



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:32 pm BST

PDB ID : 2Q30  
Title : Crystal structure of a rmlc-like cupin protein (dde\_2303) from *desulfovibrio desulfuricans* subsp. at 1.94 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2007-05-29  
Resolution : 1.94 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

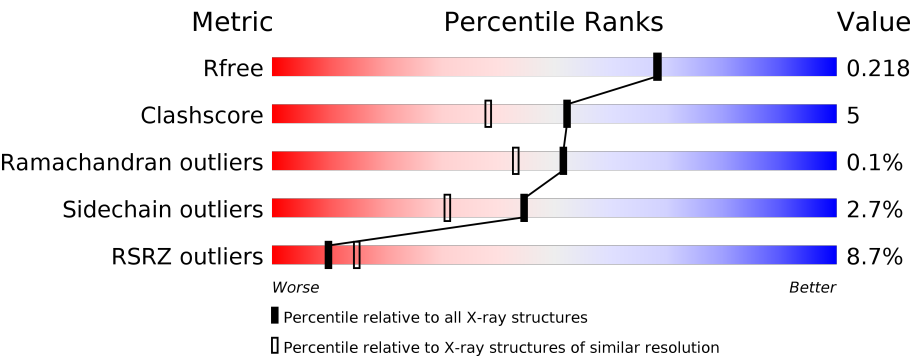
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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))
$R_{free}$	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 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  $\leq 5\%$ . 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	110	<div><div>5%</div><div><div></div><div>83%</div><div>13%</div><div>• •</div></div></div>
1	B	110	<div><div>3%</div><div><div></div><div>85%</div><div>10%</div><div>5%</div></div></div>
1	C	110	<div><div>%</div><div><div></div><div>82%</div><div>13%</div><div>• 5%</div></div></div>
1	D	110	<div><div>2%</div><div><div></div><div>85%</div><div>11%</div><div>• •</div></div></div>
1	E	110	<div><div>8%</div><div><div></div><div>88%</div><div>6%</div><div>5%</div></div></div>
1	F	110	<div><div>15%</div><div><div></div><div>81%</div><div>13%</div><div>• 5%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	110	
1	H	110	

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	EDO	C	110	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7119 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	Se	0	4	0
			815	527	135	150	3			
1	B	105	Total	C	N	O	Se	0	0	0
			800	512	134	151	3			
1	C	105	Total	C	N	O	Se	0	3	0
			816	525	137	150	4			
1	D	106	Total	C	N	O	Se	0	2	0
			822	526	139	153	4			
1	E	104	Total	C	N	O	Se	0	1	0
			795	511	136	146	2			
1	F	104	Total	C	N	O	Se	0	1	0
			798	511	135	150	2			
1	G	104	Total	C	N	O	Se	0	1	0
			794	510	135	147	2			
1	H	104	Total	C	N	O	Se	0	2	0
			792	511	134	145	2			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q30YZ6
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
A	5	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
A	23	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
A	99	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
B	0	GLY	-	LEADER SEQUENCE	UNP Q30YZ6
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
B	5	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
B	23	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
B	99	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
C	0	GLY	-	LEADER SEQUENCE	UNP Q30YZ6
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
C	5	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
C	99	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
D	0	GLY	-	LEADER SEQUENCE	UNP Q30YZ6
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
D	5	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
D	23	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
D	99	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
E	0	GLY	-	LEADER SEQUENCE	UNP Q30YZ6
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
E	5	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
E	23	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
E	99	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
F	0	GLY	-	LEADER SEQUENCE	UNP Q30YZ6
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
F	5	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
F	23	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
F	99	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
G	0	GLY	-	LEADER SEQUENCE	UNP Q30YZ6
G	1	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
G	5	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
G	23	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
G	99	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
H	0	GLY	-	LEADER SEQUENCE	UNP Q30YZ6
H	1	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
H	5	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
H	23	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6
H	99	MSE	MET	MODIFIED RESIDUE	UNP Q30YZ6

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



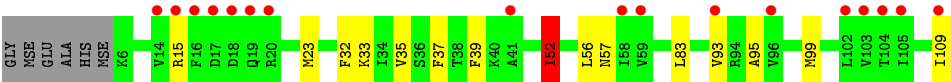
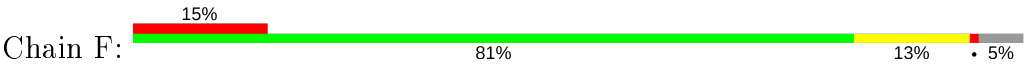
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

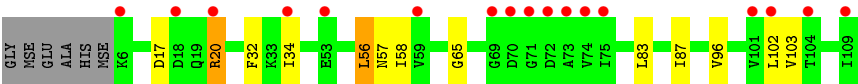
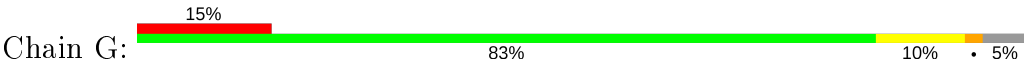
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	97	Total	O	0	0
			97	97		
4	C	96	Total	O	0	0
			96	96		
4	D	82	Total	O	0	0
			82	82		
4	E	76	Total	O	0	0
			76	76		
4	F	66	Total	O	0	0
			66	66		
4	G	69	Total	O	0	0
			69	69		
4	H	77	Total	O	0	0
			77	77		



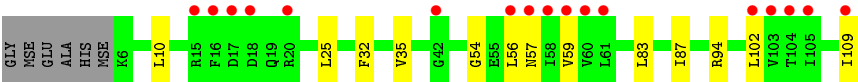
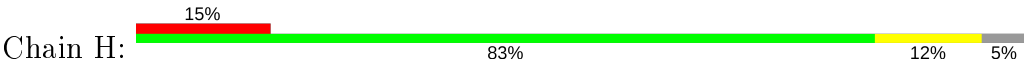




• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.14Å 133.95Å 74.66Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	29.02 – 1.94 29.02 – 1.94	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.02-1.94) 96.4 (29.02-1.94)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, $R_{free}$	0.167 , 0.212 0.175 , 0.218	Depositor DCC
$R_{free}$ test set	3173 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7119	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 4.71% 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, EDO

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	0.67	0/841	0.92	2/1137 (0.2%)
1	B	0.73	0/815	0.94	2/1104 (0.2%)
1	C	0.67	0/840	0.87	1/1136 (0.1%)
1	D	0.70	0/843	0.90	0/1139
1	E	0.68	0/813	0.87	0/1102
1	F	0.62	0/816	0.87	1/1106 (0.1%)
1	G	0.64	0/812	0.87	1/1101 (0.1%)
1	H	0.66	0/813	0.84	1/1104 (0.1%)
All	All	0.67	0/6593	0.89	8/8929 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	94	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	94	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	15	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	G	20	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	94	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	H	94	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	52	ILE	CB-CA-C	-5.02	101.56	111.60

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	815	0	823	20	0
1	B	800	0	796	5	0
1	C	816	0	830	10	0
1	D	822	0	822	7	0
1	E	795	0	801	7	0
1	F	798	0	793	12	0
1	G	794	0	797	6	0
1	H	792	0	795	6	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
2	E	4	0	6	0	0
2	F	4	0	6	0	0
2	H	4	0	6	0	0
3	D	5	0	0	0	0
4	A	91	0	0	0	0
4	B	97	0	0	1	0
4	C	96	0	0	0	0
4	D	82	0	0	1	0
4	E	76	0	0	0	0
4	F	66	0	0	0	0
4	G	69	0	0	0	0
4	H	77	0	0	0	0
All	All	7119	0	6499	71	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 5.

All (71) 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:93:VAL:CG1	1:A:99:MSE:HE1	2.00	0.92
1:A:52:ILE:HD11	1:A:109:ILE:HD12	1.52	0.90
1:D:95:ALA:HB2	1:D:99[A]:MSE:HE2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CD2	1:A:99:MSE:HE2	2.15	0.82
1:F:52:ILE:CD1	1:F:109:ILE:HD12	2.10	0.81
1:A:93:VAL:HG11	1:A:99:MSE:HE1	1.61	0.81
1:F:52:ILE:HD11	1:F:109:ILE:HD12	1.63	0.80
1:A:87:ILE:HD13	1:A:109:ILE:HD11	1.66	0.77
1:A:99:MSE:HE3	1:A:101:VAL:HG13	1.68	0.76
1:A:87:ILE:HG21	1:A:109:ILE:HD11	1.68	0.74
1:A:52:ILE:HD11	1:A:109:ILE:HG23	1.69	0.74
1:F:95:ALA:HB2	1:F:99:MSE:HE2	1.72	0.72
1:E:52:ILE:HD11	1:E:109:ILE:CD1	2.20	0.71
1:F:52:ILE:HD11	1:F:109:ILE:HG23	1.71	0.70
1:C:95:ALA:HB2	1:C:99[A]:MSE:HE2	1.75	0.68
1:E:52:ILE:HD11	1:E:109:ILE:HD12	1.81	0.62
1:A:99:MSE:HE3	1:A:101:VAL:CG1	2.29	0.62
1:B:87:ILE:HG21	1:B:109:ILE:HD11	1.81	0.61
1:A:93:VAL:HG12	1:A:99:MSE:HE1	1.82	0.60
1:D:23:MSE:HE2	1:D:37:PHE:HE2	1.68	0.59
1:E:52:ILE:HD11	1:E:109:ILE:HD13	1.84	0.58
1:C:93:VAL:HG12	1:C:99[A]:MSE:HE1	1.83	0.58
1:D:93:VAL:HG12	1:D:99[A]:MSE:HE1	1.85	0.58
1:A:39:PHE:CE2	1:A:99:MSE:HE2	2.41	0.56
1:C:89:THR:HG21	1:D:5:MSE:HG2	1.89	0.55
1:F:39:PHE:CD2	1:F:99:MSE:HE3	2.42	0.55
1:F:93:VAL:HG12	1:F:99:MSE:HE1	1.89	0.54
1:F:52:ILE:CD1	1:F:109:ILE:HG23	2.36	0.53
1:A:52:ILE:CD1	1:A:109:ILE:HG23	2.39	0.53
1:E:52:ILE:HD13	1:E:109:ILE:HG23	1.88	0.53
1:F:52:ILE:HD12	1:F:109:ILE:HD12	1.86	0.53
1:A:87:ILE:HD13	1:A:109:ILE:CD1	2.37	0.53
1:E:52:ILE:CD1	1:E:109:ILE:HG23	2.40	0.52
1:C:34:ILE:HG22	1:C:102:LEU:HD11	1.91	0.52
1:A:25:LEU:HA	1:A:35[A]:VAL:HG12	1.92	0.52
1:C:52:ILE:HD11	1:C:109:ILE:HD12	1.92	0.52
1:C:52:ILE:HD11	1:C:109:ILE:CD1	2.41	0.51
1:A:52:ILE:HD11	1:A:109:ILE:CD1	2.34	0.51
1:G:56:LEU:HD12	1:G:87:ILE:HA	1.93	0.51
1:H:87:ILE:HG21	1:H:109:ILE:HD11	1.94	0.50
1:C:87:ILE:HD13	1:C:109:ILE:CD1	2.43	0.49
1:B:57:ASN:HA	1:B:83:LEU:O	2.12	0.48
1:D:57:ASN:HA	1:D:83:LEU:O	2.14	0.47
1:H:10:LEU:CD1	1:H:102:LEU:HD13	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:ILE:HG12	1:G:103:VAL:HG22	1.97	0.47
1:H:25:LEU:HA	1:H:35[A]:VAL:HG12	1.97	0.47
1:A:34:ILE:HG22	1:A:102:LEU:HD11	1.97	0.46
1:B:87:ILE:CG2	1:B:109:ILE:HD11	2.46	0.45
1:D:99[B]:MSE:HE2	1:D:101:VAL:CG1	2.46	0.45
1:E:56:LEU:HD21	1:E:91:HIS:CE1	2.52	0.45
1:D:10:LEU:CD1	1:D:102:LEU:HD13	2.47	0.45
1:G:65:GLY:HA2	1:G:96:VAL:HG23	1.99	0.45
1:F:57:ASN:HA	1:F:83:LEU:O	2.17	0.45
1:G:57:ASN:HA	1:G:83:LEU:O	2.17	0.45
1:A:93:VAL:HG11	1:A:99:MSE:CE	2.41	0.44
1:C:34:ILE:CG2	1:C:102:LEU:HD11	2.48	0.44
1:C:57:ASN:HA	1:C:83:LEU:O	2.17	0.43
4:B:150:HOH:O	1:F:23:MSE:HE3	2.18	0.43
1:F:33:LYS:HE2	1:F:35:VAL:HG11	2.00	0.43
1:B:23:MSE:HE2	1:B:37:PHE:HE2	1.84	0.43
1:H:57:ASN:HA	1:H:83:LEU:O	2.19	0.42
1:H:59[B]:VAL:HG12	1:H:102:LEU:HB3	2.00	0.42
1:A:39:PHE:CE2	1:A:99:MSE:CE	3.03	0.42
1:A:6[A]:LYS:HZ2	1:B:84:VAL:HB	1.85	0.42
1:G:34:ILE:HG22	1:G:102:LEU:HD11	2.02	0.41
1:G:17:ASP:HB3	1:G:20:ARG:O	2.21	0.41
1:E:58:ILE:HG12	1:E:103:VAL:HG22	2.02	0.41
1:F:23:MSE:HG3	1:F:37:PHE:CE2	2.56	0.41
1:A:87:ILE:HG21	1:A:109:ILE:CD1	2.45	0.41
1:C:5:MSE:HE1	4:D:124:HOH:O	2.21	0.40
1:H:54:GLY:HA3	1:H:87:ILE:HD12	2.01	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	108/110 (98%)	105 (97%)	2 (2%)	1 (1%)	17	7
1	B	103/110 (94%)	103 (100%)	0	0	100	100
1	C	106/110 (96%)	105 (99%)	1 (1%)	0	100	100
1	D	106/110 (96%)	105 (99%)	1 (1%)	0	100	100
1	E	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
1	F	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
1	G	103/110 (94%)	101 (98%)	2 (2%)	0	100	100
1	H	104/110 (94%)	102 (98%)	2 (2%)	0	100	100
All	All	836/880 (95%)	825 (99%)	10 (1%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	MSE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/88 (101%)	86 (97%)	3 (3%)	37	22
1	B	88/88 (100%)	86 (98%)	2 (2%)	50	38
1	C	91/88 (103%)	88 (97%)	3 (3%)	38	24
1	D	91/88 (103%)	88 (97%)	3 (3%)	38	24
1	E	87/88 (99%)	86 (99%)	1 (1%)	73	67
1	F	87/88 (99%)	83 (95%)	4 (5%)	27	12
1	G	87/88 (99%)	85 (98%)	2 (2%)	50	38
1	H	86/88 (98%)	84 (98%)	2 (2%)	50	38
All	All	706/704 (100%)	686 (97%)	20 (3%)	44	29

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6[A]	LYS
1	A	6[B]	LYS
1	A	32	PHE
1	B	32	PHE
1	B	72	ASP
1	C	5	MSE
1	C	32	PHE
1	C	72	ASP
1	D	5	MSE
1	D	6	LYS
1	D	32	PHE
1	E	32	PHE
1	F	15	ARG
1	F	32	PHE
1	F	52	ILE
1	F	56	LEU
1	G	32	PHE
1	G	56	LEU
1	H	32	PHE
1	H	56	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

8 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	EDO	D	111	-	3,3,3	0.51	0	2,2,2	0.31	0
2	EDO	E	110	-	3,3,3	0.57	0	2,2,2	0.22	0
2	EDO	F	110	-	3,3,3	0.43	0	2,2,2	0.20	0
2	EDO	C	110	-	3,3,3	0.57	0	2,2,2	0.07	0
3	SO4	D	110	-	4,4,4	0.13	0	6,6,6	0.22	0
2	EDO	A	110	-	3,3,3	0.37	0	2,2,2	0.14	0
2	EDO	B	110	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	H	110	-	3,3,3	0.58	0	2,2,2	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	EDO	D	111	-	-	1/1/1/1	-
2	EDO	E	110	-	-	0/1/1/1	-
2	EDO	F	110	-	-	1/1/1/1	-
2	EDO	C	110	-	-	1/1/1/1	-
2	EDO	A	110	-	-	0/1/1/1	-
2	EDO	B	110	-	-	1/1/1/1	-
2	EDO	H	110	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	111	EDO	O1-C1-C2-O2
2	H	110	EDO	O1-C1-C2-O2
2	F	110	EDO	O1-C1-C2-O2
2	C	110	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	110	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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	103/110 (93%)	0.69	5 (4%) 29 37	28, 32, 41, 55	0
1	B	102/110 (92%)	0.51	3 (2%) 51 59	28, 32, 42, 50	0
1	C	102/110 (92%)	0.64	1 (0%) 82 86	28, 32, 42, 52	0
1	D	103/110 (93%)	0.59	2 (1%) 66 72	28, 32, 44, 70	0
1	E	102/110 (92%)	0.81	9 (8%) 10 15	28, 32, 44, 54	0
1	F	102/110 (92%)	1.07	17 (16%) 1 2	29, 32, 42, 49	0
1	G	102/110 (92%)	1.04	17 (16%) 1 2	27, 32, 42, 49	0
1	H	102/110 (92%)	0.94	17 (16%) 1 2	28, 32, 42, 52	0
All	All	818/880 (92%)	0.79	71 (8%) 10 15	27, 32, 43, 70	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ILE	9.3
1	E	109	ILE	8.1
1	D	4	HIS	6.8
1	C	109	ILE	6.1
1	H	15	ARG	5.7
1	G	70	ASP	5.7
1	F	15	ARG	5.4
1	A	4	HIS	5.3
1	F	19	GLN	5.1
1	G	73	ALA	5.0
1	F	18	ASP	4.9
1	E	13	ALA	4.7
1	G	72	ASP	4.2
1	E	72	ASP	4.1
1	F	96	VAL	4.1
1	H	59[A]	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	41	ALA	4.0
1	H	109	ILE	4.0
1	H	20	ARG	3.9
1	G	102	LEU	3.8
1	H	105	ILE	3.8
1	G	59	VAL	3.6
1	B	109	ILE	3.6
1	F	103	VAL	3.6
1	G	71	GLY	3.6
1	F	16	PHE	3.5
1	A	52	ILE	3.5
1	H	16	PHE	3.5
1	F	102	LEU	3.4
1	H	17	ASP	3.4
1	G	109	ILE	3.2
1	H	102	LEU	3.2
1	G	69	GLY	3.1
1	F	93	VAL	3.0
1	F	104	THR	3.0
1	H	104	THR	2.9
1	A	70	ASP	2.9
1	E	51	ASN	2.9
1	H	103	VAL	2.9
1	G	53	GLU	2.7
1	H	56	LEU	2.7
1	F	105	ILE	2.6
1	E	73	ALA	2.6
1	E	19	GLN	2.6
1	F	14	VAL	2.6
1	F	17	ASP	2.6
1	H	58	ILE	2.5
1	H	60	VAL	2.5
1	E	59	VAL	2.5
1	G	101	VAL	2.5
1	F	20	ARG	2.4
1	G	34	ILE	2.4
1	F	59	VAL	2.4
1	G	20	ARG	2.4
1	E	71	GLY	2.4
1	H	42	GLY	2.4
1	G	18	ASP	2.3
1	E	74	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	60	VAL	2.3
1	G	104	THR	2.2
1	H	57	ASN	2.2
1	G	75	ILE	2.2
1	B	102	LEU	2.2
1	H	18	ASP	2.1
1	G	6	LYS	2.1
1	B	53	GLU	2.1
1	G	74	VAL	2.1
1	F	58	ILE	2.1
1	F	109	ILE	2.0
1	H	61	LEU	2.0
1	A	89	THR	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	EDO	C	110	4/4	0.49	0.41	49,61,62,66	0
3	SO4	D	110	5/5	0.81	0.48	79,79,84,89	0
2	EDO	B	110	4/4	0.84	0.17	39,41,45,47	0
2	EDO	D	111	4/4	0.85	0.22	55,57,57,59	0
2	EDO	F	110	4/4	0.86	0.21	45,47,48,48	0
2	EDO	E	110	4/4	0.90	0.16	42,48,48,51	0
2	EDO	H	110	4/4	0.93	0.16	45,48,48,50	0
2	EDO	A	110	4/4	0.95	0.15	30,33,35,38	0

## 6.5 Other polymers

There are no such residues in this entry.