



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:15 PM UTC

PDB ID : 2D2A / pdb_00002d2a
Title : Crystal Structure of Escherichia coli SufA Involved in Biosynthesis of Iron-sulfur Clusters
Authors : Wada, K.; Hasegawa, Y.; Gong, Z.; Minami, Y.; Fukuyama, K.; Takahashi, Y.
Deposited on : 2005-09-05
Resolution : 2.70 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
Xtrriage (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

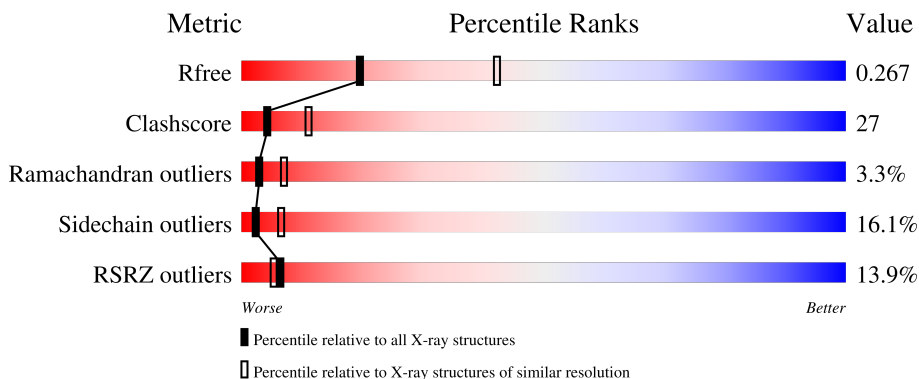
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	145	
1	B	145	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 1677 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 SufA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	114	854	546	143	160	5	0	0	0
1	B	102	786	510	131	143	2	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP P77667
A	-21	GLY	-	expression tag	UNP P77667
A	-20	HIS	-	expression tag	UNP P77667
A	-19	HIS	-	expression tag	UNP P77667
A	-18	HIS	-	expression tag	UNP P77667
A	-17	HIS	-	expression tag	UNP P77667
A	-16	HIS	-	expression tag	UNP P77667
A	-15	HIS	-	expression tag	UNP P77667
A	-14	HIS	-	expression tag	UNP P77667
A	-13	HIS	-	expression tag	UNP P77667
A	-12	HIS	-	expression tag	UNP P77667
A	-11	HIS	-	expression tag	UNP P77667
A	-10	SER	-	expression tag	UNP P77667
A	-9	SER	-	expression tag	UNP P77667
A	-8	GLY	-	expression tag	UNP P77667
A	-7	HIS	-	expression tag	UNP P77667
A	-6	ILE	-	expression tag	UNP P77667
A	-5	ASP	-	expression tag	UNP P77667
A	-4	ASP	-	expression tag	UNP P77667
A	-3	ASP	-	expression tag	UNP P77667
A	-2	ASP	-	expression tag	UNP P77667
A	-1	LEU	-	expression tag	UNP P77667
A	0	HIS	-	expression tag	UNP P77667
B	-22	MET	-	expression tag	UNP P77667
B	-21	GLY	-	expression tag	UNP P77667

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP P77667
B	-19	HIS	-	expression tag	UNP P77667
B	-18	HIS	-	expression tag	UNP P77667
B	-17	HIS	-	expression tag	UNP P77667
B	-16	HIS	-	expression tag	UNP P77667
B	-15	HIS	-	expression tag	UNP P77667
B	-14	HIS	-	expression tag	UNP P77667
B	-13	HIS	-	expression tag	UNP P77667
B	-12	HIS	-	expression tag	UNP P77667
B	-11	HIS	-	expression tag	UNP P77667
B	-10	SER	-	expression tag	UNP P77667
B	-9	SER	-	expression tag	UNP P77667
B	-8	GLY	-	expression tag	UNP P77667
B	-7	HIS	-	expression tag	UNP P77667
B	-6	ILE	-	expression tag	UNP P77667
B	-5	ASP	-	expression tag	UNP P77667
B	-4	ASP	-	expression tag	UNP P77667
B	-3	ASP	-	expression tag	UNP P77667
B	-2	ASP	-	expression tag	UNP P77667
B	-1	LEU	-	expression tag	UNP P77667
B	0	HIS	-	expression tag	UNP P77667

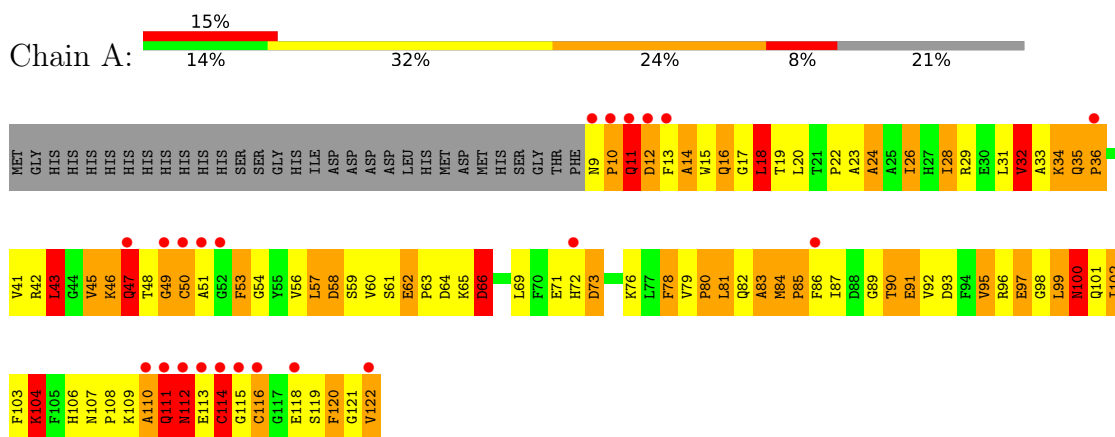
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	18	Total O 18 18	0	0
2	B	19	Total O 19 19	0	0

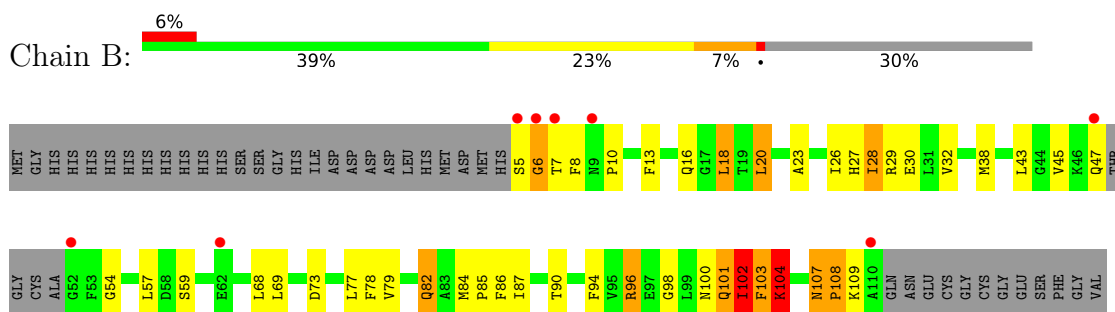
3 Residue-property plots [i](#)

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: SufA protein



- Molecule 1: SufA protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	25.16Å 88.50Å 122.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.60 – 2.70 41.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.60-2.70) 95.2 (41.60-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.272 0.229 , 0.267	Depositor DCC
R_{free} test set	861 reflections (10.64%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1677	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.12% 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

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	3.56	132/875 (15.1%)	2.70	82/1187 (6.9%)
1	B	0.95	6/806 (0.7%)	1.23	10/1093 (0.9%)
All	All	2.65	138/1681 (8.2%)	2.13	92/2280 (4.0%)

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	2

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ASP	CB-CG	12.57	1.83	1.52
1	A	47	GLN	CG-CD	12.04	1.82	1.52
1	A	118	GLU	C-O	-12.01	1.08	1.24
1	A	66	ASP	CB-CG	11.51	1.80	1.52
1	A	58	ASP	CG-OD1	11.35	1.47	1.25
1	A	19	THR	C-O	-11.01	1.09	1.23
1	A	16	GLN	CA-C	-10.53	1.39	1.52
1	A	32	VAL	CA-CB	-10.41	1.39	1.54
1	A	36	PRO	C-O	10.38	1.35	1.23
1	A	14	ALA	CA-C	10.29	1.66	1.52
1	A	73	ASP	C-O	-10.11	1.10	1.23
1	A	11	GLN	CG-CD	10.04	1.77	1.52
1	A	92	VAL	CA-CB	-9.84	1.42	1.54
1	A	102	ILE	C-O	-9.47	1.12	1.23
1	A	10	PRO	CA-C	9.46	1.65	1.52
1	A	45	VAL	C-O	-9.32	1.14	1.24
1	A	29	ARG	CZ-NH2	9.30	1.45	1.33
1	A	59	SER	C-O	9.12	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	SER	N-CA	8.98	1.58	1.46
1	A	71	GLU	C-O	-8.97	1.13	1.24
1	A	63	PRO	C-O	-8.94	1.13	1.23
1	A	11	GLN	CB-CG	8.89	1.79	1.52
1	A	49	GLY	CA-C	8.89	1.66	1.51
1	A	95	VAL	C-O	-8.41	1.15	1.24
1	A	107	ASN	CA-C	8.38	1.62	1.52
1	A	28	ILE	N-CA	-8.13	1.36	1.46
1	A	65	LYS	CA-CB	7.97	1.66	1.53
1	A	95	VAL	CA-CB	7.94	1.64	1.54
1	A	76	LYS	C-O	-7.86	1.14	1.24
1	A	58	ASP	CA-C	-7.73	1.43	1.52
1	A	11	GLN	N-CA	7.73	1.56	1.46
1	A	46	LYS	CA-C	7.72	1.61	1.52
1	A	48	THR	CA-C	7.71	1.62	1.52
1	A	112	ASN	CA-C	7.70	1.65	1.52
1	A	46	LYS	CA-CB	7.66	1.71	1.53
1	A	116	CYS	C-O	7.63	1.33	1.24
1	A	86	PHE	CA-C	7.59	1.63	1.52
1	A	17	GLY	C-O	7.57	1.32	1.23
1	A	36	PRO	N-CD	7.56	1.58	1.47
1	A	121	GLY	C-O	7.42	1.33	1.23
1	B	104	LYS	N-CA	-7.29	1.37	1.46
1	A	62	GLU	CA-CB	7.27	1.63	1.53
1	A	34	LYS	C-O	-7.22	1.14	1.24
1	A	106	HIS	CA-CB	7.21	1.64	1.53
1	A	120	PHE	CA-C	7.20	1.60	1.52
1	A	11	GLN	CA-C	7.18	1.62	1.52
1	A	60	VAL	CA-CB	7.17	1.67	1.55
1	A	61	SER	C-O	-7.13	1.12	1.23
1	A	104	LYS	N-CA	-7.13	1.37	1.45
1	A	35	GLN	N-CA	-7.13	1.39	1.46
1	A	106	HIS	CB-CG	7.10	1.60	1.50
1	A	93	ASP	CG-OD1	7.08	1.38	1.25
1	A	62	GLU	CD-OE2	7.08	1.38	1.25
1	A	107	ASN	N-CA	7.02	1.56	1.46
1	A	119	SER	CA-C	6.96	1.61	1.52
1	A	18	LEU	CA-C	-6.92	1.44	1.52
1	A	18	LEU	C-O	-6.92	1.15	1.23
1	A	28	ILE	C-O	-6.91	1.15	1.24
1	A	41	VAL	CA-CB	-6.88	1.44	1.54
1	A	23	ALA	CA-C	6.86	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	ILE	CA-CB	6.84	1.63	1.54
1	A	87	ILE	C-O	6.84	1.32	1.24
1	A	97	GLU	N-CA	-6.83	1.38	1.46
1	A	60	VAL	CA-C	-6.82	1.44	1.52
1	A	19	THR	C-N	-6.75	1.24	1.33
1	A	86	PHE	CA-CB	6.72	1.65	1.53
1	A	56	VAL	N-CA	6.71	1.54	1.46
1	A	72	HIS	C-O	-6.64	1.16	1.24
1	A	113	GLU	C-O	6.59	1.31	1.23
1	A	93	ASP	CA-C	6.57	1.60	1.52
1	A	73	ASP	CG-OD2	6.55	1.37	1.25
1	A	12	ASP	CB-CG	6.50	1.68	1.52
1	A	79	VAL	C-O	-6.50	1.17	1.23
1	A	54	GLY	CA-C	-6.45	1.46	1.52
1	A	63	PRO	CA-C	-6.42	1.44	1.52
1	A	112	ASN	CA-CB	6.41	1.63	1.53
1	A	95	VAL	CA-C	-6.37	1.44	1.52
1	A	102	ILE	N-CA	-6.36	1.38	1.46
1	A	47	GLN	CB-CG	6.36	1.71	1.52
1	A	111	GLN	C-O	6.36	1.31	1.24
1	B	104	LYS	CE-NZ	6.33	1.68	1.49
1	A	51	ALA	CA-CB	6.32	1.61	1.53
1	A	66	ASP	CA-C	6.32	1.61	1.52
1	A	49	GLY	N-CA	6.30	1.54	1.45
1	A	90	THR	CA-CB	-6.29	1.43	1.53
1	A	101	GLN	CA-CB	-6.29	1.44	1.53
1	A	86	PHE	CB-CG	6.25	1.65	1.50
1	A	76	LYS	CA-C	6.25	1.60	1.52
1	B	104	LYS	CD-CE	6.25	1.71	1.52
1	A	59	SER	CB-OG	-6.19	1.29	1.42
1	A	73	ASP	CA-CB	6.19	1.63	1.53
1	B	102	ILE	CA-CB	6.14	1.62	1.54
1	A	26	ILE	CB-CG1	6.13	1.65	1.53
1	A	116	CYS	CA-C	-6.12	1.44	1.52
1	A	119	SER	C-O	-6.11	1.16	1.23
1	A	84	MET	SD-CE	-6.10	1.64	1.79
1	A	53	PHE	CB-CG	6.09	1.64	1.50
1	A	84	MET	N-CA	-6.06	1.41	1.46
1	A	73	ASP	CA-C	6.06	1.60	1.53
1	A	65	LYS	N-CA	6.01	1.53	1.46
1	A	33	ALA	N-CA	-6.01	1.38	1.46
1	A	86	PHE	CD1-CE1	6.00	1.56	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	THR	N-CA	5.97	1.55	1.46
1	A	90	THR	N-CA	5.97	1.53	1.46
1	A	59	SER	CA-CB	-5.89	1.43	1.53
1	A	9	ASN	CA-CB	5.84	1.65	1.53
1	A	112	ASN	C-N	5.82	1.41	1.33
1	A	36	PRO	CB-CG	5.81	1.78	1.49
1	A	100	ASN	CA-C	-5.79	1.45	1.52
1	A	65	LYS	CA-C	5.78	1.60	1.52
1	B	109	LYS	CA-C	5.69	1.61	1.52
1	A	13	PHE	CA-C	5.63	1.60	1.52
1	A	108	PRO	C-O	-5.62	1.16	1.24
1	A	89	GLY	C-N	5.62	1.41	1.33
1	A	104	LYS	CA-CB	-5.61	1.43	1.53
1	A	79	VAL	CA-CB	-5.61	1.50	1.54
1	A	108	PRO	CA-C	5.59	1.61	1.52
1	A	69	LEU	C-O	-5.59	1.17	1.24
1	A	91	GLU	CD-OE1	5.58	1.35	1.25
1	A	49	GLY	C-O	5.56	1.31	1.24
1	A	43	LEU	C-O	-5.49	1.17	1.24
1	A	36	PRO	N-CA	5.42	1.53	1.47
1	A	110	ALA	CA-CB	-5.41	1.45	1.53
1	B	103	PHE	CB-CG	5.37	1.63	1.50
1	A	53	PHE	CG-CD2	5.32	1.50	1.38
1	A	78	PHE	CA-C	-5.31	1.46	1.52
1	A	101	GLN	CB-CG	-5.28	1.36	1.52
1	A	29	ARG	C-N	-5.24	1.26	1.33
1	A	106	HIS	CA-C	-5.23	1.46	1.53
1	A	24	ALA	N-CA	-5.22	1.40	1.46
1	A	43	LEU	CA-CB	-5.21	1.46	1.53
1	A	83	ALA	CA-CB	-5.21	1.46	1.54
1	A	31	LEU	CA-CB	-5.15	1.45	1.53
1	A	122	VAL	CA-C	5.11	1.63	1.52
1	A	107	ASN	CG-OD1	5.11	1.33	1.23
1	A	43	LEU	C-N	-5.09	1.28	1.33
1	A	51	ALA	C-O	5.02	1.30	1.24
1	A	15	TRP	CA-C	-5.01	1.46	1.52

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ILE	N-CA-C	11.93	125.48	108.42
1	A	29	ARG	NE-CZ-NH1	-11.65	109.85	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASP	CA-CB-CG	11.32	123.92	112.60
1	A	29	ARG	NE-CZ-NH2	11.32	129.39	119.20
1	A	33	ALA	N-CA-C	-10.77	99.65	113.12
1	A	119	SER	N-CA-C	9.48	124.47	109.50
1	A	118	GLU	CA-C-O	9.32	130.94	119.95
1	A	36	PRO	CB-CA-C	-9.18	98.95	110.98
1	A	76	LYS	N-CA-C	9.18	124.36	109.76
1	A	89	GLY	CA-C-O	-9.07	109.97	118.95
1	A	111	GLN	O-C-N	-8.89	110.77	122.59
1	B	8	PHE	N-CA-C	8.74	119.79	108.34
1	A	54	GLY	N-CA-C	-8.61	96.13	111.19
1	A	119	SER	N-CA-CB	-8.53	95.84	111.37
1	A	109	LYS	N-CA-C	-8.49	102.94	113.38
1	B	107	ASN	CB-CA-C	8.33	119.30	109.47
1	A	81	LEU	N-CA-C	8.30	125.07	111.37
1	A	28	ILE	N-CA-C	-8.28	101.98	111.00
1	A	110	ALA	CA-C-O	-8.14	110.07	119.60
1	A	19	THR	CA-C-O	7.86	130.63	121.44
1	A	49	GLY	N-CA-C	7.75	125.45	111.34
1	A	19	THR	N-CA-C	7.70	121.46	109.52
1	A	96	ARG	NE-CZ-NH1	-7.68	113.82	121.50
1	A	113	GLU	CA-C-O	-7.53	112.94	121.07
1	A	85	PRO	N-CD-CG	-7.52	91.91	103.20
1	A	72	HIS	CA-C-N	7.52	132.83	122.07
1	A	72	HIS	C-N-CA	7.52	132.83	122.07
1	A	89	GLY	N-CA-C	7.39	125.34	115.59
1	A	63	PRO	CB-CA-C	-7.26	102.10	111.46
1	A	35	GLN	CA-C-O	7.15	126.86	119.49
1	A	16	GLN	CB-CA-C	-7.13	97.65	110.70
1	A	11	GLN	CB-CG-CD	7.02	124.54	112.60
1	A	47	GLN	N-CA-C	-6.89	100.08	110.28
1	A	109	LYS	CB-CG-CD	6.89	127.15	111.30
1	A	19	THR	O-C-N	-6.85	114.24	123.15
1	A	114	CYS	CA-CB-SG	-6.68	99.04	114.40
1	A	50	CYS	N-CA-CB	6.63	121.69	110.49
1	A	122	VAL	CB-CA-C	-6.61	98.85	111.40
1	A	95	VAL	N-CA-CB	6.56	120.47	111.41
1	A	53	PHE	CA-C-N	6.56	126.70	122.18
1	A	53	PHE	C-N-CA	6.56	126.70	122.18
1	A	79	VAL	CB-CA-C	-6.45	103.65	110.16
1	A	73	ASP	O-C-N	-6.35	114.09	122.40
1	A	47	GLN	CB-CG-CD	6.32	123.34	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	PRO	CA-C-O	-6.30	114.16	121.34
1	B	16	GLN	N-CA-C	-6.19	104.64	111.82
1	A	26	ILE	CA-CB-CG1	6.17	120.89	110.40
1	A	16	GLN	N-CA-CB	6.11	119.30	110.20
1	A	100	ASN	CA-CB-CG	6.08	118.68	112.60
1	B	108	PRO	CB-CA-C	-6.08	102.72	112.21
1	A	66	ASP	CB-CG-OD2	6.07	132.36	118.40
1	A	104	LYS	CG-CD-CE	5.96	125.01	111.30
1	A	26	ILE	N-CA-C	-5.96	104.70	110.42
1	A	47	GLN	CB-CA-C	5.93	119.79	109.65
1	B	101	GLN	N-CA-C	-5.85	97.64	107.99
1	A	11	GLN	N-CA-CB	5.85	120.37	110.49
1	A	99	LEU	CD1-CG-CD2	-5.80	98.03	110.80
1	A	99	LEU	CA-CB-CG	5.78	136.52	116.30
1	A	81	LEU	CB-CA-C	-5.76	101.17	110.74
1	A	80	PRO	CA-C-O	-5.76	115.23	121.27
1	A	66	ASP	OD1-CG-OD2	-5.75	109.09	122.90
1	A	10	PRO	N-CA-C	5.72	124.26	112.47
1	A	119	SER	CA-C-N	5.72	130.73	122.44
1	A	119	SER	C-N-CA	5.72	130.73	122.44
1	A	9	ASN	CA-C-N	5.69	126.95	119.84
1	A	9	ASN	C-N-CA	5.69	126.95	119.84
1	B	28	ILE	N-CA-C	-5.64	105.22	110.53
1	A	110	ALA	O-C-N	-5.63	114.37	122.36
1	A	50	CYS	CA-C-N	-5.58	114.23	122.83
1	A	50	CYS	C-N-CA	-5.58	114.23	122.83
1	A	87	ILE	N-CA-C	5.57	120.93	109.34
1	A	36	PRO	CB-CG-CD	-5.55	88.35	106.10
1	A	93	ASP	CB-CG-OD1	5.55	131.16	118.40
1	A	76	LYS	CA-C-O	5.54	127.01	120.69
1	A	12	ASP	CB-CA-C	5.53	121.41	110.42
1	B	102	ILE	CA-CB-CG2	5.51	119.86	110.50
1	A	90	THR	CB-CA-C	-5.47	100.89	109.70
1	A	73	ASP	N-CA-C	-5.44	104.14	111.54
1	A	76	LYS	O-C-N	-5.42	116.70	123.04
1	A	48	THR	N-CA-C	5.39	115.24	108.45
1	A	73	ASP	CB-CG-OD1	5.39	130.79	118.40
1	A	64	ASP	CA-C-N	5.36	128.24	120.79
1	A	64	ASP	C-N-CA	5.36	128.24	120.79
1	B	101	GLN	CA-C-N	-5.30	115.62	122.99
1	B	101	GLN	C-N-CA	-5.30	115.62	122.99
1	A	59	SER	N-CA-CB	-5.29	101.85	109.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ASN	CB-CA-C	5.24	120.85	110.42
1	B	109	LYS	CA-CB-CG	5.07	124.25	114.10
1	A	73	ASP	OD1-CG-OD2	-5.07	110.74	122.90
1	A	97	GLU	CB-CA-C	5.05	118.39	109.80
1	A	104	LYS	CA-CB-CG	5.03	124.17	114.10
1	A	114	CYS	CB-CA-C	-5.00	101.64	109.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	VAL	Peptide
1	A	49	GLY	Peptide

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	854	0	808	57	0
1	B	786	0	759	33	0
2	A	18	0	0	4	0
2	B	19	0	0	0	0
All	All	1677	0	1567	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 27.

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:11:GLN:CB	1:A:11:GLN:CG	1.79	1.59
1:A:11:GLN:CG	1:A:11:GLN:CD	1.77	1.58
1:B:104:LYS:NZ	1:B:104:LYS:CE	1.68	1.54
1:A:66:ASP:CB	1:A:66:ASP:CG	1.80	1.53
1:A:36:PRO:CB	1:A:36:PRO:CG	1.78	1.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:CD	1:A:47:GLN:CG	1.82	1.52
1:A:73:ASP:CB	1:A:73:ASP:CG	1.83	1.50
1:A:11:GLN:CG	1:A:12:ASP:H	1.37	1.34
1:A:11:GLN:CG	1:A:12:ASP:N	2.17	1.07
1:A:11:GLN:HG3	1:A:12:ASP:H	1.17	1.07
1:A:11:GLN:HG3	1:A:12:ASP:N	1.69	1.05
1:A:110:ALA:O	1:A:111:GLN:O	1.92	0.88
1:A:104:LYS:HG2	2:A:139:HOH:O	1.74	0.87
1:A:114:CYS:SG	1:A:115:GLY:N	2.44	0.87
1:A:18:LEU:HD13	1:A:90:THR:HB	1.63	0.79
1:A:102:ILE:HG12	2:A:139:HOH:O	1.82	0.79
1:A:114:CYS:SG	1:A:116:CYS:N	2.58	0.77
1:B:26:ILE:HG22	1:B:29:ARG:NH2	2.03	0.72
1:A:11:GLN:CD	1:A:12:ASP:H	1.99	0.71
1:A:110:ALA:O	1:A:111:GLN:C	2.33	0.70
1:A:47:GLN:HE21	1:A:47:GLN:H	1.39	0.70
1:A:112:ASN:HD22	1:A:112:ASN:C	2.01	0.69
1:A:114:CYS:SG	1:A:115:GLY:C	2.78	0.67
1:A:100:ASN:HB2	1:A:120:PHE:CZ	2.30	0.66
1:B:26:ILE:O	1:B:30:GLU:HG3	1.96	0.65
1:A:110:ALA:C	1:A:111:GLN:O	2.39	0.64
1:B:38:MET:HE3	1:B:59:SER:HA	1.78	0.64
1:A:20:LEU:HD11	1:A:28:ILE:HD12	1.81	0.63
1:B:85:PRO:HG2	1:B:86:PHE:CD1	2.33	0.63
1:B:79:VAL:HG11	1:B:87:ILE:HD11	1.80	0.63
1:A:28:ILE:O	1:A:32:VAL:HG23	2.00	0.61
1:B:20:LEU:HD11	1:B:77:LEU:HD22	1.83	0.60
1:A:103:PHE:H	1:B:100:ASN:HD21	1.50	0.60
1:B:26:ILE:HG22	1:B:29:ARG:HH22	1.66	0.60
1:B:94:PHE:HZ	1:B:101:GLN:HB3	1.67	0.59
1:A:103:PHE:C	2:A:139:HOH:O	2.47	0.57
1:A:102:ILE:HG23	2:A:139:HOH:O	2.04	0.57
1:B:69:LEU:HD13	1:B:78:PHE:CE1	2.41	0.56
1:A:120:PHE:CE2	1:B:57:LEU:HB2	2.41	0.56
1:A:11:GLN:NE2	1:A:12:ASP:HA	2.21	0.55
1:A:114:CYS:SG	1:A:115:GLY:CA	2.94	0.55
1:A:20:LEU:CD1	1:A:28:ILE:HD12	2.37	0.54
1:A:43:LEU:O	1:A:80:PRO:HD2	2.07	0.54
1:B:29:ARG:HD3	1:B:73:ASP:O	2.08	0.53
1:A:81:LEU:C	1:A:83:ALA:H	2.17	0.53
1:B:96:ARG:HH11	1:B:96:ARG:HG2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:H	1:A:47:GLN:NE2	2.06	0.52
1:A:112:ASN:O	1:A:112:ASN:ND2	2.30	0.50
1:B:102:ILE:HD12	1:B:103:PHE:O	2.12	0.49
1:A:66:ASP:CG	1:A:66:ASP:C	2.81	0.49
1:A:11:GLN:CG	1:A:11:GLN:NE2	2.67	0.48
1:A:35:GLN:HA	1:A:36:PRO:HD2	1.73	0.47
1:A:24:ALA:O	1:A:28:ILE:HG13	2.15	0.47
1:A:81:LEU:C	1:A:83:ALA:N	2.72	0.47
1:B:68:LEU:HD12	1:B:84:MET:HG3	1.97	0.47
1:B:94:PHE:CZ	1:B:101:GLN:HB3	2.48	0.47
1:A:100:ASN:HB2	1:A:120:PHE:CE1	2.50	0.47
1:A:100:ASN:CB	1:A:120:PHE:CZ	2.97	0.47
1:B:10:PRO:HA	1:B:13:PHE:CG	2.50	0.47
1:A:42:ARG:HA	1:A:78:PHE:O	2.15	0.46
1:A:66:ASP:C	1:A:66:ASP:OD1	2.58	0.46
1:A:11:GLN:CD	1:A:12:ASP:N	2.72	0.46
1:A:122:VAL:OXT	1:A:122:VAL:HG23	2.16	0.46
1:B:84:MET:N	1:B:85:PRO:HD2	2.30	0.46
1:A:84:MET:HB2	1:A:85:PRO:HD2	1.98	0.45
1:B:87:ILE:O	1:B:90:THR:OG1	2.30	0.45
1:B:28:ILE:O	1:B:32:VAL:HG23	2.17	0.45
1:A:22:PRO:O	1:A:26:ILE:HG12	2.18	0.44
1:B:5:SER:O	1:B:6:GLY:C	2.59	0.44
1:A:11:GLN:HG2	1:A:81:LEU:HD13	2.00	0.43
1:B:45:VAL:HA	1:B:54:GLY:O	2.18	0.43
1:B:107:ASN:OD1	1:B:108:PRO:HD2	2.18	0.43
1:A:46:LYS:O	1:A:53:PHE:HA	2.19	0.43
1:B:82:GLN:H	1:B:82:GLN:CD	2.26	0.43
1:A:90:THR:HG22	1:A:91:GLU:N	2.34	0.43
1:B:5:SER:O	1:B:7:THR:HG22	2.18	0.42
1:B:28:ILE:HD13	1:B:28:ILE:HA	1.87	0.42
1:A:112:ASN:C	1:A:112:ASN:ND2	2.75	0.42
1:A:57:LEU:O	1:B:98:GLY:HA3	2.20	0.42
1:B:18:LEU:HD21	1:B:87:ILE:HD12	2.02	0.42
1:B:23:ALA:O	1:B:27:HIS:HD2	2.02	0.42
1:A:11:GLN:CG	1:A:11:GLN:C	2.89	0.41
1:A:11:GLN:HG3	1:A:11:GLN:C	2.41	0.41
1:B:18:LEU:HD13	1:B:90:THR:HB	2.02	0.41
1:B:69:LEU:HD13	1:B:78:PHE:CZ	2.56	0.41
1:A:11:GLN:CD	1:A:12:ASP:HA	2.46	0.40
1:B:107:ASN:OD1	1:B:107:ASN:C	2.65	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	112/145 (77%)	93 (83%)	13 (12%)	6 (5%)	1	2
1	B	98/145 (68%)	93 (95%)	4 (4%)	1 (1%)	12	32
All	All	210/290 (72%)	186 (89%)	17 (8%)	7 (3%)	3	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	111	GLN
1	B	6	GLY
1	A	14	ALA
1	A	11	GLN
1	A	50	CYS
1	A	98	GLY

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	87/120 (72%)	68 (78%)	19 (22%)	1	3
1	B	81/120 (68%)	73 (90%)	8 (10%)	7	19
All	All	168/240 (70%)	141 (84%)	27 (16%)	2	6

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	16	GLN
1	A	18	LEU
1	A	34	LYS
1	A	43	LEU
1	A	45	VAL
1	A	47	GLN
1	A	57	LEU
1	A	58	ASP
1	A	62	GLU
1	A	66	ASP
1	A	82	GLN
1	A	95	VAL
1	A	97	GLU
1	A	99	LEU
1	A	100	ASN
1	A	104	LYS
1	A	112	ASN
1	A	114	CYS
1	B	18	LEU
1	B	20	LEU
1	B	43	LEU
1	B	47	GLN
1	B	82	GLN
1	B	96	ARG
1	B	102	ILE
1	B	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	B	9	ASN
1	B	27	HIS
1	B	35	GLN
1	B	100	ASN
1	B	106	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](#)

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

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	114/145 (78%)	0.54	22 (19%) 3 3	15, 29, 87, 96	0
1	B	102/145 (70%)	0.33	8 (7%) 19 16	12, 28, 58, 74	0
All	All	216/290 (74%)	0.44	30 (13%) 6 5	12, 29, 74, 96	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	GLN	5.7
1	A	9	ASN	5.2
1	A	115	GLY	4.3
1	A	11	GLN	4.2
1	A	51	ALA	4.1
1	B	5	SER	3.9
1	A	113	GLU	3.9
1	A	49	GLY	3.9
1	A	50	CYS	3.7
1	A	114	CYS	3.7
1	A	10	PRO	3.7
1	A	118	GLU	3.7
1	B	9	ASN	3.3
1	A	12	ASP	3.1
1	B	6	GLY	3.0
1	A	112	ASN	2.8
1	A	110	ALA	2.8
1	B	110	ALA	2.8
1	A	13	PHE	2.7
1	B	47	GLN	2.7
1	B	7	THR	2.5
1	B	52	GLY	2.5
1	A	47	GLN	2.4
1	A	86	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	52	GLY	2.3
1	A	116	CYS	2.2
1	A	72	HIS	2.1
1	A	36	PRO	2.1
1	B	62	GLU	2.0
1	A	122	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.