



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:29 PM BST

PDB ID : 6RO6  
Title : Crystal structure of the C-terminal dimerization domain of the essential repressor DdrO from radiation-resistant *Deinococcus* bacteria (*Deinococcus deserti*)  
Authors : Pignol, D.; Arnoux, P.; Siponen, M.I.; Brandelet, G.; De Groot, A.; Blanchard, L.  
Deposited on : 2019-05-10  
Resolution : 1.41 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 : 2.13.1  
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) : 2.13.1

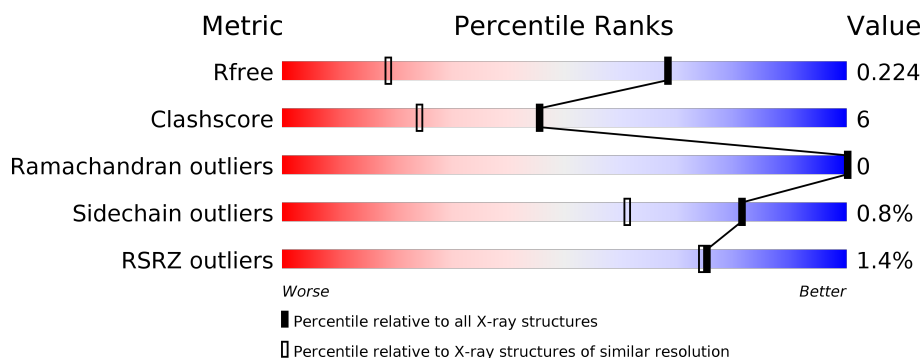
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.41 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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	58	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	B	58	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div></div> </div> <div></div> </div>
1	C	58	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div></div> </div> <div></div> </div>
1	D	58	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div></div> </div> <div></div> </div>
1	E	58	<div> <div></div> <div> <div></div> <div>88%</div> <div>5%</div> <div></div> </div> <div></div> </div>
1	F	58	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>5%</div> <div>9%</div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	58	<div> <div></div> <div>2%</div> <div>79%</div> <div>14%</div> <div>5%</div> </div>
1	H	58	<div> <div></div> <div>86%</div> <div>7%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7795 atoms, of which 3905 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 HTH-type transcriptional regulator DdrOC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	H	N	O	0	2	0
			977	306	497	89	85			
1	B	57	Total	C	H	N	O	0	3	0
			984	309	500	87	88			
1	C	56	Total	C	H	N	O	0	0	0
			939	295	479	84	81			
1	D	56	Total	C	H	N	O	0	1	0
			946	297	483	84	82			
1	E	55	Total	C	H	N	O	0	1	0
			934	294	478	83	79			
1	F	53	Total	C	H	N	O	0	1	0
			917	289	470	81	77			
1	G	55	Total	C	H	N	O	0	2	0
			961	302	494	84	81			
1	H	55	Total	C	H	N	O	0	3	0
			977	306	504	84	83			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	MET	-	initiating methionine	UNP C1CYP4
B	72	MET	-	initiating methionine	UNP C1CYP4
C	72	MET	-	initiating methionine	UNP C1CYP4
D	72	MET	-	initiating methionine	UNP C1CYP4
E	72	MET	-	initiating methionine	UNP C1CYP4
F	72	MET	-	initiating methionine	UNP C1CYP4
G	72	MET	-	initiating methionine	UNP C1CYP4
H	72	MET	-	initiating methionine	UNP C1CYP4

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	17	Total	O	0	0
			17	17		

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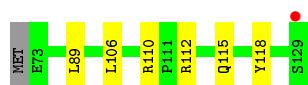
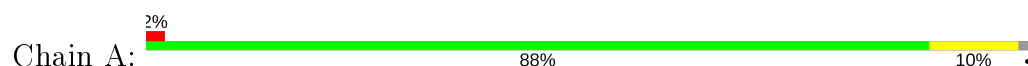
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	12	Total 12	O 12	0	0
3	D	13	Total 13	O 13	0	0
3	E	18	Total 18	O 18	0	0
3	F	9	Total 9	O 9	0	0
3	G	12	Total 12	O 12	0	0
3	H	14	Total 14	O 14	0	0

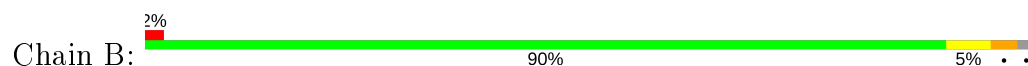
### 3 Residue-property plots [i](#)

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 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.

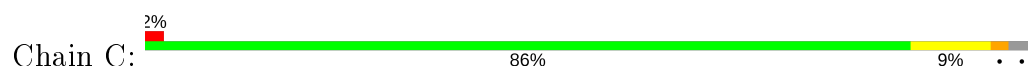
- Molecule 1: HTH-type transcriptional regulator DdrOC



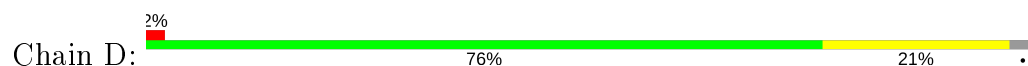
- Molecule 1: HTH-type transcriptional regulator DdrOC



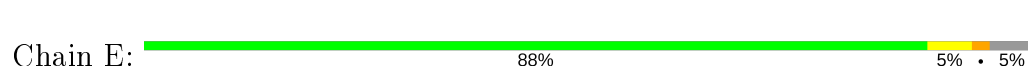
- Molecule 1: HTH-type transcriptional regulator DdrOC



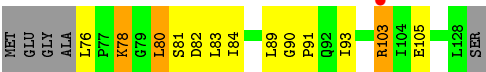
- Molecule 1: HTH-type transcriptional regulator DdrOC



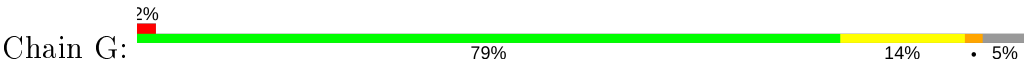
- Molecule 1: HTH-type transcriptional regulator DdrOC



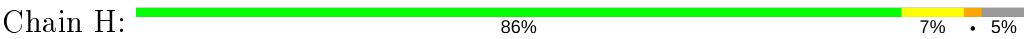
- Molecule 1: HTH-type transcriptional regulator DdrOC



• Molecule 1: HTH-type transcriptional regulator DdrOC



• Molecule 1: HTH-type transcriptional regulator DdrOC





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.91Å 76.80Å 102.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 1.41 61.42 – 1.41	Depositor EDS
% Data completeness (in resolution range)	92.4 (60.00-1.41) 92.4 (61.42-1.41)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.41Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.195 , 0.224 0.195 , 0.224	Depositor DCC
$R_{free}$ test set	4003 reflections (5.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 40.9	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	0.97	EDS
Total number of atoms	7795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0448e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.53	0/495	0.72	1/668 (0.1%)
1	B	1.37	5/506 (1.0%)	1.45	4/684 (0.6%)
1	C	0.57	0/471	0.77	1/637 (0.2%)
1	D	0.53	0/477	0.74	0/645
1	E	0.63	1/470 (0.2%)	1.13	3/637 (0.5%)
1	F	0.68	1/461 (0.2%)	0.91	3/625 (0.5%)
1	G	1.10	3/484 (0.6%)	0.98	3/655 (0.5%)
1	H	0.67	1/496 (0.2%)	0.99	4/671 (0.6%)
All	All	0.82	11/3860 (0.3%)	0.99	19/5222 (0.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	LYS	CD-CE	20.91	2.03	1.51
1	G	107	ARG	CB-CG	13.27	1.88	1.52
1	B	112	ARG	CZ-NH2	-11.82	1.17	1.33
1	G	107	ARG	NE-CZ	10.98	1.47	1.33
1	B	78	LYS	CG-CD	10.59	1.88	1.52
1	G	107	ARG	CD-NE	-10.51	1.28	1.46
1	F	103	ARG	CG-CD	-7.43	1.33	1.51
1	H	103	ARG	CG-CD	7.41	1.70	1.51
1	B	78	LYS	CB-CG	6.85	1.71	1.52
1	B	112	ARG	NE-CZ	-5.79	1.25	1.33
1	E	99	ARG	CG-CD	5.29	1.65	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	NE-CZ-NH1	19.23	129.91	120.30
1	B	78	LYS	CD-CE-NZ	18.91	155.18	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	NE-CZ-NH2	-17.44	111.58	120.30
1	E	99	ARG	NE-CZ-NH2	-16.59	112.00	120.30
1	E	99	ARG	NE-CZ-NH1	14.16	127.38	120.30
1	H	103	ARG	CB-CA-C	11.57	133.55	110.40
1	G	107	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	H	103	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	G	107	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	F	80	LEU	CB-CG-CD2	7.59	123.90	111.00
1	F	103	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	E	99	ARG	CG-CD-NE	-6.77	97.58	111.80
1	H	103	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	F	103	ARG	CB-CG-CD	-6.49	94.73	111.60
1	H	103	ARG	CG-CD-NE	6.07	124.54	111.80
1	C	103	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	110	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	G	107	ARG	CG-CD-NE	5.41	123.16	111.80
1	B	112	ARG	CG-CD-NE	-5.38	100.51	111.80

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	480	497	494	5	0
1	B	484	500	494	6	7
1	C	460	479	478	7	0
1	D	463	483	483	8	0
1	E	456	478	478	3	3
1	F	447	470	470	12	0
1	G	467	494	494	10	4
1	H	473	504	504	5	0
2	A	10	0	0	0	0
2	C	10	0	0	1	0
2	D	15	0	0	0	0
2	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	5	0	0	0	0
2	G	5	0	0	1	0
3	A	15	0	0	2	0
3	B	17	0	0	1	0
3	C	12	0	0	0	0
3	D	13	0	0	0	0
3	E	18	0	0	1	0
3	F	9	0	0	2	0
3	G	12	0	0	2	0
3	H	14	0	0	2	0
All	All	3890	3905	3895	49	7

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 6.

All (49) 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:B:78:LYS:CD	1:B:78:LYS:CG	1.88	1.50
1:G:107:ARG:CB	1:G:107:ARG:CG	1.88	1.50
1:B:78:LYS:CE	1:B:78:LYS:CD	2.03	1.36
1:B:112:ARG:NH2	3:B:201:HOH:O	1.78	1.16
1:H:125:LYS:NZ	3:H:201:HOH:O	1.91	1.03
1:A:112:ARG:NH2	3:A:301:HOH:O	2.07	0.87
1:G:125:LYS:NZ	3:G:301:HOH:O	1.59	0.86
1:C:107:ARG:NH2	2:C:201:SO4:O3	2.10	0.84
1:G:110:ARG:NH2	3:G:302:HOH:O	2.11	0.83
1:G:115[B]:GLN:OE1	1:H:118:TYR:OH	1.97	0.82
1:F:81[A]:SER:OG	3:F:301:HOH:O	1.96	0.79
1:F:81[B]:SER:OG	3:F:301:HOH:O	1.96	0.79
1:A:112:ARG:CZ	3:A:301:HOH:O	2.43	0.65
1:F:103:ARG:HD2	1:F:103:ARG:O	2.02	0.60
1:D:95:PRO:O	1:D:99:ARG:HG3	2.01	0.60
1:F:103:ARG:HD2	1:F:103:ARG:C	2.23	0.58
1:G:107:ARG:NH2	2:G:201:SO4:O4	2.39	0.56
1:F:76:LEU:HD22	1:F:80:LEU:HD13	1.90	0.54
1:F:103:ARG:CD	1:F:103:ARG:O	2.56	0.53
1:F:83:LEU:HG	1:F:93:ILE:HD12	1.91	0.53
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.74	0.52
1:C:99:ARG:HD3	1:C:103:ARG:NH2	2.27	0.50
1:F:78:LYS:HD3	1:F:82:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:GLU:OE1	3:E:301:HOH:O	2.20	0.48
1:D:99:ARG:HG2	1:E:81[A]:SER:OG	2.13	0.48
1:H:115[B]:GLN:HG2	3:H:209:HOH:O	2.13	0.48
1:F:80:LEU:HD22	1:F:84:ILE:HD11	1.97	0.46
1:G:106:LEU:HD23	1:G:109:LYS:HE3	1.99	0.45
1:C:110:ARG:NH1	1:C:110:ARG:HG2	2.31	0.44
1:A:89:LEU:HD22	1:A:118:TYR:CZ	2.53	0.44
1:D:77:PRO:HB3	1:D:110:ARG:HD3	1.99	0.44
1:B:73:GLU:OE1	1:B:105[A]:GLU:OE2	2.36	0.43
1:H:78:LYS:HB2	1:H:78:LYS:HE2	1.91	0.43
1:D:78:LYS:HA	1:D:78:LYS:HD2	1.85	0.43
1:D:89:LEU:O	1:D:92:GLN:HG2	2.18	0.43
1:F:80:LEU:O	1:F:84:ILE:HG13	2.20	0.42
1:D:90:GLY:N	1:D:91:PRO:CD	2.83	0.42
1:A:115:GLN:OE1	1:D:118:TYR:OH	2.37	0.42
1:B:115[B]:GLN:OE1	1:C:125:LYS:NZ	2.53	0.42
1:G:110:ARG:HB2	1:G:112:ARG:HH12	1.86	0.41
1:G:83[A]:LEU:HD11	1:G:89:LEU:HB3	2.03	0.41
1:B:115[A]:GLN:OE1	1:C:125:LYS:NZ	2.53	0.41
1:D:97:TRP:CZ2	1:D:125:LYS:HA	2.56	0.41
1:H:78:LYS:CE	1:H:78:LYS:H	2.34	0.41
1:E:89:LEU:HD21	1:F:89:LEU:HD21	2.03	0.40
1:F:90:GLY:N	1:F:91:PRO:CD	2.85	0.40
1:A:106:LEU:HD22	1:C:97:TRP:CZ2	2.56	0.40
1:G:83[A]:LEU:HD12	1:G:89:LEU:HB2	2.04	0.40

All (7) 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:B:78:LYS:HZ3	1:G:107:ARG:HG2[2_555]	1.27	0.33
1:B:78:LYS:CE	1:G:107:ARG:NE[2_555]	2.02	0.18
1:B:112:ARG:HH12	1:E:99:ARG:NH2[4_455]	1.45	0.15
1:B:112:ARG:O	1:G:107:ARG:NH1[2_555]	2.14	0.06
1:B:78:LYS:CD	1:G:107:ARG:HE[2_555]	1.57	0.03
1:B:112:ARG:NH1	1:E:99:ARG:NH2[4_455]	2.17	0.03
1:B:112:ARG:NH1	1:E:99:ARG:CZ[4_455]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	57/58 (98%)	55 (96%)	2 (4%)	0	100	100
1	B	58/58 (100%)	58 (100%)	0	0	100	100
1	C	54/58 (93%)	54 (100%)	0	0	100	100
1	D	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
1	E	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
1	F	52/58 (90%)	52 (100%)	0	0	100	100
1	G	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
1	H	57/58 (98%)	55 (96%)	2 (4%)	0	100	100
All	All	442/464 (95%)	435 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	52/52 (100%)	52 (100%)	0	100	100
1	B	54/52 (104%)	54 (100%)	0	100	100
1	C	50/52 (96%)	50 (100%)	0	100	100
1	D	51/52 (98%)	51 (100%)	0	100	100
1	E	50/52 (96%)	50 (100%)	0	100	100
1	F	50/52 (96%)	48 (96%)	2 (4%)	31	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	52/52 (100%)	52 (100%)	0	100	100
1	H	54/52 (104%)	53 (98%)	1 (2%)	57	24
All	All	413/416 (99%)	410 (99%)	3 (1%)	81	65

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	78	LYS
1	F	105	GLU
1	H	78	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	92	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

10 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	D	201	-	4,4,4	0.22	0	6,6,6	1.02	1 (16%)
2	SO4	D	203	-	4,4,4	0.16	0	6,6,6	0.28	0
2	SO4	C	202	-	4,4,4	0.14	0	6,6,6	0.24	0
2	SO4	A	202	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	G	201	-	4,4,4	0.21	0	6,6,6	0.57	0
2	SO4	E	201	-	4,4,4	0.25	0	6,6,6	0.35	0
2	SO4	F	201	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	C	201	-	4,4,4	0.14	0	6,6,6	0.47	0
2	SO4	A	201	-	4,4,4	0.22	0	6,6,6	0.19	0
2	SO4	D	202	-	4,4,4	0.15	0	6,6,6	0.21	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	201	SO4	O4-S-O1	2.08	120.17	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	201	SO4	1	0
2	C	201	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](#)

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	57/58 (98%)	-0.28	1 (1%) 68 68	17, 28, 59, 92	0
1	B	57/58 (98%)	-0.32	1 (1%) 68 68	17, 27, 65, 72	0
1	C	56/58 (96%)	-0.34	1 (1%) 68 68	16, 33, 62, 97	0
1	D	56/58 (96%)	-0.34	1 (1%) 68 68	17, 31, 57, 130	0
1	E	55/58 (94%)	-0.23	0 100 100	22, 33, 67, 76	0
1	F	53/58 (91%)	-0.29	1 (1%) 66 66	19, 37, 60, 83	0
1	G	55/58 (94%)	-0.40	1 (1%) 68 68	18, 29, 58, 104	0
1	H	55/58 (94%)	-0.23	0 100 100	20, 34, 66, 76	0
All	All	444/464 (95%)	-0.31	6 (1%) 75 74	16, 32, 64, 130	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	129	SER	4.0
1	F	103	ARG	3.2
1	A	129	SER	2.9
1	C	129	SER	2.2
1	G	107	ARG	2.0
1	B	78	LYS	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 monosaccharides 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	201	5/5	0.69	0.30	66,69,83,95	0
2	SO4	F	201	5/5	0.79	0.16	86,98,104,105	0
2	SO4	A	202	5/5	0.90	0.23	75,89,98,101	0
2	SO4	C	202	5/5	0.92	0.10	51,67,71,75	0
2	SO4	E	201	5/5	0.95	0.07	30,30,44,63	0
2	SO4	D	203	5/5	0.96	0.11	45,62,72,81	0
2	SO4	D	202	5/5	0.97	0.07	49,49,55,65	5
2	SO4	D	201	5/5	0.99	0.09	24,24,27,27	5
2	SO4	A	201	5/5	0.99	0.05	27,29,33,37	0
2	SO4	G	201	5/5	0.99	0.06	27,29,34,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.