



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2017 – 02:52 AM EDT

PDB ID : 1TK6  
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 : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

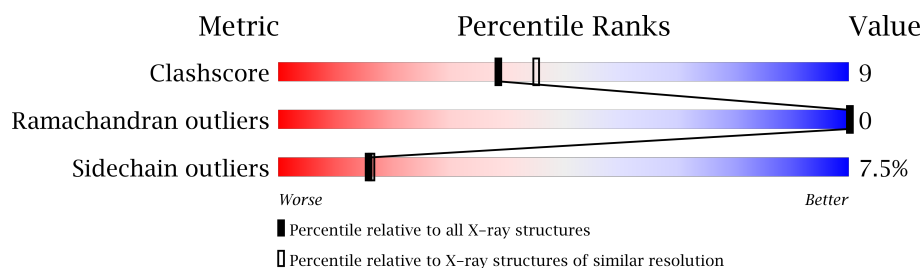
# 1 Overall quality at a glance

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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	182	
1	B	182	
1	C	182	
1	D	182	

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
1	A	180	Total	C	N	O	S	0	0	0
			1394	852	242	296	4			
1	B	175	Total	C	N	O	S	0	0	0
			1355	830	234	287	4			
1	C	175	Total	C	N	O	S	0	0	0
			1355	830	234	287	4			
1	D	175	Total	C	N	O	S	0	0	0
			1355	830	234	287	4			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is water.

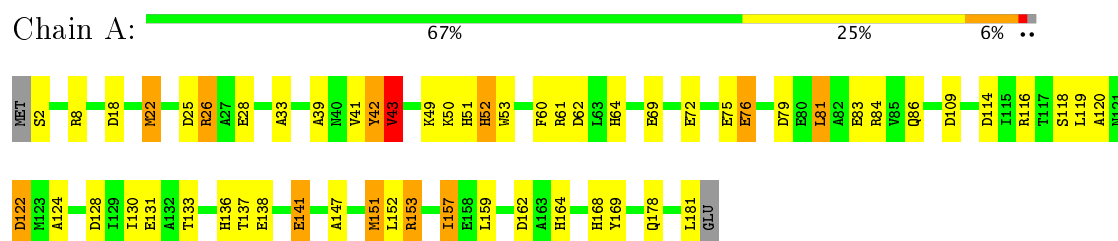
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total 58	O 58	0	0
6	B	68	Total 68	O 68	0	0
6	C	67	Total 67	O 67	0	0
6	D	77	Total 77	O 77	0	0

### 3 Residue-property plots [i](#)

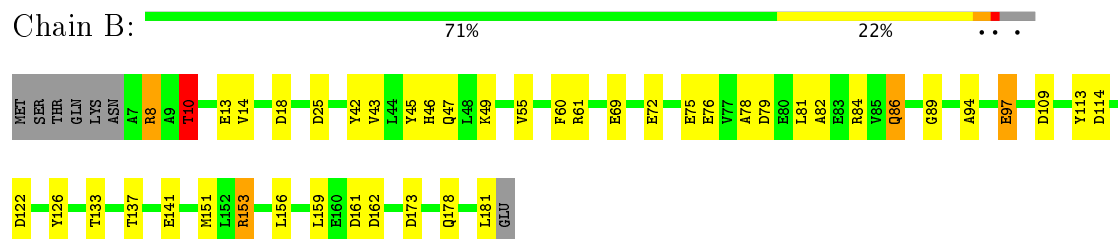
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

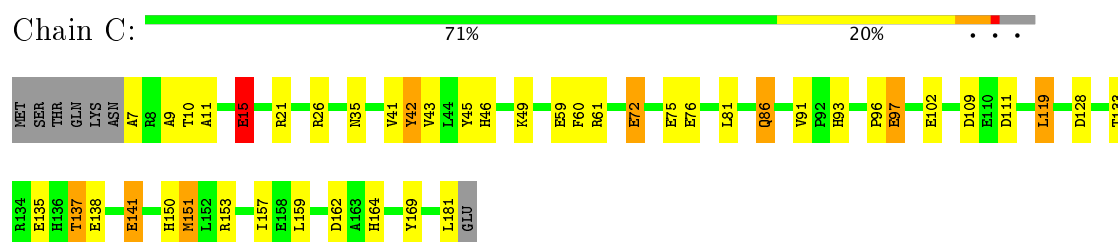
#### • Molecule 1: Iron-rich dpsA-homolog protein



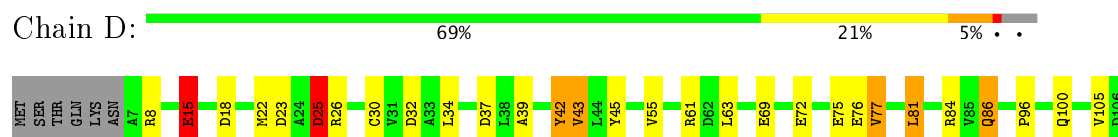
#### • Molecule 1: Iron-rich dpsA-homolog protein

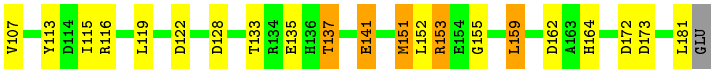


#### • Molecule 1: Iron-rich dpsA-homolog protein



#### • Molecule 1: Iron-rich dpsA-homolog protein





## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$	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.	Xtriage
Total number of atoms	5751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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: NA, MG, FE, SO4

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	1.68	20/1415 (1.4%)	1.42	21/1923 (1.1%)
1	B	1.63	14/1376 (1.0%)	1.30	13/1871 (0.7%)
1	C	2.58	21/1376 (1.5%)	1.93	16/1871 (0.9%)
1	D	2.23	16/1376 (1.2%)	1.75	27/1871 (1.4%)
All	All	2.07	71/5543 (1.3%)	1.62	77/7536 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	GLU	CB-CG	48.00	2.43	1.52
1	D	15	GLU	CB-CG	44.06	2.35	1.52
1	C	15	GLU	CB-CG	41.90	2.31	1.52
1	D	15	GLU	CG-CD	31.45	1.99	1.51
1	C	15	GLU	CG-CD	30.52	1.97	1.51
1	C	141	GLU	CG-CD	20.95	1.83	1.51
1	D	141	GLU	CD-OE2	13.64	1.40	1.25
1	B	141	GLU	CD-OE2	10.37	1.37	1.25
1	A	141	GLU	CD-OE2	10.26	1.36	1.25
1	C	43	VAL	CB-CG2	-10.10	1.31	1.52
1	A	43	VAL	CB-CG2	-9.21	1.33	1.52
1	A	72	GLU	CG-CD	7.88	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	GLU	CD-OE1	7.79	1.34	1.25
1	A	75	GLU	CD-OE1	7.75	1.34	1.25
1	B	97	GLU	CD-OE2	7.67	1.34	1.25
1	C	45	TYR	CD2-CE2	-7.28	1.28	1.39
1	A	76	GLU	CD-OE1	7.10	1.33	1.25
1	C	42	TYR	CD1-CE1	-7.07	1.28	1.39
1	A	141	GLU	CG-CD	6.89	1.62	1.51
1	D	25	ASP	CB-CG	6.55	1.65	1.51
1	D	76	GLU	CD-OE1	6.52	1.32	1.25
1	A	69	GLU	CD-OE1	6.51	1.32	1.25
1	A	147	ALA	CA-CB	-6.43	1.39	1.52
1	B	49	LYS	CE-NZ	6.28	1.64	1.49
1	A	69	GLU	CG-CD	6.25	1.61	1.51
1	C	135	GLU	CD-OE1	6.22	1.32	1.25
1	D	105	VAL	CB-CG2	6.21	1.65	1.52
1	C	9	ALA	CA-CB	6.19	1.65	1.52
1	B	97	GLU	CD-OE1	6.16	1.32	1.25
1	C	42	TYR	CD2-CE2	-6.14	1.30	1.39
1	C	97	GLU	CG-CD	6.07	1.61	1.51
1	C	61	ARG	CD-NE	-5.96	1.36	1.46
1	B	49	LYS	CD-CE	-5.96	1.36	1.51
1	C	41	VAL	CB-CG2	5.93	1.65	1.52
1	D	113	TYR	CE2-CZ	-5.90	1.30	1.38
1	C	153	ARG	CD-NE	-5.80	1.36	1.46
1	C	138	GLU	CD-OE2	5.74	1.31	1.25
1	C	42	TYR	CE1-CZ	-5.73	1.31	1.38
1	C	72	GLU	CD-OE2	5.71	1.31	1.25
1	A	53	TRP	CE2-CZ2	-5.63	1.30	1.39
1	B	8	ARG	CB-CG	-5.63	1.37	1.52
1	D	77	VAL	CB-CG1	5.58	1.64	1.52
1	A	120	ALA	CA-CB	-5.57	1.40	1.52
1	C	59	GLU	CG-CD	5.56	1.60	1.51
1	D	135	GLU	CD-OE2	5.53	1.31	1.25
1	D	69	GLU	CD-OE1	5.50	1.31	1.25
1	A	28	GLU	CD-OE2	5.47	1.31	1.25
1	A	42	TYR	CD1-CE1	5.45	1.47	1.39
1	C	169	TYR	CD2-CE2	-5.39	1.31	1.39
1	A	124	ALA	CA-CB	5.36	1.63	1.52
1	D	86	GLN	C-O	5.33	1.33	1.23
1	B	113	TYR	CD1-CE1	-5.31	1.31	1.39
1	A	138	GLU	CD-OE2	5.26	1.31	1.25
1	A	72	GLU	CD-OE1	5.24	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	91	VAL	CB-CG2	-5.23	1.41	1.52
1	D	45	TYR	CZ-OH	-5.21	1.28	1.37
1	A	41	VAL	CB-CG2	-5.21	1.42	1.52
1	D	42	TYR	CB-CG	-5.17	1.43	1.51
1	A	49	LYS	CD-CE	-5.16	1.38	1.51
1	D	72	GLU	CD-OE2	5.14	1.31	1.25
1	B	126	TYR	CD1-CE1	-5.12	1.31	1.39
1	C	109	ASP	C-O	-5.11	1.13	1.23
1	D	75	GLU	CD-OE1	5.11	1.31	1.25
1	B	55	VAL	CB-CG2	5.11	1.63	1.52
1	B	78	ALA	CA-CB	-5.09	1.41	1.52
1	B	141	GLU	CD-OE1	5.08	1.31	1.25
1	B	10	THR	CB-CG2	-5.08	1.35	1.52
1	B	82	ALA	CA-CB	-5.07	1.41	1.52
1	B	69	GLU	CD-OE2	5.04	1.31	1.25
1	A	83	GLU	CD-OE1	5.01	1.31	1.25
1	D	135	GLU	CG-CD	5.00	1.59	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	GLU	CG-CD-OE1	-46.63	25.03	118.30
1	C	15	GLU	CG-CD-OE1	-32.19	53.92	118.30
1	D	15	GLU	CG-CD-OE1	-31.49	55.33	118.30
1	D	15	GLU	CG-CD-OE2	23.85	166.00	118.30
1	C	15	GLU	CG-CD-OE2	23.78	165.87	118.30
1	C	141	GLU	CG-CD-OE2	15.96	150.22	118.30
1	A	61	ARG	NE-CZ-NH2	-15.84	112.38	120.30
1	D	61	ARG	NE-CZ-NH1	-14.96	112.82	120.30
1	D	153	ARG	NE-CZ-NH2	-12.79	113.90	120.30
1	A	153	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	C	15	GLU	CA-CB-CG	11.17	137.97	113.40
1	B	153	ARG	NE-CZ-NH2	-10.89	114.85	120.30
1	A	162	ASP	CB-CG-OD2	10.02	127.32	118.30
1	D	159	LEU	CB-CG-CD2	-9.97	94.05	111.00
1	A	153	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	D	15	GLU	CA-CB-CG	9.61	134.54	113.40
1	B	153	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	D	162	ASP	CB-CG-OD2	9.56	126.90	118.30
1	A	114	ASP	CB-CG-OD2	9.36	126.72	118.30
1	D	153	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	D	81	LEU	CB-CG-CD2	-8.80	96.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	ASP	CB-CG-OD2	8.76	126.19	118.30
1	D	23	ASP	CB-CG-OD2	8.36	125.83	118.30
1	B	61	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	A	116	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	A	162	ASP	CB-CG-OD1	-8.06	111.05	118.30
1	D	61	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	A	61	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	C	141	GLU	CA-CB-CG	7.68	130.31	113.40
1	D	116	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	109	ASP	CB-CG-OD2	7.59	125.13	118.30
1	D	116	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	C	81	LEU	CB-CG-CD2	-7.24	98.69	111.00
1	C	153	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	D	18	ASP	CB-CG-OD2	7.14	124.72	118.30
1	D	25	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	151	MET	CG-SD-CE	-7.08	88.87	100.20
1	A	81	LEU	CA-CB-CG	7.04	131.49	115.30
1	A	81	LEU	CB-CG-CD1	7.00	122.90	111.00
1	B	79	ASP	CB-CG-OD2	6.96	124.57	118.30
1	A	128	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	122	ASP	CB-CG-OD2	6.86	124.47	118.30
1	D	18	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	B	81	LEU	CB-CG-CD2	-6.62	99.75	111.00
1	C	109	ASP	CB-CG-OD2	6.57	124.21	118.30
1	C	151	MET	CG-SD-CE	-6.56	89.71	100.20
1	A	116	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	D	137	THR	OG1-CB-CG2	-6.33	95.43	110.00
1	D	172	ASP	CB-CG-OD2	6.31	123.98	118.30
1	D	37	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	61	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	159	LEU	CB-CG-CD1	6.17	121.50	111.00
1	C	61	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	119	LEU	CB-CG-CD1	6.10	121.38	111.00
1	D	173	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	8	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	25	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	109	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	128	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	111	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	122	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	18	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	128	ASP	CB-CG-OD2	5.58	123.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	ASP	CB-CG-OD2	5.56	123.31	118.30
1	D	32	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	156	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	B	114	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	151	MET	CG-SD-CE	-5.33	91.67	100.20
1	B	161	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	18	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	15	GLU	CB-CG-CD	5.27	128.44	114.20
1	B	173	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	79	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	15	GLU	CB-CG-CD	5.06	127.86	114.20
1	A	130	ILE	CG1-CB-CG2	-5.04	100.32	111.40
1	A	8	ARG	CG-CD-NE	-5.04	101.22	111.80
1	D	8	ARG	CG-CD-NE	-5.00	101.30	111.80

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

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	32	0
1	B	1355	0	1253	15	0
1	C	1355	0	1253	24	0
1	D	1355	0	1253	24	0
2	A	5	0	0	2	0
2	B	5	0	0	1	8
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
6	D	77	0	0	6	0
All	All	5751	0	5051	90	8

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 (90) 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
1:D:15:GLU:OE1	1:D:15:GLU:CG	1.64	1.44
1:D:15:GLU:CD	1:D:15:GLU:CG	1.99	1.31
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:CG	1:C:141:GLU:CB	2.43	0.96
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:B:133:THR:O	1:B:137:THR:HG23	1.89	0.71
1:D:22:MET:HE3	1:D:26:ARG:HG2	1.72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:GLU:CD	1:D:153:ARG:HH22	1.98	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:C:35:ASN:CG	1:C:93:HIS:CD2	2.70	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:A:51:HIS:CD2	1:A:118:SER:HB3	2.37	0.57
1:D:22:MET:CE	1:D:26:ARG:HG2	2.35	0.56
1:D:77:VAL:HG21	1:D:159:LEU:CD1	2.34	0.56
1:D:84:ARG:HB2	1:D:151:MET:HE1	1.88	0.56
1:A:131:GLU:OE1	1:C:21:ARG:NH1	2.31	0.56
1:B:84:ARG:HB2	1:B:151:MET:HE1	1.89	0.55
1:C:35:ASN:CG	1:C:93:HIS:HD2	2.09	0.55
1:A:84:ARG:HB2	1:A:151:MET:HE1	1.89	0.54
1:C:133:THR:O	1:C:137:THR:HG23	2.08	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:A:157:ILE:HD13	1:A:157:ILE:C	2.29	0.52
1:D:30:CYS:O	1:D:34:LEU:HG	2.10	0.51
1:A:22:MET:HE2	1:A:26:ARG:NH2	2.26	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:C:151:MET:HE1	6:C:1337:HOH:O	2.11	0.49
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: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:A:2:SER:CA	6:A:1347:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:49:LYS:HE3	6:D:1370:HOH:O	2.18	0.44
1:A:22:MET:HE2	1:A:22:MET:HA	1.99	0.43
1:A:33:ALA:HB1	1:A:136:HIS:CD2	2.53	0.43
1:C:35:ASN:HB3	1:C:93:HIS:NE2	2.33	0.43
1:A:33:ALA:HB1	1:A:136:HIS:CG	2.54	0.42
1:B:86:GLN:HB3	1:B:86:GLN:HE21	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:C:10:THR:O	1:C:11:ALA:C	2.58	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 (8) 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
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
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%)	11	11
1	B	138/145 (95%)	127 (92%)	11 (8%)	14	14
1	C	138/145 (95%)	127 (92%)	11 (8%)	14	14
1	D	138/145 (95%)	131 (95%)	7 (5%)	28	33
All	All	557/580 (96%)	515 (92%)	42 (8%)	16	16

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	26	ARG

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Mol	Chain	Res	Type
1	A	42	TYR
1	A	43	VAL
1	A	52	HIS
1	A	60	PHE
1	A	81	LEU
1	A	86	GLN
1	A	119	LEU
1	A	157	ILE
1	A	159	LEU
1	A	178	GLN
1	A	181	LEU
1	B	8	ARG
1	B	10	THR
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	159	LEU
1	B	178	GLN
1	B	181	LEU
1	C	26	ARG
1	C	42	TYR
1	C	60	PHE
1	C	75	GLU
1	C	86	GLN
1	C	97	GLU
1	C	119	LEU
1	C	137	THR
1	C	157	ILE
1	C	159	LEU
1	C	181	LEU
1	D	25	ASP
1	D	42	TYR
1	D	43	VAL
1	D	86	GLN
1	D	107	VAL
1	D	119	LEU
1	D	181	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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
1	B	86	GLN
1	B	142	ASN
1	B	165	HIS
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 carbohydrates 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	0.60	0	6,6,6	0.77	0
2	SO4	B	1202	1	4,4,4	0.54	0	6,6,6	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1201	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1202	1	-	0/0/0/0	0/0/0/0

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 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	SO4	2	0
2	B	1202	SO4	1	8

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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.