



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:08 AM UTC

PDB ID : 6S3J / pdb_00006s3j
Title : Crystal Structure of lipase from *Geobacillus stearothermophilus* T6 variant E134C/F149C
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Deposited on : 2019-06-25
Resolution : 1.90 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

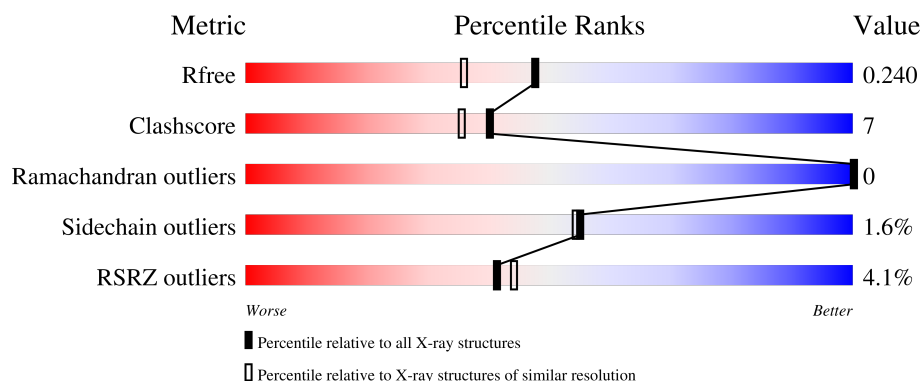
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	392	4% 50% 43% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3444 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 Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3099	1964	555	570	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	CYS	GLU	engineered mutation	UNP Q93A71
A	149	CYS	PHE	engineered mutation	UNP Q93A71
A	323	ALA	THR	conflict	UNP Q93A71
A	390	HIS	-	expression tag	UNP Q93A71
A	391	HIS	-	expression tag	UNP Q93A71
A	392	HIS	-	expression tag	UNP Q93A71
A	393	HIS	-	expression tag	UNP Q93A71
A	394	HIS	-	expression tag	UNP Q93A71
A	395	HIS	-	expression tag	UNP Q93A71

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

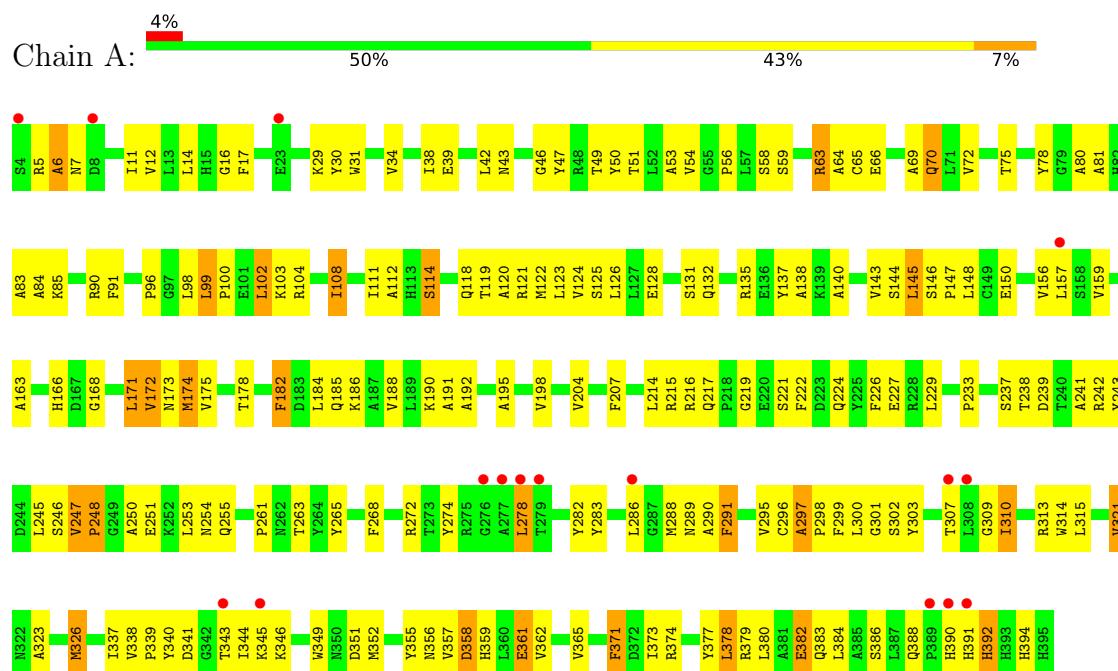
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	343	Total 343	O 343	0	0

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: Lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.59Å 71.59Å 113.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.56 – 1.90 44.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.56-1.90) 98.0 (44.56-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.240 0.225 , 0.240	Depositor DCC
R_{free} test set	1585 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3444	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: ZN, 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	2.17	160/3188 (5.0%)	1.24	12/4335 (0.3%)

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	SER	C-O	-9.69	1.15	1.24
1	A	111	ILE	C-O	-8.83	1.14	1.24
1	A	297	ALA	C-O	-8.59	1.16	1.24
1	A	126	LEU	C-O	-8.38	1.14	1.24
1	A	321	VAL	C-O	-8.37	1.15	1.24
1	A	268	PHE	C-O	-8.32	1.14	1.24
1	A	224	GLN	C-O	-8.27	1.14	1.24
1	A	51	THR	C-O	-8.16	1.14	1.24
1	A	300	LEU	C-O	-8.14	1.14	1.24
1	A	66	GLU	C-O	-7.86	1.15	1.24
1	A	81	ALA	C-O	-7.82	1.15	1.24
1	A	380	LEU	C-O	-7.75	1.15	1.24
1	A	313	ARG	C-O	-7.75	1.14	1.24
1	A	147	PRO	C-O	-7.74	1.14	1.24
1	A	338	VAL	C-O	-7.73	1.14	1.24
1	A	238	THR	C-O	-7.63	1.14	1.24
1	A	394	HIS	C-O	-7.61	1.14	1.23
1	A	227	GLU	C-O	-7.60	1.15	1.24
1	A	242	ARG	C-O	-7.50	1.15	1.24
1	A	148	LEU	C-O	-7.46	1.15	1.24
1	A	112	ALA	C-O	-7.43	1.14	1.24
1	A	98	LEU	C-O	-7.38	1.15	1.24
1	A	43	ASN	C-O	-7.37	1.15	1.24
1	A	251	GLU	C-O	-7.36	1.15	1.24
1	A	289	ASN	C-O	-7.36	1.15	1.23
1	A	323	ALA	C-O	-7.34	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	ALA	C-O	-7.31	1.15	1.24
1	A	207	PHE	C-O	-7.25	1.14	1.24
1	A	90	ARG	C-O	-7.20	1.15	1.24
1	A	345	LYS	C-O	-7.20	1.15	1.23
1	A	291	PHE	C-O	-7.17	1.15	1.24
1	A	361	GLU	C-O	-7.15	1.15	1.24
1	A	29	LYS	C-O	-7.14	1.15	1.24
1	A	14	LEU	C-O	-7.12	1.15	1.24
1	A	174	MET	C-O	-7.12	1.15	1.23
1	A	382	GLU	C-O	-7.09	1.15	1.24
1	A	343	THR	C-O	-7.06	1.16	1.24
1	A	84	ALA	C-O	-6.99	1.16	1.24
1	A	12	VAL	C-O	-6.97	1.16	1.24
1	A	191	ALA	C-O	-6.96	1.16	1.24
1	A	125	SER	C-O	-6.93	1.16	1.24
1	A	171	LEU	C-O	-6.92	1.16	1.24
1	A	299	PHE	C-O	-6.87	1.16	1.24
1	A	215	ARG	C-O	-6.84	1.15	1.23
1	A	122	MET	C-O	-6.76	1.16	1.24
1	A	156	VAL	C-O	-6.73	1.17	1.24
1	A	383	GLN	C-O	-6.71	1.16	1.24
1	A	96	PRO	C-O	-6.68	1.15	1.24
1	A	247	VAL	CA-C	6.67	1.58	1.52
1	A	222	PHE	C-O	-6.63	1.16	1.24
1	A	185	GLN	C-O	-6.62	1.16	1.24
1	A	146	SER	C-O	-6.61	1.15	1.23
1	A	346	LYS	C-O	-6.61	1.15	1.23
1	A	75	THR	C-O	-6.56	1.16	1.24
1	A	80	ALA	C-O	-6.55	1.16	1.24
1	A	72	VAL	C-O	-6.52	1.17	1.24
1	A	378	LEU	C-O	-6.50	1.16	1.24
1	A	69	ALA	C-O	-6.47	1.16	1.24
1	A	303	TYR	C-O	-6.46	1.16	1.24
1	A	145	LEU	C-O	-6.45	1.15	1.24
1	A	351	ASP	C-O	-6.43	1.16	1.23
1	A	282	TYR	C-O	-6.41	1.16	1.24
1	A	63	ARG	C-O	-6.40	1.16	1.24
1	A	261	PRO	C-O	-6.37	1.15	1.24
1	A	175	VAL	C-O	-6.35	1.16	1.24
1	A	344	ILE	C-O	-6.32	1.17	1.24
1	A	245	LEU	C-O	-6.30	1.15	1.24
1	A	217	GLN	C-O	-6.27	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	PHE	C-O	-6.21	1.16	1.24
1	A	365	VAL	C-O	-6.20	1.16	1.24
1	A	250	ALA	C-O	-6.17	1.17	1.24
1	A	124	VAL	C-O	-6.14	1.17	1.24
1	A	386	SER	C-O	-6.11	1.16	1.24
1	A	70	GLN	C-O	-6.08	1.16	1.24
1	A	46	GLY	C-O	-6.07	1.16	1.24
1	A	339	PRO	C-O	-6.06	1.16	1.23
1	A	254	ASN	C-O	-6.06	1.16	1.24
1	A	85	LYS	C-O	-6.03	1.17	1.24
1	A	195	ALA	C-O	-6.02	1.16	1.23
1	A	188	VAL	N-CA	-6.00	1.39	1.46
1	A	137	TYR	C-O	-5.99	1.17	1.24
1	A	272	ARG	C-O	-5.97	1.17	1.24
1	A	102	LEU	C-O	-5.97	1.17	1.24
1	A	5	ARG	C-O	-5.95	1.16	1.24
1	A	263	THR	C-O	-5.94	1.16	1.23
1	A	204	VAL	C-O	-5.93	1.17	1.24
1	A	296	CYS	C-O	-5.92	1.14	1.23
1	A	166	HIS	C-O	-5.91	1.16	1.24
1	A	64	ALA	C-O	-5.89	1.17	1.24
1	A	340	TYR	C-O	-5.85	1.16	1.23
1	A	374	ARG	C-O	-5.83	1.17	1.24
1	A	265	TYR	C-O	-5.83	1.17	1.24
1	A	302	SER	C-O	-5.82	1.16	1.24
1	A	34	VAL	C-O	-5.82	1.17	1.24
1	A	120	ALA	C-O	-5.80	1.17	1.24
1	A	248	PRO	C-O	-5.79	1.17	1.24
1	A	91	PHE	C-O	-5.79	1.17	1.23
1	A	53	ALA	C-O	-5.78	1.17	1.24
1	A	17	PHE	C-O	-5.78	1.16	1.24
1	A	337	ILE	C-O	-5.76	1.18	1.24
1	A	38	ILE	C-O	-5.74	1.17	1.24
1	A	243	TYR	C-O	-5.74	1.17	1.24
1	A	65	CYS	C-O	-5.73	1.17	1.24
1	A	214	LEU	C-O	-5.72	1.16	1.24
1	A	352	MET	C-O	-5.71	1.16	1.24
1	A	132	GLN	C-O	-5.67	1.17	1.24
1	A	172	VAL	C-O	-5.66	1.15	1.23
1	A	301	GLY	C-O	-5.66	1.16	1.23
1	A	78	TYR	C-O	-5.65	1.15	1.24
1	A	131	SER	C-O	-5.63	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	LEU	C-O	-5.63	1.17	1.24
1	A	30	TYR	C-O	-5.62	1.17	1.24
1	A	143	VAL	C-O	-5.58	1.16	1.23
1	A	237	SER	C-O	-5.54	1.16	1.23
1	A	56	PRO	C-O	-5.52	1.17	1.24
1	A	118	GLN	C-O	-5.52	1.17	1.24
1	A	384	LEU	C-O	-5.52	1.17	1.24
1	A	178	THR	C-O	-5.51	1.17	1.24
1	A	140	ALA	C-O	-5.48	1.17	1.24
1	A	254	ASN	CG-OD1	-5.47	1.13	1.23
1	A	377	TYR	C-O	-5.47	1.17	1.24
1	A	355	TYR	C-O	-5.43	1.17	1.23
1	A	253	LEU	C-O	-5.42	1.17	1.24
1	A	255	GLN	C-O	-5.41	1.17	1.24
1	A	359	HIS	C-O	-5.40	1.17	1.24
1	A	379	ARG	C-O	-5.40	1.17	1.24
1	A	198	VAL	N-CA	-5.40	1.41	1.46
1	A	119	THR	C-O	-5.39	1.17	1.24
1	A	392	HIS	C-O	-5.39	1.17	1.23
1	A	159	VAL	C-O	-5.39	1.18	1.24
1	A	192	ALA	C-O	-5.38	1.16	1.24
1	A	290	ALA	C-O	-5.38	1.17	1.24
1	A	278	LEU	C-O	-5.38	1.17	1.24
1	A	58	SER	C-O	-5.36	1.16	1.23
1	A	16	GLY	C-O	-5.34	1.16	1.23
1	A	226	PHE	C-O	-5.33	1.17	1.24
1	A	54	VAL	C-O	-5.33	1.17	1.23
1	A	31	TRP	C-O	-5.28	1.18	1.23
1	A	11	ILE	C-O	-5.28	1.17	1.24
1	A	168	GLY	C-O	-5.28	1.15	1.23
1	A	288	MET	C-O	-5.27	1.17	1.23
1	A	190	LYS	C-O	-5.24	1.18	1.24
1	A	173	ASN	C-O	-5.24	1.17	1.24
1	A	6	ALA	C-O	-5.21	1.17	1.24
1	A	108	ILE	C-O	-5.20	1.18	1.23
1	A	7	ASN	N-CA	-5.19	1.39	1.45
1	A	216	ARG	C-O	-5.18	1.17	1.23
1	A	123	LEU	C-O	-5.16	1.18	1.24
1	A	128	GLU	C-O	-5.15	1.18	1.24
1	A	233	PRO	C-O	-5.11	1.17	1.24
1	A	341	ASP	C-O	-5.10	1.16	1.24
1	A	219	GLY	C-O	-5.09	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	SER	C-O	-5.08	1.17	1.23
1	A	371	PHE	C-O	-5.07	1.18	1.24
1	A	99	LEU	N-CA	-5.06	1.40	1.46
1	A	138	ALA	C-O	-5.05	1.18	1.24
1	A	356	ASN	C-O	-5.02	1.16	1.23
1	A	221	SER	C-O	-5.01	1.17	1.23
1	A	247	VAL	C-O	-5.01	1.20	1.24
1	A	362	VAL	C-O	-5.01	1.18	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	ASP	CA-CB-CG	9.85	122.45	112.60
1	A	156	VAL	N-CA-C	9.74	121.78	107.37
1	A	326	MET	N-CA-C	7.88	123.00	113.23
1	A	373	ILE	N-CA-C	7.12	117.88	110.62
1	A	295	VAL	N-CA-C	6.05	120.88	112.35
1	A	217	GLN	N-CA-C	5.79	116.78	110.13
1	A	30	TYR	N-CA-C	-5.54	105.24	111.28
1	A	7	ASN	N-CA-C	5.44	117.34	109.07
1	A	315	LEU	N-CA-C	5.41	117.26	111.36
1	A	241	ALA	N-CA-C	-5.17	105.72	111.36
1	A	29	LYS	N-CA-C	5.11	117.89	109.76
1	A	278	LEU	N-CA-C	5.07	118.72	112.54

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	3099	0	2958	40	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	343	0	0	2	0
All	All	3444	0	2958	40	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 7.

All (40) 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:358:ASP:OD1	1:A:361:GLU:HG3	1.79	0.80
1:A:171:LEU:CD1	1:A:174:MET:HE2	2.12	0.79
1:A:171:LEU:HD11	1:A:174:MET:HE2	1.77	0.66
1:A:103:LYS:HG2	4:A:807:HOH:O	1.96	0.64
1:A:184:LEU:HB2	1:A:291:PHE:HE2	1.65	0.62
1:A:171:LEU:HD12	1:A:174:MET:HE2	1.83	0.60
1:A:157:LEU:C	1:A:157:LEU:HD23	2.28	0.59
1:A:114:SER:HA	1:A:163:ALA:O	2.04	0.57
1:A:184:LEU:HB2	1:A:291:PHE:CE2	2.40	0.57
1:A:102:LEU:HD21	1:A:108:ILE:HG23	1.88	0.55
1:A:310:ILE:HD12	1:A:314:TRP:CE2	2.42	0.55
1:A:135:ARG:HG2	1:A:145:LEU:HD21	1.88	0.55
1:A:310:ILE:HD13	1:A:310:ILE:N	2.22	0.53
1:A:157:LEU:HD23	1:A:157:LEU:O	2.10	0.52
1:A:145:LEU:HD23	1:A:150:GLU:HG2	1.93	0.50
1:A:50:TYR:CE1	1:A:99:LEU:HD21	2.47	0.50
1:A:47:TYR:OH	1:A:382:GLU:HG2	2.13	0.48
1:A:392:HIS:HA	4:A:528:HOH:O	2.14	0.47
1:A:182:PHE:O	1:A:186:LYS:HG3	2.15	0.47
1:A:39:GLU:HG3	1:A:49:THR:HG22	1.97	0.46
1:A:321:VAL:HB	1:A:326:MET:HE2	1.98	0.45
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.98	0.44
1:A:59:SER:HB3	1:A:239:ASP:C	2.43	0.43
1:A:310:ILE:HD12	1:A:314:TRP:CD2	2.53	0.43
1:A:6:ALA:HB2	1:A:388:GLN:NE2	2.33	0.42
1:A:172:VAL:HG21	1:A:246:SER:HA	2.01	0.42
1:A:274:TYR:CZ	1:A:283:TYR:HB2	2.54	0.42
1:A:388:GLN:HB2	1:A:391:HIS:CE1	2.54	0.42
1:A:309:GLY:C	1:A:310:ILE:HD13	2.45	0.42
1:A:104:ARG:HH11	1:A:104:ARG:HD3	1.68	0.41
1:A:42:LEU:HD23	1:A:378:LEU:HD23	2.02	0.41
1:A:42:LEU:CD2	1:A:378:LEU:HD23	2.49	0.41
1:A:99:LEU:HA	1:A:100:PRO:HD2	1.91	0.41
1:A:47:TYR:HH	1:A:382:GLU:HG2	1.84	0.41
1:A:70:GLN:HE21	1:A:70:GLN:HB2	1.65	0.41
1:A:297:ALA:N	1:A:298:PRO:CD	2.83	0.41
1:A:357:VAL:HG11	1:A:371:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLN:HB2	1:A:391:HIS:HE1	1.86	0.41
1:A:63:ARG:HH11	1:A:63:ARG:HD2	1.74	0.40
1:A:121:ARG:HD2	1:A:349:TRP:CZ2	2.56	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	390/392 (100%)	376 (96%)	14 (4%)	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	320/320 (100%)	315 (98%)	5 (2%)	55	54

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	LEU
1	A	286	LEU
1	A	307	THR

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Mol	Chain	Res	Type
1	A	310	ILE
1	A	390	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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	392/392 (100%)	0.29	16 (4%) 41 44	10, 15, 31, 67	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	ALA	4.5
1	A	390	HIS	3.9
1	A	4	SER	3.6
1	A	278	LEU	3.3
1	A	276	GLY	3.2
1	A	8	ASP	3.2
1	A	308	LEU	3.2
1	A	23	GLU	3.1
1	A	389	PRO	2.8
1	A	391	HIS	2.5
1	A	307	THR	2.5
1	A	157	LEU	2.3
1	A	279	THR	2.3
1	A	343	THR	2.2
1	A	286	LEU	2.1
1	A	345	LYS	2.0

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($\text{\AA}^2$)	Q<0.9
3	CA	A	402	1/1	0.92	0.10	36,36,36,36	0
2	ZN	A	401	1/1	0.97	0.07	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.