



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:26 PM UTC

PDB ID : 1TK6 / pdb_00001tk6
Title : Iron-oxo clusters biomineralizing on protein surfaces. Structural analysis of H.salinarum DpsA in its low and high iron states
Authors : Zeth, K.; Offermann, S.; Essen, L.O.; Oesterhelt, D.
Deposited on : 2004-06-08
Resolution : 2.20 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

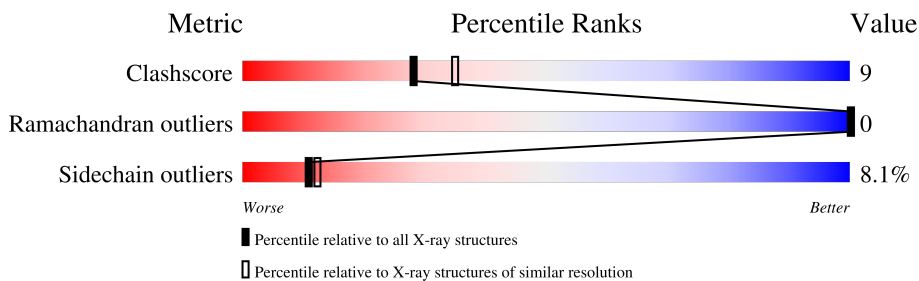
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	182	67% 26% . . .
1	B	182	66% 24% 6% . .
1	C	182	66% 25% . . .
1	D	182	66% 24% . . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1201	-	-	X	-
2	SO4	B	1202	-	-	X	-

2 Entry composition [i](#)

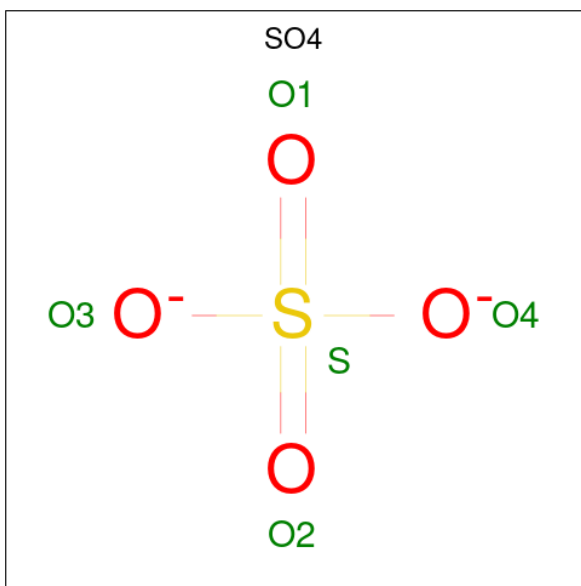
There are 6 unique types of molecules in this entry. The entry contains 5751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-rich dpsA-homolog protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	180	Total 1394	C 852	N 242	O 296	S 4	0	0	0
1	B	175	Total 1355	C 830	N 234	O 287	S 4	0	0	0
1	C	175	Total 1355	C 830	N 234	O 287	S 4	0	0	0
1	D	175	Total 1355	C 830	N 234	O 287	S 4	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	58	Total O 58 58	0	0
6	B	68	Total O 68 68	0	0
6	C	67	Total O 67 67	0	0
6	D	77	Total O 77 77	0	0

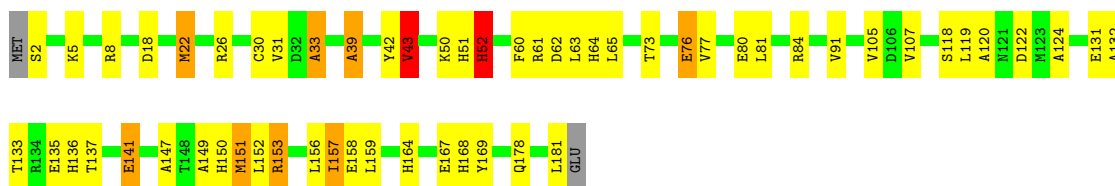
3 Residue-property plots

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.

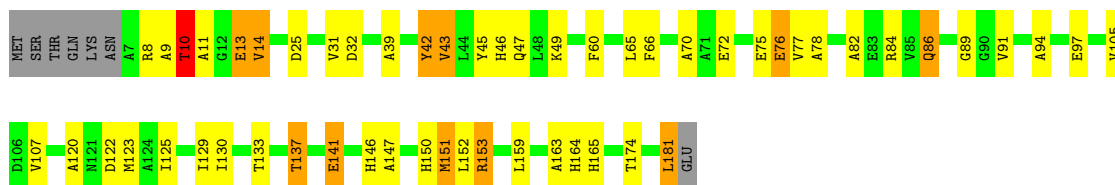
- Molecule 1: Iron-rich dpsA-homolog protein

Chain A: 



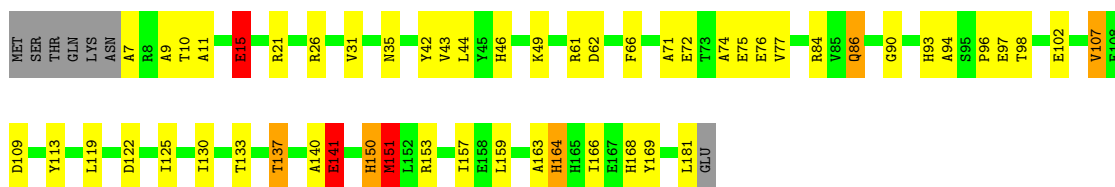
- Molecule 1: Iron-rich dpsA-homolog protein

Chain B: 



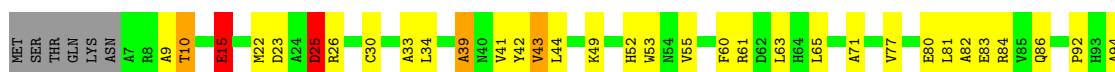
- Molecule 1: Iron-rich dpsA-homolog protein

Chain C: 



- Molecule 1: Iron-rich dpsA-homolog protein

Chain D: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.11Å 91.11Å 150.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	158.11 – 2.20	Depositor
% Data completeness (in resolution range)	99.7 (158.11-2.20)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.172 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5751	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, NA, 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	2.07	32/1415 (2.3%)	1.42	7/1923 (0.4%)
1	B	2.02	35/1376 (2.5%)	1.42	8/1871 (0.4%)
1	C	2.38	35/1376 (2.5%)	1.92	10/1871 (0.5%)
1	D	2.23	36/1376 (2.6%)	1.69	11/1871 (0.6%)
All	All	2.18	138/5543 (2.5%)	1.62	36/7536 (0.5%)

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	C	0	1
1	D	0	1
All	All	0	2

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	GLU	CB-CG	30.30	2.43	1.52
1	D	15	GLU	CB-CG	27.81	2.35	1.52
1	C	15	GLU	CB-CG	26.43	2.31	1.52
1	D	15	GLU	CG-CD	18.83	1.99	1.52
1	C	15	GLU	CG-CD	18.27	1.97	1.52
1	C	141	GLU	CG-CD	12.53	1.83	1.52
1	A	147	ALA	CA-CB	-9.29	1.39	1.53
1	C	109	ASP	C-O	-8.98	1.13	1.23
1	B	77	VAL	C-O	-8.77	1.14	1.24
1	A	150	HIS	C-O	-8.60	1.14	1.24
1	B	123	MET	SD-CE	-8.45	1.58	1.79
1	D	141	GLU	CD-OE2	8.05	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	ALA	CA-CB	-8.04	1.40	1.53
1	A	30	CYS	C-O	-8.02	1.14	1.24
1	D	86	GLN	C-O	7.87	1.33	1.24
1	D	49	LYS	C-O	-7.73	1.15	1.24
1	C	62	ASP	N-CA	-7.70	1.36	1.46
1	D	10	THR	CA-C	-7.62	1.43	1.52
1	A	158	GLU	C-O	-7.47	1.15	1.24
1	B	78	ALA	CA-CB	-7.46	1.41	1.53
1	C	130	ILE	CA-CB	-7.36	1.45	1.54
1	B	65	LEU	C-O	-7.23	1.15	1.24
1	B	82	ALA	CA-CB	-7.22	1.41	1.53
1	C	163	ALA	C-O	-7.18	1.15	1.24
1	B	66	PHE	C-O	-7.17	1.15	1.24
1	B	125	ILE	C-O	-7.11	1.16	1.24
1	C	61	ARG	CD-NE	-7.10	1.36	1.46
1	A	31	VAL	CA-CB	-7.09	1.45	1.54
1	B	146	HIS	C-O	-7.07	1.15	1.24
1	A	149	ALA	C-O	-7.05	1.16	1.24
1	D	39	ALA	CA-CB	-7.01	1.42	1.53
1	D	117	THR	C-O	-6.93	1.16	1.24
1	C	153	ARG	CD-NE	-6.91	1.36	1.46
1	B	70	ALA	CA-CB	-6.83	1.42	1.53
1	A	124	ALA	C-O	-6.78	1.16	1.24
1	D	71	ALA	CA-CB	-6.71	1.42	1.53
1	D	120	ALA	CA-C	-6.70	1.44	1.52
1	A	124	ALA	CA-CB	6.67	1.63	1.53
1	D	82	ALA	CA-CB	-6.64	1.42	1.53
1	C	9	ALA	CA-CB	6.53	1.65	1.53
1	C	94	ALA	CA-CB	-6.48	1.42	1.54
1	B	32	ASP	C-O	-6.45	1.16	1.24
1	C	71	ALA	CA-CB	-6.40	1.43	1.53
1	C	122	ASP	C-O	-6.38	1.16	1.24
1	C	113	TYR	CA-C	-6.38	1.44	1.53
1	D	33	ALA	CA-CB	-6.34	1.43	1.53
1	C	43	VAL	CB-CG2	-6.34	1.31	1.52
1	C	77	VAL	CA-C	6.28	1.60	1.52
1	C	164	HIS	C-O	6.27	1.31	1.24
1	A	33	ALA	C-O	-6.25	1.17	1.24
1	A	91	VAL	CA-CB	6.22	1.62	1.54
1	A	65	LEU	C-O	-6.22	1.16	1.24
1	A	105	VAL	C-O	-6.20	1.15	1.23
1	B	91	VAL	CA-CB	-6.19	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	31	VAL	CA-CB	-6.19	1.47	1.54
1	B	120	ALA	CA-CB	-6.17	1.43	1.53
1	C	98	THR	CA-C	-6.17	1.44	1.52
1	B	141	GLU	CD-OE2	6.16	1.37	1.25
1	C	168	HIS	C-O	-6.13	1.16	1.24
1	A	52	HIS	CE1-NE2	-6.11	1.26	1.32
1	D	52	HIS	C-O	-6.10	1.17	1.24
1	A	141	GLU	CD-OE2	6.10	1.36	1.25
1	A	77	VAL	C-O	-6.09	1.17	1.24
1	C	125	ILE	CA-CB	-6.08	1.47	1.54
1	B	31	VAL	CA-CB	-5.99	1.47	1.54
1	B	31	VAL	CA-C	-5.96	1.45	1.52
1	B	147	ALA	CA-C	-5.96	1.45	1.52
1	D	83	GLU	C-O	-5.93	1.17	1.24
1	B	9	ALA	CA-CB	-5.92	1.43	1.53
1	A	61	ARG	CD-NE	-5.92	1.38	1.46
1	B	163	ALA	C-O	-5.92	1.17	1.24
1	D	82	ALA	CA-C	-5.91	1.45	1.52
1	A	135	GLU	C-O	-5.90	1.17	1.24
1	D	60	PHE	C-O	-5.88	1.16	1.24
1	C	43	VAL	CA-C	-5.87	1.45	1.52
1	A	61	ARG	CA-CB	-5.83	1.44	1.53
1	A	43	VAL	CB-CG2	-5.77	1.33	1.52
1	C	169	TYR	C-O	-5.77	1.16	1.24
1	B	174	THR	C-O	-5.76	1.17	1.23
1	B	165	HIS	C-O	-5.73	1.17	1.24
1	D	65	LEU	C-O	-5.73	1.17	1.24
1	D	9	ALA	CA-C	-5.72	1.45	1.52
1	A	73	THR	C-O	-5.70	1.17	1.24
1	B	76	GLU	N-CA	-5.70	1.39	1.46
1	D	53	TRP	C-O	-5.69	1.17	1.24
1	D	161	ASP	CG-OD2	5.67	1.36	1.25
1	B	129	ILE	CA-CB	-5.66	1.47	1.54
1	D	133	THR	CA-C	-5.66	1.45	1.52
1	D	165	HIS	CA-CB	-5.64	1.44	1.53
1	C	9	ALA	CA-C	-5.59	1.45	1.52
1	D	153	ARG	CD-NE	-5.58	1.38	1.46
1	D	115	ILE	C-O	-5.57	1.17	1.24
1	C	61	ARG	CA-CB	-5.56	1.44	1.53
1	C	150	HIS	C-O	-5.55	1.17	1.24
1	B	14	VAL	CA-CB	-5.54	1.47	1.54
1	A	39	ALA	N-CA	-5.54	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	VAL	CA-C	-5.53	1.47	1.53
1	A	132	ALA	CA-CB	-5.53	1.44	1.53
1	B	42	TYR	CA-C	-5.51	1.45	1.52
1	C	44	LEU	CA-C	5.47	1.59	1.52
1	C	153	ARG	NE-CZ	-5.44	1.27	1.33
1	B	153	ARG	NE-CZ	-5.43	1.27	1.33
1	D	94	ALA	CA-CB	-5.43	1.44	1.54
1	C	140	ALA	CA-CB	-5.42	1.45	1.53
1	C	90	GLY	C-O	-5.42	1.16	1.23
1	D	25	ASP	CB-CG	5.38	1.65	1.52
1	B	130	ILE	CA-CB	-5.37	1.47	1.54
1	B	49	LYS	CD-CE	-5.36	1.36	1.52
1	C	66	PHE	C-O	-5.36	1.17	1.24
1	D	92	PRO	C-O	-5.34	1.18	1.23
1	A	167	GLU	C-O	-5.34	1.17	1.24
1	A	61	ARG	N-CA	-5.29	1.39	1.46
1	D	23	ASP	CA-C	-5.28	1.46	1.52
1	B	152	LEU	N-CA	-5.26	1.40	1.46
1	D	157	ILE	CA-C	5.25	1.60	1.52
1	A	80	GLU	CA-C	5.25	1.59	1.52
1	D	150	HIS	C-O	-5.24	1.18	1.24
1	B	10	THR	C-O	-5.20	1.17	1.24
1	C	125	ILE	C-O	5.19	1.29	1.24
1	A	153	ARG	C-O	-5.19	1.18	1.24
1	A	77	VAL	CA-CB	5.17	1.60	1.54
1	A	33	ALA	CA-CB	-5.17	1.45	1.53
1	A	120	ALA	C-O	-5.15	1.18	1.24
1	B	153	ARG	CD-NE	-5.14	1.39	1.46
1	B	10	THR	CB-CG2	-5.13	1.35	1.52
1	B	49	LYS	CE-NZ	5.13	1.64	1.49
1	D	10	THR	C-O	-5.13	1.17	1.24
1	A	156	LEU	CA-C	-5.12	1.46	1.52
1	B	39	ALA	CA-CB	-5.12	1.45	1.53
1	D	80	GLU	C-O	-5.11	1.18	1.24
1	D	99	LEU	C-O	-5.06	1.18	1.24
1	A	76	GLU	N-CA	-5.05	1.40	1.46
1	D	10	THR	N-CA	-5.05	1.39	1.46
1	D	41	VAL	CA-CB	-5.04	1.48	1.54
1	B	8	ARG	CB-CG	-5.03	1.37	1.52
1	C	74	ALA	C-O	-5.03	1.18	1.24
1	C	166	ILE	CA-CB	-5.02	1.48	1.54
1	D	44	LEU	CA-C	5.00	1.59	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	GLU	CG-CD-OE1	-40.59	25.03	118.40
1	C	15	GLU	CG-CD-OE1	-28.04	53.92	118.40
1	D	15	GLU	CG-CD-OE1	-27.42	55.33	118.40
1	D	15	GLU	CG-CD-OE2	20.69	166.00	118.40
1	C	15	GLU	CG-CD-OE2	20.64	165.87	118.40
1	C	141	GLU	CG-CD-OE2	13.83	150.22	118.40
1	C	15	GLU	CA-CB-CG	11.93	137.97	114.10
1	D	15	GLU	CA-CB-CG	10.22	134.54	114.10
1	D	15	GLU	CB-CG-CD	9.31	128.44	112.60
1	C	15	GLU	CB-CG-CD	8.98	127.86	112.60
1	D	61	ARG	NE-CZ-NH1	-8.68	112.82	121.50
1	C	141	GLU	CA-CB-CG	8.10	130.31	114.10
1	A	61	ARG	NE-CZ-NH2	-7.58	112.38	119.20
1	D	137	THR	OG1-CB-CG2	-6.93	95.43	109.30
1	C	141	GLU	CB-CG-CD	6.12	123.00	112.60
1	A	149	ALA	N-CA-C	5.89	117.38	111.07
1	D	153	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	D	61	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	D	23	ASP	N-CA-CB	5.58	118.23	110.04
1	D	159	LEU	CB-CG-CD2	-5.55	94.05	110.70
1	C	107	VAL	CB-CA-C	5.52	118.84	110.62
1	A	151	MET	CG-SD-CE	-5.47	88.87	100.90
1	B	11	ALA	CA-C-N	-5.42	114.80	123.31
1	B	11	ALA	C-N-CA	-5.42	114.80	123.31
1	B	43	VAL	N-CA-CB	5.32	118.56	110.58
1	A	8	ARG	N-CA-CB	-5.23	102.18	110.28
1	B	13	GLU	N-CA-CB	5.20	118.19	110.29
1	D	83	GLU	CA-CB-CG	-5.13	103.84	114.10
1	A	63	LEU	N-CA-C	5.12	116.86	111.28
1	B	137	THR	OG1-CB-CG2	-5.12	99.07	109.30
1	C	151	MET	CG-SD-CE	-5.09	89.71	100.90
1	B	164	HIS	N-CA-C	-5.08	105.83	111.36
1	B	10	THR	CB-CA-C	5.08	118.52	109.38
1	B	181	LEU	CA-C-O	-5.05	112.21	120.80
1	A	18	ASP	N-CA-CB	5.03	118.04	110.30
1	A	153	ARG	NE-CZ-NH2	-5.01	114.69	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	15	GLU	Sidechain
1	D	15	GLU	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1394	0	1292	31	0
1	B	1355	0	1253	19	1
1	C	1355	0	1253	24	0
1	D	1355	0	1253	25	0
2	A	5	0	0	2	0
2	B	5	0	0	1	9
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	58	0	0	7	0
6	B	68	0	0	3	0
6	C	67	0	0	2	0
6	D	77	0	0	6	0
All	All	5751	0	5051	94	9

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 9.

All (94) 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:52:HIS:CE1	1:A:64:HIS:CE1	1.93	1.51
1:A:52:HIS:HE1	1:A:64:HIS:CE1	1.24	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:GLU:OE1	1:D:15:GLU:CG	1.64	1.44
1:D:15:GLU:CG	1:D:15:GLU:CD	1.99	1.36
1:A:2:SER:N	6:A:1347:HOH:O	1.74	1.20
1:C:15:GLU:CB	1:C:15:GLU:CG	2.31	1.07
1:A:52:HIS:CE1	1:A:64:HIS:HE1	1.49	1.06
1:D:15:GLU:CG	1:D:15:GLU:CB	2.35	1.04
1:C:141:GLU:CB	1:C:141:GLU:CG	2.43	0.96
1:D:22:MET:HE3	1:D:26:ARG:HG2	1.49	0.93
1:A:52:HIS:ND1	1:A:64:HIS:CE1	2.42	0.86
1:D:164:HIS:HE1	6:D:1350:HOH:O	1.65	0.80
1:D:77:VAL:HG21	1:D:159:LEU:HD11	1.64	0.79
1:A:133:THR:O	1:A:137:THR:HG23	1.82	0.79
1:C:7:ALA:N	6:C:1376:HOH:O	2.16	0.78
1:A:52:HIS:ND1	1:A:64:HIS:ND1	2.31	0.78
1:A:52:HIS:CE1	1:A:64:HIS:ND1	2.50	0.77
1:D:25:ASP:CB	6:D:1338:HOH:O	2.36	0.74
1:D:141:GLU:CD	1:D:153:ARG:HH22	1.98	0.72
1:B:133:THR:O	1:B:137:THR:HG23	1.89	0.71
1:C:93:HIS:ND1	1:C:102:GLU:HG3	2.08	0.69
1:D:164:HIS:CE1	6:D:1350:HOH:O	2.40	0.69
1:C:35:ASN:CG	1:C:93:HIS:CD2	2.70	0.69
1:B:25:ASP:HB2	6:B:1327:HOH:O	1.93	0.68
1:D:25:ASP:HB3	6:D:1338:HOH:O	1.94	0.68
1:C:93:HIS:CE1	1:C:102:GLU:HG3	2.27	0.68
1:A:22:MET:HE2	1:A:26:ARG:NH2	2.10	0.67
1:A:51:HIS:CD2	1:A:122:ASP:OD2	2.48	0.67
1:A:51:HIS:HD2	1:A:122:ASP:OD2	1.78	0.67
1:D:133:THR:O	1:D:137:THR:HG23	1.96	0.66
1:A:164:HIS:HD2	6:A:1334:HOH:O	1.79	0.65
1:D:84:ARG:HB2	1:D:151:MET:HE1	1.79	0.64
1:D:137:THR:HG22	1:D:152:LEU:HB3	1.80	0.63
1:B:10:THR:HG22	1:B:13:GLU:HG3	1.81	0.63
1:A:76:GLU:HG3	6:A:1332:HOH:O	1.99	0.62
1:A:64:HIS:CD2	6:A:1335:HOH:O	2.53	0.61
1:C:164:HIS:HD2	6:C:1324:HOH:O	1.82	0.61
1:A:137:THR:HG22	1:A:152:LEU:HB3	1.82	0.61
1:C:35:ASN:CG	1:C:93:HIS:HD2	2.09	0.60
1:C:84:ARG:HB2	1:C:151:MET:HE1	1.84	0.60
1:A:51:HIS:CD2	1:A:118:SER:HB3	2.37	0.57
1:A:157:ILE:C	1:A:157:ILE:HD13	2.29	0.57
1:A:84:ARG:HB2	1:A:151:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:VAL:HG21	1:D:159:LEU:CD1	2.34	0.56
1:A:131:GLU:OE1	1:C:21:ARG:NH1	2.31	0.56
1:C:133:THR:O	1:C:137:THR:HG23	2.08	0.54
1:B:84:ARG:CG	1:B:151:MET:HE1	2.37	0.54
1:C:35:ASN:OD1	1:C:93:HIS:HD2	1.90	0.54
1:A:64:HIS:HD2	6:A:1335:HOH:O	1.90	0.54
1:B:45:TYR:HD2	1:B:46:HIS:CD2	2.26	0.54
1:A:137:THR:HG22	1:A:152:LEU:CB	2.38	0.53
2:A:1201:SO4:O3	1:C:150:HIS:CE1	2.62	0.53
1:A:50:LYS:HB2	1:B:94:ALA:HB1	1.90	0.53
1:D:30:CYS:O	1:D:34:LEU:HG	2.10	0.51
1:B:153:ARG:CD	2:B:1202:SO4:O1	2.58	0.51
1:D:39:ALA:O	1:D:43:VAL:HG13	2.11	0.51
1:C:93:HIS:CE1	1:C:102:GLU:CG	2.95	0.50
1:B:84:ARG:HB2	1:B:151:MET:HE1	1.94	0.50
1:A:39:ALA:O	1:A:43:VAL:HG13	2.13	0.49
1:B:45:TYR:HD2	1:B:46:HIS:HD2	1.59	0.49
1:B:84:ARG:HG2	1:B:151:MET:HE1	1.96	0.48
1:C:133:THR:O	1:C:137:THR:CG2	2.61	0.47
1:D:77:VAL:O	1:D:81:LEU:HD13	2.15	0.47
1:B:47:GLN:HG2	1:B:122:ASP:OD1	2.14	0.47
2:A:1201:SO4:O3	1:C:150:HIS:ND1	2.49	0.46
1:C:10:THR:O	1:C:11:ALA:C	2.58	0.46
1:A:2:SER:CA	6:A:1347:HOH:O	2.48	0.45
1:A:141:GLU:CG	1:A:153:ARG:HH22	2.29	0.45
1:B:45:TYR:CD2	1:B:46:HIS:CD2	3.05	0.45
1:A:62:ASP:OD1	1:A:169:TYR:OH	2.24	0.45
1:B:84:ARG:CB	1:B:151:MET:HE1	2.47	0.45
1:B:10:THR:CG2	6:B:1342:HOH:O	2.65	0.45
1:C:96:PRO:HD2	1:D:100:GLN:OE1	2.16	0.45
1:B:72:GLU:O	1:B:76:GLU:HG3	2.17	0.45
1:A:168:HIS:CE1	1:C:86:GLN:HE22	2.35	0.44
1:A:141:GLU:HG3	1:A:153:ARG:NH2	2.32	0.44
1:D:155:GLY:O	1:D:159:LEU:HD13	2.16	0.44
1:B:14:VAL:HA	1:B:89:GLY:O	2.18	0.44
1:D:22:MET:CE	1:D:26:ARG:HG2	2.35	0.44
1:C:49:LYS:HE3	6:D:1370:HOH:O	2.18	0.44
1:D:84:ARG:CB	1:D:151:MET:HE1	2.47	0.44
1:A:33:ALA:HB1	1:A:136:HIS:CD2	2.53	0.43
1:B:141:GLU:CD	1:B:153:ARG:HH22	2.27	0.43
1:C:35:ASN:HB3	1:C:93:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:HB1	1:A:136:HIS:CG	2.54	0.42
1:B:86:GLN:HE21	1:B:86:GLN:HB3	1.58	0.42
1:A:164:HIS:CD2	6:A:1334:HOH:O	2.62	0.42
1:C:72:GLU:O	1:C:76:GLU:HG3	2.20	0.42
1:D:63:LEU:HD13	1:D:115:ILE:HG12	2.01	0.42
1:C:46:HIS:CD2	1:D:96:PRO:HG3	2.56	0.41
1:B:25:ASP:CB	6:B:1327:HOH:O	2.63	0.41
1:D:25:ASP:HB2	6:D:1338:HOH:O	2.11	0.40
1:C:35:ASN:CB	1:C:93:HIS:CD2	3.05	0.40
1:D:55:VAL:HG23	1:D:115:ILE:HD13	2.02	0.40

All (9) 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)
2:B:1202:SO4:O2	2:B:1202:SO4:O4[2_655]	0.74	1.46
2:B:1202:SO4:O3	2:B:1202:SO4:O4[3_665]	1.24	0.96
2:B:1202:SO4:O1	2:B:1202:SO4:O4[3_665]	1.33	0.87
2:B:1202:SO4:S	2:B:1202:SO4:O2[2_655]	1.40	0.80
2:B:1202:SO4:O2	2:B:1202:SO4:O3[3_665]	1.40	0.80
2:B:1202:SO4:O1	2:B:1202:SO4:O2[2_655]	1.47	0.73
1:B:150:HIS:ND1	2:B:1202:SO4:O3[3_665]	1.82	0.38
2:B:1202:SO4:S	2:B:1202:SO4:O3[3_665]	1.87	0.33
2:B:1202:SO4:S	2:B:1202:SO4:O1[3_665]	1.88	0.32

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	178/182 (98%)	176 (99%)	2 (1%)	0	100 100
1	B	173/182 (95%)	171 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	173/182 (95%)	171 (99%)	2 (1%)	0	100	100
1	D	173/182 (95%)	173 (100%)	0	0	100	100
All	All	697/728 (96%)	691 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	143/145 (99%)	130 (91%)	13 (9%)	9	9
1	B	138/145 (95%)	127 (92%)	11 (8%)	11	13
1	C	138/145 (95%)	125 (91%)	13 (9%)	8	9
1	D	138/145 (95%)	130 (94%)	8 (6%)	18	22
All	All	557/580 (96%)	512 (92%)	45 (8%)	11	12

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	22	MET
1	A	42	TYR
1	A	43	VAL
1	A	52	HIS
1	A	60	PHE
1	A	81	LEU
1	A	107	VAL
1	A	119	LEU
1	A	157	ILE
1	A	159	LEU
1	A	178	GLN
1	A	181	LEU
1	B	10	THR

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Mol	Chain	Res	Type
1	B	42	TYR
1	B	43	VAL
1	B	60	PHE
1	B	75	GLU
1	B	86	GLN
1	B	97	GLU
1	B	107	VAL
1	B	151	MET
1	B	159	LEU
1	B	181	LEU
1	C	26	ARG
1	C	42	TYR
1	C	75	GLU
1	C	86	GLN
1	C	97	GLU
1	C	107	VAL
1	C	119	LEU
1	C	137	THR
1	C	141	GLU
1	C	151	MET
1	C	157	ILE
1	C	159	LEU
1	C	181	LEU
1	D	10	THR
1	D	25	ASP
1	D	42	TYR
1	D	43	VAL
1	D	107	VAL
1	D	119	LEU
1	D	141	GLU
1	D	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	52	HIS
1	A	64	HIS
1	A	86	GLN
1	A	142	ASN
1	A	164	HIS
1	A	165	HIS

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Mol	Chain	Res	Type
1	B	86	GLN
1	B	142	ASN
1	B	164	HIS
1	B	165	HIS
1	C	29	GLN
1	C	86	GLN
1	C	93	HIS
1	C	142	ASN
1	C	164	HIS
1	C	168	HIS
1	D	86	GLN
1	D	142	ASN
1	D	164	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](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1201	-	4,4,4	0.62	0	6,6,6	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	1202	-	4,4,4	0.57	0	6,6,6	0.24	0

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.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	SO4	2	0
2	B	1202	SO4	1	9

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.