



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:06 PM UTC

PDB ID : 6FZA / pdb_00006fza
Title : Crystal Structure of lipase from *Geobacillus stearothermophilus* T6 methanol stable variant A187F
Authors : Gihaz, S.; Kanteev, M.; Pazy, Y.; Fishman, A.
Deposited on : 2018-03-14
Resolution : 1.75 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

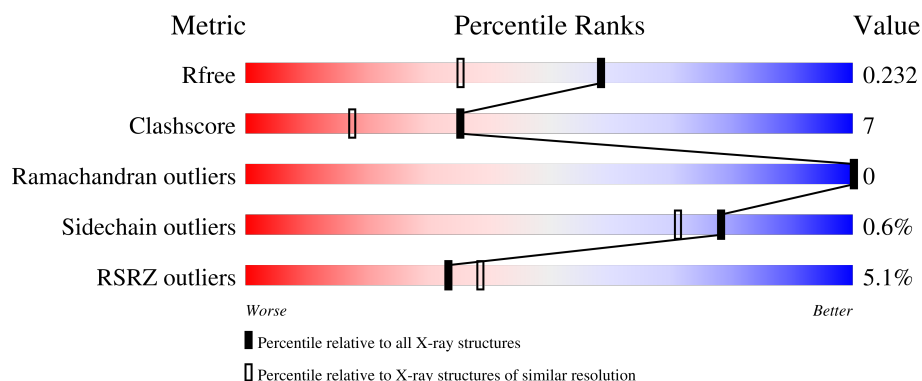
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	391	5% 48% 43% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3314 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	391	Total	C	N	O	S	0	0	0
			3107	1975	554	570	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	PHE	ALA	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		

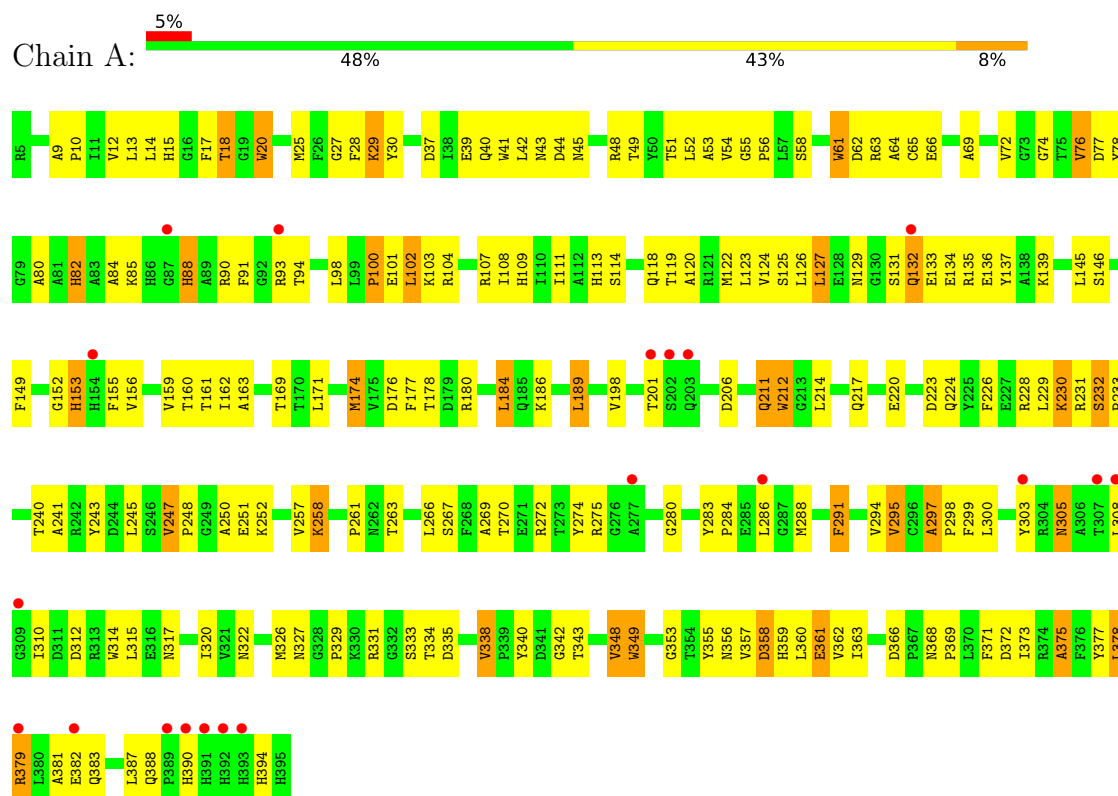
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	205	Total	O	0	0
			205	205		

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	49.47Å 71.26Å 112.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.21 – 1.75 38.21 – 1.75	Depositor EDS
% Data completeness (in resolution range)	86.5 (38.21-1.75) 86.5 (38.21-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.216 , 0.231 0.218 , 0.232	Depositor DCC
R_{free} test set	1733 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3314	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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	2.10	161/3198 (5.0%)	1.17	15/4348 (0.3%)

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	ALA	C-O	-9.56	1.15	1.24
1	A	162	ILE	C-O	-9.27	1.14	1.24
1	A	61	TRP	C-O	-8.78	1.14	1.24
1	A	229	LEU	C-O	-8.61	1.13	1.24
1	A	41	TRP	C-O	-8.56	1.14	1.24
1	A	122	MET	C-O	-8.38	1.14	1.24
1	A	320	ILE	C-O	-8.38	1.14	1.24
1	A	76	VAL	C-O	-8.31	1.15	1.24
1	A	123	LEU	C-O	-8.30	1.14	1.24
1	A	243	TYR	C-O	-8.26	1.14	1.24
1	A	52	LEU	C-O	-8.22	1.14	1.23
1	A	14	LEU	C-O	-8.21	1.14	1.23
1	A	224	GLN	C-O	-8.21	1.14	1.24
1	A	266	LEU	C-O	-8.01	1.14	1.24
1	A	77	ASP	C-O	-7.93	1.15	1.24
1	A	42	LEU	C-O	-7.79	1.15	1.24
1	A	214	LEU	C-O	-7.76	1.14	1.24
1	A	156	VAL	C-O	-7.75	1.15	1.24
1	A	291	PHE	C-O	-7.70	1.15	1.24
1	A	189	LEU	C-O	-7.66	1.15	1.24
1	A	102	LEU	C-O	-7.61	1.15	1.24
1	A	28	PHE	C-O	-7.60	1.14	1.23
1	A	355	TYR	C-O	-7.54	1.14	1.24
1	A	270	THR	C-O	-7.48	1.14	1.23
1	A	119	THR	C-O	-7.40	1.15	1.24
1	A	252	LYS	C-O	-7.35	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	VAL	C-O	-7.35	1.16	1.24
1	A	160	THR	C-O	-7.33	1.15	1.24
1	A	124	VAL	C-O	-7.32	1.15	1.24
1	A	372	ASP	C-O	-7.30	1.15	1.23
1	A	348	VAL	C-O	-7.25	1.16	1.23
1	A	118	GLN	C-O	-7.18	1.15	1.24
1	A	315	LEU	C-O	-7.14	1.14	1.24
1	A	51	THR	C-O	-7.11	1.15	1.24
1	A	247	VAL	C-O	-7.09	1.18	1.24
1	A	272	ARG	C-O	-7.02	1.16	1.24
1	A	114	SER	C-O	-7.02	1.17	1.24
1	A	80	ALA	C-O	-7.00	1.16	1.24
1	A	329	PRO	C-O	-6.99	1.15	1.23
1	A	72	VAL	C-O	-6.97	1.16	1.24
1	A	275	ARG	C-O	-6.94	1.15	1.24
1	A	294	VAL	C-O	-6.93	1.15	1.23
1	A	12	VAL	C-O	-6.83	1.16	1.24
1	A	48	ARG	C-O	-6.82	1.15	1.23
1	A	63	ARG	C-O	-6.77	1.16	1.24
1	A	109	HIS	C-O	-6.75	1.15	1.24
1	A	65	CYS	C-O	-6.70	1.16	1.24
1	A	134	GLU	C-O	-6.67	1.16	1.24
1	A	78	TYR	C-O	-6.67	1.15	1.24
1	A	82	HIS	C-O	-6.64	1.16	1.24
1	A	58	SER	C-O	-6.64	1.14	1.23
1	A	56	PRO	C-O	-6.63	1.16	1.24
1	A	40	GLN	C-O	-6.57	1.16	1.24
1	A	369	PRO	C-O	-6.56	1.15	1.24
1	A	338	VAL	C-O	-6.56	1.17	1.23
1	A	15	HIS	C-O	-6.55	1.15	1.23
1	A	39	GLU	C-O	-6.51	1.16	1.24
1	A	305	ASN	C-O	-6.50	1.16	1.23
1	A	98	LEU	C-O	-6.45	1.15	1.24
1	A	169	THR	C-O	-6.42	1.16	1.23
1	A	241	ALA	C-O	-6.42	1.16	1.24
1	A	113	HIS	C-O	-6.33	1.15	1.24
1	A	125	SER	C-O	-6.33	1.16	1.24
1	A	217	GLN	C-O	-6.33	1.17	1.23
1	A	381	ALA	C-O	-6.32	1.16	1.24
1	A	43	ASN	C-O	-6.29	1.16	1.24
1	A	177	PHE	C-O	-6.26	1.16	1.24
1	A	62	ASP	C-O	-6.26	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ALA	C-O	-6.26	1.16	1.24
1	A	261	PRO	C-O	-6.23	1.16	1.24
1	A	267	SER	C-O	-6.22	1.16	1.24
1	A	127	LEU	C-O	-6.17	1.17	1.24
1	A	300	LEU	C-O	-6.16	1.17	1.24
1	A	111	ILE	C-O	-6.16	1.17	1.24
1	A	310	ILE	C-O	-6.16	1.16	1.23
1	A	132	GLN	C-O	-6.14	1.17	1.24
1	A	288	MET	C-O	-6.13	1.16	1.23
1	A	230	LYS	C-O	-6.12	1.16	1.24
1	A	366	ASP	C-O	-6.04	1.16	1.24
1	A	356	ASN	C-O	-6.02	1.17	1.23
1	A	133	GLU	C-O	-6.00	1.17	1.24
1	A	198	VAL	C-O	-5.99	1.18	1.23
1	A	29	LYS	C-O	-5.98	1.16	1.23
1	A	53	ALA	C-O	-5.98	1.17	1.24
1	A	257	VAL	C-O	-5.97	1.14	1.23
1	A	153	HIS	C-O	-5.95	1.16	1.23
1	A	371	PHE	C-O	-5.92	1.17	1.24
1	A	312	ASP	C-O	-5.92	1.16	1.24
1	A	37	ASP	C-O	-5.92	1.17	1.23
1	A	163	ALA	C-O	-5.90	1.16	1.23
1	A	184	LEU	C-O	-5.90	1.17	1.24
1	A	378	LEU	C-O	-5.88	1.17	1.24
1	A	349	TRP	C-O	-5.87	1.16	1.24
1	A	20	TRP	C-O	-5.86	1.16	1.23
1	A	161	THR	C-O	-5.85	1.16	1.24
1	A	149	PHE	C-O	-5.85	1.16	1.24
1	A	90	ARG	C-O	-5.82	1.17	1.24
1	A	373	ILE	C-O	-5.80	1.17	1.24
1	A	375	ALA	C-O	-5.80	1.17	1.24
1	A	49	THR	C-O	-5.80	1.17	1.23
1	A	317	ASN	C-O	-5.79	1.16	1.23
1	A	379	ARG	C-O	-5.77	1.17	1.24
1	A	27	GLY	C-O	-5.75	1.16	1.24
1	A	258	LYS	C-O	-5.69	1.16	1.23
1	A	94	THR	C-O	-5.68	1.17	1.23
1	A	361	GLU	C-O	-5.68	1.17	1.24
1	A	146	SER	C-O	-5.66	1.16	1.23
1	A	327	ASN	C-O	-5.65	1.16	1.24
1	A	269	ALA	C-O	-5.64	1.17	1.23
1	A	145	LEU	C-O	-5.62	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	TRP	C-O	-5.61	1.16	1.24
1	A	263	THR	C-O	-5.60	1.16	1.24
1	A	368	ASN	C-O	-5.58	1.17	1.24
1	A	358	ASP	C-O	-5.58	1.16	1.23
1	A	101	GLU	C-O	-5.57	1.17	1.24
1	A	383	GLN	C-O	-5.56	1.17	1.24
1	A	250	ALA	C-O	-5.55	1.17	1.24
1	A	13	LEU	C-O	-5.55	1.17	1.23
1	A	155	PHE	C-O	-5.55	1.17	1.23
1	A	69	ALA	C-O	-5.54	1.17	1.24
1	A	335	ASP	C-O	-5.54	1.17	1.23
1	A	174	MET	C-O	-5.54	1.17	1.23
1	A	359	HIS	C-O	-5.53	1.17	1.24
1	A	231	ARG	C-O	-5.51	1.16	1.24
1	A	353	GLY	C-O	-5.51	1.17	1.23
1	A	120	ALA	C-O	-5.51	1.17	1.24
1	A	45	ASN	C-O	-5.50	1.16	1.24
1	A	232	SER	C-O	-5.49	1.17	1.23
1	A	178	THR	C-O	-5.46	1.17	1.24
1	A	84	ALA	C-O	-5.45	1.17	1.24
1	A	299	PHE	C-O	-5.44	1.17	1.24
1	A	360	LEU	C-O	-5.44	1.17	1.24
1	A	126	LEU	C-O	-5.44	1.17	1.24
1	A	9	ALA	C-O	-5.40	1.16	1.24
1	A	240	THR	C-O	-5.39	1.17	1.23
1	A	357	VAL	C-O	-5.38	1.17	1.23
1	A	129	ASN	C-O	-5.38	1.17	1.24
1	A	206	ASP	C-O	-5.37	1.17	1.24
1	A	152	GLY	C-O	-5.35	1.17	1.24
1	A	91	PHE	C-O	-5.34	1.17	1.23
1	A	137	TYR	C-O	-5.34	1.17	1.24
1	A	55	GLY	C-O	-5.33	1.16	1.24
1	A	284	PRO	C-O	-5.31	1.18	1.23
1	A	322	ASN	C-O	-5.26	1.17	1.24
1	A	54	VAL	C-O	-5.25	1.17	1.23
1	A	100	PRO	C-O	-5.25	1.17	1.24
1	A	245	LEU	C-O	-5.23	1.17	1.24
1	A	211	GLN	C-O	-5.21	1.17	1.24
1	A	251	GLU	C-O	-5.14	1.18	1.24
1	A	74	GLY	C-O	-5.13	1.18	1.23
1	A	314	TRP	C-O	-5.12	1.17	1.24
1	A	377	TYR	C-O	-5.11	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	THR	CA-C	5.11	1.58	1.52
1	A	343	THR	C-O	-5.10	1.18	1.24
1	A	66	GLU	C-O	-5.09	1.18	1.24
1	A	131	SER	C-O	-5.06	1.18	1.23
1	A	88	HIS	C-O	-5.04	1.17	1.23
1	A	139	LYS	C-O	-5.04	1.17	1.24
1	A	388	GLN	C-O	-5.04	1.16	1.23
1	A	387	LEU	C-O	-5.03	1.18	1.23
1	A	44	ASP	C-O	-5.01	1.17	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	MET	N-CA-C	7.72	122.80	113.23
1	A	198	VAL	N-CA-C	7.36	116.37	107.61
1	A	394	HIS	N-CA-C	6.77	119.05	108.96
1	A	294	VAL	CB-CA-C	-6.15	104.19	111.94
1	A	17	PHE	CA-C-N	-6.12	112.53	122.81
1	A	17	PHE	C-N-CA	-6.12	112.53	122.81
1	A	338	VAL	N-CA-C	6.04	114.80	107.61
1	A	201	THR	CA-C-O	5.92	126.66	119.38
1	A	295	VAL	N-CA-C	5.91	116.89	111.81
1	A	280	GLY	N-CA-C	-5.73	106.62	115.73
1	A	156	VAL	N-CA-C	5.53	115.56	107.37
1	A	303	TYR	N-CA-C	5.40	118.35	109.76
1	A	258	LYS	N-CA-C	5.32	118.66	110.42
1	A	333	SER	N-CA-C	5.16	118.23	109.76
1	A	390	HIS	CB-CA-C	-5.00	103.83	110.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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	3107	0	2964	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	205	0	0	1	0
All	All	3314	0	2964	45	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 (45) 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:93:ARG:HD3	4:A:570:HOH:O	1.81	0.81
1:A:226:PHE:O	1:A:230:LYS:HG3	1.98	0.62
1:A:305:ASN:OD1	1:A:308:LEU:HB2	2.01	0.61
1:A:220:GLU:OE2	1:A:228:ARG:HD3	2.00	0.61
1:A:132:GLN:O	1:A:136:GLU:HG3	2.02	0.60
1:A:171:LEU:CD1	1:A:174:MET:HE2	2.32	0.58
1:A:375:ALA:O	1:A:379:ARG:HG3	2.04	0.57
1:A:186:LYS:HE2	1:A:223:ASP:OD1	2.05	0.56
1:A:258:LYS:HE2	1:A:334:THR:OG1	2.06	0.55
1:A:20:TRP:CE2	1:A:25:MET:HG3	2.43	0.54
1:A:10:PRO:HD2	1:A:107:ARG:O	2.08	0.54
1:A:25:MET:HE1	1:A:189:LEU:HD23	1.90	0.53
1:A:274:TYR:CZ	1:A:283:TYR:HB2	2.42	0.53
1:A:348:VAL:HG12	1:A:349:TRP:N	2.25	0.52
1:A:85:LYS:O	1:A:85:LYS:HG3	2.12	0.50
1:A:127:LEU:HB3	1:A:153:HIS:HB2	1.92	0.49
1:A:171:LEU:HD11	1:A:174:MET:HE2	1.94	0.49
1:A:132:GLN:CD	1:A:135:ARG:HH21	2.20	0.49
1:A:76:VAL:HG23	1:A:93:ARG:O	2.13	0.48
1:A:61:TRP:CD1	1:A:82:HIS:CE1	3.01	0.48
1:A:379:ARG:O	1:A:382:GLU:HG2	2.14	0.48
1:A:340:TYR:CZ	1:A:342:GLY:HA2	2.49	0.48
1:A:297:ALA:N	1:A:298:PRO:CD	2.76	0.47
1:A:362:VAL:HG13	1:A:363:ILE:HG23	1.96	0.47
1:A:232:SER:HB2	1:A:233:PRO:HD2	1.96	0.47
1:A:283:TYR:CD1	1:A:283:TYR:N	2.83	0.47
1:A:18:THR:HG23	1:A:30:TYR:HE2	1.80	0.47
1:A:348:VAL:CG1	1:A:349:TRP:N	2.79	0.46
1:A:102:LEU:HD21	1:A:108:ILE:HG23	1.97	0.45
1:A:103:LYS:HE3	1:A:103:LYS:HB2	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ASP:OD1	1:A:361:GLU:HG3	2.17	0.45
1:A:308:LEU:O	1:A:331:ARG:NH2	2.43	0.44
1:A:176:ASP:OD2	1:A:180:ARG:NE	2.50	0.44
1:A:180:ARG:HD3	1:A:295:VAL:CG1	2.48	0.43
1:A:171:LEU:HD12	1:A:174:MET:HE2	2.00	0.43
1:A:88:HIS:HB3	1:A:212:TRP:CZ3	2.54	0.43
1:A:247:VAL:N	1:A:248:PRO:HD2	2.33	0.42
1:A:338:VAL:HG23	1:A:348:VAL:HG11	2.02	0.42
1:A:100:PRO:HB2	1:A:104:ARG:HH12	1.85	0.41
1:A:180:ARG:HD3	1:A:295:VAL:HG13	2.02	0.41
1:A:184:LEU:HB2	1:A:291:PHE:CE2	2.56	0.41
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.91	0.41
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.92	0.41
1:A:132:GLN:NE2	1:A:135:ARG:HH21	2.19	0.40
1:A:211:GLN:HG2	1:A:212:TRP:N	2.35	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	389/391 (100%)	377 (97%)	12 (3%)	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%)	318 (99%)	2 (1%)	78	71

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

Mol	Chain	Res	Type
1	A	29	LYS
1	A	286	LEU

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	60	ASN
1	A	141	HIS
1	A	173	ASN
1	A	383	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

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	391/391 (100%)	0.44	20 (5%)	33 39	11, 19, 35, 72	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	LEU	5.5
1	A	389	PRO	5.1
1	A	286	LEU	4.8
1	A	390	HIS	3.5
1	A	393	HIS	3.5
1	A	391	HIS	3.1
1	A	392	HIS	3.0
1	A	203	GLN	2.8
1	A	277	ALA	2.7
1	A	309	GLY	2.5
1	A	154	HIS	2.4
1	A	307	THR	2.4
1	A	132	GLN	2.3
1	A	303	TYR	2.3
1	A	201	THR	2.2
1	A	382	GLU	2.2
1	A	93	ARG	2.2
1	A	202	SER	2.2
1	A	87	GLY	2.1
1	A	379	ARG	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	0.93	0.06	21,21,21,21	0
2	ZN	A	401	1/1	0.99	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.