



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:29 PM UTC

PDB ID : 1MSD / pdb_00001msd
Title : COMPARISON OF THE CRYSTAL STRUCTURES OF GENETICALLY ENGINEERED HUMAN MANGANESE SUPEROXIDE DISMUTASE AND MANGANESE SUPEROXIDE DISMUTASE FROM THERMUS THERMOPHILUS. DIFFERENCES IN DIMER-DIMER INTERACTIONS.
Authors : Sussman, J.; Wagner, U.G.; Pattridge, K.A.; Ludwig, M.L.
Deposited on : 1992-11-10
Resolution : 3.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

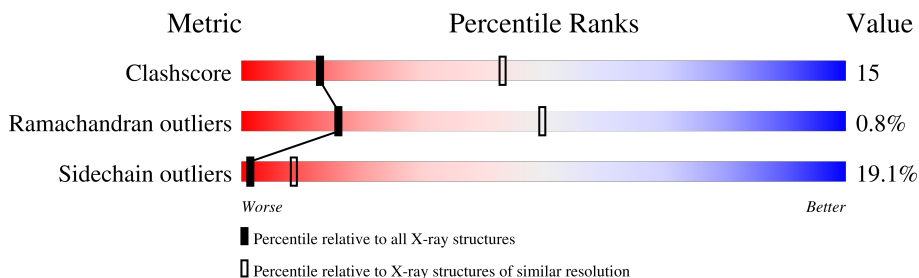
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	198	32% 46% 19% .
1	B	198	37% 39% 21% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3246 atoms, of which 98 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 MANGANESE SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	H	N	O	S	0	0	0
			1622	1008	49	275	286	4			
1	B	198	Total	C	H	N	O	S	0	0	0
			1622	1008	49	275	286	4			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

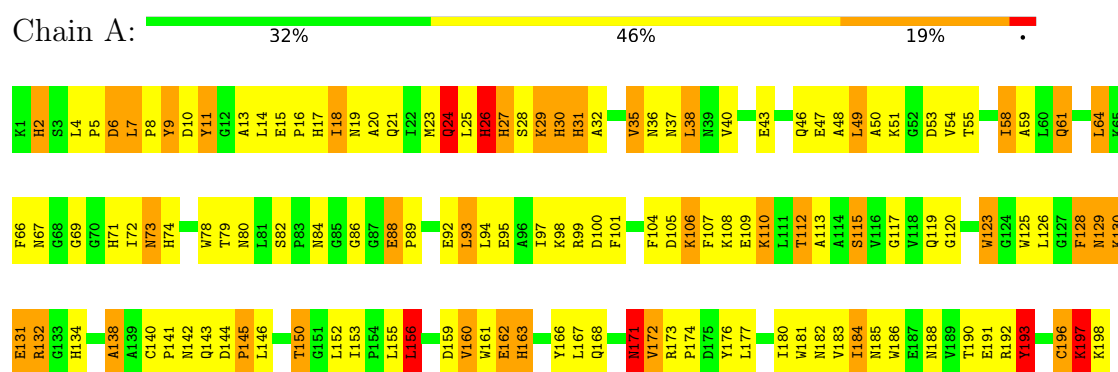
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: MANGANESE SUPEROXIDE DISMUTASE



• Molecule 1: MANGANESE SUPEROXIDE DISMUTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.80Å 74.10Å 68.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3246	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	1.47	16/1619 (1.0%)	2.42	110/2197 (5.0%)
1	B	1.49	19/1619 (1.2%)	2.44	105/2197 (4.8%)
All	All	1.48	35/3238 (1.1%)	2.43	215/4394 (4.9%)

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
1	B	0	1
All	All	0	2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	ILE	CA-CB	7.82	1.62	1.53
1	A	184	ILE	CA-CB	7.75	1.61	1.53
1	B	163	HIS	CD2-NE2	-7.59	1.29	1.37
1	B	71	HIS	CD2-NE2	-7.51	1.29	1.37
1	B	74	HIS	CG-ND1	-7.36	1.30	1.38
1	A	27	HIS	CD2-NE2	-7.30	1.29	1.37
1	B	30	HIS	CD2-NE2	-7.24	1.29	1.37
1	A	134	HIS	CD2-NE2	-7.20	1.29	1.37
1	B	74	HIS	CD2-NE2	-6.98	1.30	1.37
1	B	27	HIS	CD2-NE2	-6.87	1.30	1.37
1	A	31	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	163	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	74	HIS	CG-ND1	-6.42	1.31	1.38
1	A	17	HIS	CD2-NE2	-6.31	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	HIS	CD2-NE2	-6.30	1.30	1.37
1	B	134	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	17	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	30	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	99	ARG	NE-CZ	6.10	1.39	1.33
1	B	141	PRO	CA-CB	-5.97	1.46	1.53
1	B	79	THR	CA-CB	5.93	1.63	1.53
1	B	2	HIS	CD2-NE2	-5.85	1.31	1.37
1	A	134	HIS	CG-ND1	-5.75	1.31	1.38
1	A	74	HIS	CD2-NE2	-5.74	1.31	1.37
1	B	71	HIS	CG-ND1	-5.63	1.32	1.38
1	A	2	HIS	CD2-NE2	-5.35	1.31	1.37
1	B	163	HIS	CG-ND1	-5.33	1.32	1.38
1	B	31	HIS	CG-ND1	-5.31	1.32	1.38
1	B	31	HIS	CD2-NE2	-5.28	1.32	1.37
1	B	197	LYS	C-N	5.18	1.40	1.33
1	A	163	HIS	CG-ND1	-5.17	1.32	1.38
1	A	197	LYS	CA-C	5.17	1.59	1.52
1	B	26	HIS	CD2-NE2	-5.15	1.32	1.37
1	B	163	HIS	CE1-NE2	-5.12	1.27	1.32
1	A	141	PRO	CA-CB	-5.12	1.47	1.53

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	GLN	OE1-CD-NE2	-14.99	107.61	122.60
1	B	143	GLN	OE1-CD-NE2	-14.59	108.01	122.60
1	A	24	GLN	OE1-CD-NE2	-12.40	110.20	122.60
1	B	24	GLN	OE1-CD-NE2	-12.25	110.35	122.60
1	B	129	ASN	OD1-CG-ND2	-11.40	111.20	122.60
1	B	163	HIS	CA-CB-CG	11.04	124.84	113.80
1	A	129	ASN	OD1-CG-ND2	-10.94	111.66	122.60
1	A	172	VAL	N-CA-C	10.87	117.84	106.21
1	B	30	HIS	N-CA-C	10.71	122.92	111.03
1	B	182	ASN	OD1-CG-ND2	-10.67	111.93	122.60
1	B	19	ASN	OD1-CG-ND2	-10.24	112.36	122.60
1	A	129	ASN	CB-CG-ND2	10.22	131.73	116.40
1	A	36	ASN	CA-CB-CG	-9.87	102.73	112.60
1	B	188	ASN	OD1-CG-ND2	-9.85	112.75	122.60
1	A	30	HIS	N-CA-C	9.81	121.92	111.03
1	A	168	GLN	OE1-CD-NE2	-9.70	112.90	122.60
1	A	182	ASN	OD1-CG-ND2	-9.54	113.06	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	GLN	OE1-CD-NE2	-9.39	113.21	122.60
1	A	163	HIS	CA-CB-CG	9.28	123.08	113.80
1	B	129	ASN	CB-CG-ND2	9.25	130.27	116.40
1	B	36	ASN	CA-CB-CG	-8.71	103.89	112.60
1	B	188	ASN	CB-CG-ND2	8.61	129.31	116.40
1	B	24	GLN	CG-CD-NE2	8.18	128.67	116.40
1	A	19	ASN	OD1-CG-ND2	-8.17	114.43	122.60
1	A	197	LYS	N-CA-C	8.05	127.95	110.80
1	A	24	GLN	CG-CD-NE2	8.05	128.47	116.40
1	A	6	ASP	CA-CB-CG	8.05	120.65	112.60
1	B	197	LYS	N-CA-C	8.00	127.84	110.80
1	B	119	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	A	17	HIS	CA-CB-CG	-7.83	105.97	113.80
1	A	125	TRP	N-CA-C	7.71	120.99	108.34
1	B	163	HIS	CB-CG-ND1	7.70	134.25	122.70
1	B	6	ASP	CA-CB-CG	7.61	120.21	112.60
1	B	84	ASN	OD1-CG-ND2	-7.53	115.07	122.60
1	A	73	ASN	OD1-CG-ND2	-7.51	115.09	122.60
1	A	163	HIS	CB-CG-ND1	7.46	133.90	122.70
1	A	61	GLN	OE1-CD-NE2	-7.39	115.21	122.60
1	B	61	GLN	OE1-CD-NE2	-7.36	115.25	122.60
1	B	18	ILE	N-CA-C	-7.28	96.99	107.77
1	A	78	TRP	CG-CD2-CE3	7.27	141.17	133.90
1	B	17	HIS	CA-CB-CG	-7.21	106.59	113.80
1	A	59	ALA	O-C-N	-7.20	114.49	122.12
1	B	125	TRP	N-CA-C	7.20	120.92	108.76
1	A	80	ASN	CB-CG-ND2	7.12	127.09	116.40
1	B	27	HIS	CB-CG-CD2	-7.10	121.97	131.20
1	B	37	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	A	188	ASN	CB-CG-ND2	7.06	126.99	116.40
1	A	188	ASN	OD1-CG-ND2	-7.04	115.56	122.60
1	B	142	ASN	CB-CA-C	-7.01	108.47	116.54
1	B	145	PRO	CA-C-O	-7.00	113.44	121.56
1	A	162	GLU	N-CA-C	7.00	119.76	111.71
1	B	78	TRP	CG-CD2-CE3	6.89	140.79	133.90
1	B	182	ASN	CB-CG-ND2	6.88	126.72	116.40
1	A	18	ILE	N-CA-C	-6.79	97.72	107.77
1	A	156	LEU	O-C-N	-6.73	115.40	123.27
1	B	162	GLU	N-CA-C	6.69	119.40	111.71
1	A	130	LYS	CB-CG-CD	6.65	126.60	111.30
1	A	78	TRP	CB-CG-CD1	-6.63	116.96	126.90
1	A	142	ASN	CB-CA-C	-6.61	108.94	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	GLU	CB-CA-C	-6.60	100.71	110.95
1	A	130	LYS	CG-CD-CE	6.55	126.38	111.30
1	A	144	ASP	CA-C-N	6.51	126.49	119.78
1	A	144	ASP	C-N-CA	6.51	126.49	119.78
1	A	119	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	A	67	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	B	21	GLN	OE1-CD-NE2	-6.46	116.14	122.60
1	B	163	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	B	83	PRO	O-C-N	-6.41	114.93	122.17
1	B	59	ALA	O-C-N	-6.38	114.88	122.15
1	A	80	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	A	143	GLN	CG-CD-NE2	6.34	125.91	116.40
1	A	92	GLU	CA-CB-CG	-6.33	101.44	114.10
1	A	49	LEU	O-C-N	6.33	128.83	122.12
1	B	112	THR	N-CA-C	-6.30	104.41	111.28
1	B	84	ASN	CB-CG-ND2	6.30	125.85	116.40
1	B	73	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	B	119	GLN	CG-CD-NE2	6.26	125.80	116.40
1	B	130	LYS	CB-CG-CD	6.26	125.69	111.30
1	B	2	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	A	100	ASP	CA-C-O	6.21	125.97	119.14
1	B	109	GLU	N-CA-CB	6.20	118.98	109.98
1	A	182	ASN	CB-CG-ND2	6.13	125.60	116.40
1	B	147	GLN	OE1-CD-NE2	-6.11	116.49	122.60
1	A	46	GLN	O-C-N	-6.09	114.17	122.33
1	A	123	TRP	CG-CD2-CE3	6.01	139.91	133.90
1	A	196	CYS	N-CA-C	5.98	118.76	111.82
1	A	19	ASN	CA-CB-CG	5.97	118.57	112.60
1	B	78	TRP	CB-CG-CD1	-5.96	117.96	126.90
1	A	14	LEU	CA-C-O	5.94	126.96	119.95
1	B	141	PRO	O-C-N	-5.94	115.58	123.06
1	A	82	SER	CA-C-N	5.92	125.12	118.97
1	A	82	SER	C-N-CA	5.92	125.12	118.97
1	B	64	LEU	CA-C-O	-5.88	114.82	121.00
1	B	171	ASN	N-CA-C	5.88	119.93	112.87
1	B	88	GLU	O-C-N	-5.87	115.88	121.57
1	A	145	PRO	CA-C-O	-5.85	114.77	121.56
1	B	123	TRP	CG-CD2-CE3	5.84	139.74	133.90
1	B	130	LYS	CG-CD-CE	5.83	124.71	111.30
1	A	134	HIS	CA-CB-CG	5.83	119.63	113.80
1	B	131	GLU	CA-CB-CG	5.80	125.71	114.10
1	A	105	ASP	CA-CB-CG	-5.80	106.80	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	GLU	CA-CB-CG	5.79	125.68	114.10
1	B	80	ASN	CB-CG-ND2	5.79	125.08	116.40
1	A	181	TRP	CG-CD2-CE3	5.78	139.68	133.90
1	B	181	TRP	CG-CD2-CE3	5.75	139.65	133.90
1	A	93	LEU	CA-C-O	-5.73	114.98	121.00
1	A	150	THR	O-C-N	-5.72	115.31	122.35
1	B	134	HIS	CA-CB-CG	5.69	119.49	113.80
1	A	197	LYS	CA-CB-CG	5.69	125.47	114.10
1	B	138	ALA	O-C-N	-5.68	116.33	123.27
1	A	27	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	A	17	HIS	CA-C-O	5.68	126.44	120.42
1	B	100	ASP	CA-C-O	5.68	125.83	119.41
1	A	128	PHE	O-C-N	-5.67	116.69	123.27
1	B	40	VAL	N-CA-CB	-5.66	104.23	110.51
1	A	163	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	B	31	HIS	CB-CG-ND1	5.64	131.16	122.70
1	A	37	ASN	CA-CB-CG	5.63	118.23	112.60
1	B	197	LYS	CA-CB-CG	5.63	125.35	114.10
1	A	31	HIS	CB-CG-CD2	-5.62	123.90	131.20
1	B	144	ASP	CA-C-N	5.61	125.56	119.78
1	B	144	ASP	C-N-CA	5.61	125.56	119.78
1	A	159	ASP	CA-CB-CG	5.61	118.20	112.60
1	A	141	PRO	O-C-N	-5.60	116.00	123.06
1	A	171	ASN	N-CA-C	5.60	119.59	112.87
1	A	185	ASN	N-CA-C	5.60	118.77	108.58
1	A	112	THR	N-CA-C	-5.59	105.19	111.28
1	A	72	ILE	N-CA-C	5.58	118.07	111.09
1	A	117	GLY	O-C-N	-5.57	115.45	122.70
1	A	74	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	B	66	PHE	N-CA-C	5.56	117.78	111.11
1	B	19	ASN	CB-CG-ND2	5.55	124.72	116.40
1	B	66	PHE	CA-CB-CG	-5.54	108.26	113.80
1	A	2	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	A	88	GLU	CB-CG-CD	5.52	121.98	112.60
1	B	19	ASN	CA-CB-CG	5.51	118.11	112.60
1	B	143	GLN	CG-CD-NE2	5.50	124.66	116.40
1	B	197	LYS	CA-C-N	5.50	131.59	121.70
1	B	197	LYS	C-N-CA	5.50	131.59	121.70
1	B	92	GLU	CA-CB-CG	-5.48	103.15	114.10
1	B	110	LYS	CA-CB-CG	5.48	125.05	114.10
1	B	128	PHE	O-C-N	-5.47	116.81	123.27
1	B	159	ASP	CA-CB-CG	5.47	118.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	THR	OG1-CB-CG2	5.45	120.20	109.30
1	B	53	ASP	N-CA-C	5.45	118.03	108.56
1	A	17	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	B	86	GLY	O-C-N	5.41	130.02	123.37
1	A	40	VAL	N-CA-CB	-5.40	104.51	110.51
1	A	110	LYS	CA-CB-CG	5.40	124.90	114.10
1	B	160	VAL	CA-C-O	5.40	124.88	119.97
1	B	92	GLU	N-CA-C	5.39	120.27	111.37
1	B	30	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	37	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	71	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	B	196	CYS	N-CA-C	5.38	118.06	111.82
1	A	138	ALA	O-C-N	-5.38	116.71	123.27
1	A	40	VAL	N-CA-C	5.37	116.00	110.36
1	B	9	TYR	O-C-N	-5.36	117.47	123.48
1	A	19	ASN	CB-CG-ND2	5.35	124.43	116.40
1	B	143	GLN	CA-CB-CG	5.32	124.73	114.10
1	B	40	VAL	N-CA-C	5.30	115.93	110.36
1	B	88	GLU	CA-C-N	5.30	125.46	119.90
1	B	88	GLU	C-N-CA	5.30	125.46	119.90
1	B	195	ALA	N-CA-C	5.29	122.08	110.80
1	A	112	THR	CB-CA-C	-5.29	102.01	110.79
1	B	105	ASP	CA-CB-CG	-5.29	107.31	112.60
1	A	29	LYS	O-C-N	-5.26	116.41	122.09
1	A	31	HIS	CB-CG-ND1	5.25	130.58	122.70
1	B	109	GLU	CA-C-O	-5.25	115.49	120.90
1	A	54	VAL	O-C-N	-5.25	116.57	121.87
1	B	123	TRP	CE2-CD2-CG	-5.25	100.91	107.20
1	B	130	LYS	O-C-N	-5.24	116.09	122.22
1	B	29	LYS	O-C-N	-5.23	116.44	122.09
1	B	181	TRP	CB-CG-CD1	-5.22	119.07	126.90
1	A	11	TYR	CA-C-N	5.21	125.88	119.99
1	A	11	TYR	C-N-CA	5.21	125.88	119.99
1	B	74	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	150	THR	CB-CA-C	-5.19	100.83	109.55
1	B	78	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	B	167	LEU	O-C-N	5.19	129.62	122.46
1	A	86	GLY	O-C-N	5.18	129.75	123.37
1	A	58	ILE	N-CA-C	5.17	115.90	110.62
1	A	143	GLN	CA-CB-CG	5.17	124.44	114.10
1	A	160	VAL	CA-C-O	5.16	124.67	119.97
1	A	53	ASP	N-CA-C	5.14	117.51	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	CYS	CA-C-N	5.14	125.54	119.99
1	A	140	CYS	C-N-CA	5.14	125.54	119.99
1	A	9	TYR	O-C-N	-5.14	117.73	123.48
1	A	193	TYR	CA-C-O	5.13	126.72	121.07
1	B	181	TRP	N-CA-C	5.13	118.32	111.75
1	A	64	LEU	CA-C-O	-5.12	115.44	120.82
1	B	197	LYS	O-C-N	5.12	129.40	122.59
1	B	156	LEU	O-C-N	-5.12	117.28	123.27
1	A	112	THR	N-CA-CB	5.12	117.64	110.12
1	A	197	LYS	O-C-N	5.12	129.39	122.59
1	A	186	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	B	129	ASN	CA-C-O	5.11	127.39	121.11
1	A	115	SER	N-CA-C	5.10	116.53	111.07
1	B	168	GLN	CG-CD-NE2	5.08	124.02	116.40
1	B	143	GLN	CB-CG-CD	5.08	121.23	112.60
1	A	181	TRP	CE2-CD2-CG	-5.07	101.11	107.20
1	A	186	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	B	57	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	B	82	SER	CA-C-N	5.07	124.24	118.97
1	B	82	SER	C-N-CA	5.07	124.24	118.97
1	B	49	LEU	O-C-N	5.06	127.48	122.12
1	A	123	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	B	150	THR	O-C-N	-5.04	116.15	122.35
1	A	18	ILE	CA-C-N	-5.03	113.04	121.39
1	A	18	ILE	C-N-CA	-5.03	113.04	121.39
1	A	36	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	26	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	B	46	GLN	O-C-N	-5.02	115.61	122.33
1	A	125	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	A	191	GLU	CA-CB-CG	5.00	124.11	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	TYR	Sidechain
1	B	107	PHE	Sidechain

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	1573	49	1528	50	0
1	B	1573	49	1528	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	3148	98	3056	93	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 15.

All (93) 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:167:LEU:HD23	1:B:167:LEU:HD23	1.72	0.72
1:A:161:TRP:CH2	1:B:120:GLY:HA2	2.28	0.69
1:B:9:TYR:HB2	1:B:13:ALA:HB3	1.75	0.68
1:A:9:TYR:HB2	1:A:13:ALA:HB3	1.77	0.66
1:B:94:LEU:HG	1:B:98:LYS:HD2	1.81	0.62
1:A:120:GLY:HA2	1:B:161:TRP:CH2	2.35	0.62
1:B:89:PRO:O	1:B:94:LEU:HB2	1.99	0.62
1:A:89:PRO:O	1:A:94:LEU:HB2	2.00	0.62
1:A:94:LEU:HG	1:A:98:LYS:HD2	1.82	0.61
1:B:95:GLU:HA	1:B:98:LYS:HD3	1.82	0.60
1:A:190:THR:O	1:A:193:TYR:HB3	2.01	0.60
1:A:95:GLU:HA	1:A:98:LYS:HD3	1.85	0.59
1:B:190:THR:O	1:B:193:TYR:HB3	2.03	0.59
1:A:155:LEU:HD22	1:A:193:TYR:HA	1.87	0.56
1:A:18:ILE:HG21	1:A:23:MET:SD	2.48	0.54
1:A:8:PRO:HD2	1:A:9:TYR:CE2	2.42	0.54
1:B:155:LEU:HD22	1:B:193:TYR:HA	1.88	0.54
1:B:48:ALA:HA	1:B:51:LYS:HE2	1.89	0.53
1:A:115:SER:HB3	1:A:160:VAL:HG11	1.91	0.51
1:B:128:PHE:CD2	1:B:196:CYS:HB3	2.45	0.51
1:B:69:GLY:HA3	1:B:145:PRO:HD3	1.92	0.51
1:A:31:HIS:O	1:A:35:VAL:HG23	2.11	0.51
1:A:58:ILE:HA	1:A:61:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:TYR:HE1	1:B:23:MET:HE2	1.76	0.50
1:B:2:HIS:ND1	1:B:38:LEU:HD13	2.26	0.50
1:B:8:PRO:HD2	1:B:9:TYR:CE2	2.46	0.50
1:A:104:PHE:CE2	1:A:108:LYS:HD2	2.47	0.49
1:B:162:GLU:O	1:B:166:TYR:HB2	2.12	0.49
1:A:9:TYR:HE1	1:A:23:MET:HE2	1.77	0.49
1:A:48:ALA:HA	1:A:51:LYS:HE2	1.94	0.48
1:A:69:GLY:HA3	1:A:145:PRO:HD3	1.95	0.48
1:A:107:PHE:CE1	1:A:126:LEU:HD22	2.49	0.48
1:A:155:LEU:O	1:A:192:ARG:HD2	2.13	0.48
1:B:173:ARG:O	1:B:176:TYR:HB3	2.14	0.48
1:A:28:SER:O	1:A:32:ALA:HB3	2.14	0.48
1:B:31:HIS:O	1:B:35:VAL:HG23	2.13	0.48
1:B:58:ILE:HA	1:B:61:GLN:HG3	1.95	0.48
1:A:128:PHE:CD2	1:A:196:CYS:HB3	2.49	0.47
1:B:7:LEU:HD22	1:B:27:HIS:CE1	2.49	0.47
1:A:129:ASN:OD1	1:A:132:ARG:HB2	2.15	0.47
1:A:171:ASN:HD21	1:B:29:LYS:NZ	2.13	0.47
1:B:104:PHE:CE2	1:B:108:LYS:HD2	2.49	0.47
1:B:115:SER:HB3	1:B:160:VAL:HG11	1.96	0.47
1:B:129:ASN:HA	1:B:130:LYS:HE3	1.97	0.47
1:A:2:HIS:ND1	1:A:38:LEU:HD13	2.29	0.46
1:B:26:HIS:O	1:B:30:HIS:HB2	2.16	0.46
1:B:21:GLN:O	1:B:25:LEU:HG	2.15	0.46
1:B:107:PHE:CE1	1:B:126:LEU:HD22	2.50	0.46
1:B:18:ILE:HG21	1:B:23:MET:SD	2.55	0.46
1:A:7:LEU:HD22	1:A:27:HIS:CE1	2.51	0.46
1:B:129:ASN:OD1	1:B:132:ARG:HB2	2.16	0.46
1:B:106:LYS:O	1:B:110:LYS:HG2	2.15	0.46
1:A:21:GLN:O	1:A:25:LEU:HG	2.16	0.45
1:A:5:PRO:O	1:A:27:HIS:NE2	2.49	0.45
1:A:47:GLU:O	1:A:50:ALA:HB3	2.16	0.45
1:A:162:GLU:O	1:A:166:TYR:HB2	2.16	0.45
1:A:15:GLU:OE1	1:A:16:PRO:HA	2.16	0.45
1:A:29:LYS:NZ	1:B:171:ASN:HD21	2.14	0.45
1:B:36:ASN:O	1:B:40:VAL:HG23	2.16	0.45
1:A:101:PHE:O	1:A:106:LYS:HB3	2.17	0.45
1:A:128:PHE:CE2	1:A:196:CYS:HB3	2.52	0.45
1:A:66:PHE:HZ	1:A:161:TRP:HH2	1.64	0.44
1:A:20:ALA:O	1:A:24:GLN:HB2	2.18	0.44
1:B:7:LEU:HD21	1:B:11:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:O	1:A:176:TYR:HB3	2.18	0.44
1:A:173:ARG:N	1:A:174:PRO:HD2	2.33	0.44
1:A:29:LYS:HB3	1:B:171:ASN:OD1	2.17	0.43
1:A:58:ILE:O	1:A:61:GLN:HG3	2.18	0.43
1:B:156:LEU:HD21	1:B:184:ILE:HD12	2.00	0.43
1:B:15:GLU:OE1	1:B:16:PRO:HA	2.19	0.43
1:A:106:LYS:O	1:A:110:LYS:HG2	2.19	0.43
1:B:128:PHE:CE2	1:B:196:CYS:HB3	2.53	0.43
1:B:89:PRO:HG3	1:B:97:ILE:HD12	2.01	0.43
1:B:31:HIS:HD2	1:B:78:TRP:HE1	1.67	0.42
1:B:66:PHE:HZ	1:B:161:TRP:HH2	1.65	0.42
1:A:73:ASN:HB3	1:A:123:TRP:CZ2	2.54	0.42
1:B:73:ASN:HB3	1:B:123:TRP:CZ2	2.54	0.42
1:B:47:GLU:O	1:B:50:ALA:HB3	2.18	0.42
1:B:101:PHE:O	1:B:106:LYS:HB3	2.20	0.42
1:A:138:ALA:HB3	1:A:146:LEU:HD11	2.01	0.42
1:A:7:LEU:HD21	1:A:11:TYR:CE1	2.55	0.42
1:A:89:PRO:HG3	1:A:97:ILE:HD12	2.01	0.42
1:A:163:HIS:HB3	1:B:162:GLU:OE2	2.20	0.41
1:B:45:TYR:O	1:B:49:LEU:HB2	2.20	0.41
1:A:109:GLU:O	1:A:113:ALA:HB2	2.20	0.41
1:B:7:LEU:H	1:B:7:LEU:HD23	1.86	0.41
1:B:88:GLU:HG2	1:B:104:PHE:CE2	2.56	0.41
1:A:156:LEU:HD21	1:A:184:ILE:HD12	2.01	0.40
1:B:138:ALA:HB3	1:B:146:LEU:HD11	2.03	0.40
1:A:153:ILE:HG21	1:A:196:CYS:SG	2.61	0.40
1:B:5:PRO:O	1:B:27:HIS:NE2	2.54	0.40
1:B:58:ILE:O	1:B:61:GLN:HG3	2.21	0.40
1:A:26:HIS:O	1:A:30:HIS:HB2	2.21	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	196/198 (99%)	176 (90%)	19 (10%)	1 (0%)	24	59
1	B	196/198 (99%)	174 (89%)	20 (10%)	2 (1%)	12	45
All	All	392/396 (99%)	350 (89%)	39 (10%)	3 (1%)	16	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	LYS
1	B	197	LYS
1	B	13	ALA

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	162/162 (100%)	131 (81%)	31 (19%)	1	9
1	B	162/162 (100%)	131 (81%)	31 (19%)	1	9
All	All	324/324 (100%)	262 (81%)	62 (19%)	1	9

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	ASP
1	A	7	LEU
1	A	10	ASP
1	A	24	GLN
1	A	26	HIS
1	A	35	VAL
1	A	38	LEU
1	A	43	GLU
1	A	49	LEU
1	A	55	THR
1	A	64	LEU
1	A	79	THR

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Mol	Chain	Res	Type
1	A	84	ASN
1	A	88	GLU
1	A	93	LEU
1	A	106	LYS
1	A	112	THR
1	A	130	LYS
1	A	131	GLU
1	A	132	ARG
1	A	150	THR
1	A	152	LEU
1	A	156	LEU
1	A	171	ASN
1	A	172	VAL
1	A	177	LEU
1	A	180	ILE
1	A	183	VAL
1	A	197	LYS
1	A	198	LYS
1	B	4	LEU
1	B	6	ASP
1	B	7	LEU
1	B	10	ASP
1	B	24	GLN
1	B	26	HIS
1	B	35	VAL
1	B	38	LEU
1	B	43	GLU
1	B	49	LEU
1	B	54	VAL
1	B	55	THR
1	B	64	LEU
1	B	79	THR
1	B	84	ASN
1	B	93	LEU
1	B	106	LYS
1	B	112	THR
1	B	130	LYS
1	B	131	GLU
1	B	132	ARG
1	B	150	THR
1	B	152	LEU
1	B	156	LEU

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Mol	Chain	Res	Type
1	B	171	ASN
1	B	172	VAL
1	B	177	LEU
1	B	180	ILE
1	B	183	VAL
1	B	197	LYS
1	B	198	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	37	ASN
1	A	57	GLN
1	A	134	HIS
1	A	143	GLN
1	A	171	ASN
1	A	185	ASN
1	B	31	HIS
1	B	57	GLN
1	B	67	ASN
1	B	134	HIS
1	B	143	GLN
1	B	171	ASN
1	B	185	ASN

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 oligosaccharides 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.