



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 05:48 AM UTC

PDB ID : 6FZD / pdb_00006fzd
Title : Crystal Structure of lipase from *Geobacillus stearothermophilus* T6 variant
L184F/A187F/L360F
Authors : Gihaz, S.; Kanteev, M.; Pazy, Y.; Fishman, A.
Deposited on : 2018-03-14
Resolution : 1.80 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

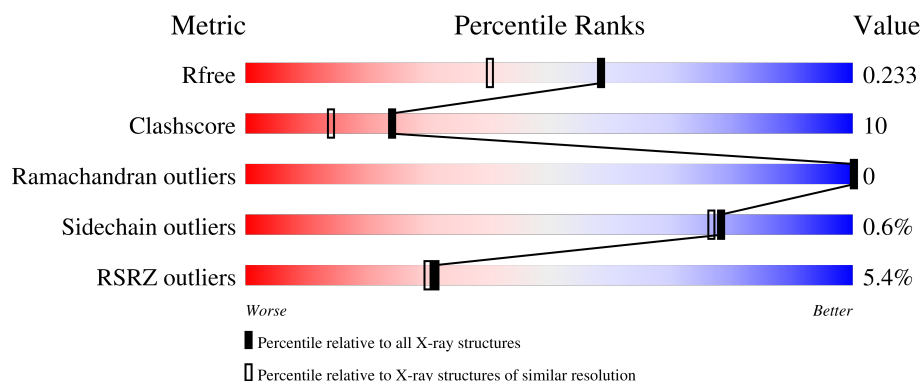
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	5% 52% 43% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3392 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
			3119	1984	555	572	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	PHE	LEU	engineered mutation	UNP Q93A71
A	187	PHE	ALA	engineered mutation	UNP Q93A71
A	323	ALA	THR	conflict	UNP Q93A71
A	360	PHE	LEU	engineered mutation	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		

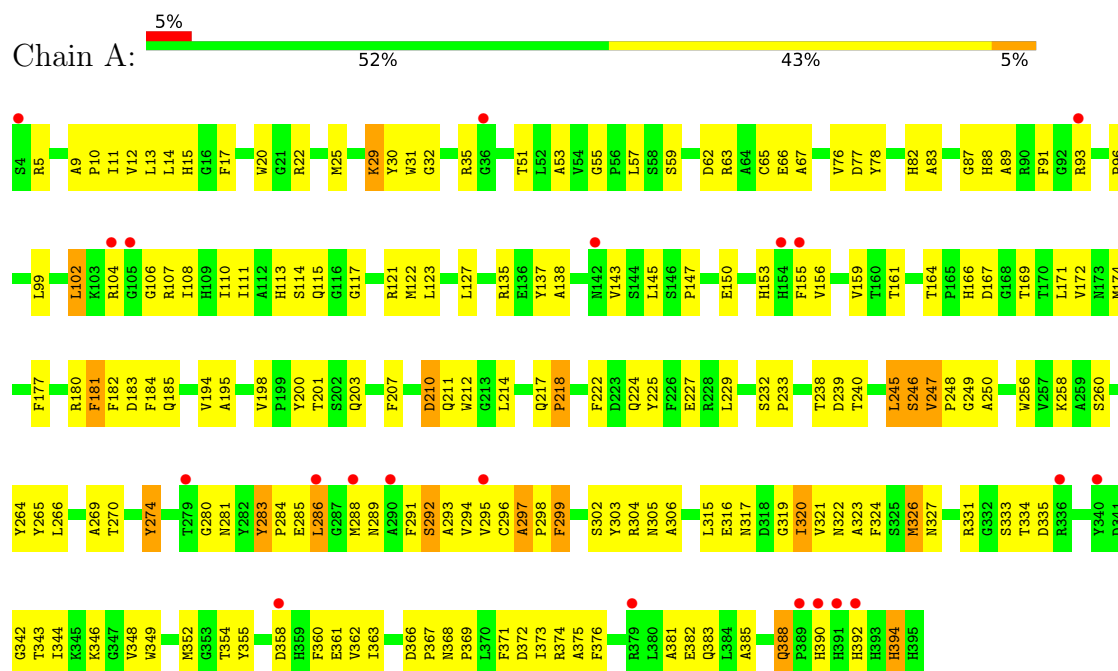
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	271	Total 271	O 271	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: Lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.86Å 70.88Å 113.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.63 – 1.80 45.63 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.63-1.80) 98.8 (45.63-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.97 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.212 , 0.229 0.215 , 0.233	Depositor DCC
R_{free} test set	1873 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3392	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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](#)

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	1.93	132/3212 (4.1%)	1.11	12/4366 (0.3%)

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	LEU	C-O	-8.51	1.14	1.23
1	A	82	HIS	C-O	-8.51	1.14	1.24
1	A	371	PHE	C-O	-8.45	1.14	1.24
1	A	111	ILE	C-O	-8.28	1.15	1.24
1	A	135	ARG	C-O	-8.22	1.14	1.24
1	A	355	TYR	C-O	-8.15	1.14	1.23
1	A	376	PHE	C-O	-7.95	1.15	1.24
1	A	122	MET	C-O	-7.91	1.14	1.24
1	A	372	ASP	C-O	-7.89	1.14	1.23
1	A	322	ASN	C-O	-7.85	1.14	1.23
1	A	198	VAL	C-O	-7.85	1.16	1.23
1	A	388	GLN	C-O	-7.75	1.14	1.24
1	A	229	LEU	C-O	-7.74	1.15	1.24
1	A	13	LEU	C-O	-7.69	1.14	1.23
1	A	200	TYR	C-O	-7.67	1.14	1.23
1	A	138	ALA	C-O	-7.63	1.15	1.24
1	A	225	TYR	C-O	-7.63	1.15	1.24
1	A	156	VAL	C-O	-7.58	1.16	1.24
1	A	51	THR	C-O	-7.31	1.15	1.24
1	A	77	ASP	C-O	-7.28	1.15	1.23
1	A	110	ILE	C-O	-7.22	1.16	1.24
1	A	65	CYS	C-O	-7.22	1.15	1.24
1	A	102	LEU	C-O	-7.21	1.15	1.24
1	A	17	PHE	C-O	-7.20	1.14	1.24
1	A	114	SER	C-O	-7.19	1.15	1.24
1	A	123	LEU	C-O	-7.12	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	ALA	C-O	-7.11	1.14	1.23
1	A	284	PRO	C-O	-7.10	1.16	1.23
1	A	181	PHE	C-O	-7.06	1.16	1.24
1	A	183	ASP	C-O	-7.06	1.15	1.24
1	A	227	GLU	C-O	-7.03	1.15	1.24
1	A	159	VAL	C-O	-7.02	1.16	1.24
1	A	137	TYR	C-O	-6.95	1.15	1.24
1	A	269	ALA	C-O	-6.75	1.15	1.23
1	A	266	LEU	C-O	-6.73	1.15	1.24
1	A	145	LEU	C-O	-6.68	1.16	1.24
1	A	333	SER	C-O	-6.66	1.15	1.23
1	A	161	THR	C-O	-6.57	1.15	1.24
1	A	11	ILE	C-O	-6.56	1.15	1.24
1	A	323	ALA	C-O	-6.54	1.16	1.24
1	A	127	LEU	C-O	-6.53	1.16	1.24
1	A	62	ASP	C-O	-6.50	1.16	1.24
1	A	270	THR	C-O	-6.48	1.16	1.23
1	A	53	ALA	C-O	-6.45	1.16	1.23
1	A	99	LEU	N-CA	-6.45	1.39	1.46
1	A	297	ALA	C-O	-6.44	1.18	1.24
1	A	15	HIS	C-O	-6.44	1.15	1.23
1	A	383	GLN	C-O	-6.37	1.16	1.24
1	A	256	TRP	C-O	-6.33	1.16	1.24
1	A	296	CYS	C-O	-6.32	1.16	1.24
1	A	218	PRO	C-O	-6.30	1.15	1.23
1	A	250	ALA	C-O	-6.29	1.16	1.24
1	A	113	HIS	C-O	-6.27	1.16	1.24
1	A	224	GLN	C-O	-6.26	1.17	1.24
1	A	260	SER	C-O	-6.25	1.15	1.24
1	A	194	VAL	C-O	-6.22	1.17	1.24
1	A	258	LYS	C-O	-6.19	1.16	1.23
1	A	367	PRO	C-O	-6.18	1.16	1.23
1	A	89	ALA	C-O	-6.17	1.16	1.23
1	A	222	PHE	C-O	-6.13	1.16	1.24
1	A	249	GLY	C-O	-6.12	1.16	1.23
1	A	240	THR	C-O	-6.08	1.16	1.23
1	A	368	ASN	C-O	-6.07	1.16	1.24
1	A	369	PRO	C-O	-6.04	1.16	1.24
1	A	348	VAL	C-O	-6.02	1.17	1.23
1	A	265	TYR	C-O	-5.98	1.16	1.24
1	A	9	ALA	C-O	-5.97	1.16	1.24
1	A	184	PHE	C-O	-5.95	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	LEU	C-O	-5.92	1.16	1.23
1	A	29	LYS	C-O	-5.92	1.16	1.23
1	A	394	HIS	C-O	-5.90	1.16	1.23
1	A	381	ALA	C-O	-5.89	1.17	1.24
1	A	354	THR	C-O	-5.84	1.17	1.24
1	A	12	VAL	C-O	-5.83	1.17	1.24
1	A	214	LEU	C-O	-5.83	1.16	1.24
1	A	169	THR	C-O	-5.81	1.16	1.23
1	A	382	GLU	C-O	-5.79	1.17	1.24
1	A	305	ASN	C-O	-5.77	1.18	1.23
1	A	66	GLU	C-O	-5.75	1.17	1.24
1	A	334	THR	C-O	-5.73	1.16	1.23
1	A	342	GLY	C-O	-5.72	1.16	1.24
1	A	210	ASP	C-O	-5.72	1.17	1.24
1	A	303	TYR	C-O	-5.69	1.17	1.24
1	A	304	ARG	C-O	-5.69	1.16	1.23
1	A	285	GLU	C-O	-5.63	1.16	1.23
1	A	150	GLU	C-O	-5.62	1.16	1.24
1	A	374	ARG	C-O	-5.62	1.17	1.24
1	A	352	MET	C-O	-5.61	1.16	1.24
1	A	164	THR	C-O	-5.61	1.16	1.24
1	A	299	PHE	C-O	-5.56	1.17	1.24
1	A	87	GLY	C-O	-5.55	1.16	1.24
1	A	280	GLY	C-O	-5.53	1.16	1.24
1	A	201	THR	C-O	-5.53	1.17	1.24
1	A	171	LEU	C-O	-5.51	1.17	1.24
1	A	274	TYR	C-O	-5.49	1.16	1.23
1	A	245	LEU	C-O	-5.47	1.16	1.24
1	A	335	ASP	C-O	-5.45	1.17	1.23
1	A	55	GLY	C-O	-5.44	1.16	1.24
1	A	78	TYR	C-O	-5.43	1.16	1.24
1	A	291	PHE	C-O	-5.43	1.17	1.24
1	A	264	TYR	C-O	-5.42	1.17	1.23
1	A	283	TYR	C-O	-5.41	1.17	1.24
1	A	315	LEU	C-O	-5.41	1.17	1.24
1	A	366	ASP	C-O	-5.40	1.17	1.24
1	A	331	ARG	C-O	-5.38	1.17	1.24
1	A	106	GLY	C-O	-5.32	1.17	1.23
1	A	324	PHE	C-O	-5.31	1.17	1.24
1	A	238	THR	C-O	-5.28	1.17	1.24
1	A	349	TRP	C-O	-5.26	1.17	1.24
1	A	83	ALA	C-O	-5.25	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	VAL	C-O	-5.24	1.18	1.24
1	A	177	PHE	C-O	-5.23	1.18	1.24
1	A	30	TYR	C-O	-5.21	1.18	1.24
1	A	67	ALA	C-O	-5.21	1.18	1.24
1	A	203	GLN	C-O	-5.20	1.18	1.24
1	A	292	SER	C-O	-5.20	1.17	1.24
1	A	343	THR	C-O	-5.17	1.18	1.24
1	A	88	HIS	C-O	-5.16	1.17	1.23
1	A	316	GLU	C-O	-5.15	1.17	1.23
1	A	31	TRP	C-O	-5.14	1.17	1.23
1	A	302	SER	C-O	-5.14	1.17	1.23
1	A	207	PHE	C-O	-5.13	1.16	1.24
1	A	246	SER	C-O	-5.13	1.17	1.23
1	A	375	ALA	C-O	-5.12	1.18	1.24
1	A	335	ASP	CG-OD1	-5.11	1.15	1.25
1	A	63	ARG	C-O	-5.09	1.17	1.24
1	A	327	ASN	CG-OD1	-5.08	1.14	1.23
1	A	281	ASN	C-O	-5.07	1.17	1.23
1	A	167	ASP	C-O	-5.07	1.17	1.24
1	A	346	LYS	C-O	-5.05	1.17	1.23
1	A	320	ILE	C-O	-5.03	1.18	1.24
1	A	96	PRO	C-O	-5.00	1.18	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	MET	N-CA-C	7.91	123.26	112.90
1	A	293	ALA	N-CA-C	7.73	121.20	111.69
1	A	29	LYS	N-CA-C	6.53	119.95	110.28
1	A	156	VAL	N-CA-C	6.19	116.53	107.37
1	A	306	ALA	N-CA-C	5.33	117.09	111.28
1	A	155	PHE	CB-CA-C	-5.27	100.50	109.03
1	A	333	SER	N-CA-C	5.15	118.14	109.95
1	A	240	THR	N-CA-C	5.12	116.86	109.07
1	A	143	VAL	CB-CA-C	-5.10	105.98	111.59
1	A	317	ASN	N-CA-C	5.09	116.03	108.60
1	A	294	VAL	N-CA-C	5.08	115.23	110.30
1	A	373	ILE	N-CA-C	5.02	115.74	110.62

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	3119	0	2965	61	0
2	A	1	0	0	0	0
3	A	1	0	0	1	0
4	A	271	0	0	2	0
All	All	3392	0	2965	61	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 10.

All (61) 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:117:GLY:O	1:A:121:ARG:HG3	1.67	0.94
1:A:93:ARG:CD	1:A:210:ASP:OD2	2.18	0.92
1:A:358:ASP:OD2	1:A:361:GLU:N	2.16	0.78
1:A:93:ARG:HD3	1:A:210:ASP:CG	2.11	0.75
1:A:358:ASP:OD2	1:A:361:GLU:CB	2.35	0.74
1:A:93:ARG:HD3	1:A:210:ASP:OD2	1.85	0.74
1:A:5:ARG:HG3	1:A:385:ALA:HB1	1.71	0.72
1:A:180:ARG:HD2	1:A:295:VAL:HG11	1.70	0.71
1:A:232:SER:HB2	1:A:233:PRO:HD2	1.75	0.68
1:A:289:ASN:OD1	1:A:292:SER:N	2.25	0.68
1:A:358:ASP:OD2	1:A:361:GLU:HB2	1.93	0.67
1:A:358:ASP:OD2	1:A:361:GLU:HG3	1.94	0.67
1:A:361:GLU:OE2	3:A:402:CA:CA	1.71	0.67
1:A:76:VAL:HG23	1:A:93:ARG:O	1.97	0.65
1:A:358:ASP:OD2	1:A:361:GLU:CG	2.46	0.64
1:A:362:VAL:HG13	1:A:363:ILE:HG23	1.80	0.63
1:A:172:VAL:HG21	1:A:246:SER:HA	1.82	0.61
1:A:93:ARG:HD2	1:A:210:ASP:OD2	2.02	0.58
1:A:297:ALA:HB3	1:A:298:PRO:HD3	1.84	0.58
1:A:180:ARG:CD	1:A:295:VAL:HG11	2.34	0.57
1:A:10:PRO:HD2	1:A:107:ARG:O	2.05	0.57
1:A:182:PHE:O	1:A:185:GLN:HB2	2.05	0.56
1:A:232:SER:HB2	1:A:233:PRO:CD	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.88	0.55
1:A:115:GLN:OE1	1:A:245:LEU:CG	2.55	0.54
1:A:93:ARG:CG	1:A:210:ASP:OD2	2.55	0.54
1:A:320:ILE:HD11	1:A:360:PHE:HE2	1.72	0.53
1:A:93:ARG:HG2	1:A:210:ASP:OD2	2.08	0.52
1:A:93:ARG:HD3	1:A:210:ASP:OD1	2.10	0.52
1:A:32:GLY:O	1:A:35:ARG:HB2	2.10	0.52
1:A:321:VAL:HB	1:A:326:MET:HE2	1.92	0.51
1:A:358:ASP:CG	1:A:361:GLU:HG3	2.37	0.50
1:A:288:MET:HE1	1:A:319:GLY:CA	2.42	0.50
1:A:115:GLN:OE1	1:A:245:LEU:HD21	2.12	0.50
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.77	0.49
1:A:22:ARG:HG2	1:A:22:ARG:NH1	2.27	0.49
1:A:115:GLN:OE1	1:A:245:LEU:HG	2.13	0.49
1:A:20:TRP:CE2	1:A:25:MET:HG3	2.48	0.48
1:A:174:MET:HG2	1:A:299:PHE:CD2	2.49	0.48
1:A:115:GLN:OE1	1:A:245:LEU:HD11	2.14	0.48
1:A:388:GLN:HG3	1:A:390:HIS:O	2.13	0.48
1:A:93:ARG:CD	1:A:210:ASP:CG	2.80	0.47
1:A:392:HIS:O	1:A:392:HIS:ND1	2.47	0.47
1:A:147:PRO:O	1:A:153:HIS:HE1	1.97	0.47
1:A:217:GLN:HB3	1:A:218:PRO:HD2	1.97	0.47
1:A:320:ILE:HD11	1:A:360:PHE:CE2	2.49	0.46
1:A:29:LYS:NZ	4:A:518:HOH:O	2.46	0.45
1:A:10:PRO:HG2	1:A:108:ILE:HG22	2.00	0.44
1:A:57:LEU:CD2	1:A:181:PHE:HE2	2.31	0.44
1:A:211:GLN:HG2	1:A:212:TRP:N	2.33	0.43
1:A:274:TYR:CZ	1:A:283:TYR:HB2	2.52	0.43
1:A:172:VAL:HG21	1:A:246:SER:CA	2.47	0.43
1:A:59:SER:HB3	1:A:239:ASP:C	2.44	0.42
1:A:102:LEU:HD21	1:A:108:ILE:HG23	2.02	0.42
1:A:76:VAL:O	1:A:91:PHE:HA	2.19	0.42
1:A:217:GLN:NE2	4:A:528:HOH:O	2.53	0.41
1:A:121:ARG:HD2	1:A:166:HIS:CE1	2.55	0.41
1:A:392:HIS:CE1	1:A:394:HIS:CD2	3.09	0.41
1:A:104:ARG:NH1	1:A:104:ARG:HG3	2.36	0.41
1:A:288:MET:CE	1:A:319:GLY:CA	2.99	0.41
1:A:392:HIS:ND1	1:A:392:HIS:C	2.80	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	390/392 (100%)	375 (96%)	15 (4%)	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	321/321 (100%)	319 (99%)	2 (1%)	78	77

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	LEU
1	A	344	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	141	HIS
1	A	173	ASN
1	A	203	GLN

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 [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	392/392 (100%)	0.41	21 (5%) 31 30	10, 18, 31, 65	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	392	HIS	5.3
1	A	390	HIS	5.2
1	A	391	HIS	4.5
1	A	4	SER	4.2
1	A	295	VAL	4.0
1	A	340	TYR	3.9
1	A	286	LEU	3.6
1	A	358	ASP	3.1
1	A	154	HIS	3.1
1	A	105	GLY	2.9
1	A	104	ARG	2.9
1	A	36	GLY	2.8
1	A	288	MET	2.6
1	A	155	PHE	2.4
1	A	93	ARG	2.4
1	A	336	ARG	2.4
1	A	290	ALA	2.3
1	A	279	THR	2.3
1	A	142	ASN	2.1
1	A	379	ARG	2.1
1	A	389	PRO	2.1

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	0.90	0.14	33,33,33,33	0
2	ZN	A	401	1/1	0.99	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.