



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:52 PM UTC

PDB ID : 6FZ9 / pdb_00006fz9
Title : Crystal Structure of lipase from *Geobacillus stearothermophilus* T6 methanol stable variant A187F/L360F
Authors : Gihaz, S.; Kanteev, M.; Pazy, Y.; Fishman, A.
Deposited on : 2018-03-14
Resolution : 1.25 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

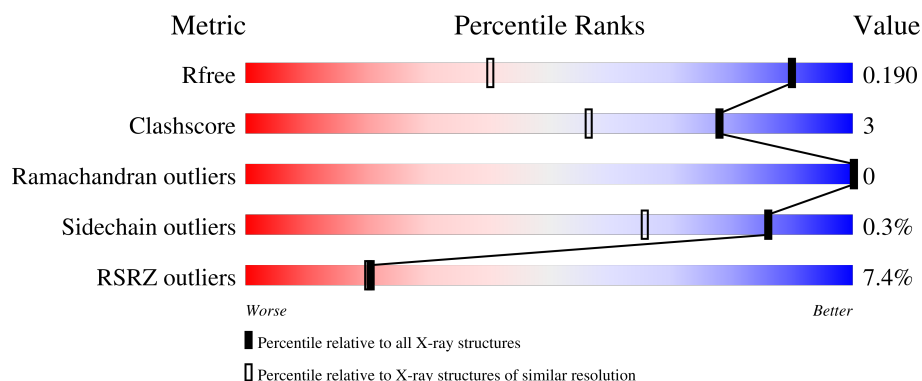
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1630 (1.26-1.22)
Clashscore	190562	1668 (1.26-1.22)
Ramachandran outliers	187476	1635 (1.26-1.22)
Sidechain outliers	187428	1633 (1.26-1.22)
RSRZ outliers	180081	1630 (1.26-1.22)

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	7% 65% 33% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3571 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
			3116	1981	555	572	8			

There are 9 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	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 CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

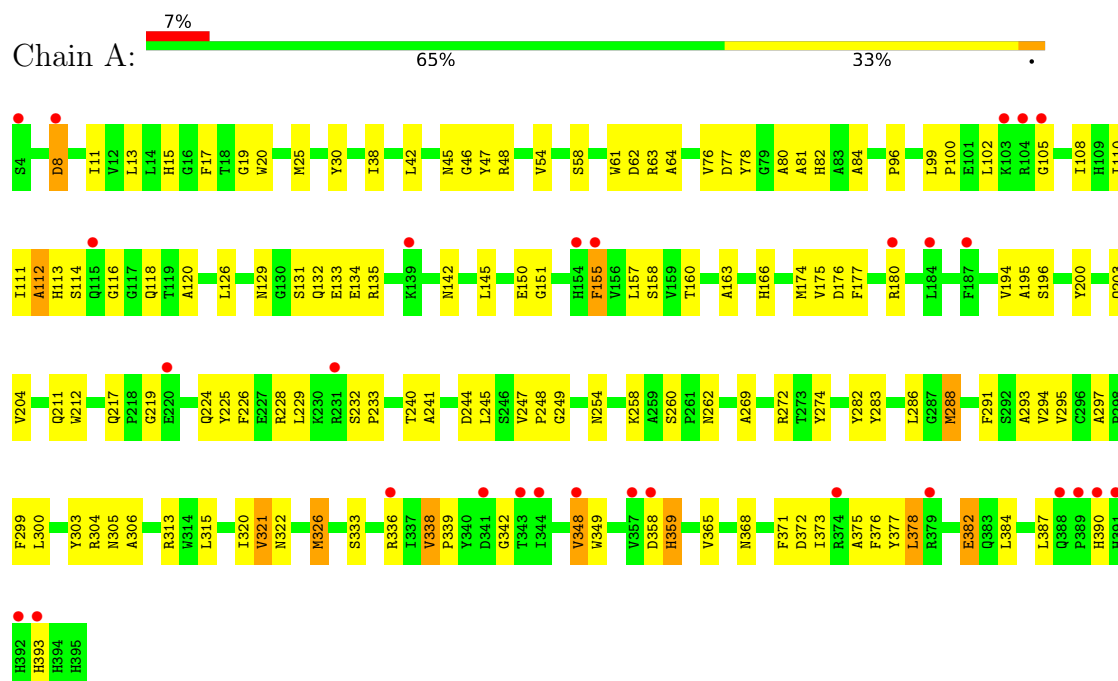
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	453	Total 453	O 453	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	49.96Å 71.26Å 113.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.72 – 1.25 45.72 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.72-1.25) 99.7 (45.72-1.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.25Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.158 , 0.177 0.172 , 0.190	Depositor DCC
R_{free} test set	5733 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.8	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	0.96	EDS
Total number of atoms	3571	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 4.50% 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, ZN

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	1.87	123/3208 (3.8%)	1.00	6/4361 (0.1%)

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	ALA	C-O	-10.30	1.14	1.24
1	A	272	ARG	C-O	-10.04	1.15	1.24
1	A	348	VAL	C-O	-8.40	1.14	1.23
1	A	371	PHE	C-O	-8.12	1.14	1.24
1	A	105	GLY	C-O	-7.97	1.15	1.24
1	A	111	ILE	C-O	-7.76	1.15	1.24
1	A	305	ASN	C-O	-7.53	1.14	1.23
1	A	322	ASN	C-O	-7.52	1.15	1.23
1	A	174	MET	C-O	-7.48	1.14	1.23
1	A	313	ARG	C-O	-7.37	1.14	1.24
1	A	195	ALA	C-O	-7.18	1.14	1.23
1	A	368	ASN	C-O	-7.09	1.15	1.24
1	A	244	ASP	C-O	-7.08	1.15	1.24
1	A	48	ARG	C-O	-6.94	1.15	1.23
1	A	63	ARG	C-O	-6.91	1.16	1.24
1	A	100	PRO	C-O	-6.88	1.15	1.24
1	A	283	TYR	C-O	-6.86	1.15	1.24
1	A	62	ASP	C-O	-6.82	1.16	1.24
1	A	320	ILE	C-O	-6.80	1.16	1.24
1	A	76	VAL	C-O	-6.61	1.17	1.24
1	A	376	PHE	C-O	-6.60	1.16	1.24
1	A	377	TYR	C-O	-6.59	1.15	1.24
1	A	64	ALA	C-O	-6.56	1.16	1.24
1	A	102	LEU	C-O	-6.55	1.15	1.24
1	A	110	ILE	C-O	-6.49	1.17	1.24
1	A	384	LEU	C-O	-6.49	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	ALA	C-O	-6.46	1.16	1.24
1	A	13	LEU	C-O	-6.44	1.16	1.23
1	A	365	VAL	C-O	-6.43	1.15	1.24
1	A	375	ALA	C-O	-6.43	1.16	1.24
1	A	387	LEU	C-O	-6.36	1.16	1.23
1	A	200	TYR	C-O	-6.31	1.16	1.23
1	A	249	GLY	C-O	-6.31	1.16	1.23
1	A	293	ALA	C-O	-6.29	1.16	1.24
1	A	245	LEU	C-O	-6.28	1.15	1.24
1	A	177	PHE	C-O	-6.25	1.16	1.24
1	A	82	HIS	C-O	-6.25	1.17	1.24
1	A	304	ARG	C-O	-6.23	1.15	1.23
1	A	157	LEU	C-O	-6.18	1.16	1.24
1	A	378	LEU	C-O	-6.18	1.16	1.24
1	A	295	VAL	C-O	-6.16	1.16	1.24
1	A	131	SER	C-O	-6.14	1.17	1.24
1	A	226	PHE	C-O	-6.10	1.16	1.24
1	A	282	TYR	C-O	-6.09	1.16	1.24
1	A	212	TRP	C-O	-6.09	1.16	1.24
1	A	300	LEU	C-O	-6.08	1.17	1.24
1	A	163	ALA	C-O	-6.06	1.16	1.23
1	A	294	VAL	C-O	-6.02	1.16	1.23
1	A	224	GLN	C-O	-6.02	1.17	1.24
1	A	126	LEU	C-O	-6.00	1.17	1.24
1	A	248	PRO	C-O	-5.99	1.16	1.24
1	A	160	THR	C-O	-5.96	1.16	1.24
1	A	118	GLN	C-O	-5.95	1.17	1.24
1	A	306	ALA	C-O	-5.89	1.17	1.24
1	A	247	VAL	C-O	-5.87	1.19	1.24
1	A	269	ALA	C-O	-5.87	1.16	1.23
1	A	393	HIS	C-O	-5.86	1.16	1.23
1	A	84	ALA	C-O	-5.86	1.17	1.24
1	A	135	ARG	C-O	-5.86	1.17	1.24
1	A	175	VAL	C-O	-5.86	1.17	1.24
1	A	217	GLN	C-O	-5.83	1.16	1.23
1	A	99	LEU	C-O	-5.82	1.17	1.24
1	A	17	PHE	C-O	-5.80	1.16	1.24
1	A	260	SER	C-O	-5.79	1.16	1.23
1	A	96	PRO	C-O	-5.79	1.17	1.24
1	A	45	ASN	C-O	-5.76	1.16	1.24
1	A	155	PHE	CA-CB	-5.74	1.44	1.53
1	A	372	ASP	C-O	-5.72	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	GLN	C-O	-5.69	1.17	1.24
1	A	132	GLN	C-O	-5.69	1.17	1.24
1	A	390	HIS	C-O	-5.68	1.17	1.23
1	A	8	ASP	C-O	-5.64	1.16	1.24
1	A	274	TYR	C-O	-5.64	1.16	1.23
1	A	77	ASP	C-O	-5.61	1.17	1.24
1	A	299	PHE	C-O	-5.60	1.17	1.24
1	A	150	GLU	C-O	-5.56	1.16	1.24
1	A	373	ILE	C-O	-5.55	1.17	1.24
1	A	229	LEU	C-O	-5.55	1.17	1.24
1	A	145	LEU	C-O	-5.53	1.17	1.23
1	A	114	SER	C-O	-5.50	1.19	1.24
1	A	158	SER	C-O	-5.50	1.17	1.23
1	A	120	ALA	C-O	-5.49	1.17	1.24
1	A	315	LEU	C-O	-5.47	1.17	1.24
1	A	342	GLY	C-O	-5.46	1.16	1.24
1	A	321	VAL	C-O	-5.44	1.18	1.24
1	A	108	ILE	C-O	-5.43	1.17	1.23
1	A	46	GLY	C-O	-5.40	1.17	1.24
1	A	81	ALA	C-O	-5.38	1.17	1.24
1	A	288	MET	C-O	-5.38	1.17	1.23
1	A	38	ILE	C-O	-5.37	1.17	1.24
1	A	286	LEU	C-O	-5.37	1.17	1.23
1	A	303	TYR	C-O	-5.36	1.17	1.24
1	A	142	ASN	C-O	-5.36	1.16	1.23
1	A	194	VAL	C-O	-5.35	1.18	1.24
1	A	113	HIS	C-O	-5.34	1.17	1.24
1	A	151	GLY	C-O	-5.33	1.17	1.23
1	A	196	SER	C-O	-5.32	1.16	1.23
1	A	80	ALA	C-O	-5.30	1.18	1.24
1	A	240	THR	C-O	-5.30	1.17	1.23
1	A	291	PHE	C-O	-5.28	1.18	1.24
1	A	134	GLU	C-O	-5.26	1.17	1.24
1	A	54	VAL	C-O	-5.25	1.17	1.23
1	A	11	ILE	C-O	-5.21	1.17	1.24
1	A	219	GLY	C-O	-5.18	1.16	1.24
1	A	338	VAL	C-O	-5.18	1.19	1.23
1	A	225	TYR	C-O	-5.16	1.18	1.24
1	A	58	SER	C-O	-5.16	1.17	1.23
1	A	129	ASN	C-O	-5.16	1.17	1.24
1	A	254	ASN	C-O	-5.14	1.17	1.24
1	A	333	SER	C-O	-5.14	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	PHE	C-O	-5.12	1.17	1.24
1	A	258	LYS	C-O	-5.10	1.17	1.23
1	A	133	GLU	C-O	-5.10	1.18	1.24
1	A	359	HIS	C-O	-5.09	1.17	1.24
1	A	232	SER	C-O	-5.08	1.18	1.23
1	A	61	TRP	C-O	-5.06	1.18	1.24
1	A	78	TYR	C-O	-5.06	1.17	1.24
1	A	382	GLU	C-O	-5.04	1.18	1.24
1	A	112	ALA	C-O	-5.04	1.17	1.24
1	A	233	PRO	C-O	-5.03	1.17	1.24
1	A	204	VAL	C-O	-5.03	1.18	1.24
1	A	166	HIS	C-O	-5.01	1.17	1.24
1	A	228	ARG	C-O	-5.00	1.18	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	MET	N-CA-C	6.99	121.89	113.23
1	A	30	TYR	N-CA-C	-6.32	104.48	111.36
1	A	100	PRO	N-CA-C	-5.55	106.62	113.84
1	A	294	VAL	CB-CA-C	-5.44	105.09	111.94
1	A	306	ALA	N-CA-C	5.24	116.67	111.07
1	A	339	PRO	CA-C-O	-5.01	115.87	121.23

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	3116	0	2967	17	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	453	0	0	1	0
All	All	3571	0	2967	17	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 3.

All (17) 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:288:MET:HG3	1:A:358:ASP:OD1	1.88	0.73
1:A:176:ASP:OD2	1:A:180:ARG:NH2	2.25	0.69
1:A:176:ASP:OD2	1:A:180:ARG:CZ	2.44	0.65
1:A:338:VAL:HG23	1:A:348:VAL:HG11	1.82	0.62
1:A:336:ARG:O	1:A:348:VAL:HG13	2.03	0.59
1:A:8:ASP:OD1	1:A:8:ASP:N	2.35	0.58
1:A:358:ASP:OD2	1:A:359:HIS:N	2.44	0.50
1:A:348:VAL:HG12	1:A:349:TRP:N	2.29	0.46
1:A:47:TYR:OH	1:A:382:GLU:HG2	2.17	0.44
1:A:42:LEU:HD23	1:A:378:LEU:HD23	2.00	0.44
1:A:20:TRP:CE2	1:A:25:MET:HG3	2.53	0.43
1:A:155:PHE:C	1:A:155:PHE:CD1	2.96	0.43
1:A:321:VAL:HB	1:A:326:MET:HE2	2.01	0.43
1:A:15:HIS:CG	1:A:19:GLY:HA3	2.55	0.42
1:A:112:ALA:HB1	1:A:116:GLY:C	2.45	0.41
1:A:336:ARG:C	1:A:348:VAL:HG13	2.46	0.40
1:A:262:ASN:OD1	4:A:502:HOH:O	2.22	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%)	378 (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	321/321 (100%)	320 (100%)	1 (0%)	86	66

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	GLN

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	154	HIS
1	A	383	GLN
1	A	390	HIS
1	A	392	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](#)

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

6.1 Protein, DNA and RNA chains

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%)	0.44	29 (7%)	20 20	10, 15, 27, 39	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	ASP	9.9
1	A	392	HIS	5.0
1	A	154	HIS	4.5
1	A	391	HIS	4.2
1	A	4	SER	4.2
1	A	390	HIS	4.1
1	A	231	ARG	3.5
1	A	115	GLN	3.3
1	A	357	VAL	3.3
1	A	187	PHE	3.2
1	A	220	GLU	3.1
1	A	393	HIS	2.9
1	A	379	ARG	2.9
1	A	104	ARG	2.9
1	A	105	GLY	2.8
1	A	389	PRO	2.8
1	A	155	PHE	2.7
1	A	139	LYS	2.6
1	A	103	LYS	2.5
1	A	184	LEU	2.5
1	A	341	ASP	2.4
1	A	180	ARG	2.3
1	A	8	ASP	2.3
1	A	343	THR	2.2
1	A	344	ILE	2.2
1	A	374	ARG	2.2
1	A	348	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	336	ARG	2.1
1	A	388	GLN	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	ZN	A	402	1/1	0.98	0.03	12,12,12,12	0
2	CA	A	401	1/1	1.00	0.02	17,17,17,17	1

6.5 Other polymers [i](#)

There are no such residues in this entry.