



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:26 PM UTC

PDB ID : 1IDS / pdb_00001ids
Title : X-RAY STRUCTURE ANALYSIS OF THE IRON-DEPENDENT SUPER-OXIDE DISMUTASE FROM MYCOBACTERIUM TUBERCULOSIS AT 2.0 ANGSTROMS RESOLUTIONS REVEALS NOVEL DIMER-DIMER INTERACTIONS
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Deposited on : 1994-09-29
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

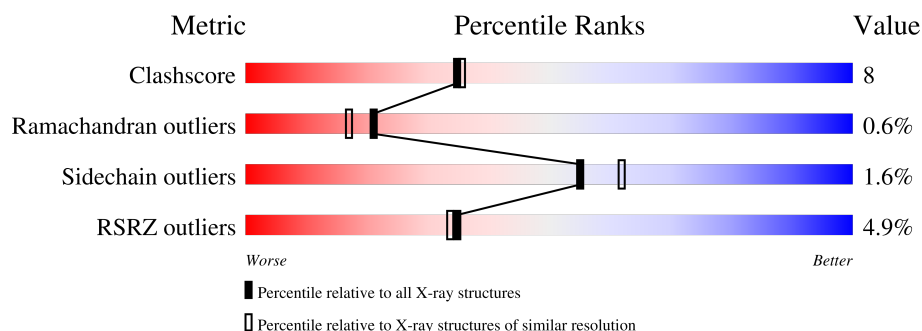
1 Overall quality at a glance

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))
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	207	5% 71% 20% . .
1	B	207	5% 71% 21% . .
1	C	207	5% 67% 25% . .
1	D	207	4% 71% 22% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6932 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 IRON SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1568	1012	269	286	1			
1	B	198	Total	C	N	O	S	0	0	0
			1568	1012	269	286	1			
1	C	198	Total	C	N	O	S	0	0	0
			1568	1012	269	286	1			
1	D	198	Total	C	N	O	S	0	0	0
			1568	1012	269	286	1			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

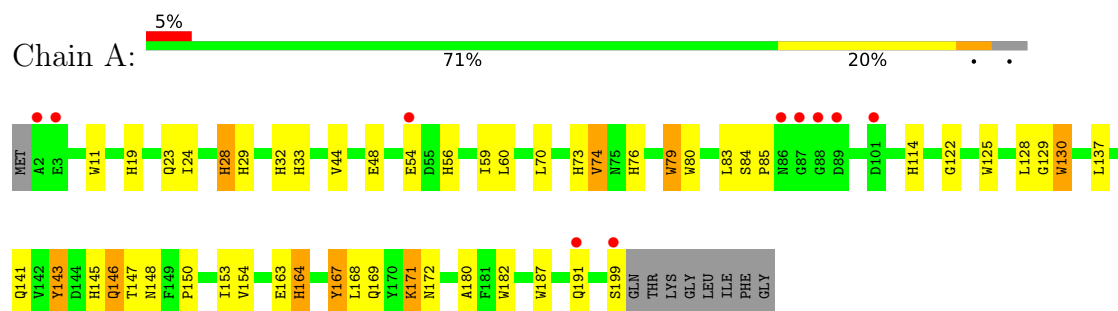
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total	O	0	0
			180	180		
3	B	168	Total	O	0	0
			168	168		
3	C	153	Total	O	0	0
			153	153		
3	D	155	Total	O	0	0
			155	155		

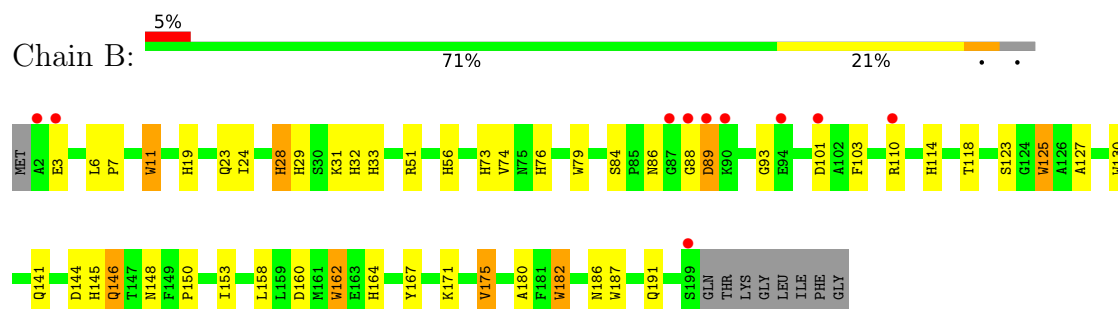
3 Residue-property plots [i](#)

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.

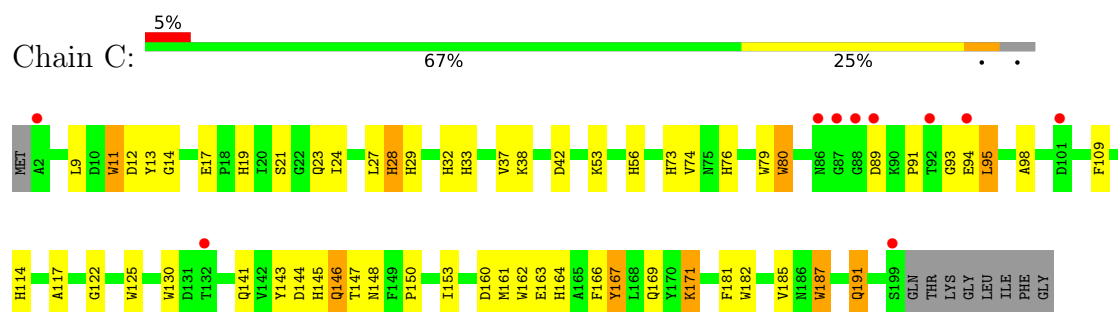
• Molecule 1: IRON SUPEROXIDE DISMUTASE



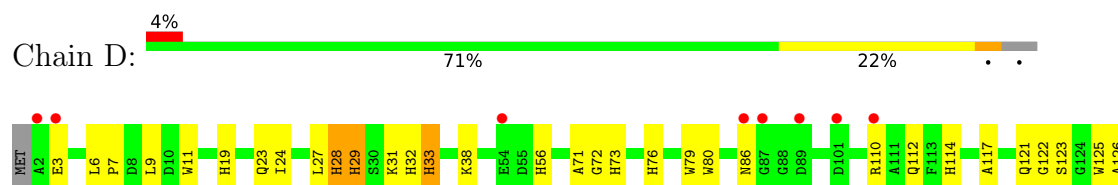
• Molecule 1: IRON SUPEROXIDE DISMUTASE

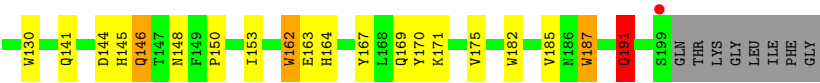


• Molecule 1: IRON SUPEROXIDE DISMUTASE



• Molecule 1: IRON SUPEROXIDE DISMUTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.65Å 85.40Å 66.35Å 90.00° 99.86° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 67.64 – 2.01	Depositor EDS
% Data completeness (in resolution range)	80.4 ((Not available)-2.00) 79.8 (67.64-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.00Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.167 , (Not available) 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 12.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6932	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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: FE

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	1.38	34/1617 (2.1%)	1.55	10/2206 (0.5%)
1	B	1.39	32/1617 (2.0%)	1.56	19/2206 (0.9%)
1	C	1.39	33/1617 (2.0%)	1.52	14/2206 (0.6%)
1	D	1.40	37/1617 (2.3%)	1.52	7/2206 (0.3%)
All	All	1.39	136/6468 (2.1%)	1.54	50/8824 (0.6%)

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	76	HIS	CE1-NE2	7.59	1.40	1.32
1	D	114	HIS	CE1-NE2	7.42	1.40	1.32
1	C	32	HIS	CE1-NE2	7.34	1.39	1.32
1	C	56	HIS	ND1-CE1	7.31	1.39	1.32
1	B	19	HIS	CE1-NE2	7.21	1.39	1.32
1	B	114	HIS	CE1-NE2	7.20	1.39	1.32
1	C	19	HIS	ND1-CE1	7.18	1.39	1.32
1	A	19	HIS	CE1-NE2	7.16	1.39	1.32
1	B	114	HIS	ND1-CE1	7.16	1.39	1.32
1	A	32	HIS	CE1-NE2	7.12	1.39	1.32
1	B	76	HIS	CE1-NE2	7.11	1.39	1.32
1	D	32	HIS	ND1-CE1	7.10	1.39	1.32
1	A	145	HIS	ND1-CE1	7.10	1.39	1.32
1	A	56	HIS	ND1-CE1	7.08	1.39	1.32
1	B	29	HIS	ND1-CE1	7.05	1.39	1.32
1	D	56	HIS	CE1-NE2	7.05	1.39	1.32
1	D	19	HIS	CE1-NE2	7.04	1.39	1.32
1	A	73	HIS	CE1-NE2	7.04	1.39	1.32
1	A	73	HIS	ND1-CE1	7.04	1.39	1.32
1	D	19	HIS	ND1-CE1	7.03	1.39	1.32
1	D	164	HIS	CE1-NE2	7.02	1.39	1.32
1	A	164	HIS	CE1-NE2	7.01	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	145	HIS	ND1-CE1	7.01	1.39	1.32
1	C	32	HIS	ND1-CE1	7.00	1.39	1.32
1	C	56	HIS	CE1-NE2	6.98	1.39	1.32
1	C	164	HIS	CE1-NE2	6.96	1.39	1.32
1	B	32	HIS	CE1-NE2	6.96	1.39	1.32
1	B	164	HIS	CE1-NE2	6.94	1.39	1.32
1	B	32	HIS	ND1-CE1	6.91	1.39	1.32
1	D	33	HIS	CE1-NE2	6.90	1.39	1.32
1	C	33	HIS	ND1-CE1	6.89	1.39	1.32
1	D	73	HIS	CE1-NE2	6.88	1.39	1.32
1	C	73	HIS	ND1-CE1	6.87	1.39	1.32
1	B	56	HIS	CE1-NE2	6.87	1.39	1.32
1	C	19	HIS	CE1-NE2	6.87	1.39	1.32
1	C	28	HIS	CE1-NE2	6.86	1.39	1.32
1	B	29	HIS	CE1-NE2	6.84	1.39	1.32
1	B	76	HIS	ND1-CE1	6.84	1.39	1.32
1	C	76	HIS	CE1-NE2	6.83	1.39	1.32
1	C	33	HIS	CE1-NE2	6.80	1.39	1.32
1	A	29	HIS	ND1-CE1	6.80	1.39	1.32
1	B	73	HIS	CE1-NE2	6.78	1.39	1.32
1	B	33	HIS	CE1-NE2	6.78	1.39	1.32
1	A	33	HIS	CE1-NE2	6.77	1.39	1.32
1	A	164	HIS	ND1-CE1	6.74	1.39	1.32
1	A	32	HIS	ND1-CE1	6.74	1.39	1.32
1	D	29	HIS	ND1-CE1	6.72	1.39	1.32
1	C	114	HIS	CE1-NE2	6.72	1.39	1.32
1	D	164	HIS	ND1-CE1	6.68	1.39	1.32
1	B	73	HIS	ND1-CE1	6.67	1.39	1.32
1	B	145	HIS	ND1-CE1	6.65	1.39	1.32
1	A	28	HIS	ND1-CE1	6.64	1.39	1.32
1	A	33	HIS	ND1-CE1	6.64	1.39	1.32
1	D	33	HIS	ND1-CE1	6.63	1.39	1.32
1	D	73	HIS	ND1-CE1	6.63	1.39	1.32
1	D	32	HIS	CE1-NE2	6.62	1.39	1.32
1	A	19	HIS	ND1-CE1	6.61	1.39	1.32
1	D	145	HIS	CE1-NE2	6.61	1.39	1.32
1	D	114	HIS	ND1-CE1	6.60	1.39	1.32
1	A	76	HIS	CE1-NE2	6.58	1.39	1.32
1	D	28	HIS	ND1-CE1	6.55	1.39	1.32
1	C	73	HIS	CE1-NE2	6.53	1.39	1.32
1	B	28	HIS	ND1-CE1	6.53	1.39	1.32
1	A	114	HIS	CE1-NE2	6.51	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	29	HIS	CE1-NE2	6.51	1.39	1.32
1	B	19	HIS	ND1-CE1	6.50	1.39	1.32
1	D	56	HIS	ND1-CE1	6.42	1.39	1.32
1	A	28	HIS	CE1-NE2	6.42	1.39	1.32
1	A	29	HIS	CE1-NE2	6.41	1.39	1.32
1	C	164	HIS	ND1-CE1	6.40	1.39	1.32
1	B	28	HIS	CE1-NE2	6.38	1.39	1.32
1	A	56	HIS	CE1-NE2	6.37	1.39	1.32
1	B	145	HIS	CE1-NE2	6.37	1.39	1.32
1	C	76	HIS	ND1-CE1	6.34	1.38	1.32
1	C	114	HIS	ND1-CE1	6.33	1.38	1.32
1	C	28	HIS	ND1-CE1	6.32	1.38	1.32
1	B	33	HIS	ND1-CE1	6.30	1.38	1.32
1	C	29	HIS	CE1-NE2	6.20	1.38	1.32
1	D	28	HIS	CE1-NE2	6.19	1.38	1.32
1	B	56	HIS	ND1-CE1	6.12	1.38	1.32
1	C	29	HIS	ND1-CE1	6.10	1.38	1.32
1	C	145	HIS	CE1-NE2	6.08	1.38	1.32
1	B	164	HIS	ND1-CE1	6.01	1.38	1.32
1	A	145	HIS	CE1-NE2	6.00	1.38	1.32
1	C	80	TRP	NE1-CE2	-6.00	1.30	1.37
1	A	76	HIS	ND1-CE1	5.98	1.38	1.32
1	A	114	HIS	ND1-CE1	5.96	1.38	1.32
1	D	80	TRP	NE1-CE2	-5.96	1.30	1.37
1	D	76	HIS	ND1-CE1	5.83	1.38	1.32
1	D	182	TRP	NE1-CE2	-5.80	1.31	1.37
1	C	145	HIS	ND1-CE1	5.79	1.38	1.32
1	C	11	TRP	NE1-CE2	-5.79	1.31	1.37
1	D	79	TRP	NE1-CE2	-5.76	1.31	1.37
1	B	79	TRP	NE1-CE2	-5.75	1.31	1.37
1	B	182	TRP	NE1-CE2	-5.72	1.31	1.37
1	D	11	TRP	NE1-CE2	-5.68	1.31	1.37
1	B	130	TRP	NE1-CE2	-5.64	1.31	1.37
1	C	191	GLN	CD-OE1	5.61	1.34	1.23
1	B	11	TRP	NE1-CE2	-5.59	1.31	1.37
1	B	125	TRP	NE1-CE2	-5.54	1.31	1.37
1	B	162	TRP	NE1-CE2	-5.53	1.31	1.37
1	C	79	TRP	NE1-CE2	-5.53	1.31	1.37
1	C	23	GLN	CD-OE1	5.52	1.34	1.23
1	D	187	TRP	NE1-CE2	-5.48	1.31	1.37
1	A	130	TRP	NE1-CE2	-5.47	1.31	1.37
1	A	125	TRP	NE1-CE2	-5.45	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	TRP	NE1-CE2	-5.43	1.31	1.37
1	D	191	GLN	CD-OE1	5.43	1.33	1.23
1	A	191	GLN	CD-OE1	5.41	1.33	1.23
1	C	182	TRP	NE1-CE2	-5.39	1.31	1.37
1	A	79	TRP	NE1-CE2	-5.38	1.31	1.37
1	A	182	TRP	NE1-CE2	-5.37	1.31	1.37
1	A	187	TRP	NE1-CE2	-5.35	1.31	1.37
1	B	23	GLN	CD-OE1	5.35	1.33	1.23
1	A	23	GLN	CD-OE1	5.34	1.33	1.23
1	D	125	TRP	NE1-CE2	-5.34	1.31	1.37
1	B	191	GLN	CD-OE1	5.32	1.33	1.23
1	D	169	GLN	CD-OE1	5.32	1.33	1.23
1	C	187	TRP	NE1-CE2	-5.29	1.31	1.37
1	A	11	TRP	NE1-CE2	-5.29	1.31	1.37
1	D	23	GLN	CD-OE1	5.27	1.33	1.23
1	C	162	TRP	NE1-CE2	-5.25	1.31	1.37
1	D	162	TRP	NE1-CE2	-5.24	1.31	1.37
1	B	187	TRP	NE1-CE2	-5.22	1.31	1.37
1	A	169	GLN	CD-OE1	5.17	1.33	1.23
1	D	121	GLN	CD-OE1	5.15	1.33	1.23
1	A	146	GLN	CD-OE1	5.14	1.33	1.23
1	B	141	GLN	CD-OE1	5.13	1.33	1.23
1	C	130	TRP	NE1-CE2	-5.11	1.31	1.37
1	C	169	GLN	CD-OE1	5.11	1.33	1.23
1	A	141	GLN	CD-OE1	5.09	1.33	1.23
1	D	146	GLN	CD-OE1	5.09	1.33	1.23
1	A	80	TRP	NE1-CE2	-5.06	1.31	1.37
1	C	141	GLN	CD-OE1	5.06	1.33	1.23
1	D	141	GLN	CD-OE1	5.04	1.33	1.23
1	D	86	ASN	CG-OD1	5.03	1.33	1.23

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	TYR	N-CA-C	7.06	119.58	111.11
1	B	19	HIS	CA-CB-CG	-7.00	106.80	113.80
1	B	175	VAL	CA-CB-CG2	6.58	121.59	110.40
1	B	31	LYS	CA-C-N	6.55	129.29	120.65
1	B	31	LYS	C-N-CA	6.55	129.29	120.65
1	C	167	TYR	N-CA-C	6.25	118.61	111.11
1	A	167	TYR	N-CA-C	6.24	118.59	111.11
1	C	93	GLY	CA-C-N	6.20	129.41	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	GLY	C-N-CA	6.20	129.41	120.79
1	D	167	TYR	N-CA-C	6.19	118.58	111.02
1	A	180	ALA	CA-C-N	6.17	128.88	120.54
1	A	180	ALA	C-N-CA	6.17	128.88	120.54
1	D	72	GLY	N-CA-C	-6.14	105.38	112.50
1	C	89	ASP	O-C-N	-6.11	114.46	122.59
1	B	171	LYS	CB-CA-C	-6.00	109.67	116.63
1	D	146	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	A	19	HIS	CA-CB-CG	-5.98	107.82	113.80
1	B	146	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	C	56	HIS	CA-CB-CG	-5.84	107.96	113.80
1	A	129	GLY	O-C-N	5.63	128.50	123.60
1	D	175	VAL	CA-CB-CG2	5.60	119.92	110.40
1	B	74	VAL	CA-CB-CG2	5.58	119.89	110.40
1	A	128	LEU	CA-C-N	-5.56	117.15	121.82
1	A	128	LEU	C-N-CA	-5.56	117.15	121.82
1	B	191	GLN	CA-C-N	5.51	127.67	120.28
1	B	191	GLN	C-N-CA	5.51	127.67	120.28
1	B	86	ASN	CA-C-N	5.51	128.61	122.55
1	B	86	ASN	C-N-CA	5.51	128.61	122.55
1	C	144	ASP	CB-CA-C	-5.45	109.81	117.23
1	B	93	GLY	CA-C-N	5.45	127.89	120.54
1	B	93	GLY	C-N-CA	5.45	127.89	120.54
1	C	27	LEU	CA-C-N	5.41	127.84	120.54
1	C	27	LEU	C-N-CA	5.41	127.84	120.54
1	B	180	ALA	CA-C-N	5.33	127.68	120.38
1	B	180	ALA	C-N-CA	5.33	127.68	120.38
1	D	144	ASP	CB-CA-C	-5.31	110.00	117.23
1	D	19	HIS	CA-CB-CG	-5.27	108.53	113.80
1	B	56	HIS	CA-CB-CG	-5.25	108.56	113.80
1	C	37	VAL	CA-CB-CG2	5.24	119.31	110.40
1	C	146	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	C	74	VAL	CA-CB-CG2	5.13	119.12	110.40
1	A	143	TYR	CA-C-O	-5.12	115.12	120.80
1	A	146	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	74	VAL	CA-CB-CG2	5.12	119.10	110.40
1	D	122	GLY	N-CA-C	-5.09	106.41	111.56
1	B	144	ASP	CB-CA-C	-5.08	110.32	117.23
1	B	103	PHE	CA-CB-CG	-5.06	108.74	113.80
1	C	109	PHE	CA-C-N	5.04	127.04	120.28
1	C	109	PHE	C-N-CA	5.04	127.04	120.28
1	C	141	GLN	OE1-CD-NE2	-5.00	117.60	122.60

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	1568	0	1489	20	0
1	B	1568	0	1489	23	0
1	C	1568	0	1489	30	0
1	D	1568	0	1489	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	180	0	0	0	0
3	B	168	0	0	2	0
3	C	153	0	0	4	0
3	D	155	0	0	2	0
All	All	6932	0	5956	92	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 8.

All (92) 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:C:95:LEU:HD12	1:C:95:LEU:O	1.79	0.82
1:B:88:GLY:O	1:B:89:ASP:HB2	1.78	0.81
1:B:3:GLU:HB2	3:B:1611:HOH:O	1.86	0.75
1:B:101:ASP:HB3	3:B:1498:HOH:O	1.94	0.67
1:A:44:VAL:O	1:A:48:GLU:HG3	1.97	0.65
1:D:27:LEU:O	1:D:31:LYS:HB2	2.00	0.62
1:C:191:GLN:HG2	3:C:1585:HOH:O	2.00	0.61
1:B:24:ILE:O	1:B:28:HIS:HB2	2.01	0.60
1:B:127:ALA:HB2	1:B:158:LEU:HD23	1.84	0.59
3:C:1637:HOH:O	1:D:171:LYS:HE3	2.02	0.59
1:D:123:SER:HB3	1:D:162:TRP:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:O	1:A:28:HIS:HB2	2.04	0.57
1:B:150:PRO:HD2	1:B:153:ILE:HG13	1.86	0.57
1:C:143:TYR:HB2	1:C:147:THR:HB	1.88	0.56
1:D:185:VAL:HG11	1:D:187:TRP:CE2	2.41	0.55
1:B:88:GLY:O	1:B:89:ASP:CB	2.49	0.55
1:C:122:GLY:HA2	1:D:162:TRP:CH2	2.42	0.55
1:D:150:PRO:HG2	1:D:153:ILE:HD11	1.89	0.55
1:D:6:LEU:HD12	1:D:7:PRO:HD2	1.89	0.55
1:D:171:LYS:N	1:D:171:LYS:HD3	2.21	0.55
1:B:125:TRP:CZ3	1:B:160:ASP:HB2	2.43	0.54
1:D:146:GLN:N	1:D:146:GLN:OE1	2.34	0.54
1:D:24:ILE:O	1:D:28:HIS:HB2	2.08	0.54
1:B:51:ARG:HD3	1:D:112:GLN:OE1	2.07	0.53
1:A:150:PRO:HG2	1:A:153:ILE:CG1	2.38	0.53
1:B:150:PRO:HB3	1:D:71:ALA:HA	1.91	0.53
1:D:191:GLN:HG2	3:D:1584:HOH:O	2.09	0.53
1:A:122:GLY:HA2	1:B:162:TRP:CH2	2.44	0.52
1:B:127:ALA:CB	1:B:158:LEU:HD23	2.39	0.52
1:C:95:LEU:HD12	1:C:95:LEU:C	2.29	0.52
1:B:127:ALA:HB2	1:B:158:LEU:CD2	2.39	0.52
1:D:9:LEU:HD21	1:D:29:HIS:CD2	2.46	0.51
1:D:150:PRO:HG2	1:D:153:ILE:CG1	2.40	0.51
1:B:110:ARG:HG3	1:B:182:TRP:CZ2	2.45	0.51
1:D:33:HIS:O	1:D:33:HIS:HD2	1.94	0.51
1:C:163:GLU:HB2	1:D:163:GLU:HB2	1.92	0.50
1:C:9:LEU:HD12	1:C:13:TYR:CE1	2.47	0.50
1:D:146:GLN:O	1:D:146:GLN:HG2	2.10	0.50
1:C:95:LEU:CD1	1:C:98:ALA:HB3	2.42	0.49
1:B:118:THR:HG21	1:B:175:VAL:HG12	1.94	0.49
1:C:38:LYS:HE2	1:C:42:ASP:OD2	2.12	0.49
1:B:123:SER:HB3	1:B:162:TRP:CE2	2.48	0.49
1:D:123:SER:HB3	1:D:162:TRP:CD2	2.48	0.49
1:B:125:TRP:CE3	1:B:160:ASP:HA	2.48	0.49
1:A:143:TYR:HB2	1:A:147:THR:HB	1.94	0.48
1:C:150:PRO:HD2	1:C:153:ILE:HG13	1.96	0.48
1:A:164:HIS:CD2	1:A:164:HIS:C	2.91	0.48
1:C:146:GLN:O	1:C:146:GLN:HG2	2.13	0.48
1:D:117:ALA:HB2	1:D:126:ALA:HB2	1.95	0.48
1:C:9:LEU:HD12	1:C:13:TYR:CD1	2.49	0.48
1:C:24:ILE:O	1:C:28:HIS:HB2	2.13	0.48
1:C:17:GLU:OE1	1:C:21:SER:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLY:O	1:C:17:GLU:HG3	2.14	0.47
1:C:95:LEU:HD12	1:C:98:ALA:HB3	1.97	0.47
1:C:163:GLU:O	1:C:167:TYR:HB2	2.15	0.47
1:B:146:GLN:OE1	1:B:146:GLN:N	2.46	0.47
1:A:163:GLU:O	1:A:167:TYR:HB2	2.15	0.47
1:A:146:GLN:O	1:A:146:GLN:HG2	2.15	0.47
1:A:79:TRP:CE2	1:A:83:LEU:HD11	2.50	0.46
1:C:146:GLN:OE1	1:C:146:GLN:N	2.45	0.46
1:D:33:HIS:O	1:D:33:HIS:CD2	2.68	0.46
1:B:84:SER:HB2	1:B:186:ASN:HB2	1.98	0.46
1:D:3:GLU:H	1:D:3:GLU:HG3	1.60	0.45
1:B:123:SER:HB3	1:B:162:TRP:CD2	2.52	0.45
1:D:170:TYR:O	1:D:171:LYS:HB2	2.16	0.44
1:A:150:PRO:HG2	1:A:153:ILE:HD11	1.99	0.44
1:A:130:TRP:HB3	1:A:154:VAL:HB	2.00	0.44
1:C:181:PHE:CZ	1:C:185:VAL:HG22	2.52	0.43
1:C:9:LEU:CD1	1:C:13:TYR:CE1	3.01	0.43
1:C:53:LYS:HD3	3:C:1475:HOH:O	2.18	0.43
1:C:166:PHE:CD1	1:C:166:PHE:C	2.97	0.43
1:C:117:ALA:O	1:C:161:MET:HG3	2.19	0.42
1:C:80:TRP:HA	1:C:80:TRP:CE3	2.54	0.42
1:C:95:LEU:HD13	1:C:95:LEU:HA	1.85	0.42
1:A:70:LEU:O	1:A:74:VAL:HG23	2.20	0.42
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.91	0.42
1:B:118:THR:CG2	1:B:175:VAL:HG12	2.50	0.42
1:C:91:PRO:HB3	1:C:187:TRP:CE3	2.55	0.42
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.92	0.41
1:C:125:TRP:CZ3	1:C:160:ASP:HB2	2.55	0.41
1:B:6:LEU:HD12	1:B:7:PRO:HD2	2.01	0.41
1:D:150:PRO:HG2	1:D:153:ILE:CD1	2.50	0.41
1:B:110:ARG:HG3	1:B:182:TRP:CE2	2.55	0.41
1:A:146:GLN:N	1:A:146:GLN:OE1	2.49	0.41
1:A:59:ILE:HG23	1:A:60:LEU:N	2.35	0.41
1:A:84:SER:HA	1:A:85:PRO:HD3	1.81	0.41
1:A:79:TRP:CZ2	1:A:83:LEU:HD11	2.56	0.40
1:A:171:LYS:HB3	1:A:172:ASN:H	1.58	0.40
1:C:38:LYS:HE2	1:C:42:ASP:CG	2.47	0.40
1:C:171:LYS:HE2	3:D:1393:HOH:O	2.21	0.40
1:A:143:TYR:HE2	3:C:1565:HOH:O	2.04	0.40
1:C:11:TRP:HE3	1:C:12:ASP:O	2.03	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	196/207 (95%)	187 (95%)	8 (4%)	1 (0%)	24	21
1	B	196/207 (95%)	186 (95%)	8 (4%)	2 (1%)	12	8
1	C	196/207 (95%)	186 (95%)	9 (5%)	1 (0%)	24	21
1	D	196/207 (95%)	185 (94%)	10 (5%)	1 (0%)	24	21
All	All	784/828 (95%)	744 (95%)	35 (4%)	5 (1%)	21	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	148	ASN
1	A	148	ASN
1	B	148	ASN
1	C	148	ASN
1	B	89	ASP

5.3.2 Protein sidechains

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	156/163 (96%)	153 (98%)	3 (2%)	50	56
1	B	156/163 (96%)	155 (99%)	1 (1%)	78	85
1	C	156/163 (96%)	153 (98%)	3 (2%)	50	56
1	D	156/163 (96%)	153 (98%)	3 (2%)	50	56
All	All	624/652 (96%)	614 (98%)	10 (2%)	55	62

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	171	LYS
1	A	199	SER
1	B	11	TRP
1	C	94	GLU
1	C	95	LEU
1	C	171	LYS
1	D	38	LYS
1	D	110	ARG
1	D	191	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	135	ASN
1	A	141	GLN
1	B	62	ASN
1	B	69	ASN
1	B	191	GLN
1	C	23	GLN
1	C	141	GLN
1	C	148	ASN
1	D	23	GLN
1	D	148	ASN

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

Of 4 ligands modelled in this entry, 4 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

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	198/207 (95%)	0.21	10 (5%) 33 32	0, 0, 1, 1	0
1	B	198/207 (95%)	0.24	10 (5%) 33 32	0, 0, 1, 1	0
1	C	198/207 (95%)	0.29	10 (5%) 33 32	0, 0, 1, 1	0
1	D	198/207 (95%)	0.23	9 (4%) 38 37	0, 0, 1, 1	0
All	All	792/828 (95%)	0.24	39 (4%) 35 34	0, 0, 1, 1	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ALA	5.7
1	A	199	SER	5.4
1	B	87	GLY	5.1
1	C	87	GLY	4.9
1	B	101	ASP	4.8
1	C	89	ASP	4.5
1	B	89	ASP	4.4
1	B	199	SER	4.4
1	D	199	SER	4.0
1	D	89	ASP	4.0
1	A	2	ALA	3.9
1	C	199	SER	3.7
1	A	89	ASP	3.4
1	B	3	GLU	3.4
1	A	101	ASP	3.3
1	B	88	GLY	3.2
1	B	2	ALA	3.1
1	C	132	THR	3.1
1	C	2	ALA	2.9
1	C	94	GLU	2.8
1	A	88	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	94	GLU	2.7
1	B	110	ARG	2.7
1	B	90	LYS	2.7
1	A	191	GLN	2.6
1	A	54	GLU	2.6
1	C	101	ASP	2.6
1	D	101	ASP	2.6
1	C	86	ASN	2.5
1	D	110	ARG	2.5
1	A	87	GLY	2.4
1	D	54	GLU	2.3
1	D	86	ASN	2.3
1	A	3	GLU	2.2
1	C	88	GLY	2.2
1	D	87	GLY	2.1
1	A	86	ASN	2.1
1	D	3	GLU	2.1
1	C	92	THR	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
2	FE	C	208	1/1	0.98	0.06	0,0,0,0	0
2	FE	D	208	1/1	0.98	0.09	0,0,0,0	0
2	FE	A	208	1/1	0.99	0.10	0,0,0,0	0
2	FE	B	208	1/1	0.99	0.09	0,0,0,0	0

6.5 Other polymers [i](#)

There are no such residues in this entry.