



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:13 PM UTC

PDB ID : 6S3V / pdb_00006s3v
Title : Crystal Structure of lipase from *Geobacillus stearothermophilus* T6 methanol stable variant E251C/G332C
Authors : Gihaz, S.; Bash, Y.; Rush, I.; Shahar, A.; Pazy, Y.; Fishman, A.
Deposited on : 2019-06-26
Resolution : 2.00 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

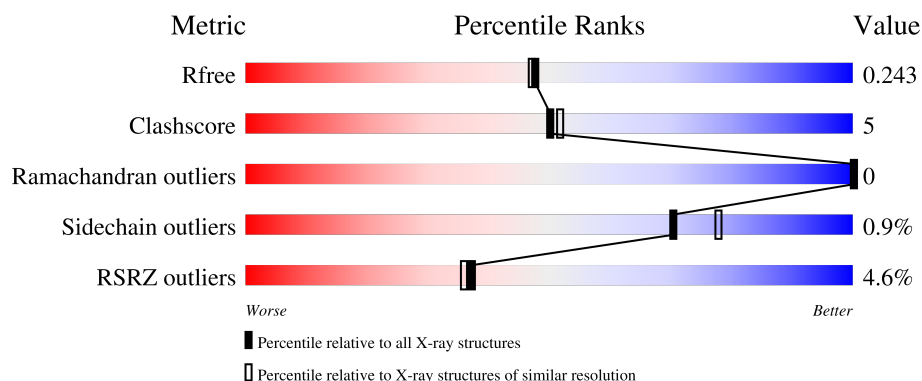
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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% 50% 45% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3351 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
			3106	1971	555	570	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	CYS	GLU	engineered mutation	UNP Q93A71
A	323	ALA	THR	conflict	UNP Q93A71
A	332	CYS	GLY	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		

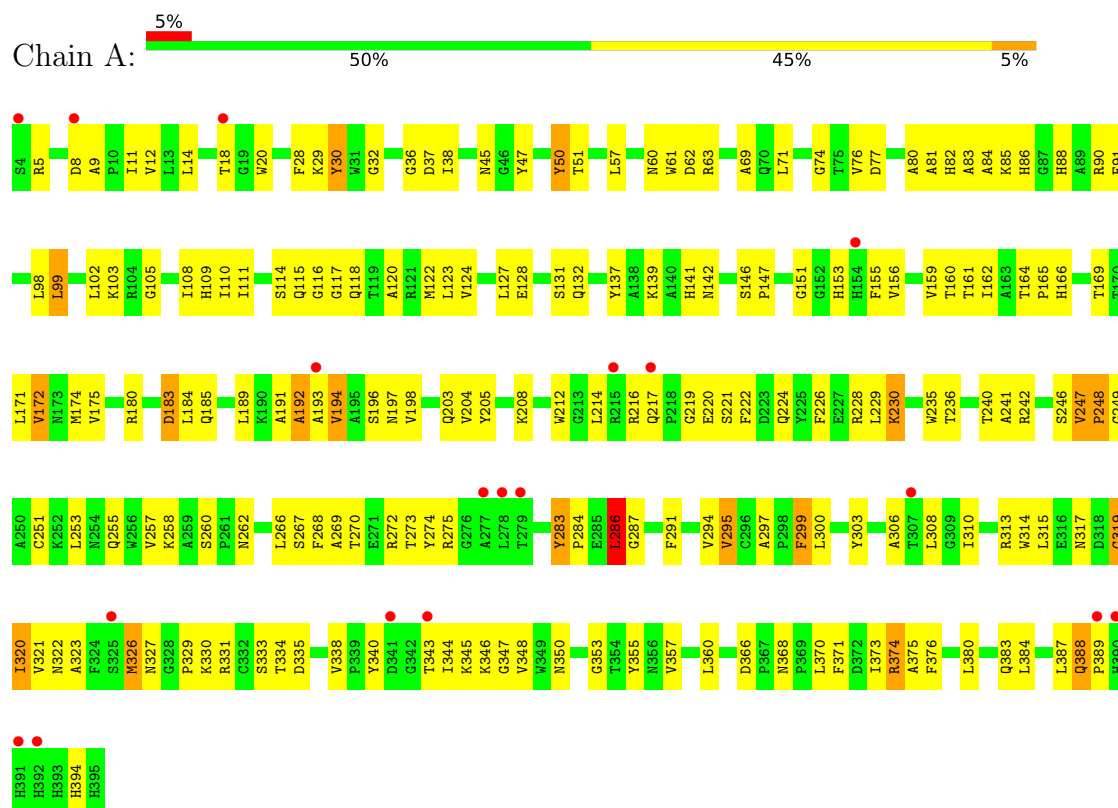
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	243	Total 243	O 243	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	49.16Å 71.97Å 112.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.32 – 2.00 56.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.32-2.00) 99.1 (56.32-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.239 0.230 , 0.243	Depositor DCC
R_{free} test set	1879 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3351	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 4.90% 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	2.20	164/3196 (5.1%)	1.22	13/4346 (0.3%)

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	VAL	C-O	-9.49	1.14	1.24
1	A	297	ALA	C-O	-9.12	1.15	1.24
1	A	108	ILE	C-O	-8.85	1.14	1.23
1	A	272	ARG	C-O	-8.75	1.14	1.24
1	A	12	VAL	C-O	-8.41	1.15	1.24
1	A	294	VAL	C-O	-8.33	1.14	1.23
1	A	80	ALA	C-O	-8.26	1.14	1.24
1	A	110	ILE	C-O	-8.10	1.15	1.24
1	A	241	ALA	C-O	-8.07	1.14	1.24
1	A	322	ASN	C-O	-7.99	1.14	1.23
1	A	105	GLY	C-O	-7.87	1.15	1.24
1	A	115	GLN	C-O	-7.81	1.14	1.24
1	A	266	LEU	C-O	-7.76	1.14	1.23
1	A	156	VAL	C-O	-7.68	1.15	1.24
1	A	172	VAL	C-O	-7.57	1.13	1.24
1	A	71	LEU	C-O	-7.50	1.15	1.24
1	A	82	HIS	C-O	-7.49	1.15	1.24
1	A	306	ALA	C-O	-7.48	1.15	1.24
1	A	299	PHE	C-O	-7.46	1.15	1.24
1	A	51	THR	C-O	-7.44	1.15	1.24
1	A	62	ASP	C-O	-7.43	1.15	1.24
1	A	137	TYR	C-O	-7.39	1.15	1.24
1	A	29	LYS	C-O	-7.37	1.14	1.23
1	A	214	LEU	C-O	-7.34	1.14	1.24
1	A	111	ILE	C-O	-7.32	1.16	1.24
1	A	260	SER	C-O	-7.19	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	THR	C-O	-7.19	1.14	1.24
1	A	230	LYS	C-O	-7.19	1.15	1.24
1	A	229	LEU	C-O	-7.16	1.15	1.24
1	A	185	GLN	C-O	-7.16	1.15	1.24
1	A	166	HIS	C-O	-7.15	1.15	1.24
1	A	159	VAL	C-O	-7.15	1.16	1.24
1	A	131	SER	C-O	-7.13	1.16	1.24
1	A	384	LEU	C-O	-7.13	1.15	1.24
1	A	205	TYR	C-O	-7.12	1.15	1.23
1	A	98	LEU	C-O	-7.09	1.15	1.24
1	A	357	VAL	C-O	-7.06	1.16	1.23
1	A	161	THR	C-O	-7.05	1.15	1.24
1	A	242	ARG	C-O	-7.05	1.16	1.24
1	A	375	ALA	C-O	-7.00	1.16	1.24
1	A	284	PRO	C-O	-6.99	1.15	1.23
1	A	20	TRP	C-O	-6.98	1.15	1.23
1	A	350	ASN	C-O	-6.97	1.15	1.23
1	A	320	ILE	C-O	-6.96	1.15	1.24
1	A	50	TYR	C-O	-6.95	1.15	1.23
1	A	224	GLN	C-O	-6.94	1.15	1.24
1	A	118	GLN	C-O	-6.93	1.15	1.24
1	A	60	ASN	C-O	-6.92	1.15	1.24
1	A	255	GLN	C-O	-6.89	1.15	1.24
1	A	90	ARG	C-O	-6.86	1.15	1.24
1	A	120	ALA	C-O	-6.76	1.16	1.24
1	A	212	TRP	C-O	-6.76	1.15	1.24
1	A	84	ALA	C-O	-6.75	1.16	1.24
1	A	348	VAL	C-O	-6.74	1.16	1.23
1	A	139	LYS	C-O	-6.73	1.16	1.24
1	A	387	LEU	C-O	-6.73	1.15	1.23
1	A	127	LEU	C-O	-6.72	1.16	1.24
1	A	222	PHE	C-O	-6.69	1.15	1.24
1	A	314	TRP	C-O	-6.62	1.15	1.24
1	A	14	LEU	C-O	-6.61	1.16	1.24
1	A	132	GLN	C-O	-6.57	1.16	1.24
1	A	171	LEU	C-O	-6.54	1.16	1.24
1	A	83	ALA	C-O	-6.52	1.16	1.24
1	A	184	LEU	C-O	-6.43	1.16	1.24
1	A	91	PHE	C-O	-6.42	1.16	1.23
1	A	38	ILE	C-O	-6.40	1.16	1.24
1	A	162	ILE	C-O	-6.37	1.17	1.24
1	A	102	LEU	C-O	-6.33	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	VAL	C-O	-6.31	1.16	1.24
1	A	253	LEU	C-O	-6.28	1.16	1.24
1	A	142	ASN	C-O	-6.26	1.15	1.23
1	A	61	TRP	C-O	-6.25	1.17	1.24
1	A	124	VAL	C-O	-6.25	1.17	1.24
1	A	88	HIS	C-O	-6.19	1.15	1.23
1	A	262	ASN	C-O	-6.17	1.15	1.24
1	A	240	THR	C-O	-6.16	1.16	1.23
1	A	85	LYS	C-O	-6.11	1.17	1.24
1	A	28	PHE	C-O	-6.10	1.16	1.24
1	A	388	GLN	C-O	-6.07	1.15	1.23
1	A	160	THR	C-O	-6.06	1.16	1.24
1	A	216	ARG	C-O	-6.05	1.16	1.23
1	A	169	THR	C-O	-6.05	1.16	1.23
1	A	315	LEU	C-O	-6.03	1.16	1.24
1	A	291	PHE	C-O	-6.00	1.17	1.24
1	A	151	GLY	C-O	-5.98	1.17	1.24
1	A	203	GLN	C-O	-5.97	1.17	1.24
1	A	346	LYS	C-O	-5.95	1.16	1.23
1	A	81	ALA	C-O	-5.93	1.17	1.24
1	A	191	ALA	C-O	-5.91	1.17	1.24
1	A	45	ASN	C-O	-5.89	1.16	1.24
1	A	258	LYS	C-O	-5.87	1.16	1.23
1	A	74	GLY	C-O	-5.87	1.17	1.23
1	A	303	TYR	C-O	-5.86	1.16	1.24
1	A	394	HIS	C-O	-5.84	1.16	1.23
1	A	128	GLU	C-O	-5.84	1.17	1.24
1	A	267	SER	C-O	-5.78	1.17	1.24
1	A	99	LEU	C-O	-5.78	1.17	1.24
1	A	228	ARG	C-O	-5.77	1.17	1.24
1	A	198	VAL	C-O	-5.72	1.18	1.23
1	A	251	CYS	C-O	-5.72	1.17	1.24
1	A	329	PRO	C-O	-5.72	1.16	1.23
1	A	376	PHE	C-O	-5.71	1.17	1.24
1	A	383	GLN	C-O	-5.71	1.17	1.24
1	A	153	HIS	C-O	-5.69	1.16	1.23
1	A	347	GLY	C-O	-5.69	1.16	1.23
1	A	374	ARG	C-O	-5.68	1.17	1.24
1	A	286	LEU	C-O	-5.63	1.17	1.23
1	A	249	GLY	C-O	-5.63	1.17	1.23
1	A	323	ALA	C-O	-5.63	1.17	1.24
1	A	273	THR	C-O	-5.62	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	LYS	C-O	-5.62	1.15	1.23
1	A	109	HIS	C-O	-5.62	1.17	1.24
1	A	355	TYR	C-O	-5.59	1.17	1.23
1	A	37	ASP	C-O	-5.58	1.17	1.23
1	A	146	SER	C-O	-5.55	1.16	1.23
1	A	353	GLY	C-O	-5.52	1.17	1.23
1	A	270	THR	C-O	-5.51	1.17	1.23
1	A	30	TYR	C-O	-5.51	1.17	1.24
1	A	194	VAL	C-O	-5.51	1.18	1.24
1	A	268	PHE	C-O	-5.49	1.17	1.24
1	A	335	ASP	C-O	-5.44	1.17	1.23
1	A	204	VAL	C-O	-5.42	1.17	1.24
1	A	340	TYR	C-O	-5.42	1.17	1.23
1	A	373	ILE	C-O	-5.42	1.17	1.24
1	A	63	ARG	C-O	-5.39	1.17	1.24
1	A	69	ALA	C-O	-5.39	1.17	1.24
1	A	247	VAL	C-O	-5.36	1.18	1.24
1	A	380	LEU	C-O	-5.36	1.18	1.24
1	A	313	ARG	C-O	-5.32	1.17	1.24
1	A	368	ASN	C-O	-5.32	1.17	1.24
1	A	269	ALA	C-O	-5.31	1.17	1.23
1	A	327	ASN	C-O	-5.31	1.17	1.24
1	A	123	LEU	C-O	-5.29	1.18	1.24
1	A	196	SER	C-O	-5.29	1.17	1.24
1	A	338	VAL	C-O	-5.29	1.18	1.23
1	A	345	LYS	CA-C	-5.28	1.46	1.52
1	A	99	LEU	N-CA	-5.25	1.41	1.46
1	A	283	TYR	C-O	-5.25	1.17	1.24
1	A	219	GLY	C-O	-5.22	1.16	1.24
1	A	300	LEU	C-O	-5.21	1.18	1.24
1	A	11	ILE	C-O	-5.20	1.17	1.24
1	A	371	PHE	C-O	-5.20	1.18	1.24
1	A	122	MET	C-O	-5.20	1.18	1.24
1	A	9	ALA	C-O	-5.19	1.17	1.24
1	A	155	PHE	C-O	-5.18	1.17	1.24
1	A	208	LYS	C-O	-5.18	1.17	1.23
1	A	366	ASP	C-O	-5.17	1.17	1.24
1	A	248	PRO	C-O	-5.16	1.18	1.24
1	A	257	VAL	C-O	-5.14	1.16	1.23
1	A	370	LEU	C-O	-5.14	1.17	1.24
1	A	308	LEU	C-O	-5.13	1.17	1.24
1	A	77	ASP	C-O	-5.11	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	LEU	C-O	-5.11	1.17	1.24
1	A	117	GLY	C-O	-5.10	1.17	1.23
1	A	319	GLY	C-O	-5.09	1.16	1.24
1	A	192	ALA	C-O	-5.09	1.17	1.24
1	A	197	ASN	C-O	-5.08	1.17	1.23
1	A	183	ASP	C-O	-5.06	1.17	1.24
1	A	360	LEU	C-O	-5.04	1.17	1.24
1	A	47	TYR	C-O	-5.02	1.18	1.24
1	A	235	TRP	C-O	-5.02	1.16	1.23
1	A	141	HIS	C-O	-5.02	1.17	1.24
1	A	147	PRO	C-O	-5.01	1.18	1.24
1	A	221	SER	C-O	-5.01	1.17	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	VAL	N-CA-C	9.62	121.78	111.58
1	A	156	VAL	N-CA-C	8.22	119.53	107.37
1	A	326	MET	N-CA-C	7.01	122.13	113.50
1	A	317	ASN	N-CA-C	6.59	118.95	109.14
1	A	5	ARG	N-CA-C	6.42	118.91	108.63
1	A	236	THR	N-CA-C	6.25	120.91	113.28
1	A	333	SER	N-CA-C	5.93	118.87	109.50
1	A	114	SER	CB-CA-C	-5.53	110.22	116.63
1	A	116	GLY	CA-C-N	5.49	126.04	119.94
1	A	116	GLY	C-N-CA	5.49	126.04	119.94
1	A	86	HIS	N-CA-C	5.36	119.82	113.28
1	A	240	THR	N-CA-C	5.11	116.96	109.24
1	A	98	LEU	N-CA-C	5.09	116.91	111.36

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	3106	0	2964	32	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	243	0	0	0	0
All	All	3351	0	2964	32	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 5.

All (32) 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:180:ARG:HD3	1:A:295:VAL:CG1	2.07	0.84
1:A:275:ARG:HH11	1:A:275:ARG:HG3	1.42	0.83
1:A:180:ARG:HD3	1:A:295:VAL:HG11	1.65	0.77
1:A:388:GLN:OE1	1:A:389:PRO:HD2	1.91	0.70
1:A:321:VAL:HB	1:A:326:MET:HE2	1.76	0.68
1:A:275:ARG:HG3	1:A:275:ARG:NH1	2.08	0.67
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.82	0.61
1:A:217:GLN:O	1:A:220:GLU:HB3	2.07	0.55
1:A:8:ASP:OD1	1:A:8:ASP:N	2.37	0.54
1:A:286:LEU:HD12	1:A:287:GLY:N	2.23	0.54
1:A:180:ARG:NH2	1:A:183:ASP:OD2	2.41	0.52
1:A:174:MET:HG2	1:A:299:PHE:CD1	2.45	0.51
1:A:321:VAL:HB	1:A:326:MET:CE	2.39	0.51
1:A:180:ARG:HD3	1:A:295:VAL:HG13	1.91	0.50
1:A:319:GLY:O	1:A:320:ILE:HD13	2.11	0.50
1:A:189:LEU:HD22	1:A:194:VAL:CG1	2.42	0.49
1:A:275:ARG:NH1	1:A:275:ARG:CG	2.71	0.48
1:A:18:THR:O	1:A:30:TYR:CE1	2.66	0.48
1:A:172:VAL:HG21	1:A:246:SER:HA	1.95	0.47
1:A:174:MET:HG2	1:A:299:PHE:CG	2.49	0.47
1:A:164:THR:HG23	1:A:165:PRO:HD2	1.97	0.47
1:A:103:LYS:HB2	1:A:103:LYS:HE3	1.84	0.46
1:A:374:ARG:HB2	1:A:374:ARG:NH1	2.30	0.46
1:A:275:ARG:HH11	1:A:275:ARG:CG	2.12	0.46
1:A:192:ALA:O	1:A:193:ALA:HB3	2.17	0.45
1:A:310:ILE:HD13	1:A:310:ILE:N	2.32	0.44
1:A:226:PHE:O	1:A:230:LYS:HG3	2.18	0.44
1:A:189:LEU:HD22	1:A:194:VAL:HG11	1.98	0.44
1:A:274:TYR:CZ	1:A:283:TYR:HB2	2.54	0.43
1:A:331:ARG:HH11	1:A:331:ARG:HD2	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:CE1	1:A:99:LEU:HD21	2.56	0.41
1:A:32:GLY:HA3	1:A:36:GLY:O	2.21	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	321/321 (100%)	318 (99%)	3 (1%)	70	78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	LEU
1	A	343	THR
1	A	344	ILE

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	255	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%)	0.30	18 (4%) 37 36	12, 20, 33, 70	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	HIS	5.8
1	A	277	ALA	4.8
1	A	4	SER	4.3
1	A	279	THR	4.1
1	A	391	HIS	3.9
1	A	18	THR	3.6
1	A	392	HIS	3.3
1	A	343	THR	2.9
1	A	389	PRO	2.8
1	A	217	GLN	2.8
1	A	193	ALA	2.6
1	A	215	ARG	2.5
1	A	154	HIS	2.5
1	A	278	LEU	2.5
1	A	325	SER	2.4
1	A	341	ASP	2.4
1	A	307	THR	2.2
1	A	8	ASP	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	0.95	0.15	41,41,41,41	0
2	ZN	A	401	1/1	0.98	0.04	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.