wwPDB X-ray Structure Validation Summary Report (i)

May 1, 2016 – 08:09 AM EDT

PDB ID	:	5CHC
Title	:	Crystal structure of the perchlorate reductase PcrAB - substrate analog SeO3 bound - from Azospira suillum PS
Authors	:	Tsai, C.-L.; Tainer, J.A.
Deposited on	:	2015-07-10
Resolution	:	2.38 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

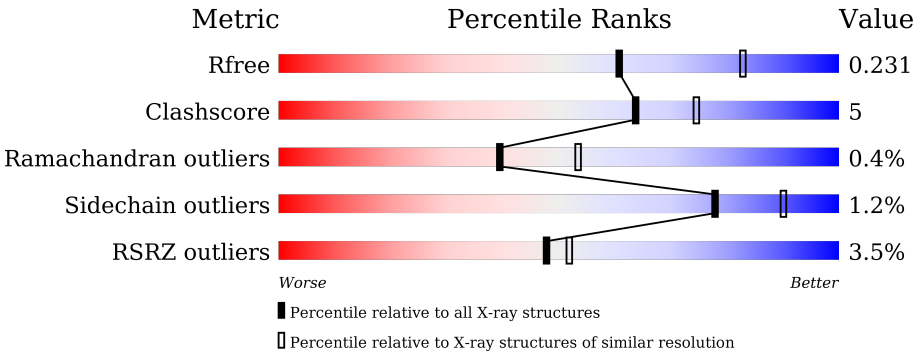
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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 <=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	2% 88% 12%
1	C	899	5% 87% 12%
1	E	899	4% 86% 12%
2	B	333	% 87% 10%
2	D	333	9% 79% 19%
2	F	333	% 88% 11%

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	NA	A	1015	-	-	-	X
10	NA	C	1011	-	-	-	X
10	NA	E	1010	-	-	-	X
13	GOL	E	1006	-	-	-	X
7	EDO	A	1005	-	-	-	X
7	EDO	A	1008	-	-	-	X
7	EDO	A	1009	-	-	-	X
7	EDO	A	1010	-	-	X	X
7	EDO	A	1012	-	-	-	X
7	EDO	A	1019	-	-	-	X
7	EDO	B	407	-	-	-	X
7	EDO	B	408	-	-	X	-
7	EDO	B	409	-	-	-	X
7	EDO	B	410	-	-	X	X
7	EDO	C	1005	-	-	-	X
7	EDO	C	1006	-	-	-	X
7	EDO	C	1007	-	-	-	X
7	EDO	E	1005	-	-	-	X
7	EDO	F	405	-	-	-	X
7	EDO	F	406	-	-	-	X
8	BSY	A	1013	-	-	X	-
8	BSY	C	1009	-	-	X	-
8	BSY	E	1008	-	-	X	-
9	SO3	A	1014	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 30958 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.

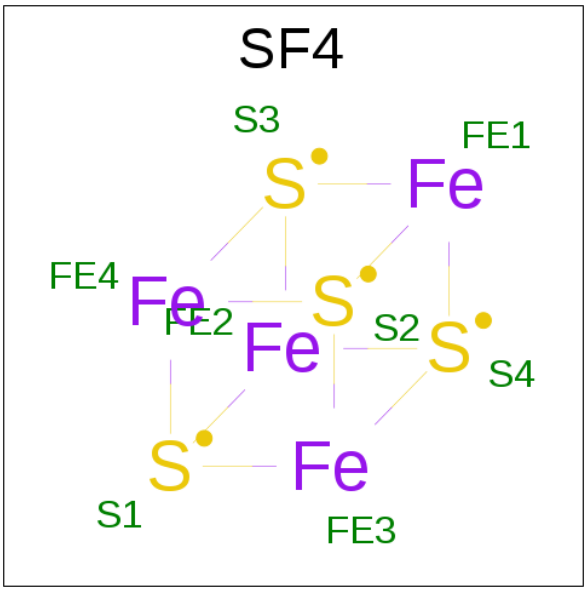
- Molecule 1 is a protein called DMSO reductase family type II enzyme, molybdopterin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	895	Total	C	N	O	S	0	1	0
			7171	4579	1243	1311	38			
1	C	892	Total	C	N	O	S	0	0	0
			7148	4563	1240	1307	38			
1	E	892	Total	C	N	O	S	0	2	0
			7163	4575	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	328	Total	C	N	O	S	0	0	0
			2556	1622	446	464	24			
2	F	328	Total	C	N	O	S	0	0	0
			2556	1622	446	464	24			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

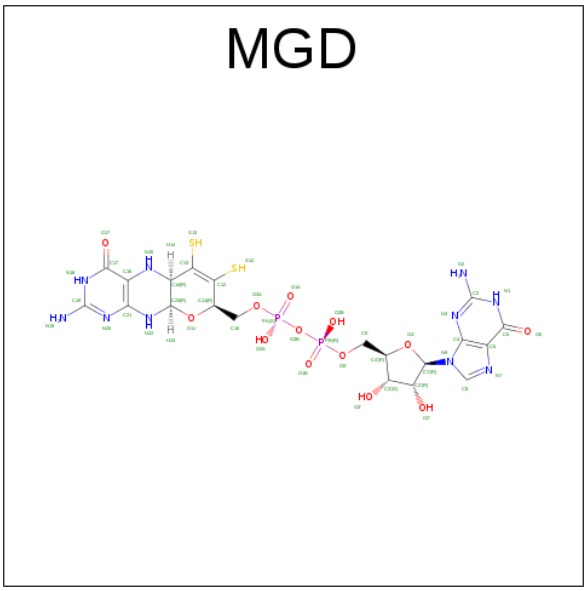


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	E	1	Total Fe S 8 4 4	0	0
3	F	1	Total Fe S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

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

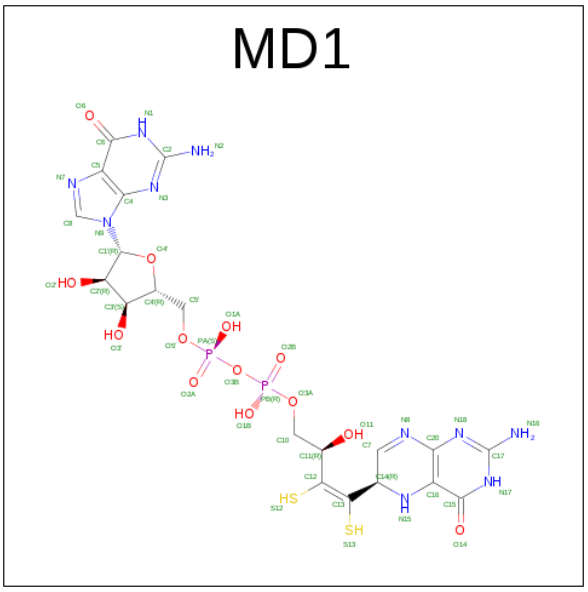
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0

- 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: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



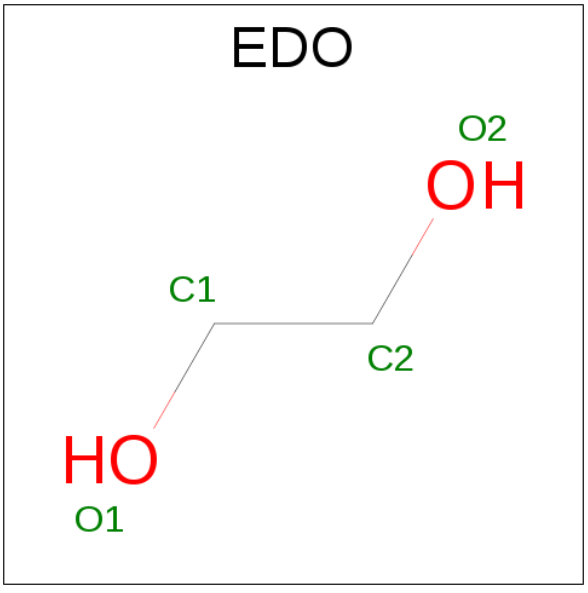
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	C	1	Total C N O P S 47 20 10 13 2 2	0	0
5	E	1	Total C N O P S 47 20 10 13 2 2	0	0

- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTERIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



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: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

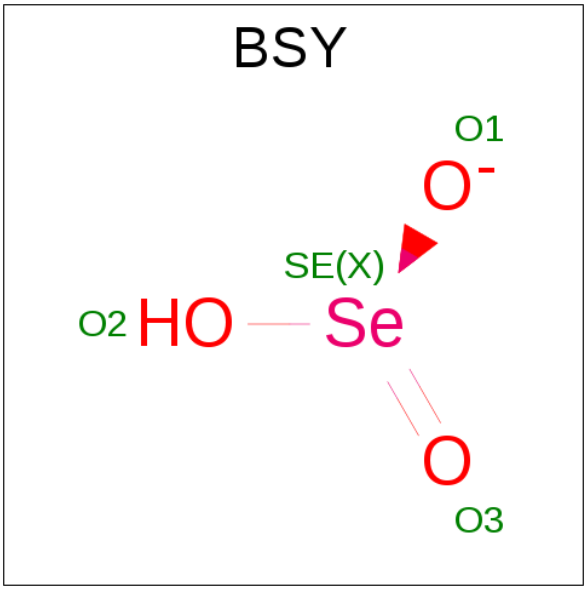
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0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

Continued on next page...

Continued from previous page...

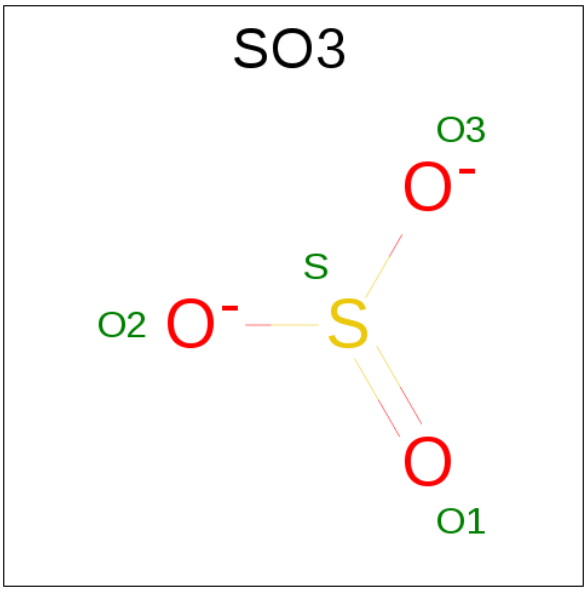
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is BISELENITE ION (three-letter code: BSY) (formula: HO_3Se).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O Se 4 3 1	0	0
8	C	1	Total O Se 4 3 1	0	0
8	E	1	Total O Se 4 3 1	0	0

- Molecule 9 is SULFITE ION (three-letter code: SO3) (formula: O_3S).



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

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Na 1 1	0	0
10	A	2	Total Na 2 2	0	0
10	C	2	Total Na 2 2	0	0
10	E	3	Total Na 3 3	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

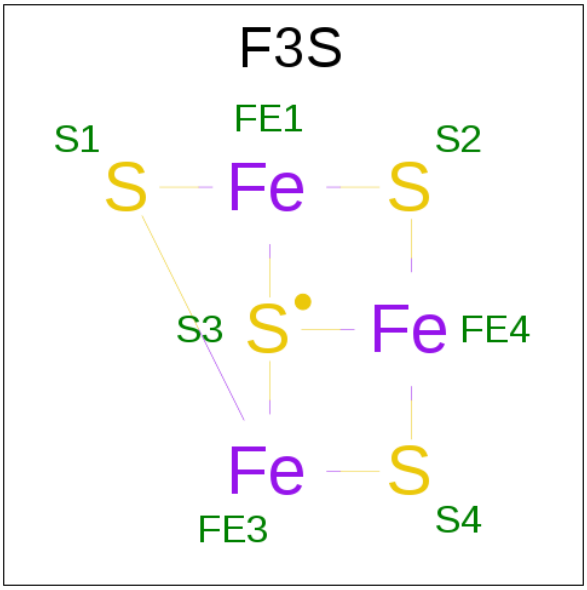
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Zn 1 1	0	0
11	C	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

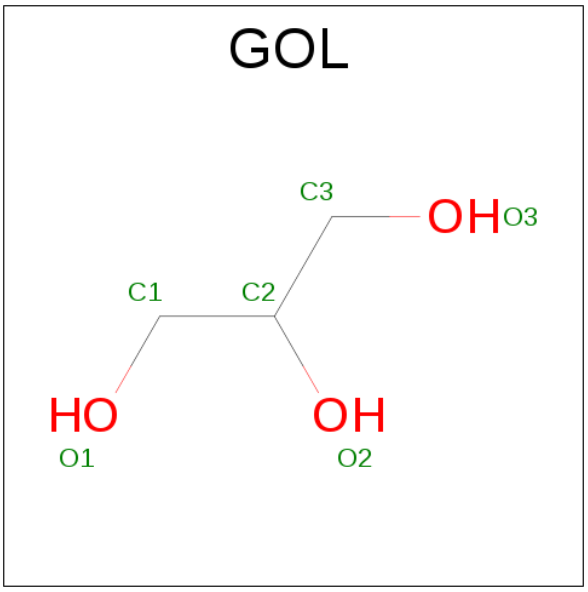
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	1	Total Zn 1 1	0	0

- 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 7 3 4	0	0
12	D	1	Total Fe S 7 3 4	0	0
12	F	1	Total Fe S 7 3 4	0	0

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	E	1	Total C O 6 3 3	0	0

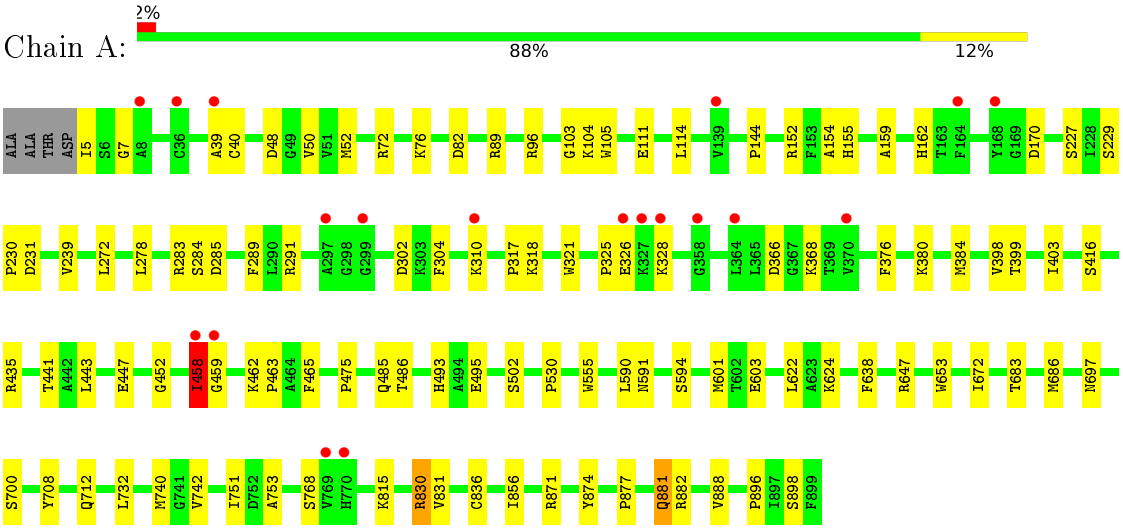
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	367	Total O 367 367	0	0
14	B	140	Total O 140 140	0	0
14	C	252	Total O 252 252	0	0
14	D	57	Total O 57 57	0	0
14	E	321	Total O 321 321	0	0
14	F	124	Total O 124 124	0	0

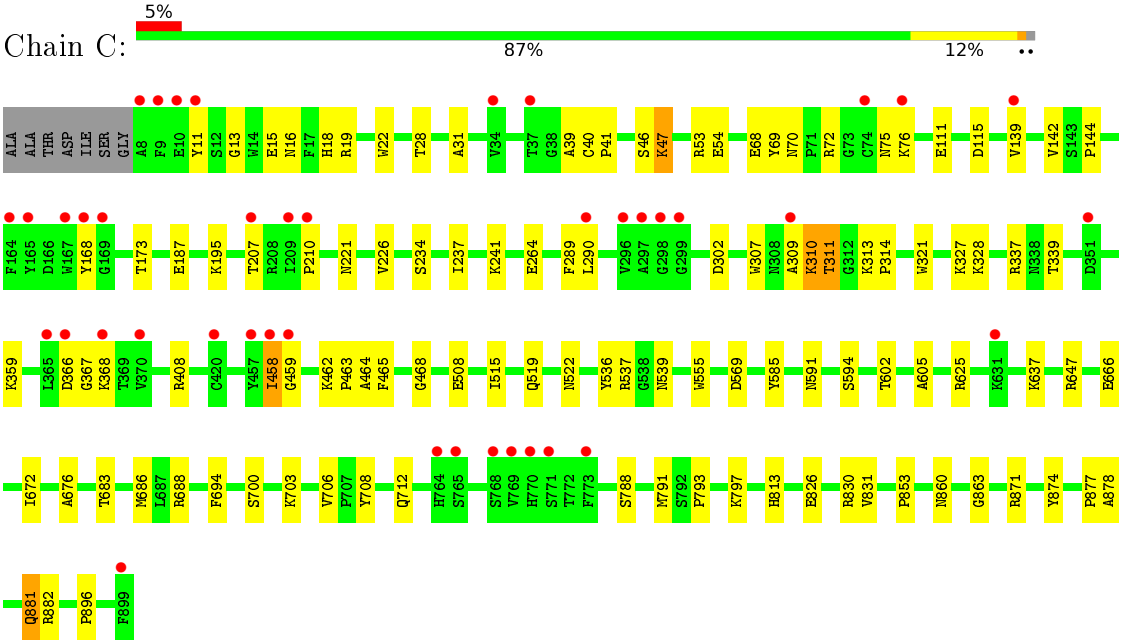
3 Residue-property plots (i)

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 (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

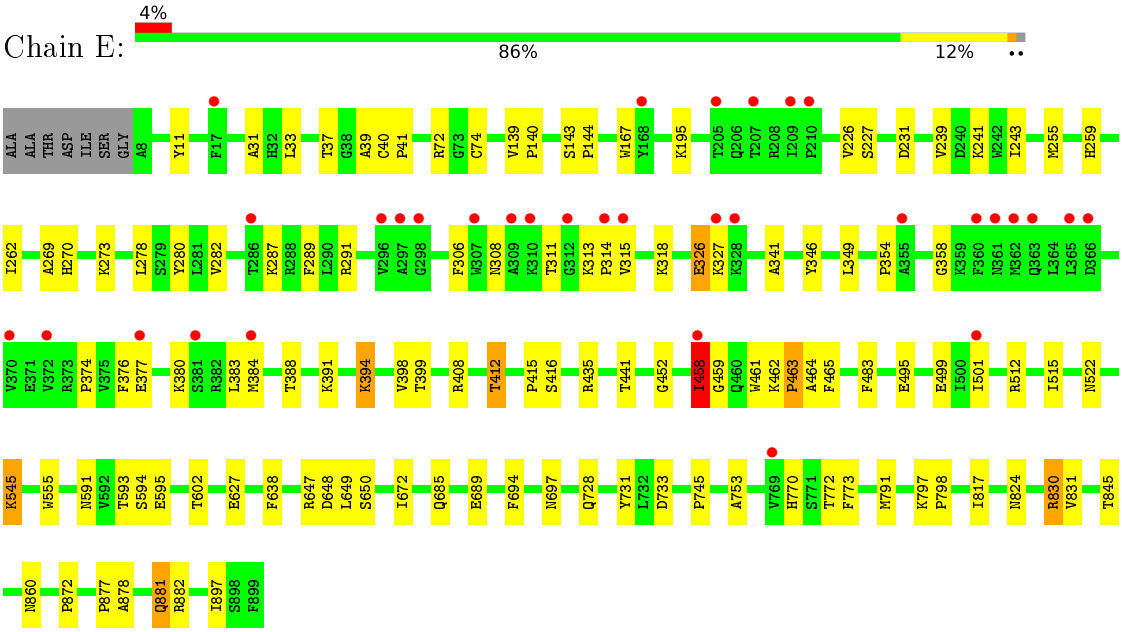


- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



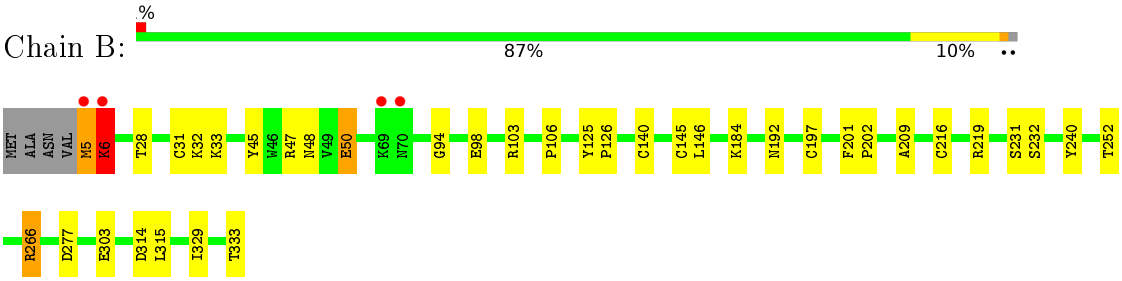
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

Chain E:



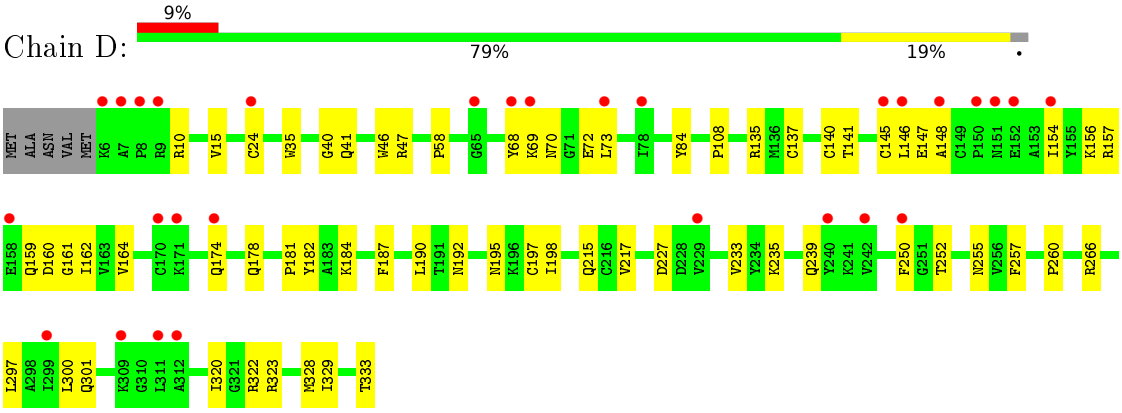
• Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit

Chain B:



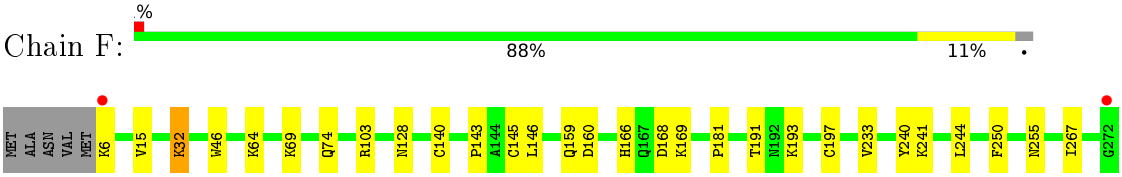
• Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit

Chain D:



• Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit

Chain F:




S275
L282
E286
V296
E305
H308
D314
T333

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	133.93Å 176.02Å 193.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.52 – 2.38 48.52 – 2.38	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.52-2.38) 100.0 (48.52-2.38)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.170 , 0.227 0.181 , 0.231	Depositor DCC
R_{free} test set	9141 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30958	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ZN, BSY, MGD, NA, SF4, EDO, SO3, F3S, 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	0.50	0/7383	0.62	1/10019 (0.0%)
1	C	0.48	0/7357	0.61	0/9984
1	E	0.51	0/7379	0.61	1/10014 (0.0%)
2	B	0.53	0/2632	0.64	1/3567 (0.0%)
2	D	0.44	0/2624	0.57	0/3557
2	F	0.49	0/2624	0.61	0/3557
All	All	0.50	0/29999	0.61	3/40698 (0.0%)

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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	830	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	830	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	B	5	MET	CA-CB-CG	5.02	121.84	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	PRO	Peptide

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	7171	0	6990	67	0
1	C	7148	0	6960	74	0
1	E	7163	0	6975	77	0
2	B	2564	0	2534	33	0
2	D	2556	0	2526	41	0
2	F	2556	0	2525	22	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	0	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	1	0
5	C	47	0	20	2	0
5	E	47	0	20	1	0
6	A	47	0	22	0	0
6	C	47	0	22	0	0
6	E	47	0	22	3	0
7	A	40	0	60	7	0
7	B	20	0	30	16	0
7	C	16	0	24	1	0
7	D	4	0	6	1	0
7	E	8	0	12	1	0
7	F	8	0	12	0	0
8	A	4	0	0	2	0
8	C	4	0	0	3	0
8	E	4	0	0	2	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
9	E	4	0	0	0	0
10	A	2	0	0	0	0
10	B	1	0	0	0	0
10	C	2	0	0	0	0
10	E	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	1	0	0	0	0
11	C	1	0	0	0	0
11	E	1	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	E	6	0	8	0	0
14	A	367	0	0	5	0
14	B	140	0	0	0	0
14	C	252	0	0	5	0
14	D	57	0	0	1	0
14	E	321	0	0	4	0
14	F	124	0	0	2	0
All	All	30958	0	28789	302	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 302 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:881:GLN:HE22	1:A:882:ARG:HE	1.22	0.86
1:E:697:ASN:HD21	7:E:1005:EDO:H11	1.42	0.83
2:F:240:TYR:OH	2:F:314:ASP:OD2	1.96	0.82
1:C:366:ASP:HB2	1:C:368:LYS:H	1.44	0.80
1:C:289:PHE:O	14:C:1101:HOH:O	2.01	0.78

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	894/899 (99%)	861 (96%)	30 (3%)	3 (0%)	46 61
1	C	890/899 (99%)	841 (94%)	44 (5%)	5 (1%)	30 40
1	E	892/899 (99%)	845 (95%)	43 (5%)	4 (0%)	39 53
2	B	327/333 (98%)	314 (96%)	12 (4%)	1 (0%)	46 61
2	D	326/333 (98%)	303 (93%)	23 (7%)	0	100 100
2	F	326/333 (98%)	308 (94%)	18 (6%)	0	100 100
All	All	3655/3696 (99%)	3472 (95%)	170 (5%)	13 (0%)	39 53

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	ILE
2	B	6	LYS
1	C	310	LYS
1	C	311	THR
1	C	47	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	767/768 (100%)	760 (99%)	7 (1%)	84 93
1	C	764/768 (100%)	757 (99%)	7 (1%)	84 93
1	E	766/768 (100%)	756 (99%)	10 (1%)	76 89
2	B	278/281 (99%)	272 (98%)	6 (2%)	60 78
2	D	277/281 (99%)	274 (99%)	3 (1%)	80 91
2	F	277/281 (99%)	273 (99%)	4 (1%)	74 88
All	All	3129/3147 (99%)	3092 (99%)	37 (1%)	78 90

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	465	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	72	GLU
2	F	32	LYS
1	C	555	TRP
1	C	788	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	860	ASN
2	F	62	GLN
1	E	308	ASN
1	C	450	ASN
1	C	881	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 66 ligands modelled in this entry, 14 are monoatomic - leaving 52 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	5.96	29 (70%)	39,81,81	3.73	17 (43%)
6	MD1	A	1004	4	40,51,51	3.74	15 (37%)	34,78,78	1.56	6 (17%)
7	EDO	A	1005	-	3,3,3	0.61	0	2,2,2	0.11	0
7	EDO	A	1006	-	3,3,3	0.49	0	2,2,2	0.53	0
7	EDO	A	1007	-	3,3,3	0.44	0	2,2,2	0.81	0
7	EDO	A	1008	-	3,3,3	0.62	0	2,2,2	0.46	0
7	EDO	A	1009	-	3,3,3	0.62	0	2,2,2	0.58	0
7	EDO	A	1010	-	3,3,3	1.12	0	2,2,2	1.18	0
7	EDO	A	1011	-	3,3,3	0.50	0	2,2,2	0.48	0
7	EDO	A	1012	-	3,3,3	0.68	0	2,2,2	0.42	0
8	BSY	A	1013	-	0,3,3	0.00	-	1,3,3	3.32	1 (100%)
9	SO3	A	1014	11	1,3,3	0.92	0	0,3,3	0.00	-
7	EDO	A	1018	-	3,3,3	0.53	0	2,2,2	0.60	0
7	EDO	A	1019	-	3,3,3	0.71	0	2,2,2	0.23	0
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	0.41	0	2,2,2	0.40	0
7	EDO	B	407	-	3,3,3	0.80	0	2,2,2	0.13	0
7	EDO	B	408	-	3,3,3	0.64	0	2,2,2	0.65	0
7	EDO	B	409	-	3,3,3	0.96	0	2,2,2	0.81	0
7	EDO	B	410	-	3,3,3	0.38	0	2,2,2	0.38	0
3	SF4	C	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	C	1003	4	41,52,52	5.88	28 (68%)	39,81,81	4.25	17 (43%)
6	MD1	C	1004	4	40,51,51	3.62	15 (37%)	34,78,78	1.45	7 (20%)
7	EDO	C	1005	-	3,3,3	0.74	0	2,2,2	0.34	0
7	EDO	C	1006	-	3,3,3	0.63	0	2,2,2	0.13	0
7	EDO	C	1007	-	3,3,3	0.50	0	2,2,2	1.33	0
7	EDO	C	1008	-	3,3,3	0.48	0	2,2,2	0.50	0
8	BSY	C	1009	-	0,3,3	0.00	-	1,3,3	4.71	1 (100%)
9	SO3	C	1010	11	1,3,3	0.65	0	0,3,3	0.00	-
12	F3S	D	401	2	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	D	402	2	0,12,12	0.00	-	0,24,24	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	-
7	EDO	D	405	-	3,3,3	0.48	0	2,2,2	0.23	0
3	SF4	E	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	E	1003	4	41,52,52	5.93	25 (60%)	39,81,81	4.02	15 (38%)
6	MD1	E	1004	4	40,51,51	3.50	15 (37%)	34,78,78	1.47	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	E	1005	-	3,3,3	0.69	0	2,2,2	0.43	0
13	GOL	E	1006	-	5,5,5	0.50	0	5,5,5	0.83	0
7	EDO	E	1007	-	3,3,3	0.44	0	2,2,2	0.93	0
8	BSY	E	1008	-	0,3,3	0.00	-	1,3,3	3.76	1 (100%)
9	SO3	E	1009	11	1,3,3	0.88	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	0.49	0	2,2,2	0.36	0
7	EDO	F	406	-	3,3,3	0.81	0	2,2,2	0.23	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
7	EDO	A	1008	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1009	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1010	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1011	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1012	-	-	0/1/1/1	0/0/0/0
8	BSY	A	1013	-	-	0/0/0/0	0/0/0/0
9	SO3	A	1014	11	-	0/0/0/0	0/0/0/0
7	EDO	A	1018	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1019	-	-	0/1/1/1	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	407	-	-	0/1/1/1	0/0/0/0
7	EDO	B	408	-	-	0/1/1/1	0/0/0/0
7	EDO	B	409	-	-	0/1/1/1	0/0/0/0
7	EDO	B	410	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
7	EDO	C	1007	-	-	0/1/1/1	0/0/0/0
7	EDO	C	1008	-	-	0/1/1/1	0/0/0/0
8	BSY	C	1009	-	-	0/0/0/0	0/0/0/0
9	SO3	C	1010	11	-	0/0/0/0	0/0/0/0
12	F3S	D	401	2	-	0/0/24/24	0/0/3/3
3	SF4	D	402	2	-	0/0/48/48	0/6/5/5
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
7	EDO	D	405	-	-	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
13	GOL	E	1006	-	-	0/4/4/4	0/0/0/0
7	EDO	E	1007	-	-	0/1/1/1	0/0/0/0
8	BSY	E	1008	-	-	0/0/0/0	0/0/0/0
9	SO3	E	1009	11	-	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
7	EDO	F	406	-	-	0/1/1/1	0/0/0/0

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1003	MGD	C23-C14	-21.24	1.37	1.53
5	A	1003	MGD	C23-C14	-20.42	1.38	1.53
5	C	1003	MGD	C23-C14	-20.41	1.38	1.53
5	C	1003	MGD	C2'-C3'	-10.29	1.25	1.53
5	A	1003	MGD	C2'-C3'	-9.98	1.26	1.53

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1003	MGD	N3-C2-N1	-7.02	118.01	127.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1003	MGD	C4'-O4'-C1'	-7.02	102.21	109.64
5	C	1003	MGD	N3-C2-N1	-6.02	119.36	127.56
5	E	1003	MGD	N3-C2-N1	-5.80	119.67	127.56
5	E	1003	MGD	C4'-O4'-C1'	-4.34	105.05	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1003	MGD	1	0
7	A	1005	EDO	1	0
7	A	1010	EDO	5	0
7	A	1012	EDO	1	0
8	A	1013	BSY	2	0
7	B	407	EDO	2	0
7	B	408	EDO	5	0
7	B	409	EDO	3	0
7	B	410	EDO	6	0
5	C	1003	MGD	2	0
7	C	1007	EDO	1	0
8	C	1009	BSY	3	0
3	D	404	SF4	1	0
7	D	405	EDO	1	0
5	E	1003	MGD	1	0
6	E	1004	MD1	3	0
7	E	1005	EDO	1	0
8	E	1008	BSY	2	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^{th} 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	895/899 (99%)	-0.09	19 (2%) 67 70	19, 32, 51, 66	0
1	C	892/899 (99%)	0.05	41 (4%) 36 41	21, 37, 58, 96	0
1	E	892/899 (99%)	-0.04	33 (3%) 45 49	18, 33, 61, 77	0
2	B	329/333 (98%)	-0.34	4 (1%) 81 83	20, 27, 41, 88	0
2	D	328/333 (98%)	0.56	29 (8%) 12 14	26, 52, 70, 92	0
2	F	328/333 (98%)	-0.15	2 (0%) 90 91	22, 35, 53, 65	0
All	All	3664/3696 (99%)	-0.01	128 (3%) 48 52	18, 34, 60, 96	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	PHE	9.6
1	C	8	ALA	8.4
2	B	5	MET	7.2
2	B	6	LYS	4.4
1	C	298	GLY	4.3

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 (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. 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^{th} 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
7	EDO	A	1010	4/4	0.69	0.47	11.96	33,35,36,40	0
7	EDO	B	409	4/4	0.79	0.25	10.46	26,28,32,33	0
7	EDO	A	1008	4/4	0.85	0.27	9.55	31,36,38,40	0
7	EDO	B	407	4/4	0.77	0.26	8.98	29,36,39,43	0
7	EDO	F	406	4/4	0.83	0.22	6.85	28,28,37,41	0
7	EDO	C	1007	4/4	0.85	0.19	6.71	26,32,34,44	0
13	GOL	E	1006	6/6	0.77	0.30	5.68	37,42,45,46	0
7	EDO	C	1006	4/4	0.86	0.26	5.35	47,49,50,52	0
7	EDO	C	1005	4/4	0.85	0.21	4.99	31,39,40,45	0
7	EDO	A	1012	4/4	0.93	0.26	4.78	24,24,27,39	0
7	EDO	F	405	4/4	0.98	0.15	4.69	25,27,30,30	0
7	EDO	A	1009	4/4	0.73	0.23	3.84	33,38,41,43	0
7	EDO	E	1005	4/4	0.82	0.23	3.52	34,35,40,43	0
10	NA	E	1010	1/1	0.99	0.18	3.17	19,19,19,19	0
7	EDO	B	410	4/4	0.95	0.23	3.10	25,30,31,31	0
10	NA	C	1011	1/1	0.99	0.24	2.99	27,27,27,27	0
10	NA	A	1015	1/1	0.96	0.18	2.80	23,23,23,23	0
7	EDO	A	1019	4/4	0.94	0.12	2.22	26,28,29,34	0
9	SO3	A	1014	4/4	0.91	0.15	2.10	50,54,61,82	0
7	EDO	A	1005	4/4	0.92	0.15	2.02	27,28,34,35	0
10	NA	B	406	1/1	0.94	0.13	1.70	44,44,44,44	0
7	EDO	A	1018	4/4	0.83	0.22	1.64	44,44,45,47	0
7	EDO	B	408	4/4	0.93	0.20	1.60	27,30,30,32	0
9	SO3	E	1009	4/4	0.91	0.13	1.32	52,52,70,86	0
8	BSY	A	1013	4/4	0.96	0.27	1.06	31,35,43,64	4
7	EDO	A	1007	4/4	0.95	0.13	0.67	28,31,33,35	0
7	EDO	B	405	4/4	0.98	0.11	0.65	22,22,24,24	0
7	EDO	A	1006	4/4	0.93	0.16	0.57	35,36,39,39	0
7	EDO	A	1011	4/4	0.96	0.12	0.54	28,28,32,32	0
8	BSY	E	1008	4/4	0.97	0.23	0.51	34,35,38,59	4
5	MGD	C	1003	47/47	0.97	0.24	0.34	18,27,32,35	0
5	MGD	A	1003	47/47	0.98	0.19	0.12	17,24,28,30	0
5	MGD	E	1003	47/47	0.96	0.19	0.11	19,28,33,36	0
6	MD1	A	1004	47/47	0.98	0.16	-0.02	20,27,31,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	EDO	E	1007	4/4	0.92	0.10	-0.04	38,42,43,43	0
6	MD1	E	1004	47/47	0.98	0.16	-0.08	19,25,32,34	0
3	SF4	F	404	8/8	0.98	0.11	-0.13	26,28,30,31	0
6	MD1	C	1004	47/47	0.97	0.17	-0.27	22,28,33,35	0
3	SF4	B	404	8/8	0.99	0.11	-0.40	22,23,24,26	0
3	SF4	B	402	8/8	0.98	0.08	-0.52	21,25,27,29	0
9	SO3	C	1010	4/4	0.88	0.12	-0.59	60,65,68,83	0
3	SF4	D	403	8/8	0.98	0.14	-0.62	40,42,48,52	0
10	NA	E	1011	1/1	0.97	0.11	-0.69	25,25,25,25	0
7	EDO	D	405	4/4	0.97	0.10	-0.88	30,32,34,36	0
3	SF4	E	1001	8/8	0.99	0.13	-1.01	21,25,28,29	0
8	BSY	C	1009	4/4	0.98	0.23	-1.27	33,35,39,51	4
3	SF4	F	403	8/8	0.98	0.13	-1.27	25,31,35,39	0
3	SF4	A	1001	8/8	0.99	0.15	-1.46	21,23,27,27	0
3	SF4	D	404	8/8	0.97	0.10	-1.46	38,45,52,53	0
3	SF4	C	1001	8/8	0.98	0.15	-1.51	32,34,36,38	0
3	SF4	B	403	8/8	0.99	0.12	-2.39	18,25,28,32	0
12	F3S	F	401	7/7	0.98	0.04	-2.61	29,33,35,36	0
12	F3S	B	401	7/7	0.99	0.05	-2.66	27,29,30,32	0
3	SF4	D	402	8/8	0.94	0.06	-2.87	37,49,57,58	0
12	F3S	D	401	7/7	0.96	0.05	-3.23	52,58,67,67	0
3	SF4	F	402	8/8	0.98	0.07	-3.24	31,34,36,37	0
4	MO	E	1002	1/1	0.99	0.10	-4.41	34,34,34,34	0
4	MO	A	1002	1/1	1.00	0.10	-4.56	35,35,35,35	0
4	MO	C	1002	1/1	1.00	0.12	-5.40	35,35,35,35	0
10	NA	A	1016	1/1	0.94	0.12	-	46,46,46,46	0
11	ZN	C	1013	1/1	0.94	0.07	-	82,82,82,82	0
10	NA	C	1012	1/1	0.96	0.18	-	42,42,42,42	0
7	EDO	C	1008	4/4	0.90	0.26	-	37,40,43,47	0
11	ZN	A	1017	1/1	0.99	0.03	-	57,57,57,57	0
10	NA	E	1012	1/1	0.87	0.18	-	48,48,48,48	0
11	ZN	E	1013	1/1	0.98	0.08	-	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.