	ASN
1	A	208	ASN
1	A	233	HIS

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 oligosaccharides 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	297/322 (92%)	0.11	7 (2%) 59 62	6, 16, 33, 46	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	5.4
1	A	20	PRO	5.3
1	A	194	VAL	3.6
1	A	21	GLY	3.6
1	A	1	MET	3.4
1	A	196	PRO	3.2
1	A	19	PRO	2.2

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.