



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:36 PM UTC

PDB ID : 1TKP / pdb\_00001tkp  
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 : 2004-06-09  
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

<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

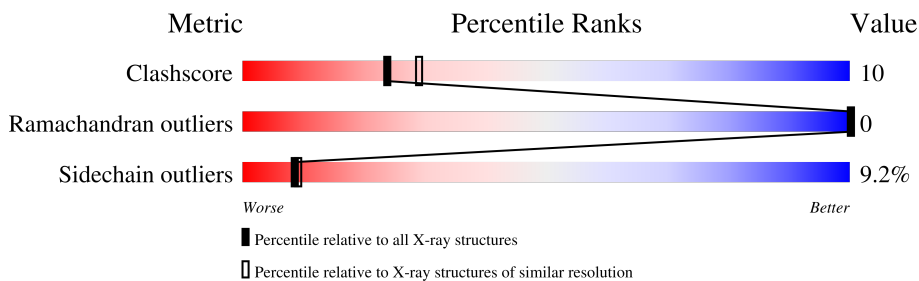
# 1 Overall quality at a glance

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  $\geq 3$ , 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	
1	B	182	
1	C	182	
1	D	182	

## 2 Entry composition [i](#)

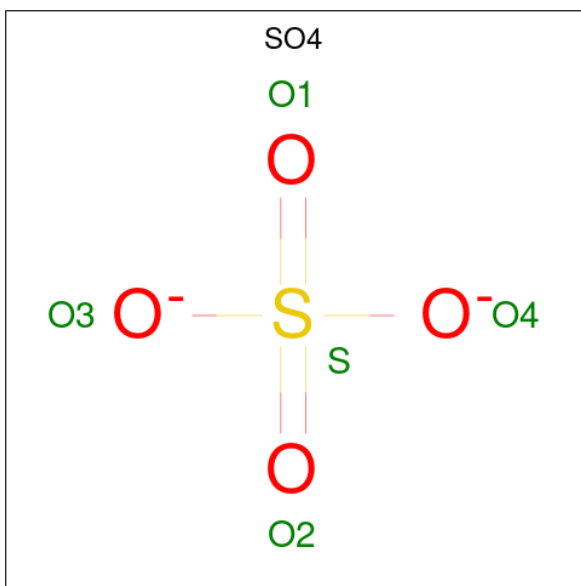
There are 5 unique types of molecules in this entry. The entry contains 5728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: O<sub>4</sub>S).



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	11	Total 11	Fe 11	0	0
3	B	9	Total 9	Fe 9	0	0
3	C	2	Total 2	Fe 2	0	0
3	D	8	Total 8	Fe 8	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	C	1	Total 1	Na 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total 50	O 50	0	0
5	B	56	Total 56	O 56	0	0
5	C	63	Total 63	O 63	0	0
5	D	58	Total 58	O 58	0	0

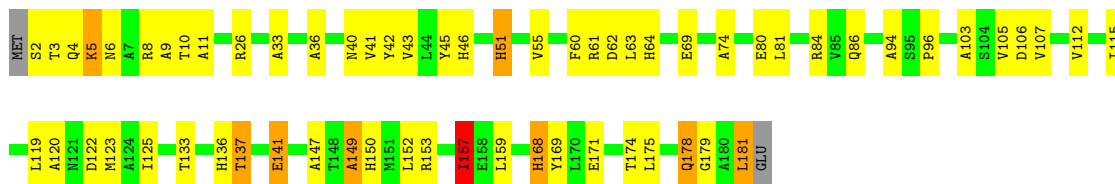
### 3 Residue-property plots [i](#)

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

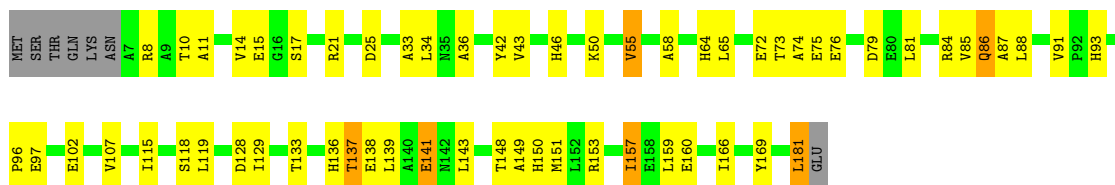
- Molecule 1: Iron-rich dpsA-homolog protein

Chain A: 



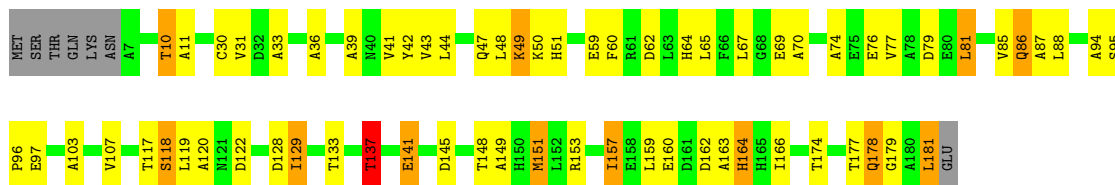
- Molecule 1: Iron-rich dpsA-homolog protein

Chain B: 



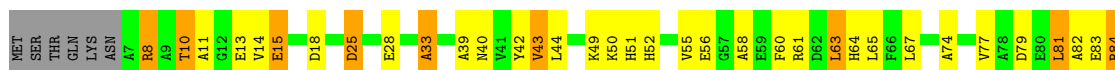
- Molecule 1: Iron-rich dpsA-homolog protein

Chain C: 



- Molecule 1: Iron-rich dpsA-homolog protein

Chain D: 





## 4 Data and refinement statistics

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)	141.42 – 2.20	Depositor
% Data completeness (in resolution range)	99.8 (141.42-2.20)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.185 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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: 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	1.86	20/1415 (1.4%)	1.56	9/1923 (0.5%)
1	B	1.90	23/1376 (1.7%)	1.55	10/1871 (0.5%)
1	C	2.09	31/1376 (2.3%)	1.61	15/1871 (0.8%)
1	D	2.00	27/1376 (2.0%)	1.62	13/1871 (0.7%)
All	All	1.96	101/5543 (1.8%)	1.58	47/7536 (0.6%)

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	151	MET	SD-CE	17.77	2.23	1.79
1	B	129	ILE	CA-CB	-9.33	1.41	1.54
1	B	93	HIS	C-O	8.79	1.34	1.23
1	A	141	GLU	CD-OE2	8.55	1.41	1.25
1	A	9	ALA	CA-CB	8.12	1.67	1.53
1	C	43	VAL	CB-CG2	-8.00	1.26	1.52
1	D	103	ALA	CA-CB	-7.92	1.40	1.53
1	B	11	ALA	CA-C	-7.74	1.43	1.52
1	B	14	VAL	CA-CB	-7.66	1.44	1.54
1	C	141	GLU	CD-OE2	7.30	1.39	1.25
1	B	79	ASP	C-O	-7.25	1.15	1.24
1	C	164	HIS	C-O	7.24	1.32	1.24
1	C	47	GLN	CA-C	7.20	1.62	1.52
1	C	70	ALA	CA-CB	7.11	1.64	1.53
1	C	177	THR	C-O	7.10	1.32	1.23
1	A	150	HIS	C-O	-7.09	1.16	1.24
1	A	149	ALA	CA-CB	7.08	1.64	1.53
1	D	154	GLU	C-O	-7.03	1.15	1.24
1	C	103	ALA	CA-C	-7.02	1.43	1.52
1	C	79	ASP	C-O	-6.90	1.16	1.24
1	D	13	GLU	CD-OE2	6.89	1.38	1.25
1	B	141	GLU	CD-OE2	6.88	1.38	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	MET	SD-CE	-6.86	1.62	1.79
1	D	44	LEU	C-O	6.84	1.32	1.24
1	D	60	PHE	C-O	-6.83	1.15	1.24
1	C	59	GLU	CA-C	-6.65	1.44	1.53
1	C	166	ILE	CA-C	6.65	1.61	1.52
1	D	63	LEU	C-O	-6.54	1.16	1.24
1	B	169	TYR	CA-C	-6.40	1.44	1.52
1	A	6	ASN	CA-C	-6.34	1.44	1.52
1	C	62	ASP	N-CA	-6.34	1.38	1.46
1	C	49	LYS	CE-NZ	6.27	1.68	1.49
1	B	166	ILE	N-CA	-6.24	1.38	1.46
1	B	150	HIS	C-O	-6.24	1.17	1.24
1	D	65	LEU	CA-C	-6.23	1.44	1.52
1	D	87	ALA	CA-CB	6.17	1.63	1.53
1	A	55	VAL	C-O	-6.14	1.17	1.24
1	A	106	ASP	C-O	6.06	1.31	1.24
1	D	160	GLU	CA-C	6.05	1.60	1.52
1	B	148	THR	CA-CB	-6.03	1.43	1.53
1	A	141	GLU	CD-OE1	6.01	1.36	1.25
1	B	74	ALA	N-CA	6.00	1.53	1.46
1	D	49	LYS	CD-CE	-5.99	1.34	1.52
1	A	103	ALA	CA-CB	-5.96	1.44	1.53
1	A	168	HIS	C-O	-5.93	1.17	1.24
1	D	67	LEU	C-O	-5.92	1.17	1.24
1	B	141	GLU	CD-OE1	5.90	1.36	1.25
1	A	69	GLU	CD-OE1	5.90	1.36	1.25
1	A	120	ALA	CA-CB	-5.88	1.44	1.53
1	D	141	GLU	CG-CD	5.88	1.66	1.52
1	C	120	ALA	CA-CB	5.87	1.62	1.53
1	B	15	GLU	CD-OE2	5.84	1.36	1.25
1	C	74	ALA	CA-CB	-5.82	1.44	1.53
1	D	107	VAL	CA-CB	5.81	1.61	1.54
1	C	160	GLU	N-CA	-5.80	1.39	1.46
1	C	122	ASP	C-O	-5.78	1.17	1.24
1	B	10	THR	CA-C	-5.77	1.45	1.52
1	B	91	VAL	CA-CB	-5.76	1.46	1.54
1	D	115	ILE	C-O	-5.74	1.17	1.24
1	C	174	THR	CB-CG2	-5.64	1.33	1.52
1	B	139	LEU	C-O	-5.64	1.17	1.24
1	A	26	ARG	CA-C	-5.63	1.45	1.52
1	D	82	ALA	CA-CB	-5.59	1.44	1.53
1	B	85	VAL	N-CA	-5.58	1.40	1.46

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	118	SER	C-O	-5.58	1.17	1.24
1	D	124	ALA	CA-CB	5.58	1.62	1.53
1	A	41	VAL	C-O	-5.57	1.17	1.24
1	A	51	HIS	C-O	-5.56	1.17	1.24
1	D	74	ALA	C-O	-5.56	1.17	1.24
1	D	147	ALA	CA-CB	5.56	1.61	1.53
1	A	157	ILE	CA-CB	5.53	1.61	1.54
1	B	118	SER	C-O	-5.50	1.17	1.24
1	D	122	ASP	CA-C	-5.49	1.45	1.52
1	D	58	ALA	CA-CB	-5.47	1.44	1.53
1	C	64	HIS	CA-C	-5.47	1.45	1.52
1	D	169	TYR	CA-CB	-5.47	1.44	1.53
1	B	157	ILE	CA-CB	-5.44	1.46	1.54
1	C	41	VAL	C-O	-5.43	1.17	1.24
1	C	50	LYS	CD-CE	5.37	1.68	1.52
1	C	178	GLN	N-CA	-5.35	1.40	1.46
1	C	129	ILE	C-O	-5.33	1.18	1.24
1	D	156	LEU	C-O	5.31	1.30	1.24
1	A	74	ALA	CA-C	-5.31	1.46	1.52
1	C	67	LEU	C-O	-5.29	1.17	1.24
1	A	40	ASN	CA-C	-5.28	1.46	1.52
1	D	107	VAL	C-O	-5.28	1.18	1.24
1	C	67	LEU	CA-CB	5.27	1.61	1.53
1	C	47	GLN	C-O	-5.26	1.17	1.24
1	C	128	ASP	C-O	-5.25	1.18	1.24
1	D	15	GLU	CD-OE2	5.24	1.35	1.25
1	D	146	HIS	N-CA	-5.24	1.39	1.46
1	D	112	VAL	C-O	-5.23	1.18	1.24
1	C	87	ALA	CA-CB	5.21	1.61	1.53
1	C	33	ALA	CA-CB	-5.20	1.45	1.53
1	B	43	VAL	CA-CB	5.15	1.61	1.54
1	D	33	ALA	CA-CB	-5.12	1.45	1.53
1	B	34	LEU	CA-CB	-5.09	1.45	1.53
1	B	55	VAL	CB-CG1	5.05	1.69	1.52
1	C	177	THR	N-CA	5.03	1.52	1.45
1	B	129	ILE	CA-C	-5.03	1.45	1.52
1	A	112	VAL	C-O	-5.02	1.18	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ALA	N-CA-C	-9.66	100.61	111.82

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	ASP	N-CA-C	9.36	121.08	111.07
1	D	25	ASP	CB-CA-C	8.42	124.21	110.90
1	C	178	GLN	N-CA-C	-8.36	101.08	111.11
1	D	107	VAL	CB-CA-C	7.42	120.44	110.42
1	B	65	LEU	N-CA-C	-7.42	103.13	111.14
1	D	40	ASN	N-CA-C	-7.37	102.62	111.69
1	C	163	ALA	N-CA-C	-7.26	103.30	111.07
1	A	64	HIS	N-CA-C	-7.12	103.60	111.36
1	A	6	ASN	N-CA-C	-6.80	104.79	113.23
1	D	137	THR	OG1-CB-CG2	-6.78	95.74	109.30
1	C	36	ALA	N-CA-C	-6.64	104.12	111.36
1	A	61	ARG	NE-CZ-NH2	6.54	125.09	119.20
1	D	18	ASP	N-CA-C	6.48	118.34	111.28
1	C	151	MET	N-CA-C	6.38	119.05	111.33
1	B	74	ALA	N-CA-C	-6.33	104.48	111.82
1	B	138	GLU	N-CA-C	-6.27	103.98	111.69
1	B	102	GLU	N-CA-C	-6.13	105.84	113.38
1	D	150	HIS	N-CA-C	6.11	118.47	111.02
1	A	74	ALA	N-CA-C	-6.09	104.72	111.36
1	A	6	ASN	N-CA-CB	6.06	119.90	110.44
1	A	61	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	D	63	LEU	N-CA-C	-5.92	104.91	111.36
1	B	73	THR	OG1-CB-CG2	-5.91	97.47	109.30
1	B	58	ALA	N-CA-C	5.91	119.31	111.75
1	D	159	LEU	N-CA-C	-5.89	104.94	111.36
1	C	137	THR	OG1-CB-CG2	-5.84	97.61	109.30
1	B	87	ALA	N-CA-C	-5.82	105.01	111.71
1	D	157	ILE	N-CA-C	-5.72	103.94	111.09
1	C	33	ALA	N-CA-C	5.71	117.50	111.28
1	A	26	ARG	CB-CA-C	-5.60	101.32	110.85
1	D	84	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	C	49	LYS	CB-CG-CD	5.50	123.95	111.30
1	C	76	GLU	N-CA-C	-5.45	105.76	112.90
1	B	36	ALA	N-CA-C	-5.44	105.43	111.36
1	D	83	GLU	CA-CB-CG	-5.37	103.35	114.10
1	B	64	HIS	N-CA-C	-5.28	105.61	111.36
1	D	141	GLU	CB-CG-CD	5.18	121.40	112.60
1	C	48	LEU	N-CA-C	-5.16	105.73	111.36
1	C	137	THR	N-CA-CB	5.15	117.78	110.16
1	C	117	THR	N-CA-C	-5.14	105.58	111.14
1	D	153	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	A	5	LYS	CA-C-O	-5.09	116.15	121.55

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	VAL	N-CA-CB	5.09	118.21	110.58
1	C	62	ASP	N-CA-C	5.07	117.19	111.11
1	C	49	LYS	N-CA-C	-5.04	105.68	111.07
1	C	39	ALA	N-CA-C	-5.03	105.88	111.36

There are no chirality outliers.

There are no planarity outliers.

## 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	36	0
1	B	1355	0	1253	28	3
1	C	1355	0	1253	30	1
1	D	1355	0	1253	26	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	11	0	0	0	0
3	B	9	0	0	0	0
3	C	2	0	0	0	0
3	D	8	0	0	0	1
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	50	0	0	2	0
5	B	56	0	0	2	1
5	C	63	0	0	0	0
5	D	58	0	0	2	0
All	All	5728	0	5051	107	5

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 10.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LYS:CE	1:C:49:LYS:NZ	1.68	1.53
1:C:151:MET:CE	1:C:151:MET:SD	2.24	1.25
1:D:141:GLU:OE1	1:D:146:HIS:ND1	2.07	0.87
1:B:55:VAL:HG23	1:B:115:ILE:HD13	1.57	0.85
1:A:157:ILE:HD12	1:A:157:ILE:O	1.76	0.83
1:B:133:THR:O	1:B:137:THR:HG22	1.80	0.82
1:D:141:GLU:OE1	1:D:146:HIS:CE1	2.32	0.82
1:B:25:ASP:HB2	5:B:423:HOH:O	1.80	0.81
1:C:49:LYS:NZ	1:C:49:LYS:CD	2.45	0.79
1:A:137:THR:HG22	1:A:152:LEU:HB3	1.65	0.78
1:B:141:GLU:CD	1:B:153:ARG:HH22	1.91	0.77
1:B:133:THR:O	1:B:137:THR:CG2	2.34	0.76
1:A:137:THR:HG22	1:A:152:LEU:CB	2.17	0.73
1:B:141:GLU:HG3	1:B:153:ARG:NH2	2.03	0.73
1:D:79:ASP:OD2	5:D:372:HOH:O	2.07	0.72
1:A:157:ILE:HD12	1:A:157:ILE:C	2.16	0.71
1:B:141:GLU:CG	1:B:153:ARG:HH22	2.03	0.70
1:A:141:GLU:CD	1:A:153:ARG:HH22	1.98	0.70
1:C:178:GLN:O	1:C:179:GLY:C	2.33	0.70
1:A:133:THR:O	1:A:137:THR:HG23	1.93	0.68
1:D:39:ALA:O	1:D:43:VAL:HG13	1.92	0.68
1:B:84:ARG:HG2	1:B:151:MET:HE1	1.77	0.67
1:A:141:GLU:CG	1:A:153:ARG:HH22	2.10	0.64
1:D:8:ARG:HG3	5:D:349:HOH:O	1.97	0.64
1:D:84:ARG:HD3	1:D:151:MET:HE1	1.78	0.64
1:A:141:GLU:HG3	1:A:153:ARG:NH2	2.13	0.63
1:A:63:LEU:HD13	1:A:115:ILE:HG12	1.82	0.62
1:B:72:GLU:O	1:B:76:GLU:HG3	2.00	0.61
1:A:46:HIS:CD2	1:B:96:PRO:HG3	2.38	0.59
1:B:84:ARG:CG	1:B:151:MET:HE1	2.33	0.58
1:A:141:GLU:HG2	1:A:149:ALA:CB	2.34	0.58
1:B:141:GLU:HG3	1:B:153:ARG:HH22	1.65	0.57
1:D:133:THR:O	1:D:137:THR:HG23	2.04	0.57
1:D:77:VAL:HG12	1:D:81:LEU:HD22	1.85	0.57
1:C:133:THR:O	1:C:137:THR:HG23	2.04	0.57
1:D:137:THR:HG22	1:D:152:LEU:HB3	1.87	0.56
1:C:157:ILE:HD13	1:C:157:ILE:O	2.06	0.56
1:D:63:LEU:HD13	1:D:115:ILE:HG12	1.89	0.55
1:D:55:VAL:HG23	1:D:115:ILE:HD13	1.88	0.55
1:C:77:VAL:HG12	1:C:81:LEU:HD22	1.89	0.54
1:C:141:GLU:HG2	1:C:149:ALA:CB	2.38	0.54
1:B:141:GLU:CG	1:B:153:ARG:NH2	2.67	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:PRO:HD2	1:D:100:GLN:OE1	2.08	0.53
1:A:62:ASP:OD2	1:D:61:ARG:NH1	2.41	0.53
1:A:62:ASP:OD1	1:A:169:TYR:OH	2.20	0.52
1:A:168:HIS:CD2	1:D:56:GLU:HG2	2.44	0.52
1:B:33:ALA:HB1	1:B:136:HIS:CD2	2.44	0.52
1:A:80:GLU:HG3	5:A:546:HOH:O	2.09	0.52
1:C:141:GLU:HG3	1:C:153:ARG:NH2	2.24	0.52
1:D:14:VAL:HG11	1:D:28:GLU:HA	1.91	0.52
1:B:55:VAL:CG2	1:B:115:ILE:HD13	2.35	0.52
1:D:178:GLN:O	1:D:179:GLY:C	2.55	0.50
1:A:96:PRO:HG3	1:B:46:HIS:CD2	2.47	0.50
1:A:137:THR:HG22	1:A:152:LEU:HB2	1.91	0.50
1:A:178:GLN:O	1:A:179:GLY:C	2.53	0.50
1:A:33:ALA:HB1	1:A:136:HIS:CD2	2.47	0.49
1:A:33:ALA:HB1	1:A:136:HIS:CG	2.46	0.49
1:D:33:ALA:HB1	1:D:136:HIS:CD2	2.48	0.49
1:A:168:HIS:CE1	1:C:86:GLN:HE22	2.31	0.49
1:C:141:GLU:HG3	1:C:153:ARG:HH22	1.79	0.48
1:C:10:THR:O	1:C:11:ALA:C	2.56	0.48
1:A:51:HIS:ND1	1:A:122:ASP:OD2	2.37	0.48
1:A:141:GLU:HG3	1:A:153:ARG:HH22	1.73	0.47
1:A:181:LEU:HD13	1:A:181:LEU:HA	1.54	0.47
1:B:141:GLU:HG2	1:B:149:ALA:CB	2.45	0.47
1:B:86:GLN:HE21	1:B:86:GLN:HB3	1.45	0.47
1:C:51:HIS:CE1	1:C:118:SER:HB3	2.49	0.47
1:C:181:LEU:HD12	1:C:181:LEU:HA	1.69	0.47
1:D:52:HIS:CE1	1:D:64:HIS:CE1	3.03	0.47
1:A:8:ARG:HG3	5:A:540:HOH:O	2.16	0.46
1:C:44:LEU:HD22	1:C:129:ILE:HD12	1.97	0.46
1:B:8:ARG:NH1	1:B:8:ARG:HG2	2.31	0.46
1:A:2:SER:C	1:A:4:GLN:H	2.22	0.46
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.67	0.46
1:C:65:LEU:O	1:C:69:GLU:HG3	2.15	0.46
1:D:133:THR:HG21	1:D:156:LEU:HB2	1.97	0.46
1:C:141:GLU:CG	1:C:153:ARG:HH22	2.30	0.45
1:C:151:MET:CE	1:C:151:MET:HB2	2.47	0.45
1:A:157:ILE:C	1:A:157:ILE:CD1	2.87	0.45
1:C:31:VAL:HG13	1:C:85:VAL:HG13	1.98	0.45
1:A:175:LEU:HD11	1:D:63:LEU:HD11	1.99	0.45
1:C:145:ASP:OD1	1:C:148:THR:OG1	2.29	0.45
1:A:105:VAL:HG11	1:A:125:ILE:HG23	1.99	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:CG	1:A:153:ARG:NH2	2.75	0.45
2:A:401:SO4:O4	1:C:153:ARG:HD3	2.17	0.44
1:B:97:GLU:HB3	5:B:442:HOH:O	2.17	0.44
1:B:8:ARG:HH11	1:B:8:ARG:CG	2.29	0.44
1:C:86:GLN:HE21	1:C:86:GLN:HB3	1.62	0.43
1:C:141:GLU:CD	1:C:153:ARG:HH22	2.27	0.43
1:C:94:ALA:CB	1:D:50:LYS:HG3	2.47	0.43
1:A:10:THR:O	1:A:11:ALA:C	2.61	0.43
1:B:8:ARG:NH1	1:B:8:ARG:CG	2.77	0.43
1:A:94:ALA:CB	1:B:50:LYS:HD2	2.49	0.42
1:B:55:VAL:HG23	1:B:115:ILE:CD1	2.39	0.42
1:A:84:ARG:NH2	1:A:147:ALA:HB3	2.34	0.42
1:B:181:LEU:HD12	1:B:181:LEU:HA	1.92	0.42
1:C:30:CYS:HB2	1:C:88:LEU:HD13	2.01	0.42
1:D:10:THR:HG22	1:D:11:ALA:O	2.20	0.42
1:C:94:ALA:HB2	1:D:50:LYS:HG3	2.01	0.42
1:C:49:LYS:NZ	1:C:49:LYS:HD3	2.30	0.41
1:A:171:GLU:HG3	1:D:56:GLU:OE2	2.21	0.41
1:A:175:LEU:HD21	1:D:119:LEU:HD22	2.01	0.41
1:B:133:THR:O	1:B:137:THR:HG23	2.16	0.41
1:C:95:SER:HA	1:C:96:PRO:HD3	1.78	0.41
1:A:45:TYR:OH	1:B:75:GLU:OE2	2.24	0.40
1:C:178:GLN:O	1:C:181:LEU:N	2.44	0.40
1:D:51:HIS:CE1	1:D:118:SER:HB3	2.56	0.40

All (5) 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:C:164:HIS:CE1	3:D:325:FE:FE[2_655]	1.91	0.29
1:B:84:ARG:NH2	1:B:160:GLU:OE1[3_665]	2.06	0.14
1:B:84:ARG:NH1	1:B:160:GLU:OE1[3_665]	2.08	0.12
5:B:414:HOH:O	5:B:435:HOH:O[3_665]	2.09	0.11
1:B:21:ARG:NH1	1:B:128:ASP:OD1[3_665]	2.13	0.07

## 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%)	168 (97%)	5 (3%)	0	100	100
1	C	173/182 (95%)	167 (96%)	6 (4%)	0	100	100
1	D	173/182 (95%)	171 (99%)	2 (1%)	0	100	100
All	All	697/728 (96%)	682 (98%)	15 (2%)	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%)	128 (90%)	15 (10%)	6	6
1	B	138/145 (95%)	127 (92%)	11 (8%)	11	13
1	C	138/145 (95%)	126 (91%)	12 (9%)	9	10
1	D	138/145 (95%)	125 (91%)	13 (9%)	8	9
All	All	557/580 (96%)	506 (91%)	51 (9%)	8	9

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	5	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	42	TYR
1	A	43	VAL
1	A	60	PHE
1	A	81	LEU
1	A	86	GLN
1	A	107	VAL
1	A	119	LEU
1	A	137	THR
1	A	157	ILE
1	A	159	LEU
1	A	174	THR
1	A	178	GLN
1	A	181	LEU
1	B	17	SER
1	B	42	TYR
1	B	81	LEU
1	B	86	GLN
1	B	107	VAL
1	B	119	LEU
1	B	137	THR
1	B	143	LEU
1	B	157	ILE
1	B	159	LEU
1	B	181	LEU
1	C	10	THR
1	C	42	TYR
1	C	60	PHE
1	C	81	LEU
1	C	86	GLN
1	C	97	GLU
1	C	107	VAL
1	C	119	LEU
1	C	137	THR
1	C	157	ILE
1	C	159	LEU
1	C	181	LEU
1	D	8	ARG
1	D	10	THR
1	D	15	GLU
1	D	25	ASP
1	D	42	TYR
1	D	43	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	81	LEU
1	D	86	GLN
1	D	107	VAL
1	D	119	LEU
1	D	157	ILE
1	D	159	LEU
1	D	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	86	GLN
1	A	142	ASN
1	B	54	ASN
1	B	86	GLN
1	B	142	ASN
1	C	86	GLN
1	C	142	ASN
1	C	164	HIS
1	C	168	HIS
1	D	142	ASN
1	D	164	HIS
1	D	168	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 34 ligands modelled in this entry, 32 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	B	402	-	4,4,4	0.29	0	6,6,6	0.14	0
2	SO4	A	401	-	4,4,4	0.26	0	6,6,6	0.63	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	1	0

## 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.