



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2018 – 01:47 PM EST

PDB ID : 2PW9  
Title : Crystal structure of a putative formate dehydrogenase accessory protein from *Desulfotalea psychrophila*  
Authors : Bonanno, J.B.; Dickey, M.; Bain, K.T.; Logan, C.; Romero, R.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-05-10  
Resolution : 2.10 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

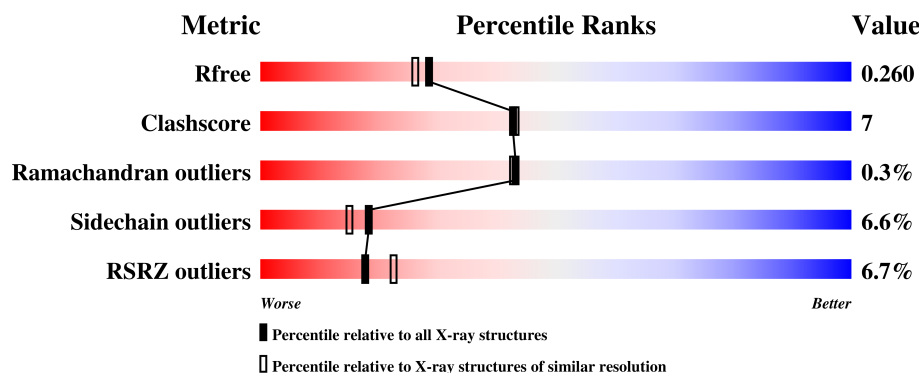
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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.

Mol	Chain	Length	Quality of chain
1	A	268	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	268	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	268	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	268	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>12%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7387 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 Putative formate dehydrogenase accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1780	1128	315	325	12			
1	B	230	Total	C	N	O	S	0	1	0
			1771	1123	314	322	12			
1	C	221	Total	C	N	O	S	0	0	0
			1693	1073	303	307	10			
1	D	237	Total	C	N	O	S	0	1	0
			1829	1157	322	338	12			

There are 44 discrepancies between the modelled and reference sequences:

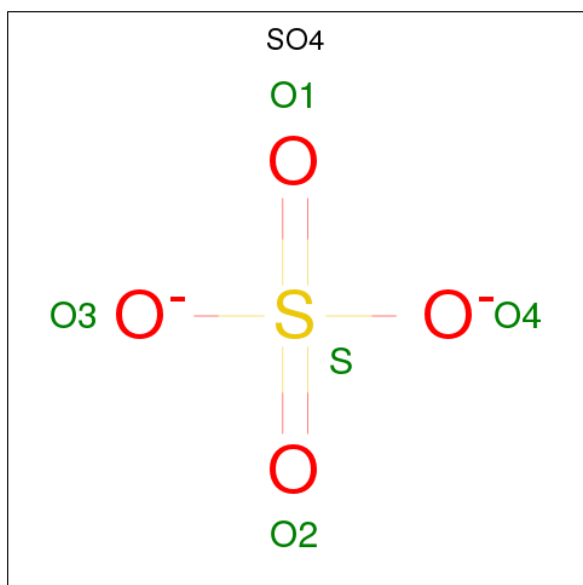
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	CLONING ARTIFACT	UNP Q6AMB9
A	0	SER	-	CLONING ARTIFACT	UNP Q6AMB9
A	1	LEU	-	CLONING ARTIFACT	UNP Q6AMB9
A	259	GLU	-	CLONING ARTIFACT	UNP Q6AMB9
A	260	GLY	-	CLONING ARTIFACT	UNP Q6AMB9
A	261	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
A	262	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
A	263	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
A	264	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
A	265	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
A	266	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
B	-1	MET	-	CLONING ARTIFACT	UNP Q6AMB9
B	0	SER	-	CLONING ARTIFACT	UNP Q6AMB9
B	1	LEU	-	CLONING ARTIFACT	UNP Q6AMB9
B	259	GLU	-	CLONING ARTIFACT	UNP Q6AMB9
B	260	GLY	-	CLONING ARTIFACT	UNP Q6AMB9
B	261	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
B	262	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
B	263	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
B	264	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
B	265	HIS	-	CLONING ARTIFACT	UNP Q6AMB9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	266	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
C	-1	MET	-	CLONING ARTIFACT	UNP Q6AMB9
C	0	SER	-	CLONING ARTIFACT	UNP Q6AMB9
C	1	LEU	-	CLONING ARTIFACT	UNP Q6AMB9
C	259	GLU	-	CLONING ARTIFACT	UNP Q6AMB9
C	260	GLY	-	CLONING ARTIFACT	UNP Q6AMB9
C	261	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
C	262	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
C	263	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
C	264	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
C	265	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
C	266	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
D	-1	MET	-	CLONING ARTIFACT	UNP Q6AMB9
D	0	SER	-	CLONING ARTIFACT	UNP Q6AMB9
D	1	LEU	-	CLONING ARTIFACT	UNP Q6AMB9
D	259	GLU	-	CLONING ARTIFACT	UNP Q6AMB9
D	260	GLY	-	CLONING ARTIFACT	UNP Q6AMB9
D	261	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
D	262	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
D	263	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
D	264	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
D	265	HIS	-	CLONING ARTIFACT	UNP Q6AMB9
D	266	HIS	-	CLONING ARTIFACT	UNP Q6AMB9

- 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	C	1	Total	O	S	0	0
			5	4	1		

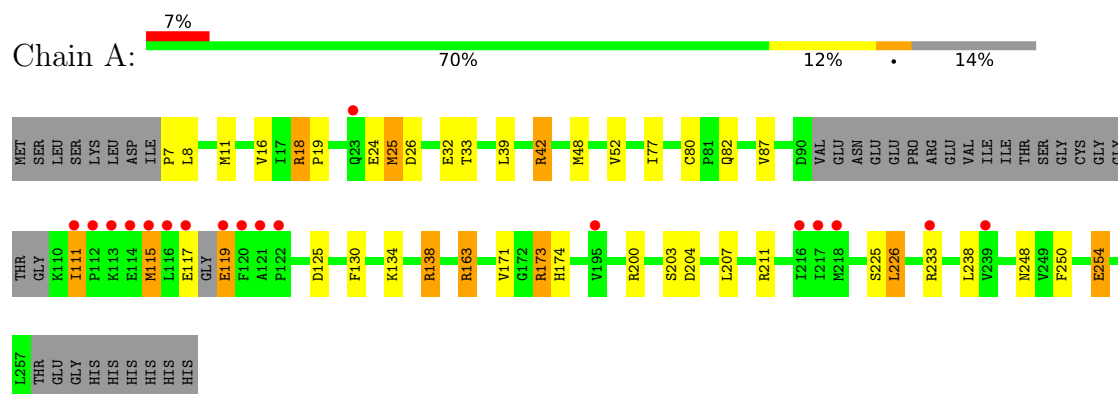
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	88	Total	O	0	0
			88	88		
3	C	55	Total	O	0	0
			55	55		
3	D	85	Total	O	0	0
			85	85		

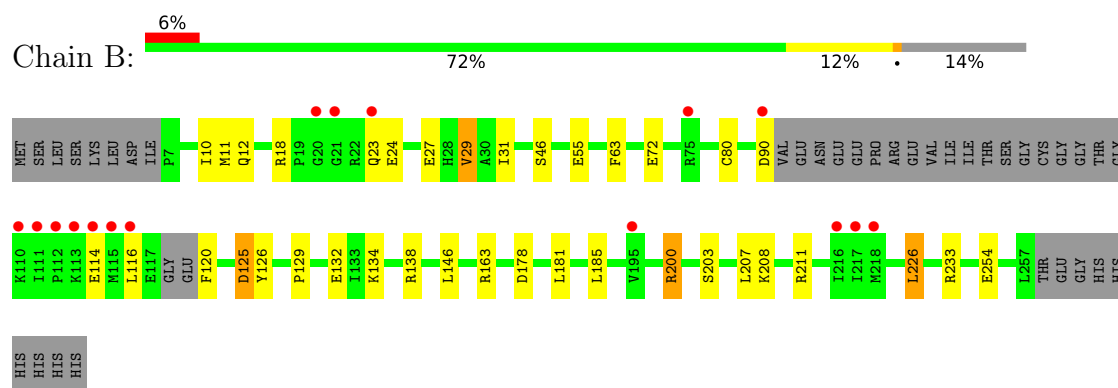
### 3 Residue-property plots [i](#)

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.

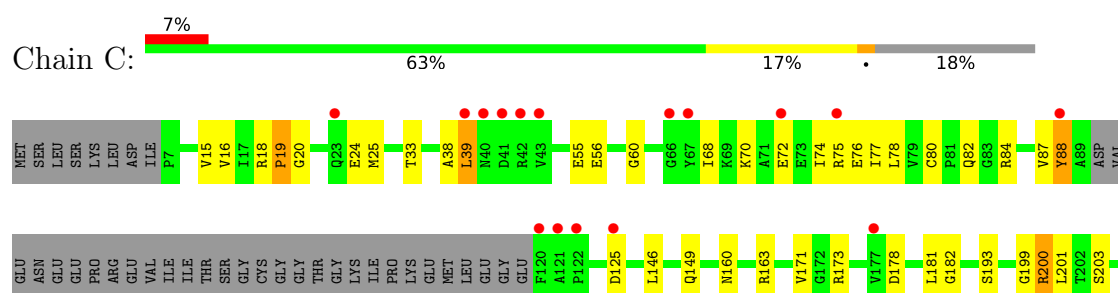
- Molecule 1: Putative formate dehydrogenase accessory protein

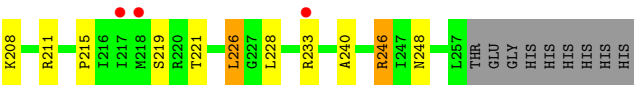


- Molecule 1: Putative formate dehydrogenase accessory protein

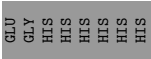
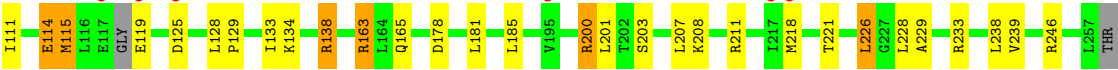


- Molecule 1: Putative formate dehydrogenase accessory protein





● Molecule 1: Putative formate dehydrogenase accessory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.99Å 99.26Å 88.50Å 90.00° 109.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 25.37 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.10) 98.2 (25.37-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.196 , 0.259 0.199 , 0.260	Depositor DCC
$R_{free}$ test set	2941 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.81	0/1816	0.84	2/2455 (0.1%)
1	B	0.81	1/1807 (0.1%)	0.86	2/2443 (0.1%)
1	C	0.73	0/1726	0.88	6/2336 (0.3%)
1	D	0.78	0/1866	0.81	2/2524 (0.1%)
All	All	0.78	1/7215 (0.0%)	0.85	12/9758 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	TYR	CD1-CE1	5.31	1.47	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	ARG	NE-CZ-NH2	-11.19	114.71	120.30
1	B	200	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	C	200	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	A	200	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	C	246	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	B	200	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	A	200	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	D	200	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	C	246	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	D	200	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	228	LEU	CB-CG-CD2	-5.88	101.00	111.00
1	C	20	GLY	N-CA-C	-5.13	100.27	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1780	0	1813	32	0
1	B	1771	0	1807	21	0
1	C	1693	0	1723	27	0
1	D	1829	0	1853	37	0
2	A	5	0	0	1	0
2	C	5	0	0	0	0
3	A	76	0	0	3	0
3	B	88	0	0	3	0
3	C	55	0	0	4	0
3	D	85	0	0	0	0
All	All	7387	0	7196	106	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 7.

All (106) 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:D:10:ILE:HD12	1:D:12:GLN:HE21	1.18	1.04
1:A:32:GLU:HG2	1:A:48:MET:HE2	1.46	0.96
1:C:55:GLU:HG3	3:C:642:HOH:O	1.71	0.90
1:D:10:ILE:HD12	1:D:12:GLN:NE2	1.89	0.86
1:C:248:ASN:ND2	1:D:27:GLU:OE2	2.19	0.76
1:C:16:VAL:HG23	1:C:25:MET:HG3	1.68	0.75
1:D:80[B]:CYS:SG	1:D:82:GLN:NE2	2.63	0.71
1:A:225:SER:HB2	1:B:10:ILE:HD11	1.74	0.68
1:C:181:LEU:HD11	1:C:208:LYS:HB3	1.76	0.68
1:C:200:ARG:HD3	3:C:605:HOH:O	1.94	0.67
1:D:163:ARG:NH2	1:D:165:GLN:HG3	2.10	0.67
1:B:125:ASP:HA	3:B:271:HOH:O	1.96	0.66
1:D:119:GLU:O	1:D:211:ARG:NH1	2.21	0.66
1:A:32:GLU:HG2	1:A:48:MET:CE	2.21	0.66
1:D:181:LEU:HD11	1:D:208:LYS:HB3	1.79	0.65
1:D:134:LYS:O	1:D:138:ARG:HD3	1.97	0.65
1:D:229:ALA:O	1:D:233:ARG:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:657:HOH:O	1:B:200:ARG:HD3	1.98	0.63
1:C:149:GLN:NE2	3:C:639:HOH:O	2.32	0.62
1:D:10:ILE:CD1	1:D:12:GLN:HE21	2.06	0.62
1:C:171:VAL:O	1:D:200:ARG:NH2	2.27	0.61
1:B:120:PHE:HA	1:B:211:ARG:HH21	1.67	0.60
1:A:134:LYS:O	1:A:138:ARG:HD3	2.01	0.60
1:C:39:LEU:HA	1:C:87:VAL:O	2.01	0.60
1:A:171:VAL:O	1:B:200:ARG:NH2	2.26	0.59
1:C:70:LYS:HE3	1:C:72:GLU:HB2	1.85	0.59
1:A:39:LEU:O	1:A:42:ARG:HG2	2.04	0.57
1:D:114:GLU:HG2	1:D:115:MET:N	2.20	0.57
3:C:645:HOH:O	1:D:200:ARG:HD3	2.03	0.57
1:D:11:MET:CE	1:D:28:HIS:CE1	2.89	0.56
1:D:18:ARG:HB3	1:D:19:PRO:HD2	1.88	0.55
1:A:80[B]:CYS:SG	1:A:82:GLN:HB2	2.46	0.55
1:D:13:LYS:HG2	1:D:24:GLU:OE2	2.07	0.55
1:D:203:SER:HB3	1:D:226:LEU:HD13	1.87	0.55
1:C:18:ARG:HH22	1:D:246:ARG:NH1	2.06	0.54
1:C:60:GLY:HA3	1:C:178:ASP:O	2.07	0.54
1:C:203:SER:HB3	1:C:226:LEU:HB3	1.88	0.54
1:D:18:ARG:HB3	1:D:19:PRO:CD	2.38	0.53
1:A:248:ASN:ND2	1:B:27:GLU:OE1	2.41	0.53
1:A:77:ILE:HG12	1:A:87:VAL:HG13	1.90	0.53
1:B:72:GLU:CD	1:B:72:GLU:H	2.13	0.52
1:B:178:ASP:OD1	3:B:340:HOH:O	2.19	0.51
1:B:181:LEU:HD11	1:B:208:LYS:HB3	1.93	0.51
1:D:17:ILE:HG12	1:D:22:ARG:HG2	1.93	0.51
1:A:163:ARG:HD2	3:A:662:HOH:O	2.10	0.51
1:C:78:LEU:HD12	1:C:88:TYR:OH	2.11	0.50
1:C:201:LEU:HG	1:C:219:SER:HB2	1.94	0.49
1:B:129:PRO:HB2	1:B:132:GLU:HG3	1.92	0.49
1:B:134:LYS:O	1:B:138:ARG:HD3	2.12	0.49
1:A:48:MET:HE3	1:A:48:MET:HA	1.92	0.49
1:D:11:MET:HE1	1:D:28:HIS:CE1	2.48	0.49
1:B:116:LEU:HD12	1:B:207:LEU:HD22	1.95	0.48
1:A:111:ILE:HG21	1:A:207:LEU:HD23	1.94	0.48
1:A:174:HIS:NE2	1:A:204:ASP:HB3	2.28	0.48
1:A:7:PRO:HB3	1:D:80[B]:CYS:SG	2.55	0.47
1:A:250:PHE:CZ	1:B:27:GLU:HG3	2.49	0.47
1:B:11:MET:HA	1:B:27:GLU:O	2.15	0.47
1:C:77:ILE:HG12	1:C:87:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:SER:HB3	1:B:226:LEU:HD13	1.97	0.47
1:D:115:MET:HB3	1:D:207:LEU:HD21	1.97	0.46
1:D:128:LEU:HD12	1:D:129:PRO:HD2	1.98	0.46
1:B:72:GLU:CD	1:B:72:GLU:N	2.69	0.46
1:A:25:MET:HG3	1:A:26:ASP:N	2.31	0.46
1:C:173:ARG:HD2	1:C:199:GLY:HA3	1.98	0.45
1:A:32:GLU:CG	1:A:48:MET:HE2	2.33	0.45
1:C:18:ARG:HB3	1:C:19:PRO:HD2	1.98	0.45
1:A:117:GLU:O	1:A:119:GLU:N	2.49	0.45
1:C:80:CYS:HB2	1:C:84:ARG:HB3	1.99	0.45
1:A:203:SER:HB3	1:A:226:LEU:HD13	1.99	0.45
1:D:200:ARG:HG3	1:D:221:THR:CG2	2.47	0.45
1:D:128:LEU:HD21	1:D:133:ILE:HG12	1.98	0.45
1:C:38:ALA:O	1:C:87:VAL:N	2.43	0.45
1:B:134:LYS:NZ	3:B:309:HOH:O	2.50	0.44
1:A:39:LEU:O	1:A:42:ARG:CG	2.66	0.44
1:C:221:THR:O	1:C:240:ALA:HB1	2.17	0.44
1:A:8:LEU:HD21	1:A:52:VAL:HB	2.00	0.44
3:A:605:HOH:O	1:B:29:VAL:HA	2.17	0.44
1:C:80:CYS:HB3	1:C:82:GLN:OE1	2.18	0.44
1:D:63:PHE:HB2	1:D:185:LEU:HD11	1.99	0.43
1:A:238:LEU:HD23	1:A:238:LEU:C	2.39	0.43
1:B:134:LYS:O	1:B:138:ARG:CD	2.66	0.43
1:D:163:ARG:HH22	1:D:165:GLN:HG3	1.81	0.43
1:A:173:ARG:HD3	2:A:601:SO4:O4	2.18	0.43
1:A:11:MET:HE1	1:D:81:PRO:HG3	2.01	0.42
1:A:18:ARG:HB2	1:A:19:PRO:CD	2.50	0.42
1:A:130:PHE:CD2	1:A:130:PHE:O	2.73	0.42
1:D:37:ILE:N	1:D:37:ILE:HD12	2.34	0.42
1:A:254:GLU:H	1:A:254:GLU:HG3	1.46	0.42
1:A:8:LEU:CD2	1:A:52:VAL:HB	2.48	0.42
1:C:246:ARG:HG2	1:C:246:ARG:HH11	1.84	0.42
1:D:60:GLY:HA3	1:D:178:ASP:O	2.19	0.42
1:B:63:PHE:HB2	1:B:185:LEU:HD11	2.02	0.41
1:C:193:SER:O	1:C:215:PRO:HD2	2.20	0.41
1:A:7:PRO:HA	1:D:80[B]:CYS:SG	2.60	0.41
1:C:68:ILE:HD13	1:C:74:ILE:HG12	2.01	0.41
1:D:13:LYS:HE3	1:D:26:ASP:OD2	2.20	0.41
1:C:56:GLU:O	1:C:182:GLY:HA3	2.20	0.41
1:A:115:MET:HB3	1:A:207:LEU:HD21	2.03	0.41
1:A:8:LEU:H	1:D:82:GLN:NE2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HD12	1:B:12:GLN:HE21	1.84	0.41
1:D:218:MET:HE3	1:D:239:VAL:HG11	2.03	0.41
1:D:201:LEU:HD13	1:D:238:LEU:HD11	2.02	0.41
1:C:160:ASN:OD1	1:C:163:ARG:NH2	2.52	0.41
1:C:146:LEU:HD23	1:C:146:LEU:HA	1.90	0.41
1:D:200:ARG:HG3	1:D:221:THR:HG21	2.04	0.40
1:A:33:THR:CA	1:A:48:MET:HE1	2.52	0.40

There are no symmetry-related clashes.

## 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	226/268 (84%)	222 (98%)	4 (2%)	0	100	100
1	B	225/268 (84%)	220 (98%)	4 (2%)	1 (0%)	36	34
1	C	217/268 (81%)	207 (95%)	8 (4%)	2 (1%)	19	13
1	D	232/268 (87%)	228 (98%)	4 (2%)	0	100	100
All	All	900/1072 (84%)	877 (97%)	20 (2%)	3 (0%)	43	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	75	ARG
1	B	23	GLN
1	C	19	PRO

### 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	194/224 (87%)	178 (92%)	16 (8%)	12	9
1	B	193/224 (86%)	177 (92%)	16 (8%)	12	8
1	C	183/224 (82%)	173 (94%)	10 (6%)	24	21
1	D	200/224 (89%)	190 (95%)	10 (5%)	27	24
All	All	770/896 (86%)	718 (93%)	52 (7%)	18	14

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	18	ARG
1	A	24	GLU
1	A	25	MET
1	A	42	ARG
1	A	111	ILE
1	A	115	MET
1	A	119	GLU
1	A	125	ASP
1	A	138	ARG
1	A	163	ARG
1	A	173	ARG
1	A	211	ARG
1	A	226	LEU
1	A	233	ARG
1	A	254	GLU
1	B	18	ARG
1	B	24	GLU
1	B	29	VAL
1	B	31	ILE
1	B	46	SER
1	B	55	GLU
1	B	80[A]	CYS
1	B	80[B]	CYS
1	B	90	ASP
1	B	114	GLU
1	B	125	ASP
1	B	146	LEU

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Mol	Chain	Res	Type
1	B	163	ARG
1	B	226	LEU
1	B	233	ARG
1	B	254	GLU
1	C	15	VAL
1	C	24	GLU
1	C	33	THR
1	C	39	LEU
1	C	76	GLU
1	C	88	TYR
1	C	125	ASP
1	C	211	ARG
1	C	226	LEU
1	C	233	ARG
1	D	26	ASP
1	D	70	LYS
1	D	111	ILE
1	D	114	GLU
1	D	115	MET
1	D	125	ASP
1	D	138	ARG
1	D	163	ARG
1	D	226	LEU
1	D	228	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	23	GLN
1	D	12	GLN
1	D	82	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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	601	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	C	602	-	4,4,4	0.28	0	6,6,6	0.52	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	601	-	-	0/0/0/0	0/0/0/0
2	SO4	C	602	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	231/268 (86%)	0.20	18 (7%)	13 17	18, 30, 50, 109	0
1	B	230/268 (85%)	0.26	16 (6%)	16 21	19, 29, 67, 108	0
1	C	221/268 (82%)	0.31	19 (8%)	10 13	22, 34, 65, 77	0
1	D	237/268 (88%)	0.04	9 (3%)	40 47	20, 30, 56, 73	0
All	All	919/1072 (85%)	0.20	62 (6%)	18 22	18, 30, 64, 109	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	ILE	7.3
1	B	20	GLY	6.5
1	B	113	LYS	5.1
1	B	116	LEU	5.1
1	D	92	GLU	4.9
1	B	112	PRO	4.6
1	B	114	GLU	4.6
1	C	67	TYR	4.5
1	A	115	MET	4.4
1	A	113	LYS	4.4
1	A	217	ILE	4.3
1	A	114	GLU	4.0
1	C	41	ASP	3.9
1	B	110	LYS	3.8
1	A	111	ILE	3.7
1	C	88	TYR	3.7
1	A	119	GLU	3.7
1	C	42	ARG	3.6
1	D	217	ILE	3.6
1	A	117	GLU	3.6
1	C	66	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	112	PRO	3.5
1	B	115	MET	3.3
1	B	21	GLY	3.1
1	C	121	ALA	3.0
1	C	217	ILE	3.0
1	A	116	LEU	3.0
1	A	239	VAL	2.8
1	C	40	ASN	2.8
1	A	233	ARG	2.7
1	A	195	VAL	2.7
1	D	195	VAL	2.6
1	B	216	ILE	2.6
1	B	217	ILE	2.6
1	D	72	GLU	2.6
1	C	120	PHE	2.5
1	C	233	ARG	2.5
1	A	121	ALA	2.4
1	C	125	ASP	2.4
1	B	75	ARG	2.4
1	C	72	GLU	2.3
1	B	218	MET	2.3
1	A	120	PHE	2.3
1	C	218	MET	2.3
1	A	218	MET	2.3
1	C	39	LEU	2.3
1	C	177	VAL	2.3
1	A	216	ILE	2.3
1	D	117	GLU	2.3
1	B	195	VAL	2.2
1	B	90	ASP	2.2
1	D	125	ASP	2.2
1	A	122	PRO	2.2
1	D	119	GLU	2.2
1	A	23	GLN	2.1
1	D	218	MET	2.1
1	B	23	GLN	2.1
1	C	23	GLN	2.1
1	C	122	PRO	2.1
1	C	75	ARG	2.0
1	D	90	ASP	2.0
1	C	43	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	602	5/5	0.99	0.09	31,33,34,35	0
2	SO4	A	601	5/5	0.99	0.08	28,29,32,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.