



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 18, 2023 – 08:11 PM 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
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) : 2.35.1

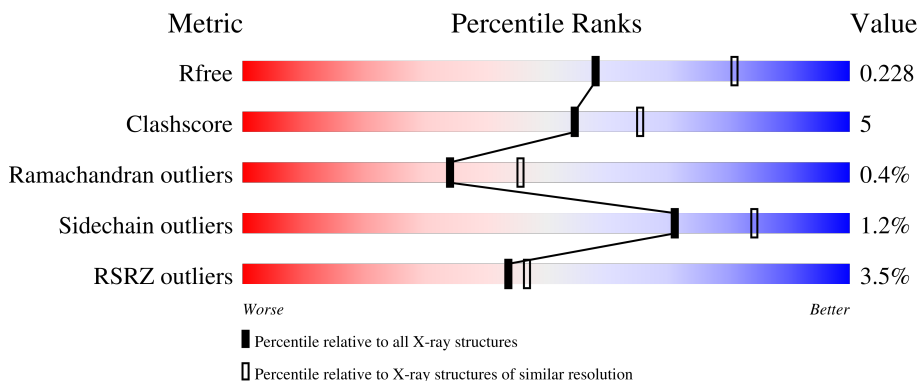
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	899	
1	C	899	
1	E	899	
2	B	333	
2	D	333	

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Mol	Chain	Length	Quality of chain
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
7	EDO	A	1010	-	-	X	X
7	EDO	B	408	-	-	X	-
7	EDO	B	410	-	-	X	-
8	BSY	A	1013	-	-	X	-
8	BSY	C	1009	-	X	X	-
8	BSY	E	1008	-	X	X	-

2 Entry composition

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
			Total	C	N	O	S			
1	A	895	Total 7171	C 4579	N 1243	O 1311	S 38	0	1	0
1	C	892	Total 7148	C 4563	N 1240	O 1307	S 38	0	0	0
1	E	892	Total 7163	C 4575	N 1240	O 1310	S 38	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	329	Total 2564	C 1627	N 447	O 465	S 25	0	0	0
2	D	328	Total 2556	C 1622	N 446	O 464	S 24	0	0	0
2	F	328	Total 2556	C 1622	N 446	O 464	S 24	0	0	0

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

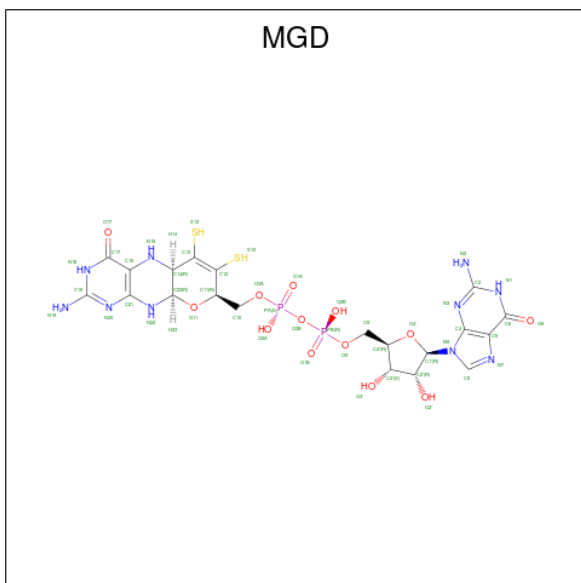


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	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 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-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

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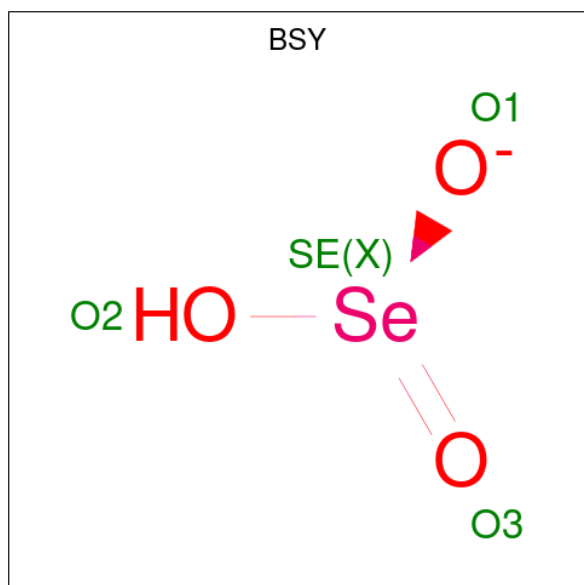
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total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

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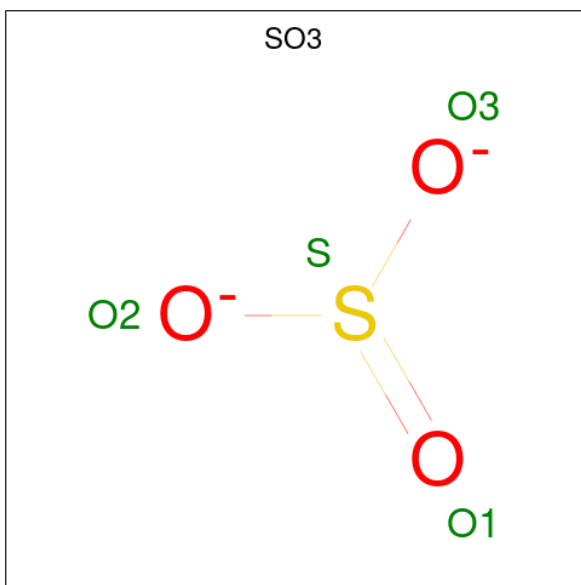
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is BISELENITE ION (three-letter code: BSY) (formula: HO₃Se).



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: O₃S).



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	A	2	Total Na 2 2	0	0
10	B	1	Total Na 1 1	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).

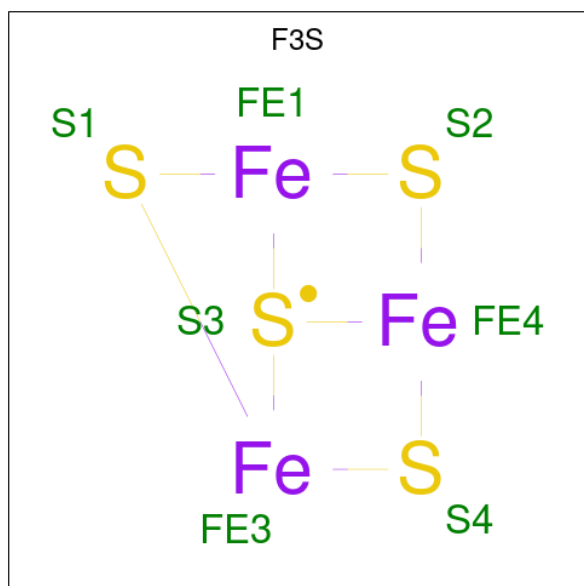
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Zn 1 1	0	0
11	C	1	Total Zn 1 1	0	0

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

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



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



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

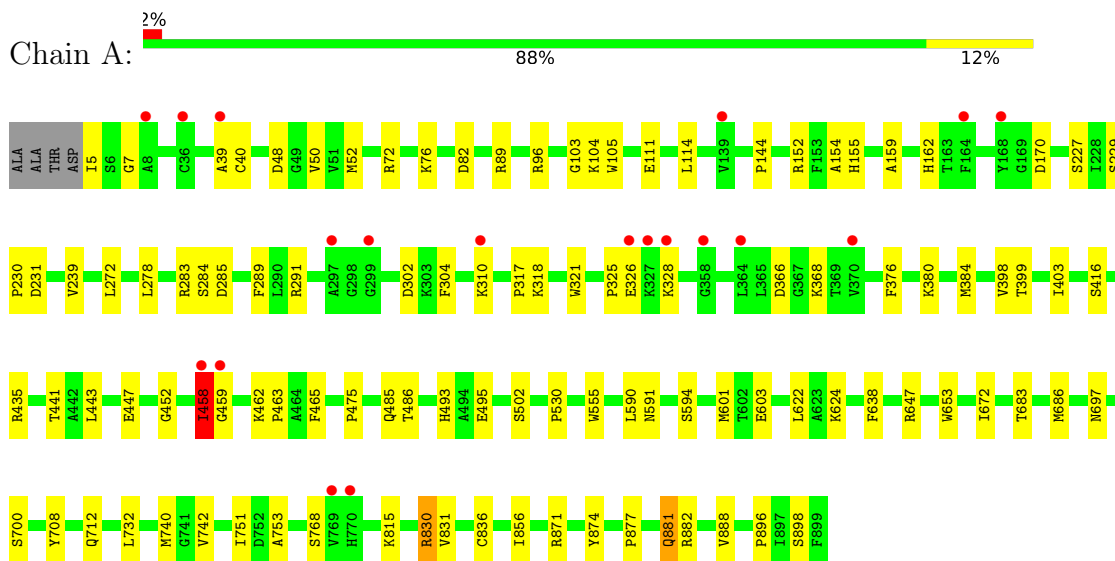
- Molecule 14 is water.

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

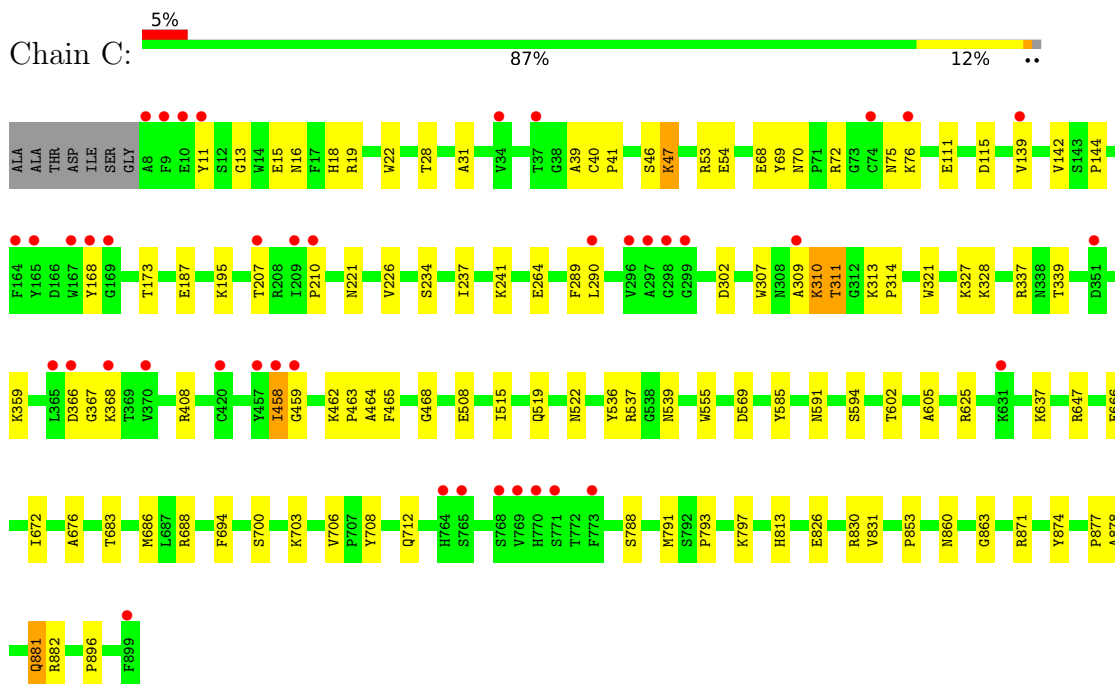
3 Residue-property plots i

These plots are drawn for all protein, RNA, 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.

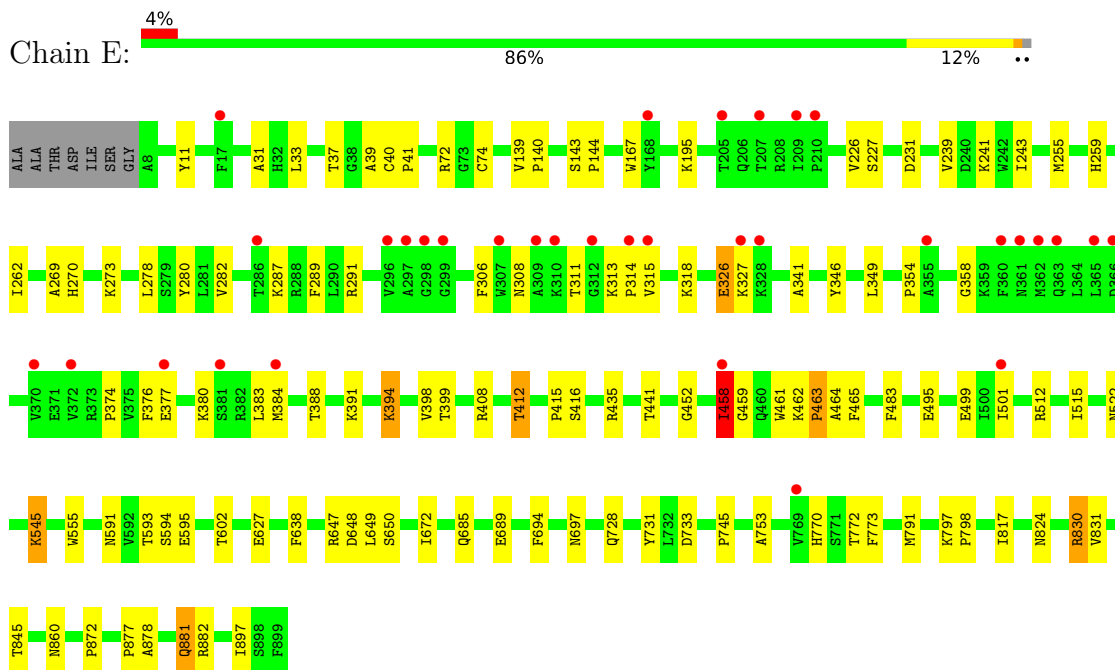
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



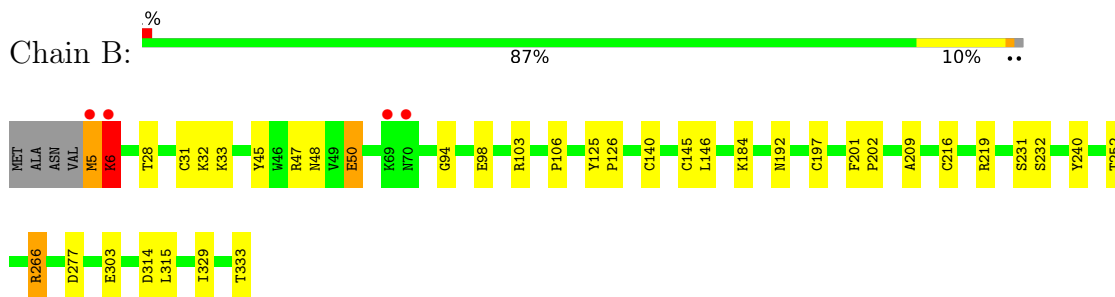
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



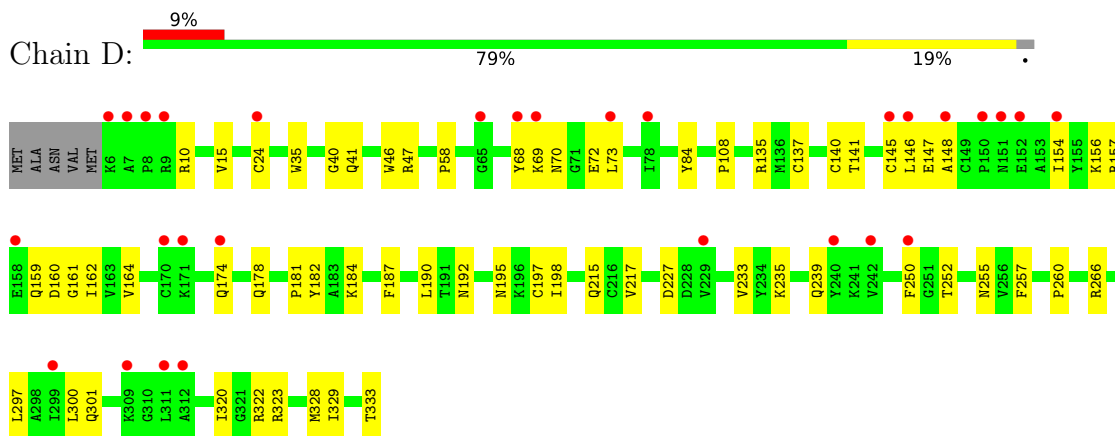
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



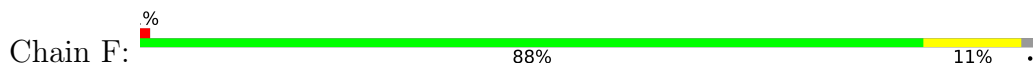
- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



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



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





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.37Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.170 , 0.227 0.173 , 0.228	Depositor DCC
R_{free} test set	9141 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtrriage
Anisotropy	0.373	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MD1, EDO, MGD, NA, BSY, SF4, MO, GOL, F3S, SO3

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($^{\circ}$)	Ideal($^{\circ}$)
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

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

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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%)	41	53
1	C	890/899 (99%)	841 (94%)	44 (5%)	5 (1%)	25	34
1	E	892/899 (99%)	845 (95%)	43 (5%)	4 (0%)	34	46
2	B	327/333 (98%)	314 (96%)	12 (4%)	1 (0%)	41	53
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%)	34	46

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%)	78	89
1	C	764/768 (100%)	757 (99%)	7 (1%)	78	89
1	E	766/768 (100%)	756 (99%)	10 (1%)	69	82
2	B	278/281 (99%)	272 (98%)	6 (2%)	52	69
2	D	277/281 (99%)	274 (99%)	3 (1%)	73	86
2	F	277/281 (99%)	273 (99%)	4 (1%)	67	81
All	All	3129/3147 (99%)	3092 (99%)	37 (1%)	71	84

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

Mol	Chain	Res	Type
1	E	458	ILE

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Mol	Chain	Res	Type
2	F	160	ASP
1	E	465	PHE
1	E	881	GLN
2	B	333	THR

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

Mol	Chain	Res	Type
2	F	62	GLN
1	E	881	GLN
1	C	881	GLN
1	C	860	ASN
1	E	308	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	1001	1	0,12,12	-	-	-		
7	EDO	B	408	-	3,3,3	0.66	0	2,2,2	0.63	0
7	EDO	F	406	-	3,3,3	0.84	0	2,2,2	0.25	0
3	SF4	D	404	2	0,12,12	-	-	-		
6	MD1	C	1004	4	39,51,51	4.14	14 (35%)	38,78,78	1.92	10 (26%)
3	SF4	D	402	2	0,12,12	-	-	-		
9	SO3	E	1009	11	1,3,3	0.77	0	0,3,3	-	-
3	SF4	D	403	2	0,12,12	-	-	-		
7	EDO	A	1011	-	3,3,3	0.52	0	2,2,2	0.41	0
3	SF4	F	404	2	0,12,12	-	-	-		
7	EDO	C	1008	-	3,3,3	0.50	0	2,2,2	0.44	0
7	EDO	F	405	-	3,3,3	0.51	0	2,2,2	0.30	0
5	MGD	C	1003	4	41,52,52	5.67	27 (65%)	40,81,81	2.49	13 (32%)
3	SF4	C	1001	1	0,12,12	-	-	-		
7	EDO	E	1007	-	3,3,3	0.45	0	2,2,2	0.84	0
3	SF4	F	402	2	0,12,12	-	-	-		
3	SF4	B	403	2	0,12,12	-	-	-		
3	SF4	F	403	2	0,12,12	-	-	-		
7	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.34	0
7	EDO	B	407	-	3,3,3	0.84	0	2,2,2	0.17	0
7	EDO	B	409	-	3,3,3	1.00	0	2,2,2	0.82	0
8	BSY	C	1009	-	3,3,3	2.00	1 (33%)	3,3,3	3.26	2 (66%)
6	MD1	A	1004	4	39,51,51	4.12	12 (30%)	38,78,78	1.86	10 (26%)
5	MGD	E	1003	4	41,52,52	5.67	26 (63%)	40,81,81	2.03	12 (30%)
7	EDO	A	1010	-	3,3,3	1.17	0	2,2,2	1.16	0
13	GOL	E	1006	-	5,5,5	0.56	0	5,5,5	0.82	0
7	EDO	A	1008	-	3,3,3	0.64	0	2,2,2	0.41	0
5	MGD	A	1003	4	41,52,52	5.78	28 (68%)	40,81,81	2.68	13 (32%)
7	EDO	A	1009	-	3,3,3	0.64	0	2,2,2	0.53	0
12	F3S	D	401	2	0,9,9	-	-	-		
7	EDO	E	1005	-	3,3,3	0.71	0	2,2,2	0.45	0
3	SF4	B	402	2	0,12,12	-	-	-		
6	MD1	E	1004	4	39,51,51	3.98	14 (35%)	38,78,78	1.95	10 (26%)
7	EDO	C	1007	-	3,3,3	0.51	0	2,2,2	1.22	0
7	EDO	B	410	-	3,3,3	0.39	0	2,2,2	0.31	0
7	EDO	D	405	-	3,3,3	0.49	0	2,2,2	0.18	0
3	SF4	B	404	2	0,12,12	-	-	-		
3	SF4	A	1001	1	0,12,12	-	-	-		
7	EDO	A	1006	-	3,3,3	0.50	0	2,2,2	0.46	0
9	SO3	A	1014	11	1,3,3	0.81	0	0,3,3	-	-
8	BSY	A	1013	-	3,3,3	1.64	1 (33%)	3,3,3	1.67	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	1005	-	3,3,3	0.63	0	2,2,2	0.08	0
9	SO3	C	1010	11	1,3,3	0.56	0	0,3,3	-	-
12	F3S	F	401	2	0,9,9	-	-	-	-	-
7	EDO	C	1005	-	3,3,3	0.77	0	2,2,2	0.36	0
7	EDO	A	1012	-	3,3,3	0.71	0	2,2,2	0.41	0
7	EDO	A	1018	-	3,3,3	0.55	0	2,2,2	0.53	0
7	EDO	A	1019	-	3,3,3	0.73	0	2,2,2	0.21	0
7	EDO	A	1007	-	3,3,3	0.45	0	2,2,2	0.73	0
7	EDO	C	1006	-	3,3,3	0.65	0	2,2,2	0.09	0
8	BSY	E	1008	-	3,3,3	1.86	1 (33%)	3,3,3	2.97	2 (66%)
12	F3S	B	401	2	0,9,9	-	-	-	-	-

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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	408	-	-	0/1/1/1	-
7	EDO	F	406	-	-	1/1/1/1	-
3	SF4	E	1001	1	-	-	0/6/5/5
3	SF4	D	404	2	-	-	0/6/5/5
6	MD1	C	1004	4	-	4/18/59/59	0/5/5/5
3	SF4	D	402	2	-	-	0/6/5/5
3	SF4	D	403	2	-	-	0/6/5/5
7	EDO	A	1011	-	-	0/1/1/1	-
7	EDO	C	1008	-	-	0/1/1/1	-
7	EDO	F	405	-	-	0/1/1/1	-
3	SF4	F	404	2	-	-	0/6/5/5
5	MGD	C	1003	4	-	2/18/66/66	0/6/6/6
3	SF4	C	1001	1	-	-	0/6/5/5
7	EDO	E	1007	-	-	1/1/1/1	-
7	EDO	B	405	-	-	0/1/1/1	-
3	SF4	B	403	2	-	-	0/6/5/5
3	SF4	F	402	2	-	-	0/6/5/5
3	SF4	F	403	2	-	-	0/6/5/5
7	EDO	B	407	-	-	0/1/1/1	-
7	EDO	B	409	-	-	0/1/1/1	-
6	MD1	A	1004	4	-	6/18/59/59	0/5/5/5
5	MGD	E	1003	4	-	3/18/66/66	0/6/6/6
7	EDO	A	1010	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GOL	E	1006	-	-	4/4/4/4	-
7	EDO	A	1008	-	-	1/1/1/1	-
5	MGD	A	1003	4	-	9/18/66/66	0/6/6/6
7	EDO	A	1009	-	-	0/1/1/1	-
12	F3S	D	401	2	-	-	0/3/3/3
7	EDO	E	1005	-	-	0/1/1/1	-
3	SF4	B	402	2	-	-	0/6/5/5
6	MD1	E	1004	4	-	2/18/59/59	0/5/5/5
7	EDO	C	1007	-	-	1/1/1/1	-
7	EDO	B	410	-	-	0/1/1/1	-
7	EDO	D	405	-	-	0/1/1/1	-
3	SF4	B	404	2	-	-	0/6/5/5
3	SF4	A	1001	1	-	-	0/6/5/5
7	EDO	A	1006	-	-	0/1/1/1	-
7	EDO	A	1005	-	-	0/1/1/1	-
12	F3S	F	401	2	-	-	0/3/3/3
7	EDO	C	1005	-	-	0/1/1/1	-
7	EDO	A	1012	-	-	0/1/1/1	-
7	EDO	A	1018	-	-	0/1/1/1	-
7	EDO	A	1019	-	-	0/1/1/1	-
7	EDO	A	1007	-	-	0/1/1/1	-
7	EDO	C	1006	-	-	0/1/1/1	-
12	F3S	B	401	2	-	-	0/3/3/3

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1003	MGD	C23-C14	-19.99	1.37	1.53
5	A	1003	MGD	C23-C14	-19.22	1.38	1.53
5	C	1003	MGD	C23-C14	-19.21	1.38	1.53
5	A	1003	MGD	C16-C21	15.19	1.64	1.38
5	E	1003	MGD	C16-C21	14.80	1.63	1.38

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	MGD	O11-C23-N22	-12.52	95.70	108.57
5	C	1003	MGD	O11-C23-N22	-10.64	97.63	108.57
5	E	1003	MGD	O11-C23-N22	-7.61	100.75	108.57
6	E	1004	MD1	N3-C2-N1	-5.89	119.37	127.22
6	C	1004	MD1	N3-C2-N1	-5.56	119.80	127.22

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1003	MGD	C5'-O5'-PB-O1B
5	A	1003	MGD	C5'-O5'-PB-O3B
6	E	1004	MD1	PB-O3B-PA-O5'
7	A	1008	EDO	O1-C1-C2-O2
13	E	1006	GOL	O1-C1-C2-C3

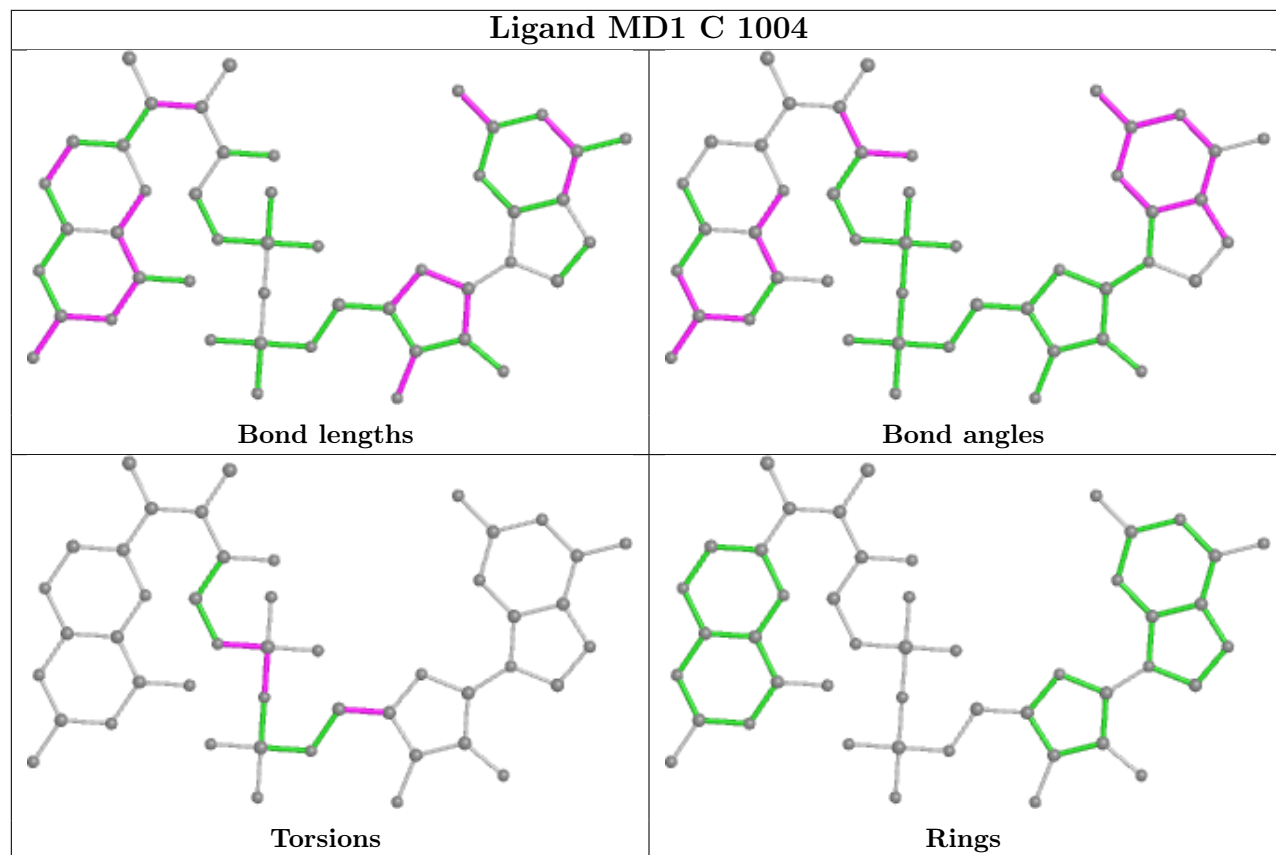
There are no ring outliers.

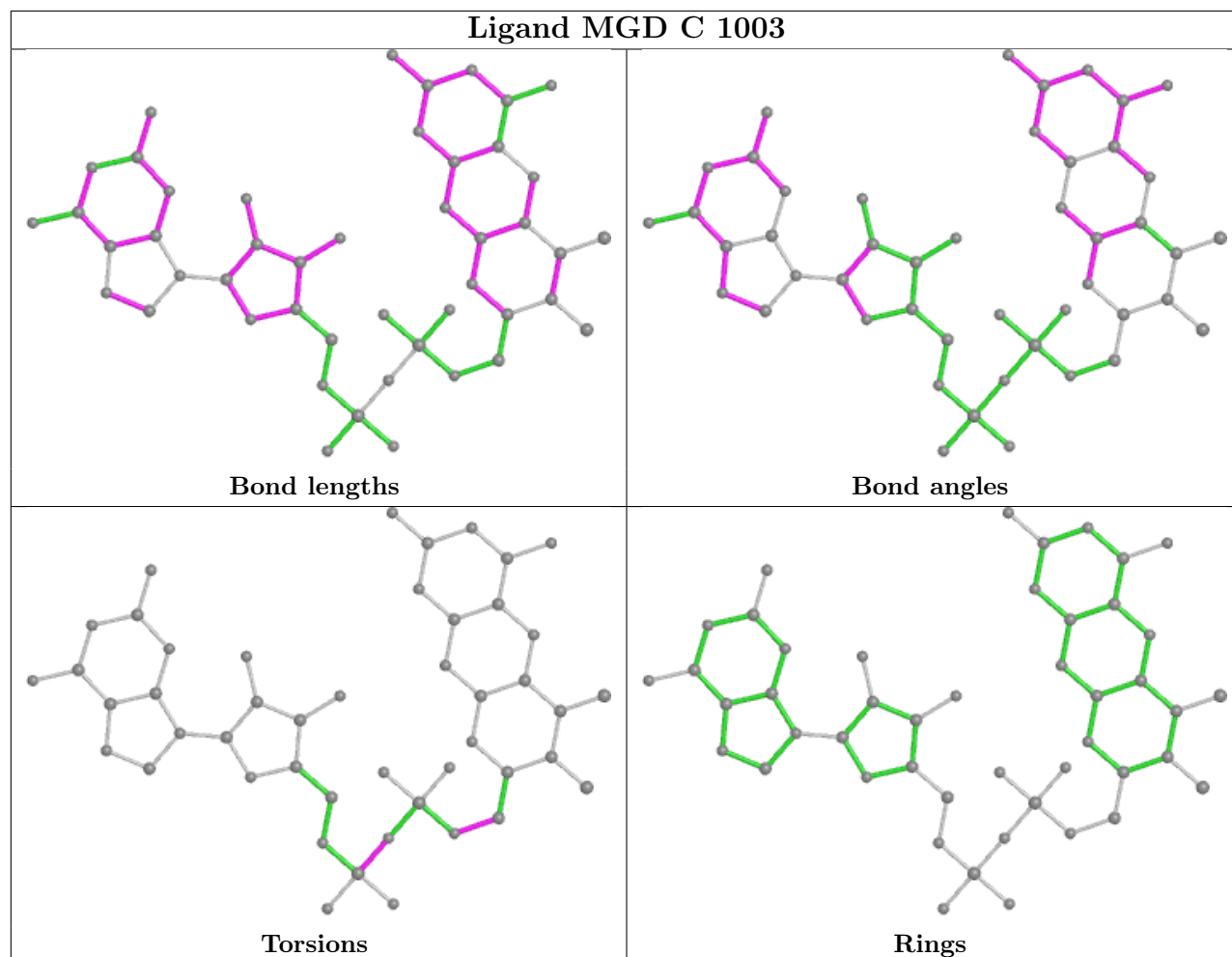
18 monomers are involved in 41 short contacts:

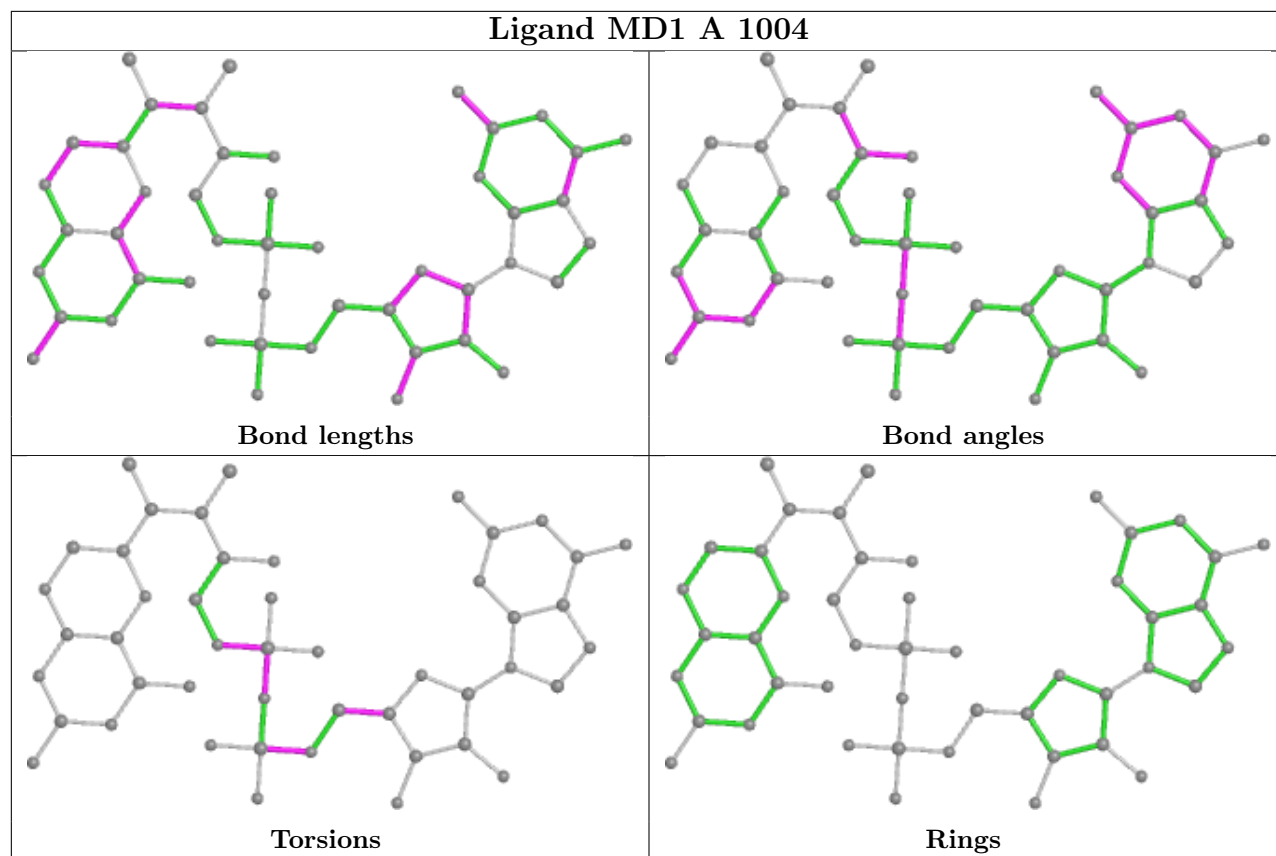
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	408	EDO	5	0
3	D	404	SF4	1	0
5	C	1003	MGD	2	0
7	B	407	EDO	2	0
7	B	409	EDO	3	0
8	C	1009	BSY	3	0
5	E	1003	MGD	1	0
7	A	1010	EDO	5	0
5	A	1003	MGD	1	0
7	E	1005	EDO	1	0
6	E	1004	MD1	3	0
7	C	1007	EDO	1	0
7	B	410	EDO	6	0
7	D	405	EDO	1	0
8	A	1013	BSY	2	0
7	A	1005	EDO	1	0
7	A	1012	EDO	1	0
8	E	1008	BSY	2	0

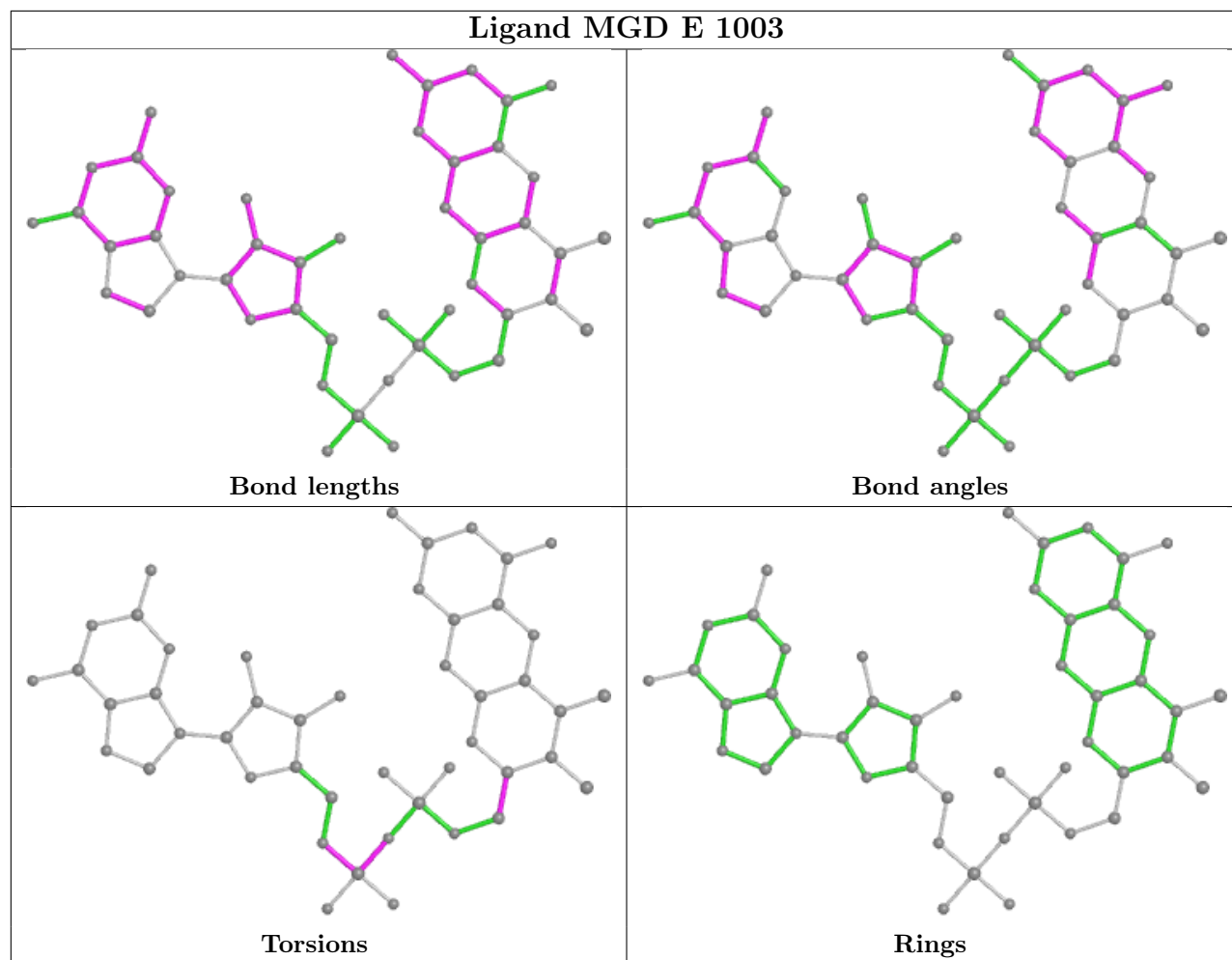
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

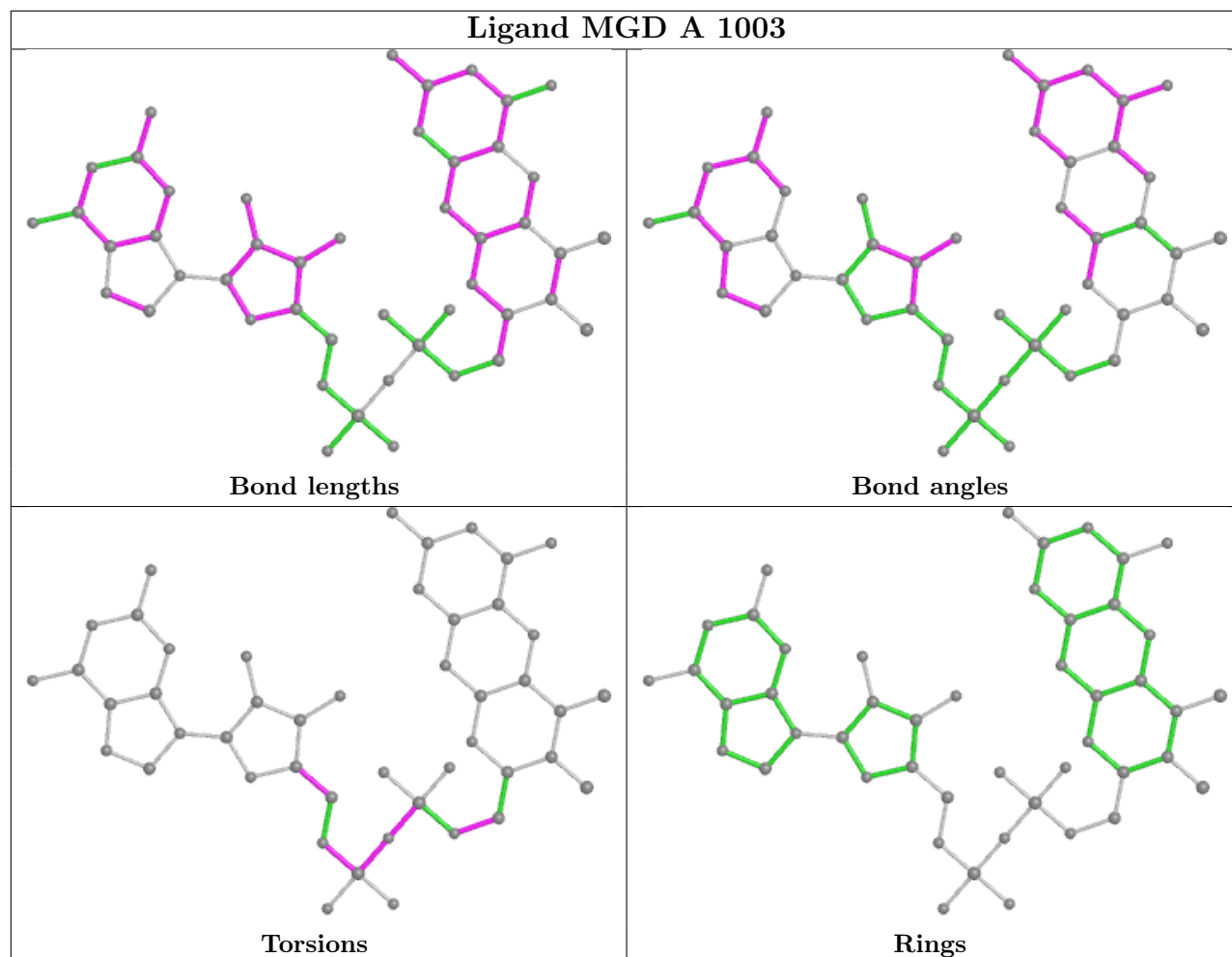
equivalents in the CSD to analyse the geometry.

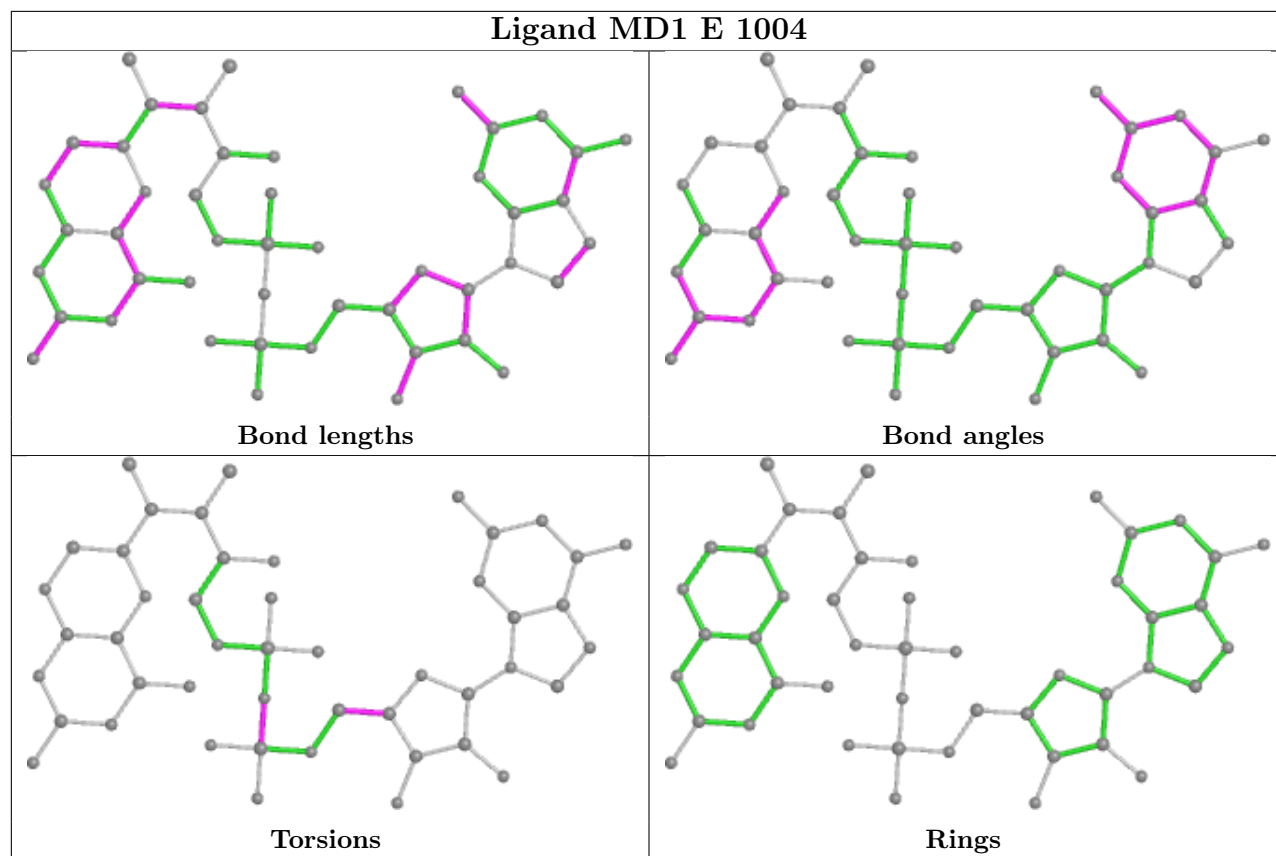












5.7 Other polymers [\(i\)](#)

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	895/899 (99%)	-0.09	19 (2%) 63 65	19, 32, 51, 66	0
1	C	892/899 (99%)	0.05	41 (4%) 32 35	21, 37, 58, 96	0
1	E	892/899 (99%)	-0.04	34 (3%) 40 43	18, 33, 61, 77	0
2	B	329/333 (98%)	-0.34	4 (1%) 79 80	20, 27, 41, 88	0
2	D	328/333 (98%)	0.56	29 (8%) 10 11	26, 52, 70, 92	0
2	F	328/333 (98%)	-0.15	2 (0%) 89 89	22, 35, 53, 65	0
All	All	3664/3696 (99%)	-0.01	129 (3%) 44 47	18, 34, 60, 96	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	PHE	9.5
1	C	8	ALA	8.4
2	B	5	MET	7.1
2	B	6	LYS	4.5
1	C	298	GLY	4.3

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, 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	B-factors(Å ²)	Q<0.9
7	EDO	A	1010	4/4	0.69	0.48	33,35,36,40	0
7	EDO	A	1009	4/4	0.73	0.22	33,38,41,43	0
7	EDO	B	407	4/4	0.77	0.26	29,36,39,43	0
13	GOL	E	1006	6/6	0.77	0.30	37,42,45,46	0
7	EDO	B	409	4/4	0.79	0.25	26,28,32,33	0
7	EDO	E	1005	4/4	0.82	0.23	34,35,40,43	0
7	EDO	F	406	4/4	0.83	0.22	28,28,37,41	0
7	EDO	A	1018	4/4	0.83	0.22	44,44,45,47	0
7	EDO	C	1007	4/4	0.85	0.19	26,32,34,44	0
7	EDO	C	1005	4/4	0.85	0.21	31,39,40,45	0
7	EDO	A	1008	4/4	0.86	0.27	31,36,38,40	0
7	EDO	C	1006	4/4	0.86	0.26	47,49,50,52	0
10	NA	E	1012	1/1	0.88	0.18	48,48,48,48	0
9	SO3	C	1010	4/4	0.88	0.12	60,65,68,83	0
7	EDO	C	1008	4/4	0.90	0.26	37,40,43,47	0
9	SO3	A	1014	4/4	0.91	0.15	50,54,61,82	0
9	SO3	E	1009	4/4	0.91	0.13	52,52,70,86	0
7	EDO	A	1005	4/4	0.92	0.15	27,28,34,35	0
7	EDO	A	1012	4/4	0.92	0.26	24,24,27,39	0
7	EDO	E	1007	4/4	0.92	0.10	38,42,43,43	0
10	NA	A	1016	1/1	0.93	0.12	46,46,46,46	0
7	EDO	B	408	4/4	0.93	0.20	27,30,30,32	0
7	EDO	A	1006	4/4	0.93	0.17	35,36,39,39	0
3	SF4	D	402	8/8	0.94	0.06	37,49,57,58	0
10	NA	B	406	1/1	0.94	0.13	44,44,44,44	0
7	EDO	B	410	4/4	0.94	0.23	25,30,31,31	0
11	ZN	C	1013	1/1	0.94	0.07	82,82,82,82	0
7	EDO	A	1019	4/4	0.94	0.12	26,28,29,34	0
7	EDO	A	1007	4/4	0.95	0.13	28,31,33,35	0
7	EDO	A	1011	4/4	0.96	0.12	28,28,32,32	0
10	NA	C	1012	1/1	0.96	0.18	42,42,42,42	0
8	BSY	A	1013	4/4	0.96	0.27	31,35,43,64	4
10	NA	A	1015	1/1	0.96	0.18	23,23,23,23	0
12	F3S	D	401	7/7	0.96	0.05	52,58,67,67	0
5	MGD	E	1003	47/47	0.96	0.19	19,28,33,36	0
3	SF4	D	404	8/8	0.97	0.10	38,45,52,53	0
10	NA	E	1011	1/1	0.97	0.10	25,25,25,25	0

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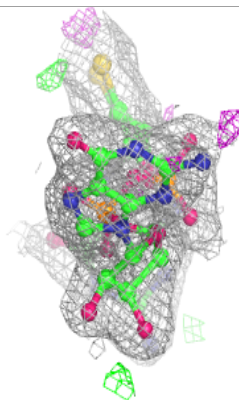
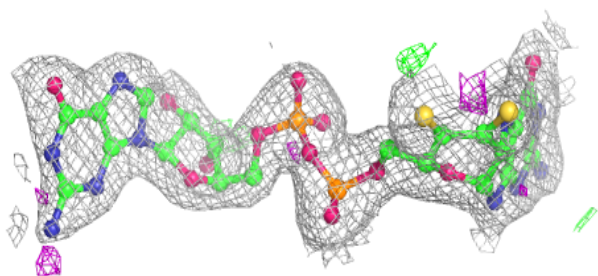
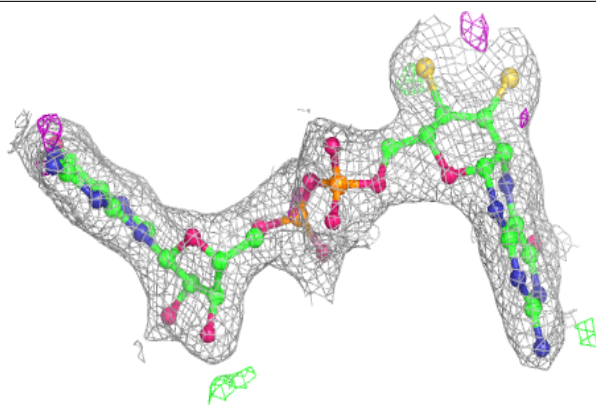
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MD1	C	1004	47/47	0.97	0.17	22,28,33,35	0
7	EDO	D	405	4/4	0.97	0.10	30,32,34,36	0
8	BSY	E	1008	4/4	0.97	0.23	34,35,38,59	4
5	MGD	C	1003	47/47	0.97	0.24	18,27,32,35	0
3	SF4	D	403	8/8	0.98	0.14	40,42,48,52	0
6	MD1	A	1004	47/47	0.98	0.17	20,27,31,35	0
3	SF4	C	1001	8/8	0.98	0.15	32,34,36,38	0
6	MD1	E	1004	47/47	0.98	0.16	19,25,32,34	0
3	SF4	F	402	8/8	0.98	0.07	31,34,36,37	0
7	EDO	B	405	4/4	0.98	0.11	22,22,24,24	0
10	NA	C	1011	1/1	0.98	0.24	27,27,27,27	0
3	SF4	F	403	8/8	0.98	0.13	25,31,35,39	0
7	EDO	F	405	4/4	0.98	0.15	25,27,30,30	0
3	SF4	F	404	8/8	0.98	0.11	26,28,30,31	0
5	MGD	A	1003	47/47	0.98	0.19	17,24,28,30	0
11	ZN	E	1013	1/1	0.98	0.08	52,52,52,52	0
8	BSY	C	1009	4/4	0.98	0.23	33,35,39,51	4
12	F3S	F	401	7/7	0.98	0.04	29,33,35,36	0
3	SF4	B	402	8/8	0.98	0.08	21,25,27,29	0
3	SF4	B	404	8/8	0.99	0.11	22,23,24,26	0
11	ZN	A	1017	1/1	0.99	0.03	57,57,57,57	0
3	SF4	A	1001	8/8	0.99	0.15	21,23,27,27	0
4	MO	E	1002	1/1	0.99	0.10	34,34,34,34	0
12	F3S	B	401	7/7	0.99	0.05	27,29,30,32	0
3	SF4	E	1001	8/8	0.99	0.13	21,25,28,29	0
10	NA	E	1010	1/1	0.99	0.18	19,19,19,19	0
3	SF4	B	403	8/8	0.99	0.12	18,25,28,32	0
4	MO	A	1002	1/1	1.00	0.10	35,35,35,35	0
4	MO	C	1002	1/1	1.00	0.12	35,35,35,35	0

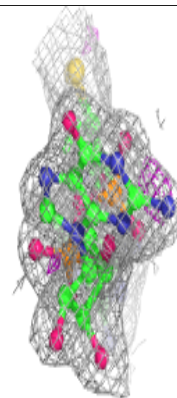
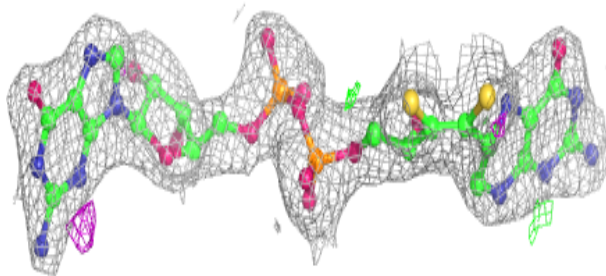
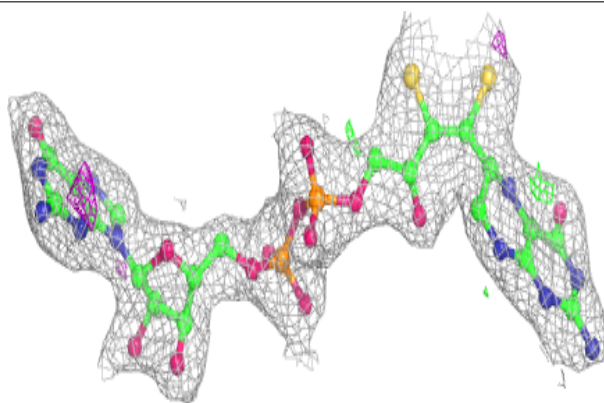
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MGD E 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

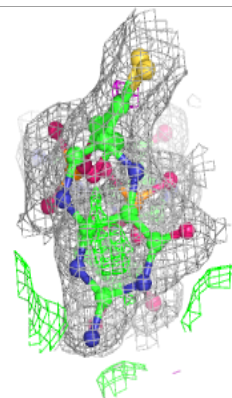
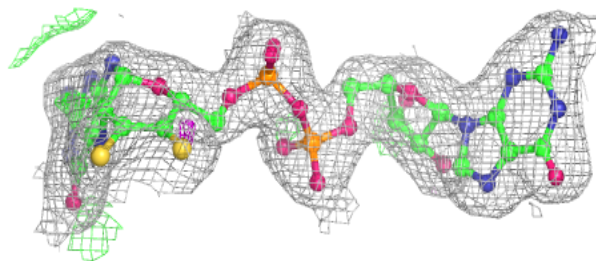
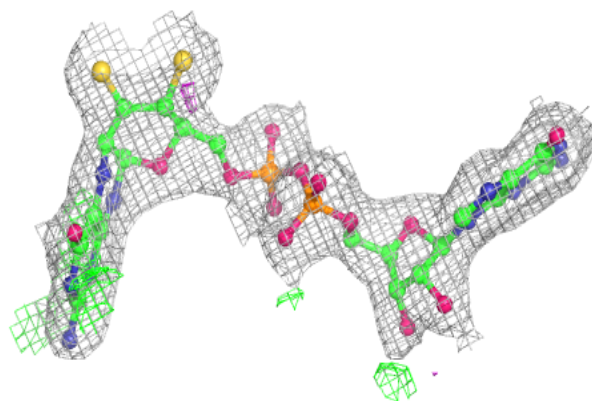
**Electron density around MD1 C 1004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

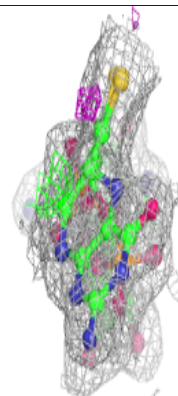
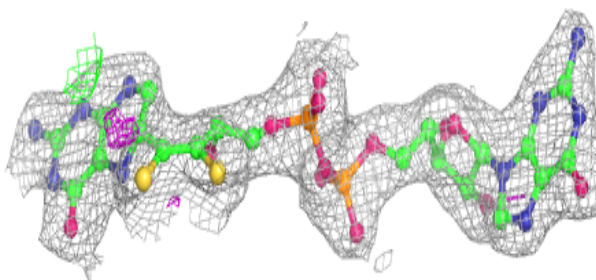
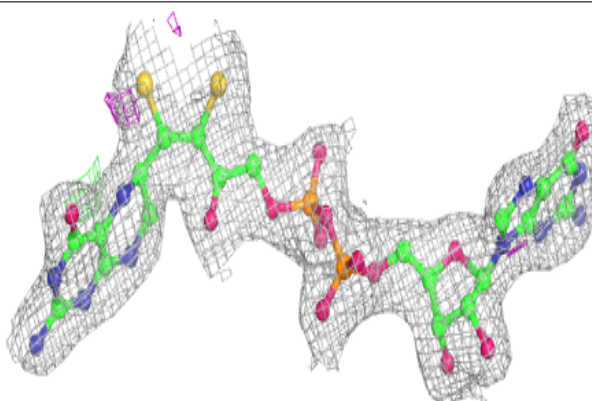


Electron density around MGD C 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

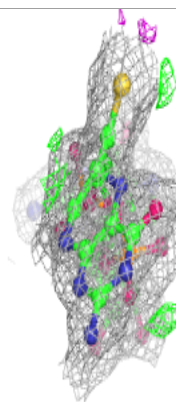
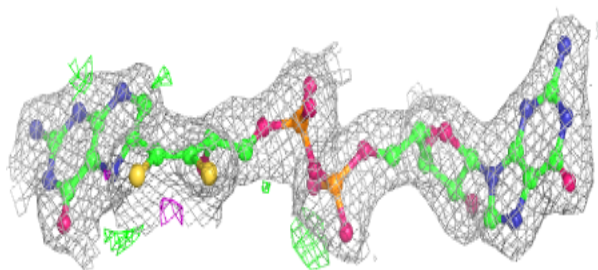
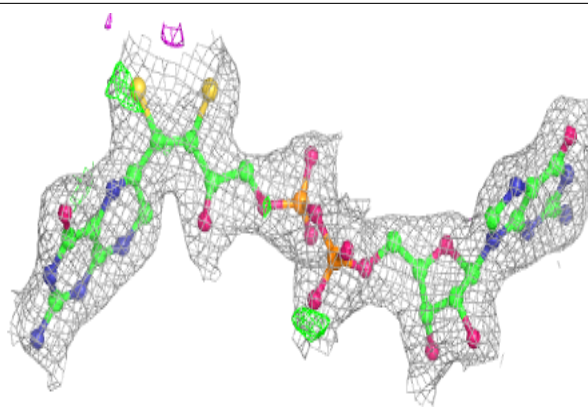
**Electron density around MD1 A 1004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

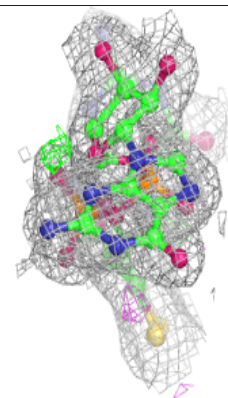
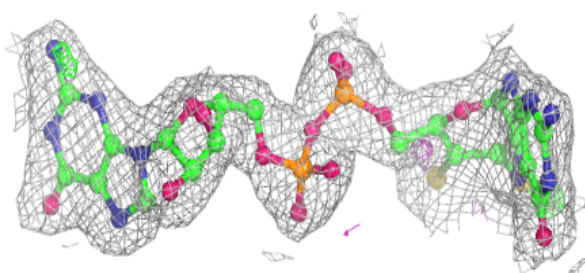
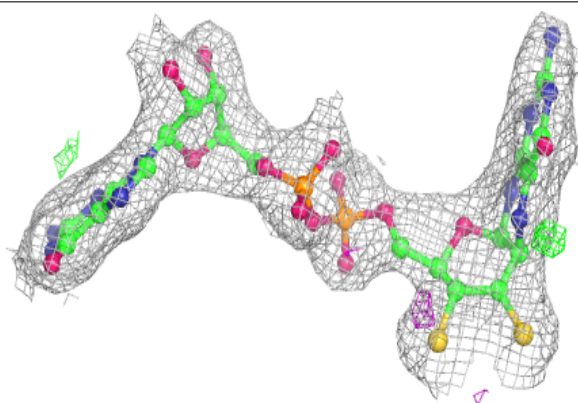


Electron density around MD1 E 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around MGD A 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.