



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:35 PM UTC

PDB ID : 3I9Y / pdb_00003i9y
Title : Crystal structure of the V. parahaemolyticus histidine kinase sensor TorS sensor domain
Authors : Moore, J.O.; Hendrickson, W.A.
Deposited on : 2009-07-13
Resolution : 2.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

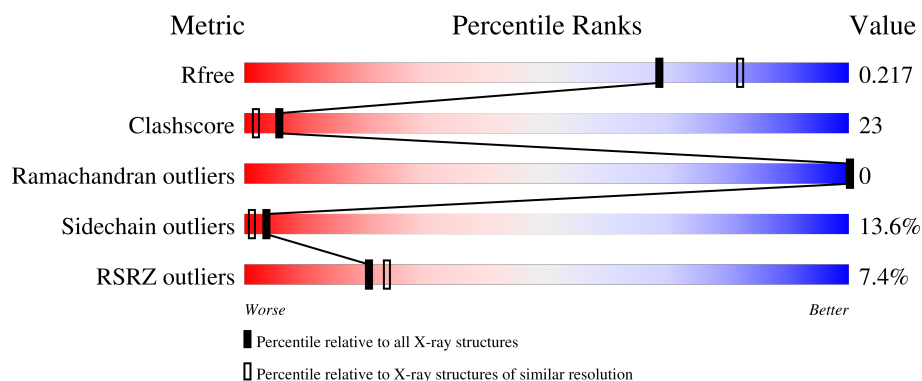
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	276	6% 22% 38% 18% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1926 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 Sensor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1854	1150	327	370	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	expression tag	UNP Q87ID1
A	48	SER	-	expression tag	UNP Q87ID1
A	49	GLY	-	expression tag	UNP Q87ID1
A	50	SER	-	expression tag	UNP Q87ID1

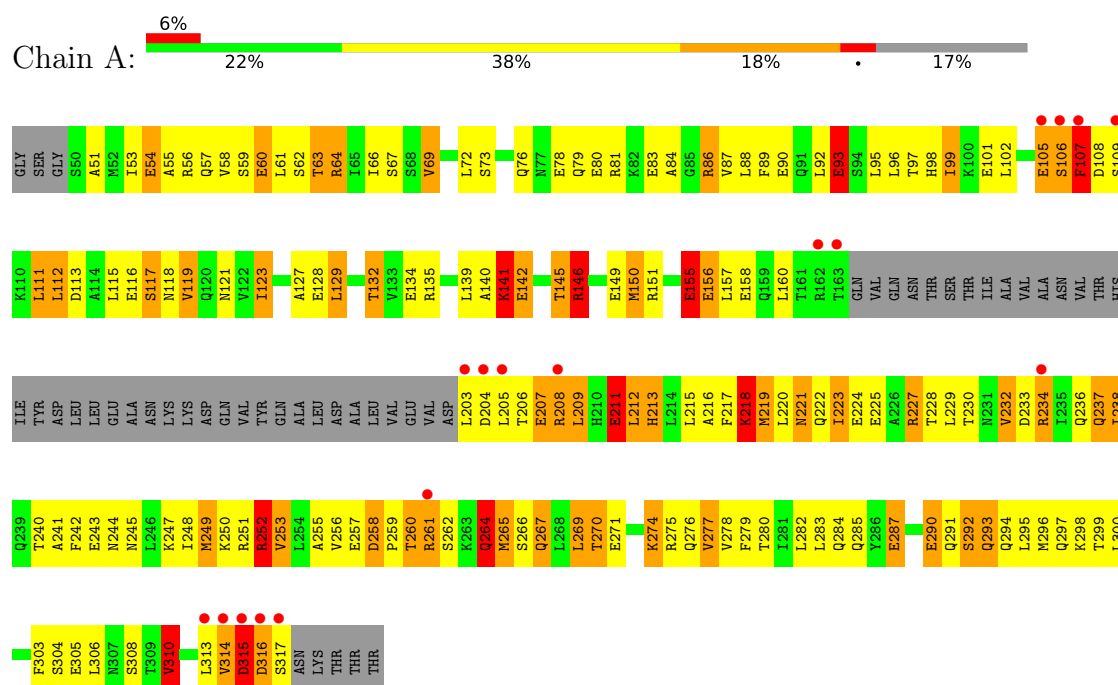
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		

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: Sensor protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	149.88Å 149.88Å 42.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 2.16 19.80 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.80-2.16) 99.8 (19.80-2.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.261 0.225 , 0.217	Depositor DCC
R_{free} test set	1519 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1926	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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 ⓘ

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	2.87	156/1865 (8.4%)	2.27	90/2507 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	MET	SD-CE	-22.27	1.23	1.79
1	A	218	LYS	CE-NZ	13.26	1.89	1.49
1	A	218	LYS	CG-CD	12.08	1.88	1.52
1	A	290	GLU	CA-C	9.90	1.65	1.52
1	A	155	GLU	CD-OE1	9.47	1.43	1.25
1	A	293	GLN	CG-CD	9.46	1.75	1.52
1	A	87	VAL	CA-C	8.92	1.64	1.52
1	A	211	GLU	CD-OE1	8.82	1.42	1.25
1	A	211	GLU	CG-CD	8.76	1.74	1.52
1	A	211	GLU	CA-C	8.61	1.63	1.52
1	A	53	ILE	CA-C	8.35	1.63	1.52
1	A	64	ARG	CZ-NH2	8.35	1.44	1.33
1	A	92	LEU	CA-C	8.34	1.63	1.52
1	A	69	VAL	CA-C	8.31	1.63	1.52
1	A	61	LEU	CA-C	8.20	1.63	1.52
1	A	93	GLU	CG-CD	8.16	1.72	1.52
1	A	117	SER	CA-C	8.12	1.63	1.52
1	A	115	LEU	CA-C	8.05	1.63	1.52
1	A	306	LEU	CA-C	8.00	1.63	1.52
1	A	291	GLN	CD-OE1	7.85	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	SER	C-O	-7.61	1.14	1.24
1	A	274	LYS	CE-NZ	7.49	1.71	1.49
1	A	64	ARG	C-O	7.47	1.32	1.24
1	A	60	GLU	CD-OE2	7.47	1.39	1.25
1	A	256	VAL	CA-C	7.40	1.61	1.52
1	A	155	GLU	CD-OE2	7.40	1.39	1.25
1	A	238	ILE	CA-C	-7.36	1.43	1.52
1	A	275	ARG	N-CA	7.34	1.55	1.46
1	A	139	LEU	CA-C	7.30	1.62	1.52
1	A	276	GLN	CA-CB	7.28	1.66	1.53
1	A	142	GLU	CB-CG	7.12	1.73	1.52
1	A	221	ASN	CA-CB	7.09	1.64	1.53
1	A	265	MET	SD-CE	-7.08	1.61	1.79
1	A	87	VAL	CB-CG2	-7.04	1.29	1.52
1	A	150	MET	C-O	6.99	1.32	1.24
1	A	112	LEU	N-CA	-6.98	1.37	1.46
1	A	255	ALA	CA-CB	-6.90	1.41	1.53
1	A	219	MET	N-CA	6.88	1.54	1.46
1	A	256	VAL	C-O	6.88	1.31	1.24
1	A	248	ILE	CA-CB	-6.86	1.46	1.54
1	A	287	GLU	CG-CD	6.80	1.69	1.52
1	A	270	THR	CA-C	6.78	1.62	1.52
1	A	127	ALA	CA-CB	6.74	1.64	1.53
1	A	132	THR	CA-CB	6.74	1.63	1.53
1	A	88	LEU	N-CA	-6.68	1.38	1.46
1	A	247	LYS	CA-C	6.65	1.61	1.52
1	A	241	ALA	CA-C	6.63	1.61	1.52
1	A	135	ARG	CA-C	6.62	1.61	1.52
1	A	293	GLN	CD-NE2	6.61	1.47	1.33
1	A	73	SER	CA-C	6.60	1.61	1.52
1	A	141	LYS	CD-CE	6.54	1.72	1.52
1	A	233	ASP	C-O	-6.53	1.16	1.24
1	A	55	ALA	CA-CB	6.53	1.63	1.53
1	A	278	VAL	N-CA	6.53	1.54	1.46
1	A	134	GLU	CA-C	6.52	1.61	1.52
1	A	216	ALA	CA-CB	6.51	1.63	1.53
1	A	151	ARG	CA-C	6.46	1.60	1.52
1	A	305	GLU	CG-CD	6.46	1.68	1.52
1	A	119	VAL	CA-C	6.45	1.61	1.52
1	A	63	THR	CB-CG2	-6.42	1.31	1.52
1	A	58	VAL	C-O	6.37	1.31	1.24
1	A	218	LYS	CB-CG	6.35	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	GLU	CA-C	6.34	1.60	1.52
1	A	224	GLU	CA-CB	6.30	1.63	1.53
1	A	132	THR	CB-CG2	-6.27	1.31	1.52
1	A	237	GLN	CA-CB	-6.25	1.43	1.53
1	A	225	GLU	CA-C	6.24	1.60	1.52
1	A	212	LEU	CA-C	6.20	1.60	1.52
1	A	208	ARG	CA-C	6.18	1.60	1.52
1	A	293	GLN	CD-OE1	6.17	1.35	1.23
1	A	282	LEU	C-O	6.06	1.31	1.24
1	A	118	ASN	CA-C	6.06	1.60	1.52
1	A	279	PHE	CA-C	6.05	1.60	1.52
1	A	218	LYS	CD-CE	6.02	1.70	1.52
1	A	156	GLU	CA-CB	-6.01	1.44	1.53
1	A	298	LYS	CE-NZ	5.99	1.67	1.49
1	A	219	MET	CA-C	5.98	1.60	1.52
1	A	249	MET	CB-CG	-5.97	1.34	1.52
1	A	266	SER	CA-C	5.97	1.60	1.52
1	A	207	GLU	CG-CD	5.94	1.66	1.52
1	A	314	VAL	CA-C	5.92	1.58	1.52
1	A	251	ARG	CZ-NH1	5.90	1.41	1.32
1	A	101	GLU	CB-CG	-5.87	1.34	1.52
1	A	215	LEU	CA-C	5.87	1.60	1.52
1	A	72	LEU	CG-CD2	5.84	1.71	1.52
1	A	291	GLN	CG-CD	5.84	1.66	1.52
1	A	310	VAL	C-O	-5.84	1.16	1.24
1	A	208	ARG	CZ-NH1	5.84	1.41	1.32
1	A	296	MET	C-N	-5.84	1.26	1.33
1	A	242	PHE	CA-C	-5.84	1.45	1.52
1	A	215	LEU	CA-CB	5.83	1.62	1.53
1	A	252	ARG	NE-CZ	5.82	1.39	1.33
1	A	243	GLU	CA-C	5.78	1.60	1.52
1	A	157	LEU	CA-CB	-5.76	1.44	1.53
1	A	66	ILE	CA-C	5.76	1.60	1.52
1	A	76	GLN	C-O	-5.73	1.16	1.24
1	A	59	SER	CA-C	5.71	1.60	1.52
1	A	218	LYS	CA-C	5.67	1.60	1.52
1	A	89	PHE	CA-CB	-5.66	1.44	1.53
1	A	305	GLU	CD-OE2	5.65	1.36	1.25
1	A	284	GLN	C-O	-5.64	1.17	1.24
1	A	155	GLU	CB-CG	5.63	1.69	1.52
1	A	113	ASP	CA-C	5.63	1.60	1.52
1	A	310	VAL	CA-CB	5.62	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	LYS	CG-CD	5.61	1.69	1.52
1	A	90	GLU	CA-C	5.61	1.60	1.52
1	A	78	GLU	N-CA	-5.60	1.39	1.46
1	A	228	THR	C-O	-5.60	1.16	1.24
1	A	303	PHE	CE2-CZ	5.59	1.55	1.38
1	A	155	GLU	CG-CD	5.58	1.66	1.52
1	A	208	ARG	NE-CZ	5.58	1.39	1.33
1	A	140	ALA	CA-CB	-5.58	1.44	1.53
1	A	305	GLU	CD-OE1	5.57	1.35	1.25
1	A	215	LEU	CG-CD1	5.57	1.71	1.52
1	A	135	ARG	CZ-NH1	5.56	1.40	1.32
1	A	119	VAL	N-CA	-5.53	1.39	1.46
1	A	117	SER	N-CA	-5.52	1.39	1.46
1	A	290	GLU	CB-CG	-5.52	1.35	1.52
1	A	267	GLN	C-O	-5.51	1.17	1.24
1	A	277	VAL	N-CA	5.50	1.53	1.46
1	A	127	ALA	C-O	-5.50	1.17	1.24
1	A	300	LEU	N-CA	5.49	1.52	1.46
1	A	62	SER	C-O	5.49	1.30	1.24
1	A	297	GLN	CD-NE2	5.49	1.44	1.33
1	A	109	SER	CA-C	5.46	1.60	1.52
1	A	245	ASN	CA-C	-5.46	1.45	1.52
1	A	57	GLN	CA-C	5.45	1.59	1.52
1	A	250	LYS	CA-C	5.45	1.60	1.52
1	A	275	ARG	CG-CD	-5.44	1.36	1.52
1	A	245	ASN	CB-CG	-5.40	1.38	1.52
1	A	156	GLU	N-CA	-5.39	1.39	1.46
1	A	123	ILE	CA-CB	5.37	1.60	1.54
1	A	249	MET	N-CA	-5.32	1.40	1.46
1	A	244	ASN	CA-C	5.32	1.59	1.52
1	A	264	GLN	CA-C	5.29	1.59	1.52
1	A	107	PHE	CB-CG	5.28	1.62	1.50
1	A	270	THR	CA-CB	5.28	1.61	1.53
1	A	63	THR	CA-CB	5.27	1.61	1.53
1	A	156	GLU	CB-CG	-5.26	1.36	1.52
1	A	227	ARG	CZ-NH2	5.26	1.40	1.33
1	A	206	THR	C-O	-5.23	1.18	1.24
1	A	219	MET	SD-CE	-5.23	1.66	1.79
1	A	79	GLN	CG-CD	5.22	1.65	1.52
1	A	142	GLU	N-CA	-5.21	1.40	1.46
1	A	128	GLU	CA-C	5.21	1.59	1.52
1	A	106	SER	CA-C	-5.20	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	ARG	CA-C	5.19	1.59	1.52
1	A	84	ALA	CA-C	5.18	1.59	1.52
1	A	142	GLU	CD-OE2	5.17	1.35	1.25
1	A	58	VAL	CA-CB	5.16	1.60	1.54
1	A	69	VAL	C-O	5.11	1.30	1.24
1	A	121	ASN	N-CA	-5.10	1.40	1.46
1	A	291	GLN	CA-C	5.09	1.59	1.52
1	A	244	ASN	N-CA	5.07	1.52	1.46
1	A	57	GLN	CA-CB	-5.05	1.45	1.53
1	A	80	GLU	CA-C	5.03	1.59	1.52

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ALA	N-CA-C	-12.86	97.34	111.36
1	A	227	ARG	NE-CZ-NH1	11.68	133.18	121.50
1	A	316	ASP	N-CA-C	-10.54	96.63	112.54
1	A	218	LYS	CG-CD-CE	9.40	132.91	111.30
1	A	315	ASP	CA-C-N	9.28	138.31	121.15
1	A	315	ASP	C-N-CA	9.28	138.31	121.15
1	A	127	ALA	N-CA-C	-9.23	100.33	111.69
1	A	86	ARG	N-CA-C	-8.50	101.96	111.14
1	A	209	LEU	N-CA-C	-8.49	102.11	111.36
1	A	81	ARG	N-CA-C	-8.44	102.03	111.14
1	A	285	GLN	N-CA-C	-8.32	102.29	111.36
1	A	67	SER	CA-CB-OG	-8.16	94.78	111.10
1	A	242	PHE	N-CA-C	-8.15	101.66	111.69
1	A	86	ARG	CA-C-N	-8.11	109.35	120.46
1	A	86	ARG	C-N-CA	-8.11	109.35	120.46
1	A	205	LEU	N-CA-C	-8.06	102.47	111.82
1	A	227	ARG	NE-CZ-NH2	-7.84	112.14	119.20
1	A	141	LYS	CB-CG-CD	-7.69	93.62	111.30
1	A	150	MET	CG-SD-CE	-7.50	84.39	100.90
1	A	151	ARG	NE-CZ-NH2	7.43	125.89	119.20
1	A	317	SER	N-CA-C	-7.35	90.41	111.00
1	A	129	LEU	N-CA-C	-7.22	103.49	111.36
1	A	258	ASP	CA-C-N	6.96	127.25	119.32
1	A	258	ASP	C-N-CA	6.96	127.25	119.32
1	A	218	LYS	CD-CE-NZ	6.88	133.92	111.90
1	A	216	ALA	N-CA-C	-6.81	103.93	111.36
1	A	142	GLU	N-CA-C	-6.71	103.89	111.07
1	A	227	ARG	NH1-CZ-NH2	-6.68	110.61	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	GLU	CG-CD-OE1	-6.66	103.08	118.40
1	A	280	THR	N-CA-C	-6.64	104.66	112.89
1	A	262	SER	CA-C-N	-6.58	109.49	120.68
1	A	262	SER	C-N-CA	-6.58	109.49	120.68
1	A	277	VAL	CG1-CB-CG2	-6.50	96.50	110.80
1	A	64	ARG	CA-CB-CG	-6.46	101.19	114.10
1	A	232	VAL	N-CA-C	6.41	119.10	111.09
1	A	208	ARG	CG-CD-NE	-6.41	97.91	112.00
1	A	275	ARG	CA-CB-CG	-6.39	101.31	114.10
1	A	87	VAL	N-CA-C	6.39	117.14	110.62
1	A	145	THR	CA-CB-OG1	-6.22	100.26	109.60
1	A	60	GLU	CB-CG-CD	-6.04	102.34	112.60
1	A	269	LEU	CA-C-N	-6.01	110.47	120.68
1	A	269	LEU	C-N-CA	-6.01	110.47	120.68
1	A	237	GLN	N-CA-CB	-5.96	101.33	110.16
1	A	101	GLU	CB-CA-C	-5.87	101.42	110.81
1	A	151	ARG	N-CA-C	-5.87	104.80	111.14
1	A	240	THR	N-CA-C	-5.87	104.84	112.23
1	A	294	GLN	CA-CB-CG	-5.83	102.43	114.10
1	A	237	GLN	CB-CG-CD	-5.83	102.69	112.60
1	A	56	ARG	N-CA-C	-5.82	104.85	111.14
1	A	315	ASP	N-CA-C	-5.80	101.53	109.71
1	A	244	ASN	N-CA-C	-5.79	105.05	111.36
1	A	291	GLN	CA-CB-CG	-5.78	102.54	114.10
1	A	300	LEU	N-CA-C	-5.74	104.94	111.14
1	A	90	GLU	CB-CA-C	-5.69	101.34	110.79
1	A	149	GLU	CB-CA-C	-5.64	101.43	110.79
1	A	257	GLU	N-CA-C	5.64	117.12	110.97
1	A	256	VAL	CA-C-N	5.63	128.08	120.65
1	A	256	VAL	C-N-CA	5.63	128.08	120.65
1	A	211	GLU	CB-CG-CD	5.59	122.10	112.60
1	A	274	LYS	N-CA-C	-5.57	105.75	112.54
1	A	157	LEU	CB-CG-CD2	-5.56	94.03	110.70
1	A	146	ARG	CD-NE-CZ	-5.55	116.63	124.40
1	A	218	LYS	CB-CG-CD	5.52	124.00	111.30
1	A	67	SER	CA-C-O	-5.48	115.07	120.82
1	A	218	LYS	CA-CB-CG	-5.45	103.20	114.10
1	A	304	SER	N-CA-C	-5.43	105.44	111.36
1	A	264	GLN	CA-C-O	-5.43	113.73	119.97
1	A	219	MET	CA-CB-CG	-5.42	103.25	114.10
1	A	296	MET	CA-CB-CG	-5.42	103.25	114.10
1	A	223	ILE	CA-C-O	-5.38	115.47	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	GLU	CB-CA-C	-5.38	102.94	111.17
1	A	140	ALA	N-CA-C	-5.35	105.53	111.36
1	A	83	GLU	CA-C-O	-5.32	115.22	120.70
1	A	63	THR	OG1-CB-CG2	5.30	119.90	109.30
1	A	299	THR	CB-CA-C	-5.28	102.03	110.79
1	A	300	LEU	CB-CA-C	-5.28	102.56	110.90
1	A	129	LEU	O-C-N	-5.24	116.18	122.15
1	A	211	GLU	CG-CD-OE2	-5.23	106.36	118.40
1	A	291	GLN	N-CA-C	-5.23	105.58	111.28
1	A	208	ARG	CD-NE-CZ	5.23	131.72	124.40
1	A	228	THR	N-CA-C	-5.21	106.32	113.30
1	A	111	LEU	CB-CA-C	-5.20	102.69	110.90
1	A	304	SER	CA-CB-OG	-5.18	100.73	111.10
1	A	127	ALA	CA-C-O	-5.13	114.54	120.24
1	A	54	GLU	CA-C-O	-5.11	115.13	120.55
1	A	99	ILE	CB-CG1-CD1	-5.11	103.07	113.80
1	A	227	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	230	THR	N-CA-C	-5.06	106.35	112.88
1	A	116	GLU	N-CA-C	-5.01	105.89	111.36
1	A	88	LEU	CD1-CG-CD2	-5.00	99.80	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	ARG	Sidechain

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	1854	0	1897	87	0
2	A	72	0	0	0	0
All	All	1926	0	1897	87	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 23.

All (87) 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:293:GLN:CD	1:A:293:GLN:CG	1.75	1.56
1:A:274:LYS:CE	1:A:274:LYS:NZ	1.71	1.50
1:A:218:LYS:CD	1:A:218:LYS:CG	1.88	1.48
1:A:218:LYS:CE	1:A:218:LYS:NZ	1.89	1.34
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.10	1.10
1:A:261:ARG:HH11	1:A:261:ARG:HB3	1.16	1.07
1:A:211:GLU:CD	1:A:252:ARG:HD3	1.79	1.06
1:A:261:ARG:HH11	1:A:261:ARG:CB	1.70	1.02
1:A:218:LYS:HD2	1:A:218:LYS:O	1.64	0.97
1:A:219:MET:SD	1:A:249:MET:HE2	2.08	0.94
1:A:252:ARG:HH11	1:A:252:ARG:CG	1.81	0.91
1:A:132:THR:CG2	1:A:292:SER:HB2	2.00	0.90
1:A:315:ASP:N	1:A:315:ASP:OD1	2.08	0.85
1:A:229:LEU:HD13	1:A:234:ARG:HB3	1.64	0.80
1:A:219:MET:SD	1:A:249:MET:CE	2.70	0.79
1:A:132:THR:HG21	1:A:292:SER:HB2	1.64	0.78
1:A:218:LYS:HD2	1:A:222:GLN:HG3	1.66	0.77
1:A:211:GLU:OE2	1:A:252:ARG:HD3	1.84	0.76
1:A:142:GLU:O	1:A:146:ARG:HD2	1.87	0.75
1:A:252:ARG:HG2	1:A:252:ARG:NH1	1.91	0.75
1:A:218:LYS:CD	1:A:218:LYS:O	2.34	0.75
1:A:261:ARG:CB	1:A:261:ARG:NH1	2.50	0.72
1:A:211:GLU:OE2	1:A:252:ARG:NE	2.22	0.72
1:A:211:GLU:OE2	1:A:252:ARG:CD	2.39	0.71
1:A:261:ARG:HH11	1:A:261:ARG:CG	2.04	0.70
1:A:108:ASP:OD1	1:A:108:ASP:C	2.35	0.69
1:A:252:ARG:CG	1:A:252:ARG:NH1	2.50	0.68
1:A:204:ASP:HB3	1:A:208:ARG:NH1	2.10	0.67
1:A:212:LEU:HD13	1:A:265:MET:HE1	1.76	0.67
1:A:209:LEU:HD21	1:A:261:ARG:HH22	1.62	0.65
1:A:261:ARG:NH1	1:A:261:ARG:CG	2.59	0.65
1:A:158:GLU:OE2	1:A:213:HIS:HD2	1.81	0.63
1:A:218:LYS:HD3	1:A:221:ASN:HB2	1.80	0.63
1:A:209:LEU:CD2	1:A:261:ARG:HH22	2.12	0.62
1:A:274:LYS:NZ	1:A:274:LYS:CG	2.62	0.61
1:A:211:GLU:CD	1:A:252:ARG:CD	2.68	0.61
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.67	0.60
1:A:261:ARG:HB3	1:A:261:ARG:NH1	2.01	0.59
1:A:249:MET:HG2	1:A:269:LEU:HD21	1.84	0.58
1:A:211:GLU:OE1	1:A:252:ARG:HD3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:HB3	1:A:112:LEU:HD21	1.85	0.58
1:A:106:SER:OG	1:A:107:PHE:N	2.37	0.57
1:A:69:VAL:HG13	1:A:129:LEU:HD21	1.87	0.57
1:A:150:MET:SD	1:A:223:ILE:HD13	2.46	0.56
1:A:316:ASP:C	1:A:316:ASP:OD1	2.49	0.56
1:A:146:ARG:HH12	1:A:277:VAL:CG2	2.19	0.55
1:A:60:GLU:OE2	1:A:64:ARG:HD3	2.07	0.55
1:A:141:LYS:HE3	1:A:141:LYS:HA	1.89	0.54
1:A:158:GLU:HG3	1:A:217:PHE:CE1	2.42	0.54
1:A:146:ARG:HH12	1:A:277:VAL:HG21	1.72	0.54
1:A:314:VAL:C	1:A:315:ASP:OD1	2.51	0.53
1:A:93:GLU:O	1:A:97:THR:HG23	2.08	0.53
1:A:146:ARG:NH1	1:A:277:VAL:CG2	2.72	0.53
1:A:69:VAL:HG13	1:A:129:LEU:CD2	2.40	0.52
1:A:155:GLU:HG2	1:A:156:GLU:N	2.24	0.52
1:A:204:ASP:HB3	1:A:208:ARG:HH12	1.73	0.52
1:A:141:LYS:HE3	1:A:141:LYS:O	2.10	0.52
1:A:60:GLU:OE2	1:A:64:ARG:CD	2.58	0.52
1:A:316:ASP:O	1:A:316:ASP:CG	2.53	0.51
1:A:258:ASP:HB3	1:A:261:ARG:HG3	1.94	0.50
1:A:274:LYS:NZ	1:A:274:LYS:CD	2.65	0.48
1:A:249:MET:HG2	1:A:269:LEU:CD2	2.44	0.48
1:A:141:LYS:HE2	1:A:145:THR:OG1	2.13	0.48
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.53	0.47
1:A:283:LEU:O	1:A:287:GLU:HG3	2.14	0.47
1:A:313:LEU:O	1:A:316:ASP:HB3	2.14	0.47
1:A:119:VAL:O	1:A:123:ILE:HG13	2.17	0.45
1:A:54:GLU:OE1	1:A:98:HIS:HD2	1.99	0.44
1:A:232:VAL:O	1:A:236:GLN:HG3	2.17	0.44
1:A:86:ARG:NH1	1:A:86:ARG:HG2	2.33	0.44
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.18	0.44
1:A:260:THR:HG23	1:A:264:GLN:NE2	2.33	0.44
1:A:249:MET:O	1:A:253:VAL:HG13	2.17	0.43
1:A:102:LEU:HD21	1:A:310:VAL:HB	2.00	0.43
1:A:86:ARG:HG2	1:A:86:ARG:HH11	1.85	0.42
1:A:234:ARG:HD2	1:A:234:ARG:HA	1.55	0.42
1:A:234:ARG:HH11	1:A:237:GLN:HE21	1.68	0.42
1:A:99:ILE:HG23	1:A:99:ILE:HD12	1.67	0.41
1:A:99:ILE:HA	1:A:99:ILE:HD13	1.80	0.41
1:A:258:ASP:C	1:A:258:ASP:OD2	2.64	0.41
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HH11	1:A:237:GLN:NE2	2.19	0.40
1:A:258:ASP:HA	1:A:259:PRO:HD2	1.80	0.40
1:A:274:LYS:NZ	1:A:274:LYS:HG3	2.36	0.40
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.76	0.40
1:A:95:LEU:O	1:A:99:ILE:HG12	2.20	0.40
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.91	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	225/276 (82%)	221 (98%)	4 (2%)	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	213/253 (84%)	184 (86%)	29 (14%)	3	1

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	93	GLU
1	A	105	GLU
1	A	107	PHE
1	A	117	SER
1	A	141	LYS
1	A	146	ARG
1	A	155	GLU
1	A	203	LEU
1	A	207	GLU
1	A	211	GLU
1	A	213	HIS
1	A	218	LYS
1	A	220	LEU
1	A	234	ARG
1	A	238	ILE
1	A	252	ARG
1	A	253	VAL
1	A	260	THR
1	A	261	ARG
1	A	264	GLN
1	A	267	GLN
1	A	270	THR
1	A	290	GLU
1	A	292	SER
1	A	295	LEU
1	A	308	SER
1	A	310	VAL
1	A	315	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	98	HIS
1	A	120	GLN
1	A	210	HIS
1	A	213	HIS
1	A	237	GLN
1	A	239	GLN
1	A	264	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](#)

There are no ligands in this entry.

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	229/276 (82%)	0.15	17 (7%) 20 23	14, 28, 58, 71	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	LEU	7.5
1	A	107	PHE	5.2
1	A	317	SER	4.5
1	A	163	THR	4.3
1	A	105	GLU	3.5
1	A	316	ASP	2.9
1	A	106	SER	2.8
1	A	204	ASP	2.8
1	A	313	LEU	2.8
1	A	314	VAL	2.7
1	A	208	ARG	2.7
1	A	234	ARG	2.5
1	A	315	ASP	2.4
1	A	261	ARG	2.3
1	A	162	ARG	2.2
1	A	109	SER	2.1
1	A	205	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.