



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:36 PM GMT

PDB ID : 1G8K  
Title : CRYSTAL STRUCTURE ANALYSIS OF ARSENITE OXIDASE FROM AL-CALIGENES FAECALIS  
Authors : Ellis, P.J.; Conrads, T.; Hille, R.; Kuhn, P.  
Deposited on : 2000-11-17  
Resolution : 1.64 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

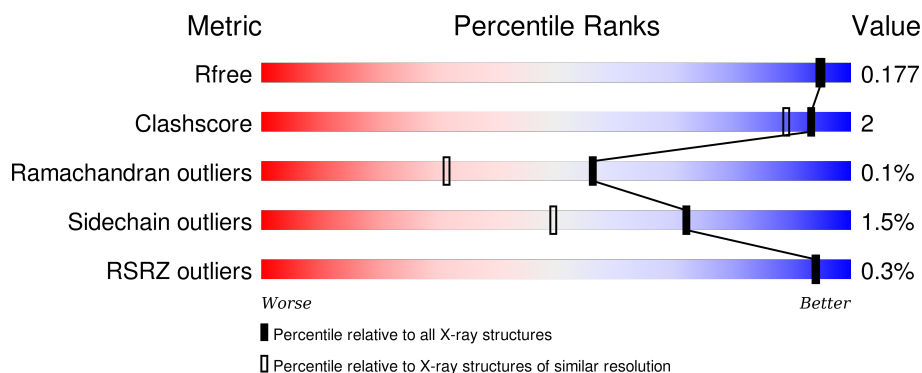
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.64 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.



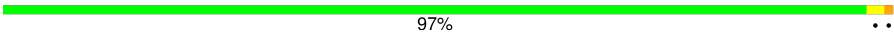
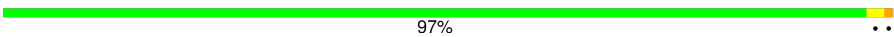
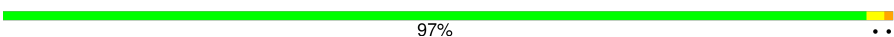
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1953 (1.66-1.62)
Clashscore	102246	2091 (1.66-1.62)
Ramachandran outliers	100387	2052 (1.66-1.62)
Sidechain outliers	100360	2052 (1.66-1.62)
RSRZ outliers	91569	1955 (1.66-1.62)

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	825	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	C	825	<div> <div></div> <div>94%</div> <div>5%</div> </div>
1	E	825	<div> <div></div> <div>93%</div> <div>6%</div> </div>
1	G	825	<div> <div></div> <div>94%</div> <div>5%</div> </div>
2	B	133	<div> <div></div> <div>98%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	133	 97% ..
2	F	133	 97% ..
2	H	133	 97% ..

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
10	EDO	A	7001	-	-	-	X
6	O	A	5003	-	-	-	X
6	O	E	5203	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 34251 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 ARSENITE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	67	0	0
			6455	4060	1136	1219	40			
1	C	822	Total	C	N	O	S	44	0	0
			6455	4060	1136	1219	40			
1	E	822	Total	C	N	O	S	37	0	0
			6455	4060	1136	1219	40			
1	G	822	Total	C	N	O	S	61	0	0
			6455	4060	1136	1219	40			

- Molecule 2 is a protein called ARSENITE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			965	604	158	195	8			
2	D	133	Total	C	N	O	S	0	0	0
			965	604	158	195	8			
2	F	133	Total	C	N	O	S	0	0	0
			965	604	158	195	8			
2	H	133	Total	C	N	O	S	0	0	0
			965	604	158	195	8			

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Hg	0	0
			2	2		
3	D	1	Total	Hg	0	0
			1	1		
3	E	2	Total	Hg	0	0
			2	2		
3	H	1	Total	Hg	0	0
			1	1		

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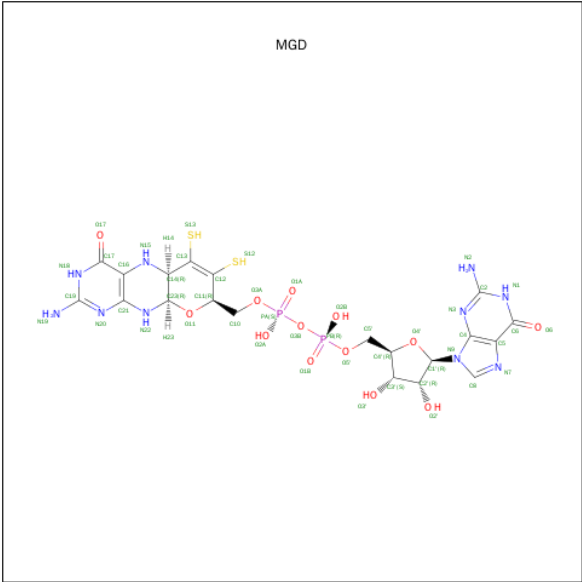
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Hg	0	0
			1	1		
3	C	2	Total	Hg	0	0
			2	2		
3	A	2	Total	Hg	0	0
			2	2		
3	F	1	Total	Hg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Ca	0	0
			2	2		
4	A	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		
4	E	2	Total	Ca	0	0
			2	2		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

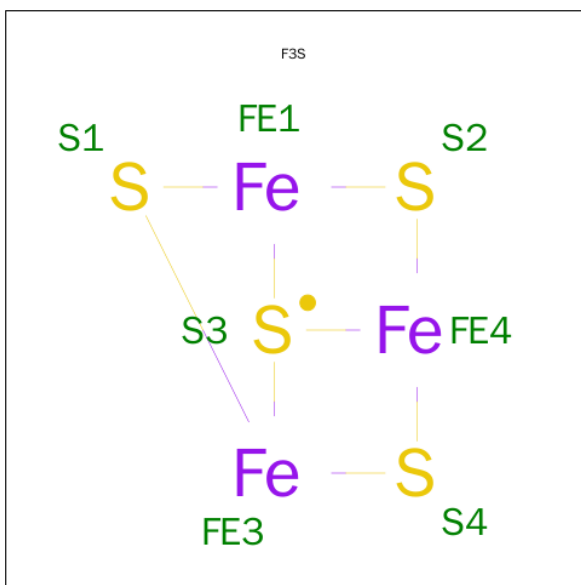
- Molecule 6 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	O	0	0
			1	1		
6	A	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	E	1	Total	O	0	0
			1	1		

- Molecule 7 is MOLYBDENUM(IV) ION (three-letter code: 4MO) (formula: Mo).

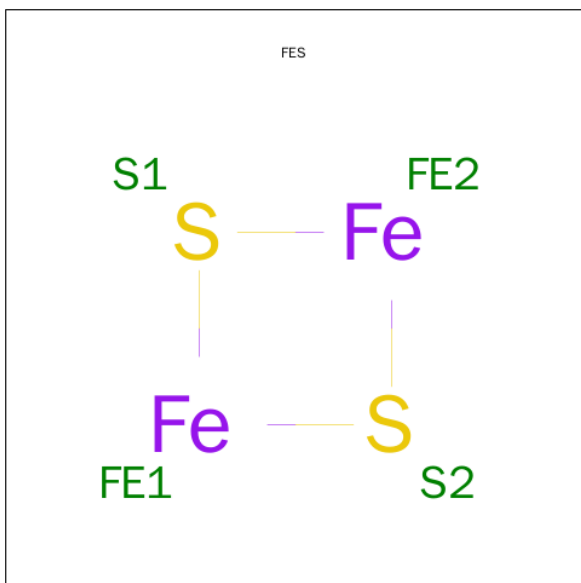
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Mo	0	0
			1	1		
7	A	1	Total	Mo	0	0
			1	1		
7	C	1	Total	Mo	0	0
			1	1		
7	E	1	Total	Mo	0	0
			1	1		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



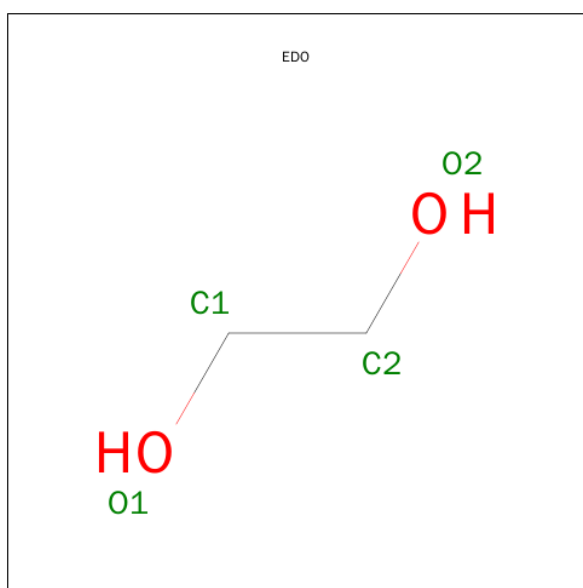
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Fe	S	0	0
			7	3	4		
8	C	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		
8	G	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			4	2	2		
9	D	1	Total	Fe	S	0	0
			4	2	2		
9	F	1	Total	Fe	S	0	0
			4	2	2		
9	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 10 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
10	A	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		
10	E	1	Total	C	O	0	0
			4	2	2		
10	G	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		
10	E	1	Total	C	O	0	0
			4	2	2		
10	G	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	O	0	0
			4	2	2		

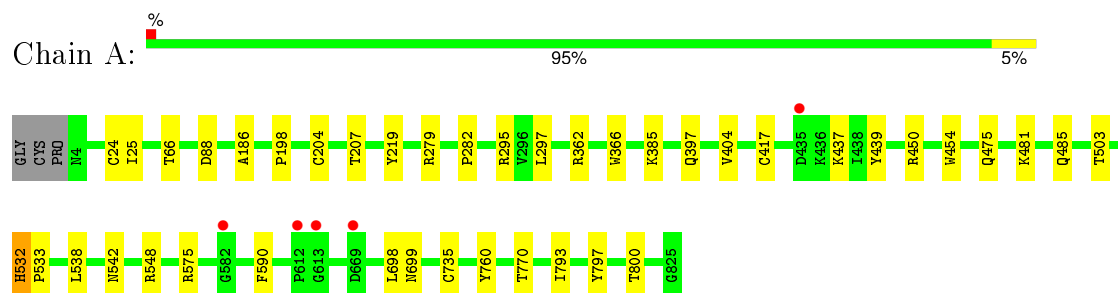
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	804	Total	O	0	0
			804	804		
11	B	165	Total	O	0	0
			165	165		
11	C	908	Total	O	0	0
			908	908		
11	D	157	Total	O	0	0
			157	157		
11	E	878	Total	O	0	0
			878	878		
11	F	162	Total	O	0	0
			162	162		
11	G	849	Total	O	0	0
			849	849		
11	H	164	Total	O	0	0
			164	164		

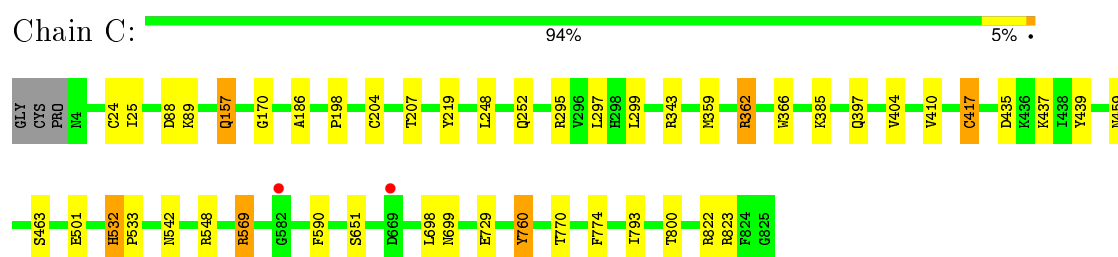
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

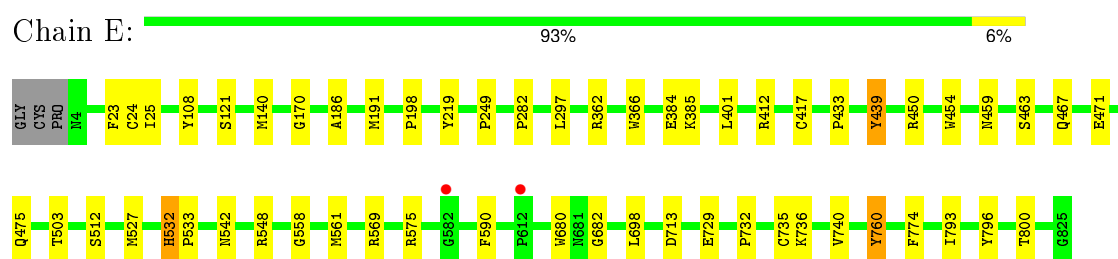
#### • Molecule 1: ARSENITE OXIDASE



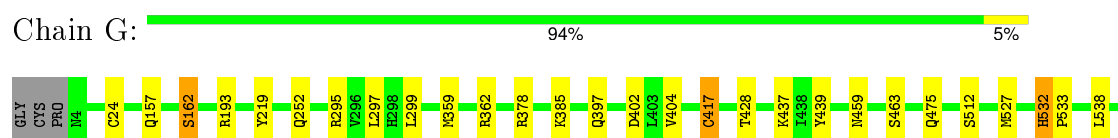
#### • Molecule 1: ARSENITE OXIDASE



#### • Molecule 1: ARSENITE OXIDASE



#### • Molecule 1: ARSENITE OXIDASE





- Molecule 2: ARSENITE OXIDASE

Chain B: 98% ..



- Molecule 2: ARSENITE OXIDASE

Chain D: 97% ..



- Molecule 2: ARSENITE OXIDASE

Chain F: 97% ..



- Molecule 2: ARSENITE OXIDASE

Chain H: 97% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.74Å 109.52Å 117.64Å 97.71° 90.00° 96.43°	Depositor
Resolution (Å)	17.80 – 1.64 17.76 – 1.64	Depositor EDS
% Data completeness (in resolution range)	(Not available) (17.80-1.64) 90.9 (17.76-1.64)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 1.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.154 , 0.179 0.153 , 0.177	Depositor DCC
$R_{free}$ test set	25621 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 509185 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: MGD, CA, EDO, O, F3S, FES, HG, 4MO

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	0.91	1/6616 (0.0%)	0.90	4/8969 (0.0%)
1	C	0.95	0/6616	0.95	8/8969 (0.1%)
1	E	1.00	5/6616 (0.1%)	0.97	5/8969 (0.1%)
1	G	0.96	0/6616	0.95	8/8969 (0.1%)
2	B	0.98	0/986	0.95	0/1349
2	D	0.93	0/986	0.94	0/1349
2	F	0.93	0/986	0.93	0/1349
2	H	0.98	0/986	0.94	0/1349
All	All	0.96	6/30408 (0.0%)	0.94	25/41272 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	E	0	2
1	G	0	2
All	All	0	7

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	735	CYS	CB-SG	-7.09	1.70	1.82
1	E	140	MET	CG-SD	5.96	1.96	1.81
1	E	108	TYR	CE1-CZ	5.50	1.45	1.38
1	E	191	MET	SD-CE	-5.48	1.47	1.77
1	E	23	PHE	CD1-CE1	5.41	1.50	1.39

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	295	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	G	295	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	343	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	295	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	E	713	ASP	CB-CG-OD2	-6.30	112.63	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	TYR	Sidechain
1	A	797	TYR	Sidechain
1	C	219	TYR	Sidechain
1	E	219	TYR	Sidechain
1	E	439	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6455	0	6220	20	0
1	C	6455	0	6221	23	0
1	E	6455	0	6220	25	0
1	G	6455	0	6221	23	0
2	B	965	0	934	3	0
2	D	965	0	933	3	0
2	F	965	0	933	2	0
2	H	965	0	933	6	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
5	A	94	0	44	2	0
5	C	94	0	44	2	0
5	E	94	0	44	2	0
5	G	94	0	44	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	A	7	0	0	0	0
8	C	7	0	0	0	0
8	E	7	0	0	0	0
8	G	7	0	0	0	0
9	B	4	0	0	0	0
9	D	4	0	0	0	0
9	F	4	0	0	0	0
9	H	4	0	0	0	0
10	A	8	0	12	0	0
10	C	8	0	12	0	0
10	E	12	0	18	0	0
10	G	8	0	12	0	0
11	A	804	0	0	3	0
11	B	165	0	0	3	0
11	C	908	0	0	5	0
11	D	157	0	0	1	0
11	E	878	0	0	2	0
11	F	162	0	0	0	0
11	G	849	0	0	8	0
11	H	164	0	0	4	0
All	All	34251	0	28845	105	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 2.

The worst 5 of 105 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:157:GLN:HG2	11:C:7662:HOH:O	1.72	0.89
1:E:561:MET:HE1	1:E:569:ARG:HH11	1.46	0.80
1:A:475:GLN:HG3	11:A:7620:HOH:O	1.89	0.73
1:E:561:MET:CE	1:E:569:ARG:HH11	2.08	0.65
2:H:100:ALA:HB3	11:H:6124:HOH:O	1.97	0.64

There are no symmetry-related clashes.

## 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	820/825 (99%)	790 (96%)	29 (4%)	1 (0%)	56	31
1	C	820/825 (99%)	792 (97%)	27 (3%)	1 (0%)	56	31
1	E	820/825 (99%)	790 (96%)	29 (4%)	1 (0%)	56	31
1	G	820/825 (99%)	792 (97%)	28 (3%)	0	100	100
2	B	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
2	D	131/133 (98%)	130 (99%)	1 (1%)	0	100	100
2	F	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
2	H	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
All	All	3804/3832 (99%)	3673 (97%)	128 (3%)	3 (0%)	56	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	793	ILE
1	E	793	ILE
1	A	793	ILE



### 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	674/676 (100%)	665 (99%)	9 (1%)	76	55
1	C	674/676 (100%)	661 (98%)	13 (2%)	65	38
1	E	674/676 (100%)	663 (98%)	11 (2%)	70	46
1	G	674/676 (100%)	666 (99%)	8 (1%)	78	58
2	B	105/105 (100%)	104 (99%)	1 (1%)	82	66
2	D	105/105 (100%)	104 (99%)	1 (1%)	82	66
2	F	105/105 (100%)	103 (98%)	2 (2%)	65	38
2	H	105/105 (100%)	104 (99%)	1 (1%)	82	66
All	All	3116/3124 (100%)	3070 (98%)	46 (2%)	72	49

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	569	ARG
1	E	249	PRO
1	G	561	MET
1	C	760	TYR
2	D	104	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	579	GLN
1	E	234	ASN
1	G	589	GLN
1	C	689	GLN
1	E	223	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 ⓘ

Of 53 ligands modelled in this entry, 28 are monoatomic - leaving 25 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$
5	MGD	A	5001	7	38,52,52	1.59	11 (28%)	43,81,81	2.51	12 (27%)
5	MGD	A	5002	7	38,52,52	1.77	5 (13%)	43,81,81	2.45	11 (25%)
8	F3S	A	5005	1	0,9,9	0.00	-	0,15,15	0.00	-
10	EDO	A	7001	-	3,3,3	1.03	0	2,2,2	0.22	0
10	EDO	A	7005	-	3,3,3	0.48	0	2,2,2	0.18	0
9	FES	B	5006	2	0,4,4	0.00	-	0,4,4	0.00	-
5	MGD	C	5101	7	38,52,52	1.66	8 (21%)	43,81,81	2.45	14 (32%)
5	MGD	C	5102	7	38,52,52	1.66	8 (21%)	43,81,81	2.37	11 (25%)
8	F3S	C	5105	1	0,9,9	0.00	-	0,15,15	0.00	-
10	EDO	C	7002	-	3,3,3	1.07	0	2,2,2	0.35	0
10	EDO	C	7006	-	3,3,3	0.65	0	2,2,2	0.16	0
9	FES	D	5106	2	0,4,4	0.00	-	0,4,4	0.00	-
5	MGD	E	5201	7	38,52,52	1.63	5 (13%)	43,81,81	2.39	10 (23%)
5	MGD	E	5202	7	38,52,52	1.75	8 (21%)	43,81,81	2.41	8 (18%)
8	F3S	E	5205	1	0,9,9	0.00	-	0,15,15	0.00	-
10	EDO	E	7003	-	3,3,3	0.72	0	2,2,2	0.20	0
10	EDO	E	7007	-	3,3,3	0.55	0	2,2,2	0.33	0
10	EDO	E	7009	-	3,3,3	0.86	0	2,2,2	0.18	0
9	FES	F	5206	2	0,4,4	0.00	-	0,4,4	0.00	-
5	MGD	G	5301	7	38,52,52	1.83	7 (18%)	43,81,81	2.47	11 (25%)
5	MGD	G	5302	7	38,52,52	1.70	6 (15%)	43,81,81	2.43	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	F3S	G	5305	1	0,9,9	0.00	-	0,15,15	0.00	-
10	EDO	G	7004	-	3,3,3	1.02	0	2,2,2	0.22	0
10	EDO	G	7008	-	3,3,3	0.77	0	2,2,2	0.21	0
9	FES	H	5306	2	0,4,4	0.00	-	0,4,4	0.00	-

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
5	MGD	A	5001	7	-	0/18/66/66	0/6/6/6
5	MGD	A	5002	7	-	0/18/66/66	0/6/6/6
8	F3S	A	5005	1	-	0/0/24/24	0/0/3/3
10	EDO	A	7001	-	-	0/1/1/1	0/0/0/0
10	EDO	A	7005	-	-	0/1/1/1	0/0/0/0
9	FES	B	5006	2	-	0/0/4/4	0/1/1/1
5	MGD	C	5101	7	-	0/18/66/66	0/6/6/6
5	MGD	C	5102	7	-	0/18/66/66	0/6/6/6
8	F3S	C	5105	1	-	0/0/24/24	0/0/3/3
10	EDO	C	7002	-	-	0/1/1/1	0/0/0/0
10	EDO	C	7006	-	-	0/1/1/1	0/0/0/0
9	FES	D	5106	2	-	0/0/4/4	0/1/1/1
5	MGD	E	5201	7	-	0/18/66/66	0/6/6/6
5	MGD	E	5202	7	-	0/18/66/66	0/6/6/6
8	F3S	E	5205	1	-	0/0/24/24	0/0/3/3
10	EDO	E	7003	-	-	0/1/1/1	0/0/0/0
10	EDO	E	7007	-	-	0/1/1/1	0/0/0/0
10	EDO	E	7009	-	-	0/1/1/1	0/0/0/0
9	FES	F	5206	2	-	0/0/4/4	0/1/1/1
5	MGD	G	5301	7	-	0/18/66/66	0/6/6/6
5	MGD	G	5302	7	-	0/18/66/66	0/6/6/6
8	F3S	G	5305	1	-	0/0/24/24	0/0/3/3
10	EDO	G	7004	-	-	0/1/1/1	0/0/0/0
10	EDO	G	7008	-	-	0/1/1/1	0/0/0/0
9	FES	H	5306	2	-	0/0/4/4	0/1/1/1

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5102	MGD	O11-C11	-3.87	1.38	1.43
5	G	5301	MGD	O11-C11	-3.65	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	5202	MGD	O11-C11	-3.52	1.38	1.43
5	E	5201	MGD	O11-C11	-2.96	1.39	1.43
5	A	5001	MGD	O11-C23	-2.81	1.39	1.43

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5301	MGD	C5-C6-N1	-9.21	111.00	123.59
5	C	5101	MGD	C5-C6-N1	-8.97	111.33	123.59
5	E	5202	MGD	C5-C6-N1	-8.95	111.35	123.59
5	A	5002	MGD	C5-C6-N1	-8.91	111.41	123.59
5	A	5001	MGD	C5-C6-N1	-8.90	111.42	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5001	MGD	1	0
5	A	5002	MGD	1	0
5	C	5101	MGD	2	0
5	E	5201	MGD	2	0
5	G	5301	MGD	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	822/825 (99%)	-0.53	5 (0%) 90 90	10, 16, 25, 36	26 (3%)
1	C	822/825 (99%)	-0.64	2 (0%) 95 94	8, 13, 22, 31	23 (2%)
1	E	822/825 (99%)	-0.65	2 (0%) 95 94	8, 13, 22, 31	28 (3%)
1	G	822/825 (99%)	-0.59	4 (0%) 91 92	9, 15, 25, 32	29 (3%)
2	B	133/133 (100%)	-0.61	0 100 100	10, 14, 20, 27	0
2	D	133/133 (100%)	-0.50	0 100 100	10, 14, 22, 28	1 (0%)
2	F	133/133 (100%)	-0.53	0 100 100	10, 14, 21, 27	1 (0%)
2	H	133/133 (100%)	-0.57	0 100 100	10, 14, 20, 27	1 (0%)
All	All	3820/3832 (99%)	-0.60	13 (0%) 94 94	8, 14, 23, 36	109 (2%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	613	GLY	3.2
1	E	582	GLY	2.9
1	A	435	ASP	2.5
1	G	669	ASP	2.4
1	A	612	PRO	2.3

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	O	A	5003	1/1	0.95	0.11	6.83	15,15,15,15	0
6	O	E	5203	1/1	0.97	0.10	6.47	9,9,9,9	0
10	EDO	A	7001	4/4	0.96	0.08	2.04	13,15,15,16	0
10	EDO	G	7004	4/4	0.98	0.07	1.47	12,13,13,15	0
10	EDO	G	7008	4/4	0.98	0.06	0.76	13,14,14,15	0
6	O	C	5103	1/1	0.99	0.06	0.32	10,10,10,10	0
10	EDO	E	7003	4/4	0.97	0.06	0.31	11,12,12,14	0
10	EDO	E	7009	4/4	0.96	0.07	0.15	14,16,17,18	0
10	EDO	C	7002	4/4	0.98	0.06	0.14	9,10,11,12	0
10	EDO	E	7007	4/4	0.99	0.05	-0.04	11,12,12,14	0
4	CA	G	5307	1/1	0.99	0.05	-0.45	18,18,18,18	0
10	EDO	A	7005	4/4	0.99	0.05	-0.55	12,14,14,15	0
4	CA	C	5107	1/1	0.99	0.05	-0.58	19,19,19,19	0
4	CA	A	5007	1/1	1.00	0.04	-0.63	18,18,18,18	0
4	CA	E	5207	1/1	1.00	0.04	-0.87	18,18,18,18	0
5	MGD	C	5101	47/47	0.99	0.05	-0.94	8,10,12,12	0
5	MGD	G	5301	47/47	0.99	0.04	-1.18	7,10,12,12	0
5	MGD	G	5302	47/47	0.99	0.04	-1.20	7,10,11,12	0
3	HG	C	6006	1/1	0.99	0.04	-1.20	15,15,15,15	1
5	MGD	C	5102	47/47	0.99	0.05	-1.22	7,9,10,11	0
5	MGD	A	5002	47/47	0.99	0.04	-1.24	9,10,12,12	0
3	HG	E	6011	1/1	0.98	0.03	-1.24	29,29,29,29	1
5	MGD	E	5201	47/47	0.99	0.04	-1.28	8,9,10,11	0
5	MGD	E	5202	47/47	0.99	0.04	-1.30	6,8,9,10	0
6	O	G	5303	1/1	1.00	0.03	-1.37	12,12,12,12	0
3	HG	A	6005	1/1	0.99	0.03	-1.41	18,18,18,18	1
3	HG	E	6007	1/1	0.99	0.04	-1.47	15,15,15,15	1
10	EDO	C	7006	4/4	0.99	0.04	-1.47	9,10,11,11	0
9	FES	D	5106	4/4	1.00	0.04	-1.71	11,11,12,12	0
5	MGD	A	5001	47/47	0.99	0.04	-1.72	10,11,13,13	0
3	HG	G	6012	1/1	0.99	0.02	-1.73	30,30,30,30	1
9	FES	H	5306	4/4	1.00	0.04	-1.78	11,12,12,13	0
4	CA	C	5108	1/1	0.99	0.03	-2.38	14,14,14,14	0
3	HG	G	6008	1/1	1.00	0.02	-2.39	17,17,17,17	1
9	FES	B	5006	4/4	1.00	0.04	-2.41	11,11,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	F3S	G	5305	7/7	1.00	0.03	-2.41	9,10,10,10	0
3	HG	A	6009	1/1	0.98	0.04	-2.69	29,29,29,29	1
9	FES	F	5206	4/4	1.00	0.03	-2.81	11,11,11,11	0
8	F3S	C	5105	7/7	1.00	0.03	-2.96	6,8,9,10	0
3	HG	C	6010	1/1	0.99	0.03	-3.14	32,32,32,32	1
3	HG	D	6002	1/1	1.00	0.03	-3.28	14,14,14,14	1
8	F3S	A	5005	7/7	1.00	0.03	-3.42	9,10,11,11	0
4	CA	G	5308	1/1	1.00	0.02	-3.44	13,13,13,13	0
8	F3S	E	5205	7/7	1.00	0.03	-3.47	8,8,8,9	0
7	4MO	G	5304	1/1	1.00	0.01	-3.74	12,12,12,12	0
7	4MO	A	5004	1/1	1.00	0.02	-3.87	12,12,12,12	0
3	HG	H	6004	1/1	1.00	0.02	-3.91	13,13,13,13	1
7	4MO	C	5104	1/1	1.00	0.01	-4.77	10,10,10,10	0
3	HG	F	6003	1/1	0.99	0.03	-5.25	13,13,13,13	1
4	CA	A	5008	1/1	0.99	0.02	-5.57	12,12,12,12	0
7	4MO	E	5204	1/1	1.00	0.01	-6.55	10,10,10,10	0
4	CA	E	5208	1/1	1.00	0.02	-7.02	12,12,12,12	0
3	HG	B	6001	1/1	0.99	0.02	-8.36	14,14,14,14	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.