Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 03:13 pm GMT

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PDB ID	:	1GN3
Title	:	H145Q mutant of Mycobacterium tuberculosis iron-superoxide dismutase.
Authors	:	Bunting, K.A.; Cooper, J.B.; Badasso, M.O.; Tickle, I.J.; Newton, M.; Wood, S.P.; Zhang, Y.; Young, D.B.
Deposited on	:	2001-10-02
Resolution	:	4.00 Å(reported)

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 4.00 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.
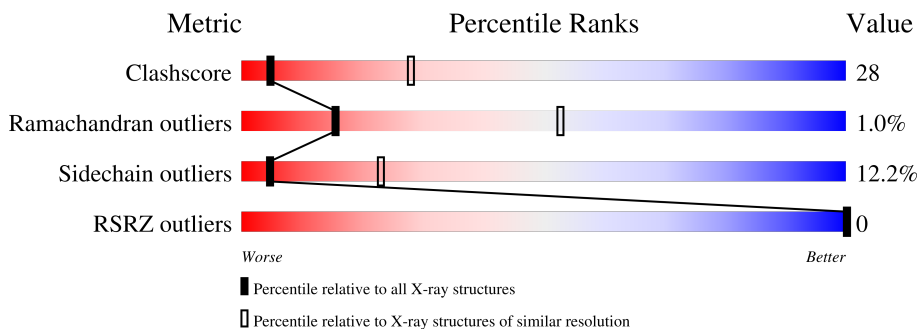
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 <=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	50% 30% 14% · ·
1	B	207	50% 32% 13% · ·

2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 3136 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 SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1567	1011	268	287	1			
1	B	198	Total	C	N	O	S	0	0	0
			1567	1011	268	287	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	145	GLN	HIS	engineered mutation	UNP P17670

- Molecule 2 is FE (III) ION (three-letter code: 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		

3 Residue-property plots ⓘ

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: SUPEROXIDE DISMUTASE

Chain A:
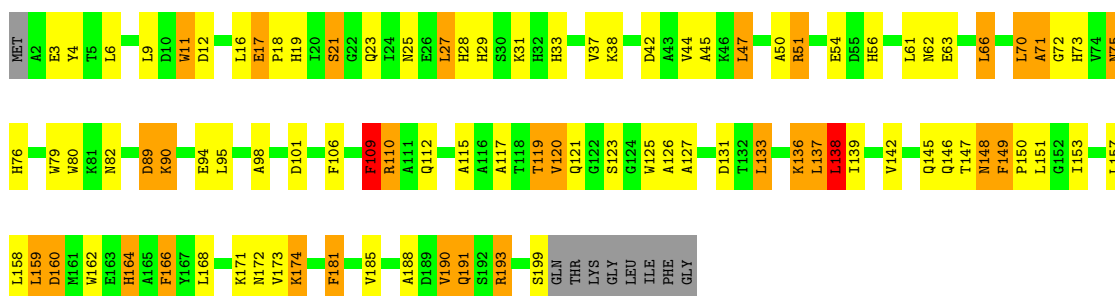
- Molecule 1: SUPEROXIDE DISMUTASE

Chain B:

4 Data and refinement statistics ⓘ

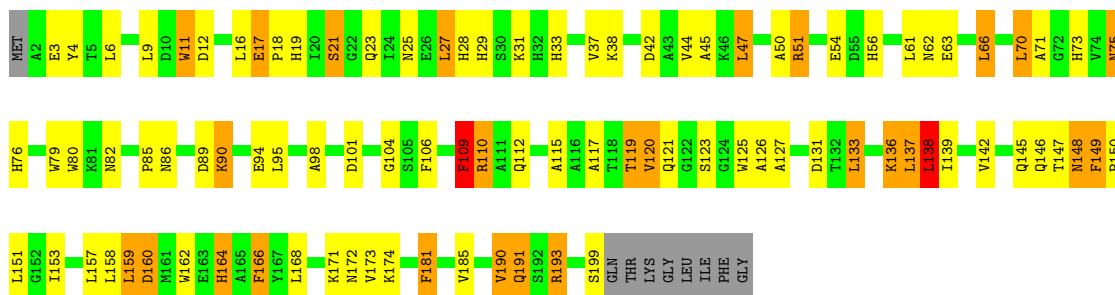| Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.88Å 103.88Å 69.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.00 15.29 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-4.00) 97.9 (15.29-3.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.70 (at 3.57Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.184 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 86.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3136	wwPDB-VP
Average B, all atoms (Å^2)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.77	0/1615	1.98	42/2203 (1.9%)
1	B	0.77	0/1615	1.98	41/2203 (1.9%)
All	All	0.77	0/3230	1.98	83/4406 (1.9%)

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	193	ARG	NE-CZ-NH2	16.76	128.68	120.30
1	A	193	ARG	NE-CZ-NH2	16.69	128.65	120.30
1	A	160	ASP	CB-CG-OD1	14.39	131.25	118.30
1	B	160	ASP	CB-CG-OD1	14.38	131.25	118.30
1	B	193	ARG	NE-CZ-NH1	-13.93	113.33	120.30
1	A	193	ARG	NE-CZ-NH1	-13.90	113.35	120.30
1	B	131	ASP	CB-CG-OD1	12.96	129.96	118.30
1	A	131	ASP	CB-CG-OD1	12.93	129.94	118.30
1	A	131	ASP	CB-CG-OD2	-10.30	109.03	118.30
1	B	131	ASP	CB-CG-OD2	-10.30	109.03	118.30
1	A	90	LYS	CD-CE-NZ	9.15	132.75	111.70
1	B	90	LYS	CD-CE-NZ	9.14	132.72	111.70
1	A	12	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	B	12	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	B	181	PHE	CG-CD2-CE2	-8.20	111.78	120.80
1	A	181	PHE	CG-CD2-CE2	-8.17	111.82	120.80
1	A	51	ARG	NE-CZ-NH1	-8.03	116.29	120.30
1	B	51	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	70	LEU	CB-CG-CD2	-7.83	97.69	111.00
1	B	70	LEU	CB-CG-CD2	-7.82	97.71	111.00
1	A	133	LEU	CA-CB-CG	-7.68	97.64	115.30
1	B	133	LEU	CA-CB-CG	-7.67	97.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	VAL	CA-CB-CG2	7.59	122.29	110.90
1	A	173	VAL	CA-CB-CG2	7.58	122.27	110.90
1	A	12	ASP	OD1-CG-OD2	7.42	137.40	123.30
1	B	12	ASP	OD1-CG-OD2	7.41	137.38	123.30
1	B	181	PHE	CZ-CE2-CD2	7.33	128.90	120.10
1	A	181	PHE	CZ-CE2-CD2	7.30	128.86	120.10
1	A	11	TRP	CA-C-O	7.29	135.41	120.10
1	B	11	TRP	CA-C-O	7.28	135.40	120.10
1	B	12	ASP	CB-CG-OD1	-7.23	111.79	118.30
1	A	12	ASP	CB-CG-OD1	-7.20	111.82	118.30
1	B	190	VAL	CA-CB-CG2	-7.07	100.29	110.90
1	A	190	VAL	CA-CB-CG2	-7.06	100.31	110.90
1	A	11	TRP	CA-C-N	-6.82	102.21	117.20
1	B	11	TRP	CA-C-N	-6.80	102.23	117.20
1	A	4	TYR	CA-C-O	-6.62	106.20	120.10
1	B	4	TYR	CA-C-O	-6.61	106.21	120.10
1	B	27	LEU	CB-CG-CD2	-6.57	99.83	111.00
1	A	27	LEU	CB-CG-CD2	-6.57	99.84	111.00
1	B	47	LEU	CA-CB-CG	-6.53	100.28	115.30
1	A	47	LEU	CA-CB-CG	-6.53	100.29	115.30
1	B	136	LYS	O-C-N	6.27	132.73	122.70
1	A	136	LYS	O-C-N	6.25	132.69	122.70
1	B	4	TYR	CB-CG-CD1	6.07	124.64	121.00
1	A	120	VAL	CA-CB-CG1	-6.07	101.80	110.90
1	B	120	VAL	CA-CB-CG1	-6.07	101.80	110.90
1	A	4	TYR	CB-CG-CD1	6.05	124.63	121.00
1	A	193	ARG	CD-NE-CZ	-5.83	115.44	123.60
1	B	193	ARG	CD-NE-CZ	-5.81	115.47	123.60
1	B	119	THR	CA-CB-CG2	-5.72	104.39	112.40
1	A	98	ALA	O-C-N	5.70	131.82	122.70
1	B	98	ALA	O-C-N	5.70	131.81	122.70
1	A	119	THR	CA-CB-CG2	-5.68	104.45	112.40
1	B	173	VAL	CG1-CB-CG2	5.67	119.97	110.90
1	A	173	VAL	CG1-CB-CG2	5.65	119.94	110.90
1	A	3	GLU	O-C-N	5.59	131.65	122.70
1	B	3	GLU	O-C-N	5.58	131.63	122.70
1	A	27	LEU	CB-CG-CD1	-5.52	101.62	111.00
1	B	27	LEU	CB-CG-CD1	-5.51	101.64	111.00
1	A	151	LEU	CB-CG-CD1	-5.46	101.73	111.00
1	B	151	LEU	CB-CG-CD1	-5.45	101.73	111.00
1	A	160	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	B	160	ASP	CB-CG-OD2	-5.43	113.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	50	ALA	CA-C-N	-5.40	105.32	117.20
1	B	109	PHE	CB-CG-CD1	-5.39	117.03	120.80
1	A	50	ALA	CA-C-N	-5.38	105.36	117.20
1	A	63	GLU	CB-CG-CD	-5.37	99.71	114.20
1	B	63	GLU	CB-CG-CD	-5.36	99.72	114.20
1	A	109	PHE	CB-CG-CD1	-5.35	117.06	120.80
1	A	61	LEU	CB-CG-CD2	-5.32	101.97	111.00
1	A	136	LYS	CA-CB-CG	5.31	125.09	113.40
1	B	136	LYS	CA-CB-CG	5.31	125.07	113.40
1	B	71	ALA	C-N-CA	-5.30	111.16	122.30
1	A	71	ALA	C-N-CA	-5.30	111.17	122.30
1	B	61	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	B	138	LEU	CB-CG-CD1	5.21	119.85	111.00
1	A	138	LEU	CB-CG-CD1	5.18	119.81	111.00
1	A	149	PHE	CA-C-O	-5.12	109.34	120.10
1	B	149	PHE	CA-C-O	-5.10	109.38	120.10
1	A	110	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	188	ALA	O-C-N	5.04	130.77	122.70
1	B	110	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	1567	0	1490	89	1
1	B	1567	0	1490	91	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	3136	0	2980	170	1

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 28.

All (170) 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:147:THR:HG23	1:B:147:THR:CG2	1.55	1.37
1:A:147:THR:CG2	1:B:147:THR:HG23	1.57	1.33
1:A:51:ARG:HD3	1:B:112:GLN:OE1	1.55	1.07
1:A:112:GLN:OE1	1:B:51:ARG:HD3	1.57	1.04
1:A:147:THR:HG23	1:B:147:THR:HG23	0.87	0.87
1:A:79:TRP:HZ3	1:A:159:LEU:HA	1.40	0.84
1:B:79:TRP:HZ3	1:B:159:LEU:HA	1.40	0.83
1:A:147:THR:CB	1:B:147:THR:HG23	2.10	0.81
1:A:147:THR:HG23	1:B:147:THR:CB	2.11	0.80
1:B:159:LEU:HD12	1:B:159:LEU:C	2.03	0.77
1:A:159:LEU:HD12	1:A:159:LEU:C	2.03	0.77
1:B:117:ALA:HB2	1:B:126:ALA:HB2	1.66	0.77
1:A:147:THR:CG2	1:B:147:THR:CG2	2.36	0.77
1:A:117:ALA:HB2	1:A:126:ALA:HB2	1.67	0.75
1:A:79:TRP:CZ3	1:A:159:LEU:HA	2.22	0.74
1:A:9:LEU:HD21	1:A:29:HIS:CD2	2.23	0.74
1:B:79:TRP:CZ3	1:B:159:LEU:HA	2.22	0.73
1:B:164:HIS:CD2	1:B:164:HIS:C	2.61	0.73
1:A:164:HIS:CD2	1:A:164:HIS:C	2.61	0.73
1:A:27:LEU:HD23	1:A:31:LYS:HG3	1.71	0.73
1:B:42:ASP:O	1:B:45:ALA:HB3	1.89	0.72
1:B:9:LEU:HD21	1:B:29:HIS:CD2	2.23	0.72
1:B:17:GLU:HB3	1:B:18:PRO:HA	1.70	0.72
1:A:42:ASP:O	1:A:45:ALA:HB3	1.89	0.71
1:A:17:GLU:HB3	1:A:18:PRO:HA	1.70	0.71
1:B:27:LEU:HD23	1:B:31:LYS:HG3	1.71	0.71
1:A:6:LEU:HD21	1:A:29:HIS:CE1	2.27	0.70
1:A:11:TRP:CH2	1:A:16:LEU:HD11	2.27	0.70
1:B:6:LEU:HD21	1:B:29:HIS:CE1	2.27	0.69
1:B:11:TRP:CH2	1:B:16:LEU:HD11	2.27	0.69
1:B:75:ASN:HB3	1:B:158:LEU:CD1	2.27	0.65
1:A:75:ASN:HB3	1:A:158:LEU:CD1	2.27	0.64
1:A:47:LEU:HD21	1:A:62:ASN:HB3	1.80	0.64
1:B:47:LEU:O	1:B:51:ARG:HG3	1.98	0.64
1:B:75:ASN:HB3	1:B:158:LEU:HD13	1.80	0.64
1:A:47:LEU:O	1:A:51:ARG:HG3	1.98	0.64
1:B:27:LEU:O	1:B:31:LYS:HB2	1.99	0.63
1:B:47:LEU:HD21	1:B:62:ASN:HB3	1.80	0.63
1:A:27:LEU:O	1:A:31:LYS:HB2	1.99	0.63
1:B:17:GLU:CB	1:B:18:PRO:HA	2.26	0.63
1:A:75:ASN:HB3	1:A:158:LEU:HD13	1.80	0.63
1:A:27:LEU:HD23	1:A:31:LYS:CG	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:HD23	1:B:31:LYS:CG	2.29	0.62
1:A:27:LEU:CD2	1:A:31:LYS:HG3	2.31	0.60
1:A:95:LEU:HD22	1:A:190:VAL:HG12	1.83	0.60
1:B:27:LEU:CD2	1:B:31:LYS:HG3	2.31	0.60
1:B:95:LEU:HD22	1:B:190:VAL:HG12	1.83	0.60
1:B:146:GLN:O	1:B:146:GLN:HG2	2.02	0.58
1:A:47:LEU:HD21	1:A:62:ASN:CB	2.34	0.58
1:A:6:LEU:HD11	1:A:33:HIS:HB3	1.86	0.57
1:A:6:LEU:HD12	1:A:33:HIS:CD2	2.39	0.57
1:B:6:LEU:HD12	1:B:33:HIS:CD2	2.39	0.57
1:A:146:GLN:HG2	1:A:146:GLN:O	2.02	0.57
1:B:47:LEU:HD21	1:B:62:ASN:CB	2.34	0.57
1:A:95:LEU:CD2	1:A:190:VAL:HG12	2.36	0.56
1:B:6:LEU:HD11	1:B:33:HIS:HB3	1.86	0.56
1:A:16:LEU:HD12	1:A:25:ASN:HD21	1.70	0.56
1:B:164:HIS:C	1:B:164:HIS:HD2	2.09	0.56
1:B:16:LEU:HD12	1:B:25:ASN:HD21	1.70	0.56
1:B:18:PRO:HD2	1:B:19:HIS:H	1.71	0.56
1:A:17:GLU:CB	1:A:18:PRO:HA	2.26	0.55
1:B:95:LEU:CD2	1:B:190:VAL:HG12	2.36	0.55
1:A:18:PRO:HD2	1:A:19:HIS:H	1.72	0.55
1:B:120:VAL:HG11	1:B:123:SER:O	2.07	0.55
1:B:159:LEU:HD12	1:B:160:ASP:N	2.22	0.54
1:A:120:VAL:HG11	1:A:123:SER:O	2.07	0.54
1:A:159:LEU:HD12	1:A:160:ASP:N	2.22	0.54
1:A:146:GLN:N	1:A:146:GLN:OE1	2.42	0.53
1:A:127:ALA:HB2	1:A:158:LEU:CD2	2.39	0.53
1:A:164:HIS:C	1:A:164:HIS:HD2	2.09	0.53
1:A:193:ARG:CG	1:A:193:ARG:HH11	2.22	0.53
1:B:37:VAL:HG22	1:B:73:HIS:CE1	2.44	0.52
1:B:127:ALA:HB2	1:B:158:LEU:CD2	2.39	0.52
1:A:37:VAL:HG22	1:A:73:HIS:CE1	2.44	0.52
1:B:117:ALA:HB2	1:B:126:ALA:CB	2.38	0.52
1:A:51:ARG:HG2	1:A:56:HIS:HE1	1.75	0.51
1:B:146:GLN:OE1	1:B:146:GLN:N	2.41	0.51
1:A:117:ALA:HB2	1:A:126:ALA:CB	2.38	0.51
1:B:28:HIS:CE1	1:B:160:ASP:OD2	2.64	0.51
1:B:51:ARG:HG2	1:B:56:HIS:CE1	2.46	0.51
1:B:21:SER:OG	1:B:23:GLN:HB3	2.11	0.51
1:B:76:HIS:HE1	1:B:145:GLN:HE22	1.59	0.50
1:A:51:ARG:HG2	1:A:56:HIS:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ARG:HG2	1:B:56:HIS:HE1	1.75	0.50
1:A:21:SER:OG	1:A:23:GLN:HB3	2.11	0.50
1:A:193:ARG:CG	1:A:193:ARG:NH1	2.74	0.50
1:A:28:HIS:CE1	1:A:160:ASP:OD2	2.64	0.49
1:A:76:HIS:HE1	1:A:145:GLN:HE22	1.59	0.49
1:B:11:TRP:CH2	1:B:16:LEU:CD1	2.96	0.48
1:A:82:ASN:OD1	1:A:157:LEU:HA	2.14	0.48
1:A:11:TRP:CH2	1:A:16:LEU:CD1	2.96	0.48
1:A:9:LEU:CD2	1:A:29:HIS:CD2	2.96	0.47
1:B:193:ARG:NH1	1:B:193:ARG:CG	2.74	0.47
1:B:193:ARG:CG	1:B:193:ARG:HH11	2.22	0.47
1:B:145:GLN:HG2	1:B:162:TRP:HZ2	1.79	0.47
1:A:33:HIS:HE2	1:A:73:HIS:CE1	2.32	0.47
1:B:27:LEU:HD23	1:B:27:LEU:HA	1.68	0.47
1:B:33:HIS:HE2	1:B:73:HIS:CE1	2.32	0.47
1:B:109:PHE:CD1	1:B:139:ILE:HD11	2.50	0.47
1:B:82:ASN:OD1	1:B:157:LEU:HA	2.14	0.46
1:B:133:LEU:HA	1:B:133:LEU:HD12	1.46	0.46
1:A:109:PHE:CD1	1:A:139:ILE:HD11	2.50	0.46
1:A:145:GLN:HG2	1:A:162:TRP:HZ2	1.79	0.46
1:A:142:VAL:HG13	1:A:149:PHE:CE1	2.50	0.46
1:A:16:LEU:HD12	1:A:25:ASN:ND2	2.31	0.46
1:B:95:LEU:HB3	1:B:191:GLN:HG3	1.98	0.46
1:A:95:LEU:HB3	1:A:191:GLN:HG3	1.98	0.46
1:B:9:LEU:CD2	1:B:29:HIS:CD2	2.96	0.46
1:A:44:VAL:O	1:A:47:LEU:HB2	2.16	0.45
1:B:16:LEU:HD12	1:B:25:ASN:ND2	2.31	0.45
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.45	0.45
1:B:18:PRO:CD	1:B:19:HIS:H	2.28	0.45
1:A:18:PRO:CD	1:A:19:HIS:H	2.28	0.45
1:A:70:LEU:HD23	1:B:150:PRO:HG3	1.97	0.45
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.46	0.45
1:A:150:PRO:HG3	1:B:70:LEU:HD23	1.98	0.45
1:B:147:THR:O	1:B:148:ASN:CB	2.64	0.45
1:B:66:LEU:O	1:B:66:LEU:HG	2.17	0.45
1:B:142:VAL:HG13	1:B:149:PHE:CE1	2.50	0.45
1:B:9:LEU:HD21	1:B:29:HIS:HD2	1.79	0.44
1:A:18:PRO:CD	1:A:19:HIS:N	2.80	0.44
1:A:181:PHE:CZ	1:A:185:VAL:HG22	2.53	0.44
1:B:44:VAL:O	1:B:47:LEU:HB2	2.16	0.44
1:B:125:TRP:CE3	1:B:160:ASP:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:HA	1:B:137:LEU:HD23	1.59	0.44
1:A:171:LYS:HB3	1:A:172:ASN:H	1.50	0.44
1:B:18:PRO:CD	1:B:19:HIS:N	2.80	0.44
1:A:71:ALA:O	1:A:72:GLY:C	2.56	0.44
1:A:106:PHE:HE2	1:A:110:ARG:NH1	2.16	0.44
1:A:147:THR:O	1:A:148:ASN:CB	2.64	0.44
1:A:147:THR:O	1:A:148:ASN:HB2	2.18	0.44
1:B:147:THR:O	1:B:148:ASN:HB2	2.18	0.43
1:A:125:TRP:CE3	1:A:160:ASP:HA	2.53	0.43
1:B:181:PHE:CZ	1:B:185:VAL:HG22	2.53	0.43
1:A:150:PRO:HG2	1:A:153:ILE:CG1	2.49	0.43
1:B:106:PHE:HE2	1:B:110:ARG:NH1	2.16	0.43
1:A:136:LYS:HD2	1:A:138:LEU:HD21	2.01	0.43
1:A:137:LEU:HA	1:A:137:LEU:HD23	1.59	0.43
1:B:171:LYS:HB3	1:B:172:ASN:H	1.49	0.43
1:B:47:LEU:HA	1:B:47:LEU:HD23	1.45	0.43
1:B:136:LYS:HD2	1:B:138:LEU:HD21	2.01	0.43
1:A:6:LEU:CD2	1:A:29:HIS:CE1	3.00	0.43
1:A:9:LEU:HD21	1:A:29:HIS:HD2	1.79	0.43
1:B:166:PHE:C	1:B:166:PHE:CD1	2.92	0.43
1:A:166:PHE:CD1	1:A:166:PHE:C	2.92	0.43
1:A:6:LEU:CD1	1:A:33:HIS:CG	3.02	0.42
1:A:66:LEU:O	1:A:66:LEU:HG	2.17	0.42
1:A:115:ALA:O	1:A:119:THR:HG23	2.19	0.42
1:A:174:LYS:H	1:A:174:LYS:HG2	1.67	0.42
1:B:150:PRO:HG2	1:B:153:ILE:CG1	2.49	0.42
1:B:6:LEU:CD1	1:B:33:HIS:CG	3.03	0.42
1:B:109:PHE:CD2	1:B:109:PHE:C	2.92	0.42
1:B:193:ARG:HH11	1:B:193:ARG:HG2	1.84	0.42
1:A:90:LYS:HG2	1:A:106:PHE:CE2	2.55	0.42
1:A:47:LEU:HB3	1:A:51:ARG:HH12	1.85	0.42
1:B:6:LEU:CD2	1:B:29:HIS:CE1	3.00	0.42
1:B:115:ALA:O	1:B:119:THR:HG23	2.19	0.42
1:B:47:LEU:HB3	1:B:51:ARG:HH12	1.85	0.41
1:B:76:HIS:O	1:B:80:TRP:CD1	2.73	0.41
1:B:117:ALA:CB	1:B:126:ALA:HB2	2.44	0.41
1:A:76:HIS:O	1:A:80:TRP:CD1	2.73	0.41
1:A:127:ALA:CB	1:A:158:LEU:CD2	2.99	0.41
1:B:85:PRO:HD2	1:B:86:ASN:H	1.85	0.41
1:B:127:ALA:CB	1:B:158:LEU:CD2	2.99	0.41
1:A:193:ARG:HH11	1:A:193:ARG:HG2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:CD1	1:B:33:HIS:HB3	2.50	0.41
1:B:106:PHE:HE2	1:B:110:ARG:HH11	1.68	0.41
1:B:90:LYS:HG2	1:B:106:PHE:CE2	2.55	0.40
1:A:106:PHE:HE2	1:A:110:ARG:HH11	1.68	0.40
1:A:109:PHE:CD2	1:A:109:PHE:C	2.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:OD1	1:B:104:GLY:O[5_664]	1.98	0.22

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%)	174 (89%)	20 (10%)	2 (1%)	15	53
1	B	196/207 (95%)	174 (89%)	20 (10%)	2 (1%)	15	53
All	All	392/414 (95%)	348 (89%)	40 (10%)	4 (1%)	15	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	B	148	ASN
1	B	166	PHE
1	A	166	PHE

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	156/163 (96%)	137 (88%)	19 (12%)	5	23
1	B	156/163 (96%)	137 (88%)	19 (12%)	5	23
All	All	312/326 (96%)	274 (88%)	38 (12%)	5	23

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	21	SER
1	A	38	LYS
1	A	54	GLU
1	A	66	LEU
1	A	75	ASN
1	A	89	ASP
1	A	94	GLU
1	A	101	ASP
1	A	109	PHE
1	A	121	GLN
1	A	137	LEU
1	A	138	LEU
1	A	159	LEU
1	A	164	HIS
1	A	168	LEU
1	A	174	LYS
1	A	191	GLN
1	A	199	SER
1	B	17	GLU
1	B	21	SER
1	B	38	LYS
1	B	54	GLU
1	B	66	LEU
1	B	75	ASN
1	B	89	ASP
1	B	94	GLU

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Mol	Chain	Res	Type
1	B	101	ASP
1	B	109	PHE
1	B	121	GLN
1	B	137	LEU
1	B	138	LEU
1	B	159	LEU
1	B	164	HIS
1	B	168	LEU
1	B	174	LYS
1	B	191	GLN
1	B	199	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	62	ASN
1	B	56	HIS
1	B	62	ASN
1	B	121	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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%)	-1.04	0	100	100	0, 5, 24, 37	0
1	B	198/207 (95%)	-1.02	0	100	100	0, 5, 24, 37	0
All	All	396/414 (95%)	-1.03	0	100	100	0, 5, 24, 37	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
2	FE	A	1200	1/1	0.99	0.08	0,0,0,0	0
2	FE	B	1200	1/1	0.99	0.03	0,0,0,0	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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