



wwPDB X-ray Structure Validation Summary Report ⓘ

May 1, 2016 – 08:07 AM EDT

PDB ID : 5CH7
Title : Crystal structure of the perchlorate reductase PcrAB - Phe164 gate switch intermediate - from Azospira suillum PS
Authors : Tsai, C.-L.; Tainer, J.A.
Deposited on : 2015-07-10
Resolution : 2.20 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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) : rb-20027457

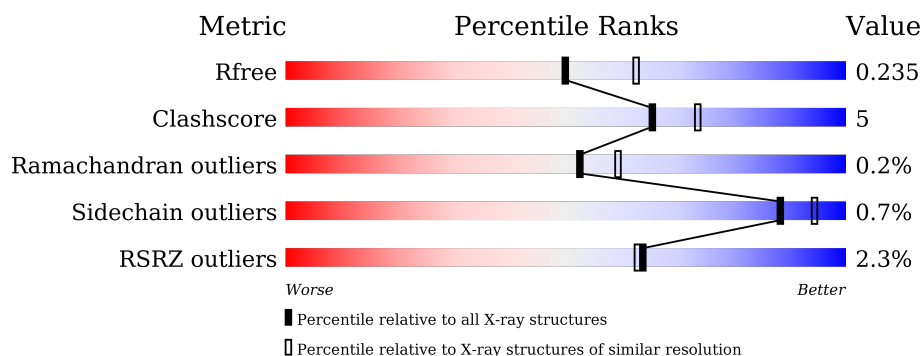
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	899	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	C	899	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>..</div> </div> </div>
1	E	899	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
2	B	333	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
2	D	333	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
2	F	333	<div> <div></div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>

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
11	SO3	A	1011	-	-	-	X
11	SO3	A	1013	-	-	-	X
11	SO3	C	1009	-	-	-	X
11	SO3	E	1008	-	-	-	X
13	ACT	C	1008	-	-	-	X
7	EDO	A	1005	-	-	-	X
7	EDO	A	1012	-	-	-	X
7	EDO	B	406	-	-	-	X
7	EDO	B	407	-	-	-	X
7	EDO	C	1005	-	-	-	X
7	EDO	E	1006	-	-	-	X
8	NA	A	1008	-	-	-	X
8	NA	C	1007	-	-	-	X
8	NA	E	1009	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31660 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.

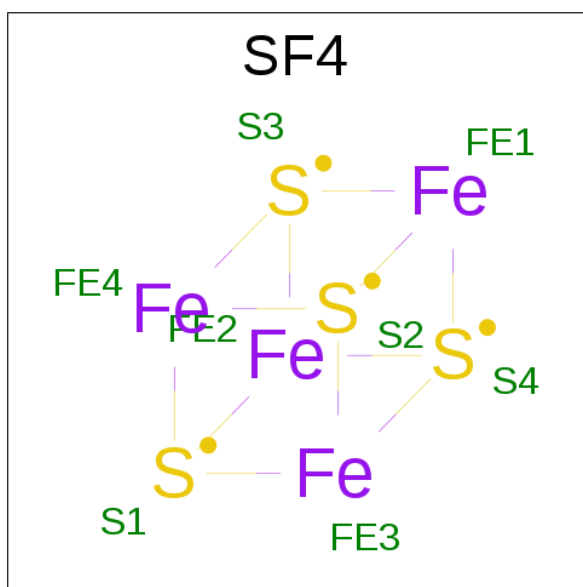
- Molecule 1 is a protein called DMSO reductase family type II enzyme, molybdopterin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	894	Total	C	N	O	S	0	3	0
			7180	4586	1246	1310	38			
1	C	891	Total	C	N	O	S	0	1	0
			7151	4568	1239	1306	38			
1	E	892	Total	C	N	O	S	0	3	0
			7171	4583	1240	1310	38			

- Molecule 2 is a protein called DMSO reductase family type II enzyme, iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	D	327	Total	C	N	O	S	0	0	0
			2547	1616	444	463	24			
2	F	328	Total	C	N	O	S	0	2	0
			2568	1631	448	465	24			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

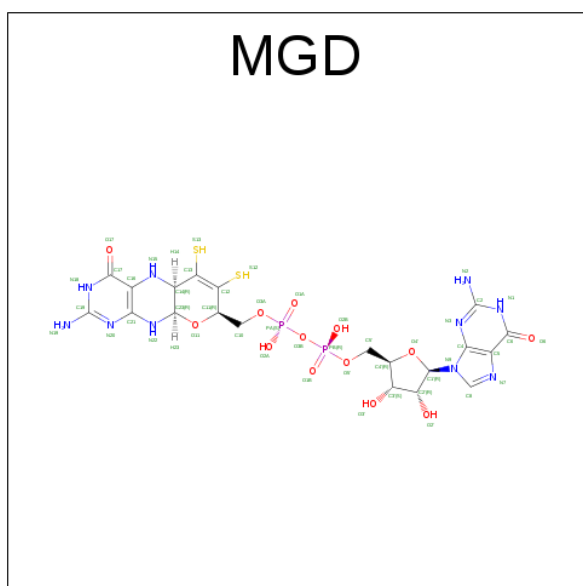


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

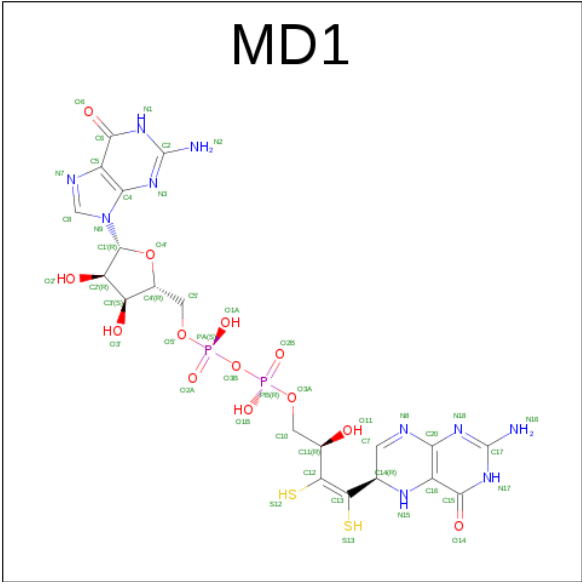
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0

- 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: C₂₀H₂₆N₁₀O₁₃P₂S₂).



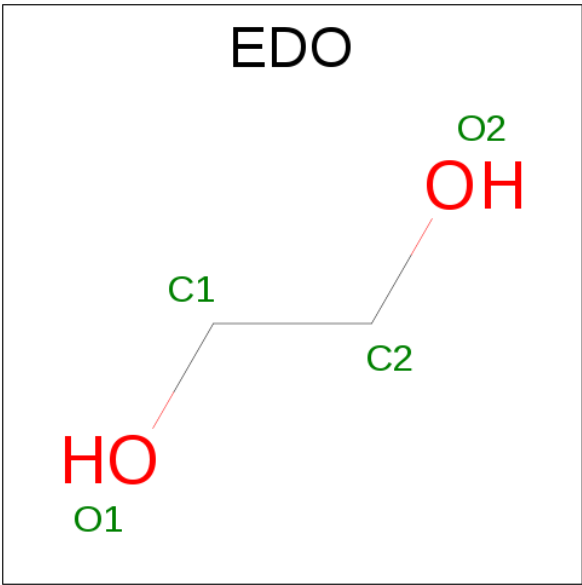
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

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

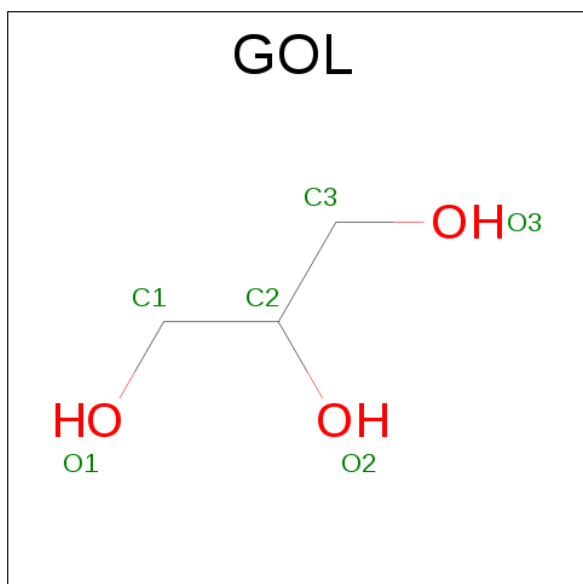
- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Na 1	0	0
8	C	1	Total 1	Na 1	0	0
8	F	1	Total 1	Na 1	0	0
8	E	1	Total 1	Na 1	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

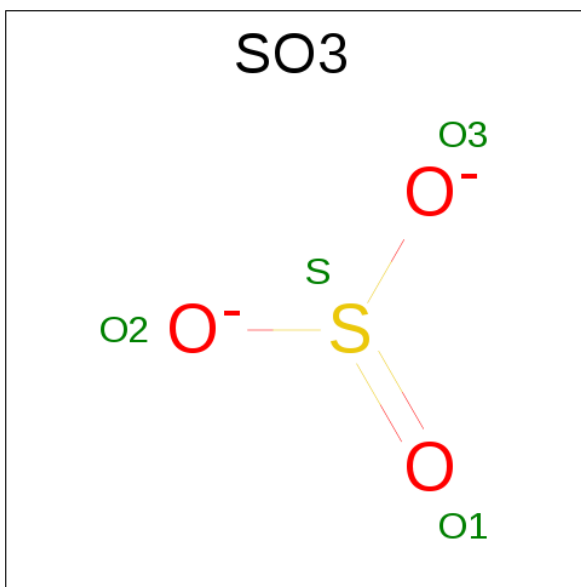
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		
9	C	1	Total	Zn	0	0
			1	1		
9	E	1	Total	Zn	0	0
			1	1		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



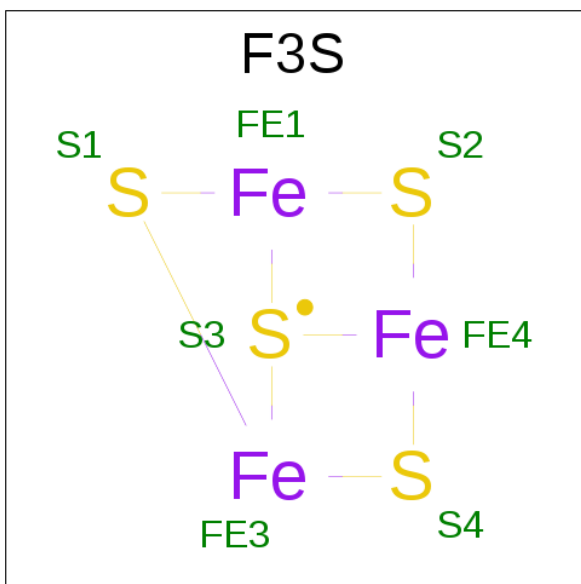
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



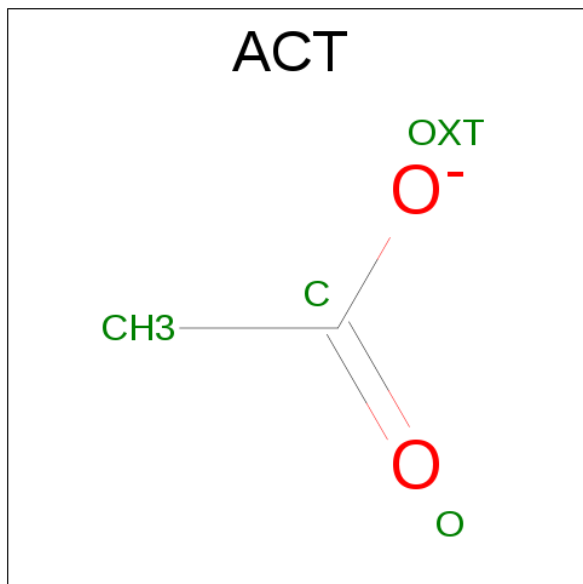
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			4	3	1		
11	A	1	Total	O	S	0	0
			4	3	1		
11	C	1	Total	O	S	0	0
			4	3	1		
11	C	1	Total	O	S	0	0
			4	3	1		
11	E	1	Total	O	S	0	0
			4	3	1		

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			7	3	4		
12	D	1	Total	Fe	S	0	0
			7	3	4		
12	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 13 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

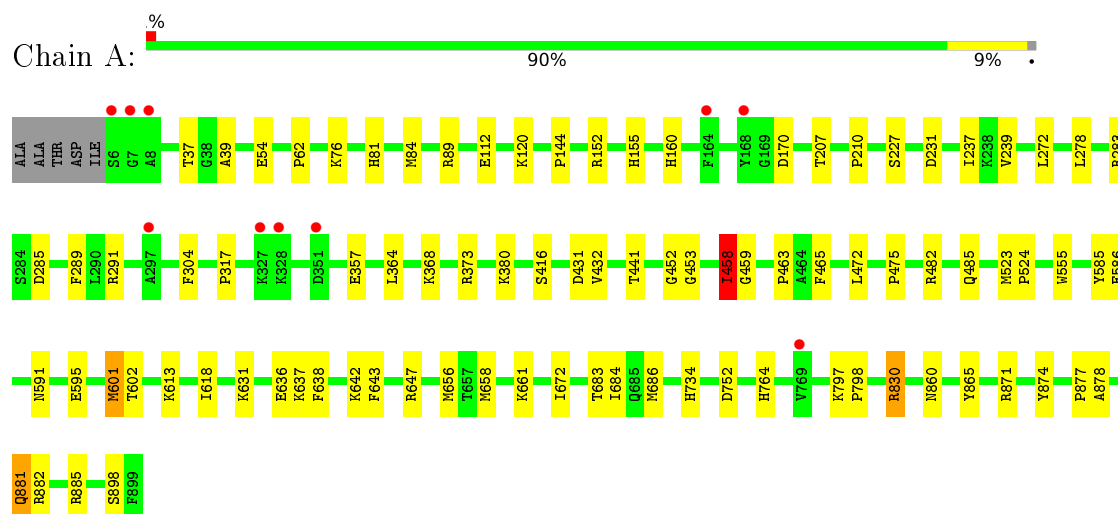
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	531	Total	O	0	0
			531	531		
14	B	273	Total	O	0	0
			273	273		
14	C	362	Total	O	0	0
			362	362		
14	D	92	Total	O	0	0
			92	92		
14	E	520	Total	O	0	0
			520	520		
14	F	198	Total	O	0	0
			198	198		

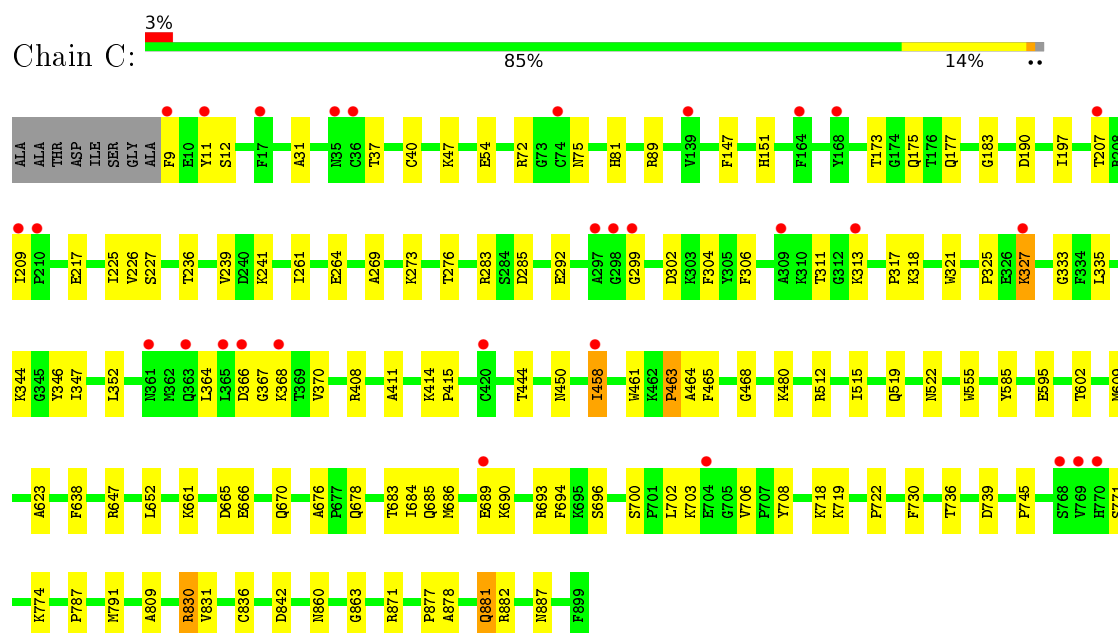
3 Residue-property plots

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: DMSO reductase family type II enzyme, molybdopterin subunit



- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.88Å 175.67Å 193.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 2.20 48.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.38-2.20) 99.9 (48.38-2.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.178 , 0.233 0.186 , 0.235	Depositor DCC
R_{free} test set	11303 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31660	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, ZN, MGD, NA, SF4, EDO, SO3, F3S, ACT, MD1, MO

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	0.56	0/7399	0.65	2/10039 (0.0%)
1	C	0.50	0/7364	0.61	1/9993 (0.0%)
1	E	0.56	0/7391	0.64	2/10030 (0.0%)
2	B	0.60	0/2632	0.67	1/3567 (0.0%)
2	D	0.43	0/2615	0.59	0/3546
2	F	0.55	0/2642	0.65	0/3580
All	All	0.54	0/30043	0.63	6/40755 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	830	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	E	830	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	830	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	B	117	ASP	CB-CG-OD1	5.62	123.36	118.30
1	E	830	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	7180	0	7003	61	0
1	C	7151	0	6964	80	0
1	E	7171	0	6984	73	0
2	B	2564	0	2534	14	0
2	D	2547	0	2513	45	0
2	F	2568	0	2546	27	0
3	A	8	0	0	0	0
3	B	24	0	0	0	0
3	C	8	0	0	0	0
3	D	24	0	0	1	0
3	E	8	0	0	0	0
3	F	24	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	47	0	21	2	0
5	C	47	0	20	2	0
5	E	47	0	20	0	0
6	A	47	0	22	1	0
6	C	47	0	22	1	0
6	E	47	0	22	1	0
7	A	16	0	24	1	0
7	B	12	0	18	1	0
7	C	8	0	12	0	0
7	D	8	0	12	0	0
7	E	12	0	18	2	0
7	F	8	0	12	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
9	E	1	0	0	0	0
10	A	6	0	8	1	0
11	A	8	0	0	0	0
11	C	8	0	0	0	0
11	E	4	0	0	0	0
12	B	7	0	0	0	0
12	D	7	0	0	0	0
12	F	7	0	0	0	0
13	C	4	0	3	0	0
14	A	531	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	273	0	0	1	0
14	C	362	0	0	7	0
14	D	92	0	0	1	0
14	E	520	0	0	12	0
14	F	198	0	0	2	0
All	All	31660	0	28778	291	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.

The worst 5 of 291 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:89:ARG:NH1	14:A:1101:HOH:O	1.94	1.01
1:E:226:VAL:HG22	1:E:241:LYS:HB3	1.56	0.87
1:E:308:ASN:HB3	1:E:311:THR:HG22	1.59	0.83
1:A:482:ARG:HB3	1:A:523:MET:HE3	1.65	0.79
1:E:860:ASN:HD22	1:E:878:ALA:H	1.32	0.77

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	895/899 (100%)	860 (96%)	33 (4%)	2 (0%)	52	59
1	C	890/899 (99%)	838 (94%)	49 (6%)	3 (0%)	46	50
1	E	893/899 (99%)	850 (95%)	41 (5%)	2 (0%)	52	59
2	B	327/333 (98%)	317 (97%)	9 (3%)	1 (0%)	46	50
2	D	325/333 (98%)	303 (93%)	21 (6%)	1 (0%)	46	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	328/333 (98%)	313 (95%)	15 (5%)	0	100	100
All	All	3658/3696 (99%)	3481 (95%)	168 (5%)	9 (0%)	52	59

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	ILE
1	C	458	ILE
2	D	205	GLU
1	E	458	ILE
2	B	6	LYS

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	768/768 (100%)	762 (99%)	6 (1%)	86	93
1	C	765/768 (100%)	758 (99%)	7 (1%)	84	92
1	E	767/768 (100%)	762 (99%)	5 (1%)	88	94
2	B	278/281 (99%)	278 (100%)	0	100	100
2	D	276/281 (98%)	273 (99%)	3 (1%)	80	89
2	F	279/281 (99%)	278 (100%)	1 (0%)	93	97
All	All	3133/3147 (100%)	3111 (99%)	22 (1%)	88	94

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	458	ILE
1	C	881	GLN
1	E	881	GLN
1	C	465	PHE
1	C	555	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	860	ASN
1	E	881	GLN
1	C	881	GLN
1	A	881	GLN
1	E	860	ASN

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 54 ligands modelled in this entry, 10 are monoatomic - leaving 44 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	$\# Z > 2$
3	SF4	A	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	A	1003	4	41,52,52	5.81	25 (60%)	39,81,81	3.80	17 (43%)
6	MD1	A	1004	4	40,51,51	3.61	14 (35%)	34,78,78	1.77	7 (20%)
7	EDO	A	1005	-	3,3,3	0.77	0	2,2,2	0.41	0
7	EDO	A	1006	-	3,3,3	0.52	0	2,2,2	0.37	0
7	EDO	A	1007	-	3,3,3	0.55	0	2,2,2	0.23	0
10	GOL	A	1010	-	5,5,5	0.22	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SO3	A	1011	9	1,3,3	1.17	0	0,3,3	0.00	-
7	EDO	A	1012	-	3,3,3	0.49	0	2,2,2	0.29	0
11	SO3	A	1013	-	1,3,3	0.99	0	0,3,3	0.00	-
12	F3S	B	401	2	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	B	402	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	B	403	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	B	404	2	0,12,12	0.00	-	0,24,24	0.00	-
7	EDO	B	405	-	3,3,3	0.30	0	2,2,2	0.75	0
7	EDO	B	406	-	3,3,3	0.56	0	2,2,2	0.36	0
7	EDO	B	407	-	3,3,3	0.73	0	2,2,2	0.24	0
3	SF4	C	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	C	1003	4	41,52,52	5.77	27 (65%)	39,81,81	4.19	17 (43%)
6	MD1	C	1004	4	40,51,51	3.50	13 (32%)	34,78,78	1.67	7 (20%)
7	EDO	C	1005	-	3,3,3	0.74	0	2,2,2	0.33	0
7	EDO	C	1006	-	3,3,3	0.55	0	2,2,2	0.31	0
13	ACT	C	1008	-	0,3,3	0.00	-	0,3,3	0.00	-
11	SO3	C	1009	-	1,3,3	0.88	0	0,3,3	0.00	-
11	SO3	C	1010	9	1,3,3	0.92	0	0,3,3	0.00	-
7	EDO	D	401	-	3,3,3	0.69	0	2,2,2	0.18	0
12	F3S	D	402	2	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	D	403	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	D	404	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	D	405	2	0,12,12	0.00	-	0,24,24	0.00	-
7	EDO	D	406	-	3,3,3	0.49	0	2,2,2	0.38	0
3	SF4	E	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	E	1003	4	41,52,52	5.75	24 (58%)	39,81,81	3.75	12 (30%)
6	MD1	E	1004	4	40,51,51	3.49	14 (35%)	34,78,78	1.62	7 (20%)
7	EDO	E	1005	-	3,3,3	0.71	0	2,2,2	0.48	0
7	EDO	E	1006	-	3,3,3	0.86	0	2,2,2	0.42	0
7	EDO	E	1007	-	3,3,3	0.54	0	2,2,2	0.39	0
11	SO3	E	1008	9	1,3,3	1.34	0	0,3,3	0.00	-
12	F3S	F	401	2	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	F	402	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	403	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	404	2	0,12,12	0.00	-	0,24,24	0.00	-
7	EDO	F	405	-	3,3,3	0.59	0	2,2,2	0.42	0
7	EDO	F	406	-	3,3,3	0.50	0	2,2,2	0.57	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
3	SF4	A	1001	1	-	0/0/48/48	0/6/5/5
5	MGD	A	1003	4	-	0/18/66/66	0/6/6/6
6	MD1	A	1004	4	-	0/21/59/59	0/5/5/5
7	EDO	A	1005	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1006	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1007	-	-	0/1/1/1	0/0/0/0
10	GOL	A	1010	-	-	0/4/4/4	0/0/0/0
11	SO3	A	1011	9	-	0/0/0/0	0/0/0/0
7	EDO	A	1012	-	-	0/1/1/1	0/0/0/0
11	SO3	A	1013	-	-	0/0/0/0	0/0/0/0
12	F3S	B	401	2	-	0/0/24/24	0/0/3/3
3	SF4	B	402	2	-	0/0/48/48	0/6/5/5
3	SF4	B	403	2	-	0/0/48/48	0/6/5/5
3	SF4	B	404	2	-	0/0/48/48	0/6/5/5
7	EDO	B	405	-	-	0/1/1/1	0/0/0/0
7	EDO	B	406	-	-	0/1/1/1	0/0/0/0
7	EDO	B	407	-	-	0/1/1/1	0/0/0/0
3	SF4	C	1001	1	-	0/0/48/48	0/6/5/5
5	MGD	C	1003	4	-	0/18/66/66	0/6/6/6
6	MD1	C	1004	4	-	0/21/59/59	0/5/5/5
7	EDO	C	1005	-	-	0/1/1/1	0/0/0/0
7	EDO	C	1006	-	-	0/1/1/1	0/0/0/0
13	ACT	C	1008	-	-	0/0/0/0	0/0/0/0
11	SO3	C	1009	-	-	0/0/0/0	0/0/0/0
11	SO3	C	1010	9	-	0/0/0/0	0/0/0/0
7	EDO	D	401	-	-	0/1/1/1	0/0/0/0
12	F3S	D	402	2	-	0/0/24/24	0/0/3/3
3	SF4	D	403	2	-	0/0/48/48	0/6/5/5
3	SF4	D	404	2	-	0/0/48/48	0/6/5/5
3	SF4	D	405	2	-	0/0/48/48	0/6/5/5
7	EDO	D	406	-	-	0/1/1/1	0/0/0/0
3	SF4	E	1001	1	-	0/0/48/48	0/6/5/5
5	MGD	E	1003	4	-	0/18/66/66	0/6/6/6
6	MD1	E	1004	4	-	0/21/59/59	0/5/5/5
7	EDO	E	1005	-	-	0/1/1/1	0/0/0/0
7	EDO	E	1006	-	-	0/1/1/1	0/0/0/0
7	EDO	E	1007	-	-	0/1/1/1	0/0/0/0
11	SO3	E	1008	9	-	0/0/0/0	0/0/0/0
12	F3S	F	401	2	-	0/0/24/24	0/0/3/3
3	SF4	F	402	2	-	0/0/48/48	0/6/5/5
3	SF4	F	403	2	-	0/0/48/48	0/6/5/5
3	SF4	F	404	2	-	0/0/48/48	0/6/5/5
7	EDO	F	405	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	F	406	-	-	0/1/1/1	0/0/0/0

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MGD	C23-C14	-20.33	1.38	1.53
5	E	1003	MGD	C23-C14	-20.22	1.38	1.53
5	C	1003	MGD	C23-C14	-19.66	1.38	1.53
5	C	1003	MGD	C2'-C3'	-10.20	1.25	1.53
5	E	1003	MGD	C2'-C3'	-9.81	1.26	1.53

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1003	MGD	N3-C2-N1	-7.02	118.00	127.56
5	A	1003	MGD	N3-C2-N1	-6.80	118.31	127.56
5	C	1003	MGD	C4'-O4'-C1'	-6.13	103.15	109.64
5	E	1003	MGD	C4'-O4'-C1'	-5.75	103.55	109.64
5	E	1003	MGD	N3-C2-N1	-5.68	119.83	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1003	MGD	2	0
6	A	1004	MD1	1	0
10	A	1010	GOL	1	0
7	A	1012	EDO	1	0
7	B	407	EDO	1	0
5	C	1003	MGD	2	0
6	C	1004	MD1	1	0
3	D	405	SF4	1	0
6	E	1004	MD1	1	0
7	E	1006	EDO	2	0
3	F	404	SF4	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, 95th 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 ²)	Q<0.9
1	A	894/899 (99%)	-0.36	10 (1%) 82 82	16, 30, 49, 68	0
1	C	891/899 (99%)	-0.04	30 (3%) 49 47	19, 39, 62, 97	0
1	E	892/899 (99%)	-0.34	14 (1%) 74 73	17, 30, 51, 70	0
2	B	329/333 (98%)	-0.62	2 (0%) 90 90	17, 24, 38, 64	0
2	D	327/333 (98%)	0.43	28 (8%) 13 12	25, 54, 71, 89	0
2	F	328/333 (98%)	-0.36	1 (0%) 94 94	18, 32, 50, 66	0
All	All	3661/3696 (99%)	-0.23	85 (2%) 64 63	16, 32, 59, 97	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	TYR	5.4
1	A	8	ALA	5.1
1	C	9	PHE	4.7
1	C	164[A]	PHE	4.6
1	E	164[A]	PHE	4.2

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 ⓘ

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, 95th 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 ²)	Q<0.9
11	SO3	A	1013	4/4	0.93	0.35	19.65	38,42,42,57	0
11	SO3	E	1008	4/4	0.44	0.25	14.57	34,38,48,71	0
7	EDO	C	1005	4/4	0.80	0.27	9.10	33,36,45,45	0
7	EDO	A	1005	4/4	0.90	0.20	8.87	25,26,31,39	0
11	SO3	C	1009	4/4	0.91	0.29	8.24	43,48,50,68	0
7	EDO	B	407	4/4	0.85	0.22	6.79	34,36,37,42	0
13	ACT	C	1008	4/4	0.88	0.14	5.62	31,36,40,44	0
7	EDO	E	1006	4/4	0.72	0.23	5.29	34,35,38,41	0
8	NA	A	1008	1/1	0.97	0.17	4.41	18,18,18,18	0
7	EDO	A	1012	4/4	0.94	0.18	2.56	21,22,27,29	0
7	EDO	B	406	4/4	0.91	0.14	2.46	32,34,40,41	0
11	SO3	A	1011	4/4	0.83	0.14	2.34	38,39,51,70	0
8	NA	C	1007	1/1	0.95	0.21	2.33	26,26,26,26	0
8	NA	E	1009	1/1	0.98	0.17	2.32	14,14,14,14	0
7	EDO	E	1005	4/4	0.94	0.11	1.84	16,20,23,23	0
10	GOL	A	1010	6/6	0.84	0.21	1.70	35,42,48,48	0
7	EDO	D	406	4/4	0.96	0.16	1.61	30,36,37,38	0
7	EDO	D	401	4/4	0.97	0.12	1.50	24,24,28,31	0
7	EDO	A	1007	4/4	0.95	0.11	1.29	26,28,29,32	0
7	EDO	F	405	4/4	0.98	0.12	1.24	23,23,23,25	0
7	EDO	A	1006	4/4	0.92	0.15	0.54	32,34,35,37	0
7	EDO	B	405	4/4	0.99	0.09	0.39	22,22,23,23	0
5	MGD	E	1003	47/47	0.97	0.18	0.29	16,24,30,31	0
5	MGD	A	1003	47/47	0.97	0.17	0.26	13,20,25,28	0
5	MGD	C	1003	47/47	0.96	0.21	0.21	21,28,32,33	0
3	SF4	B	402	8/8	0.98	0.08	0.07	22,24,24,30	0
6	MD1	A	1004	47/47	0.97	0.15	0.06	19,23,28,30	0
8	NA	F	407	1/1	0.98	0.09	0.04	41,41,41,41	0
3	SF4	F	404	8/8	0.96	0.10	-0.03	26,28,29,29	0
6	MD1	C	1004	47/47	0.97	0.16	-0.17	20,29,32,35	0
6	MD1	E	1004	47/47	0.98	0.14	-0.26	15,22,28,29	0
3	SF4	B	404	8/8	0.99	0.09	-0.33	19,21,22,23	0
3	SF4	F	403	8/8	0.98	0.14	-0.73	27,31,37,38	0
3	SF4	D	404	8/8	0.98	0.13	-0.77	45,49,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SF4	E	1001	8/8	0.98	0.12	-0.99	19,22,25,26	0
7	EDO	C	1006	4/4	0.96	0.08	-1.12	20,24,25,27	0
3	SF4	D	405	8/8	0.94	0.10	-1.38	34,48,53,54	0
3	SF4	A	1001	8/8	0.99	0.13	-1.68	20,22,26,26	0
3	SF4	C	1001	8/8	0.97	0.14	-1.87	34,36,40,42	0
3	SF4	B	403	8/8	0.99	0.10	-1.98	19,22,24,28	0
12	F3S	B	401	7/7	0.99	0.04	-2.01	26,27,28,31	0
3	SF4	F	402	8/8	0.96	0.07	-2.71	29,31,35,40	0
12	F3S	D	402	7/7	0.95	0.05	-2.75	53,58,64,74	0
12	F3S	F	401	7/7	0.98	0.04	-2.96	28,31,33,36	0
4	MO	A	1002	1/1	0.99	0.08	-3.15	33,33,33,33	0
4	MO	C	1002	1/1	0.99	0.10	-3.72	38,38,38,38	0
3	SF4	D	403	8/8	0.90	0.06	-3.74	39,45,57,57	0
4	MO	E	1002	1/1	0.99	0.11	-5.11	32,32,32,32	0
7	EDO	E	1007	4/4	0.89	0.16	-	28,40,44,49	0
9	ZN	A	1009	1/1	0.99	0.08	-	34,34,34,34	0
7	EDO	F	406	4/4	0.88	0.23	-	39,42,43,44	0
9	ZN	C	1011	1/1	0.98	0.07	-	58,58,58,58	0
11	SO3	C	1010	4/4	0.83	0.16	-	61,62,70,83	0
9	ZN	E	1010	1/1	0.97	0.07	-	33,33,33,33	0

6.5 Other polymers

There are no such residues in this entry.