



# wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 08:37 AM UTC

PDB ID : 5CH7 / pdb\_00005ch7  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

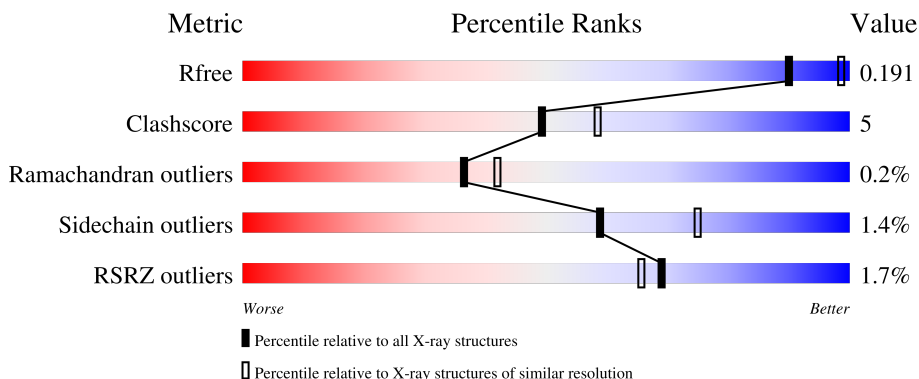
# 1 Overall quality at a glance

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.



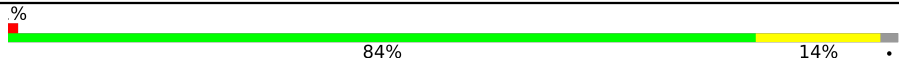
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	899	 89% 10% ..
1	C	899	 84% 15% ..
1	E	899	 86% 12% ..
2	B	333	 90% 8% .
2	D	333	 11% 74% 23% ..

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Mol	Chain	Length	Quality of chain
2	F	333	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left labeled '84%' and a yellow segment on the right labeled '14%'. A small red square is at the start of the bar, and a small grey square is at the end. A '%' symbol is positioned above the start of the bar, and a '.' symbol is positioned below the end of the bar.</p>

## 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
			Total	C	N	O	S			
1	A	894	Total 7180	C 4586	N 1246	O 1310	S 38	0	3	0
1	C	891	Total 7151	C 4568	N 1239	O 1306	S 38	0	1	0
1	E	892	Total 7171	C 4583	N 1240	O 1310	S 38	0	3	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	327	Total 2547	C 1616	N 444	O 463	S 24	0	0	0
2	F	328	Total 2568	C 1631	N 448	O 465	S 24	0	2	0

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

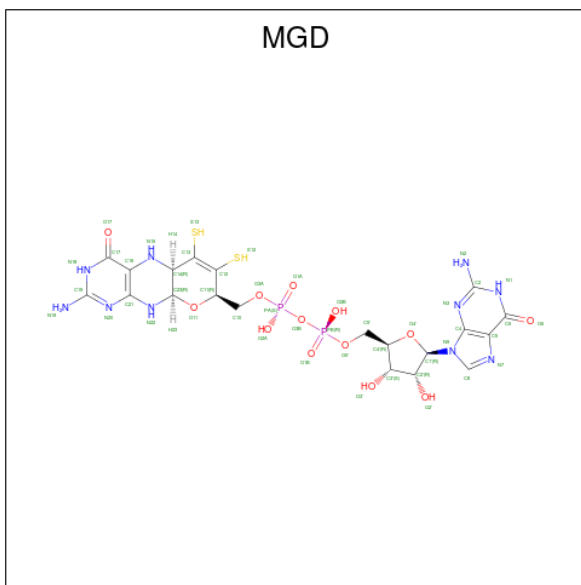


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	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 (CCD ID: MO) (formula: Mo).

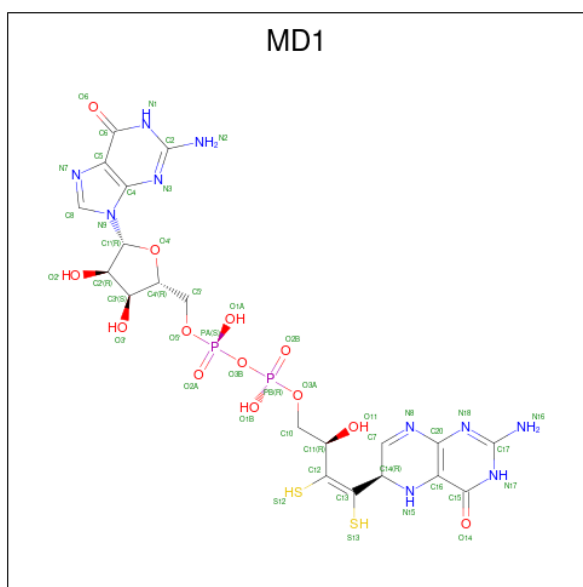
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0

- 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 (CCD ID: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



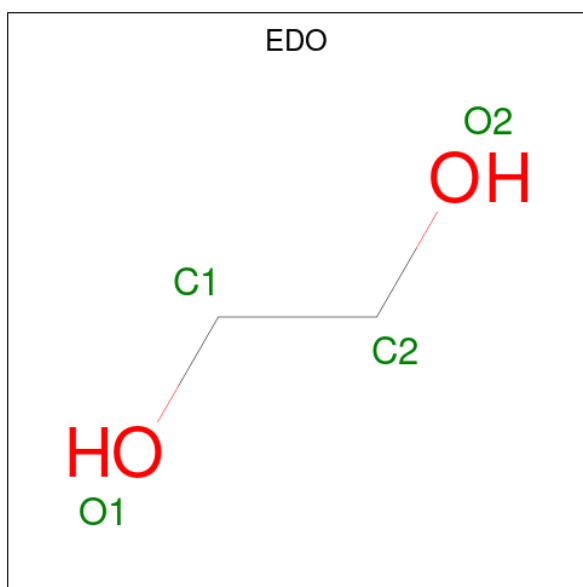
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
5	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- 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 (CCD ID: MD1) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
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 (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

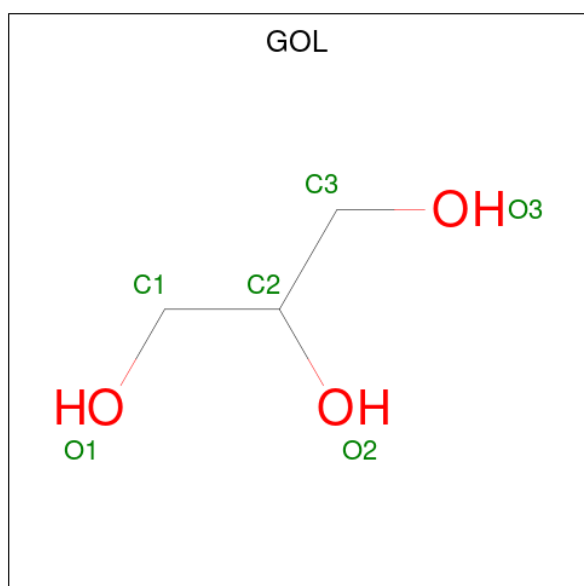
- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

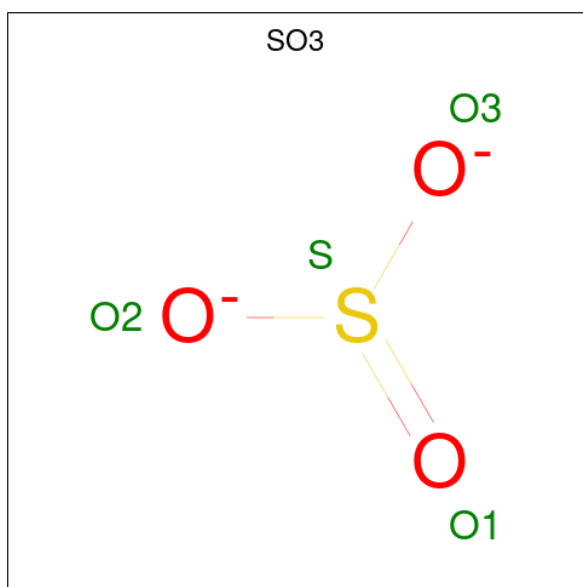
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		
9	C	1	Total	Zn	0	0
			1	1		
9	E	1	Total	Zn	0	0
			1	1		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



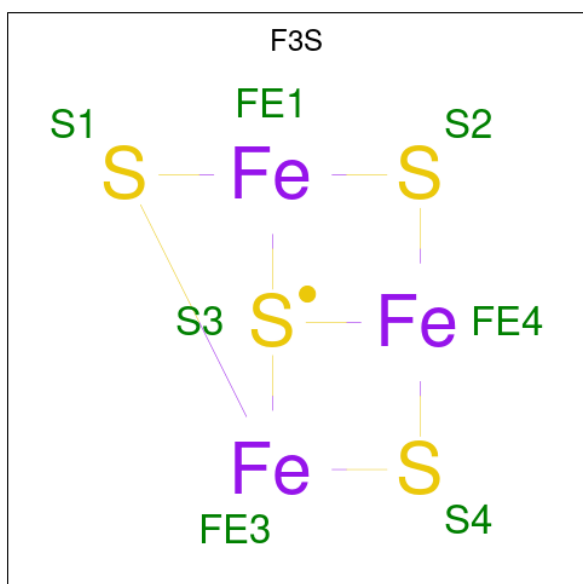
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is SULFITE ION (CCD ID: SO3) (formula: O<sub>3</sub>S).



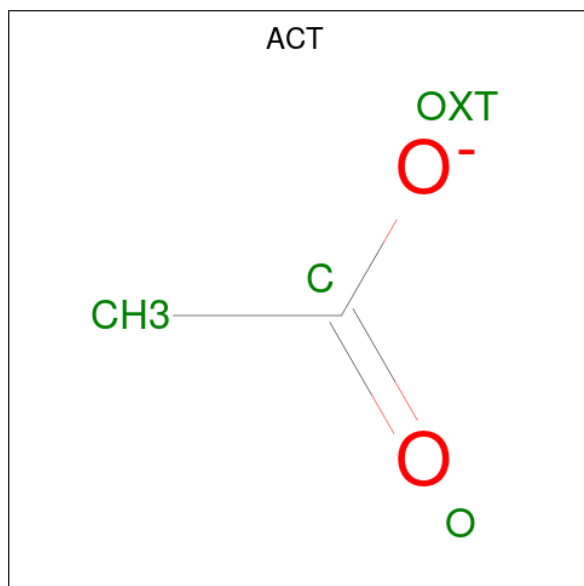
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O S 4 3 1	0	0
11	A	1	Total O S 4 3 1	0	0
11	C	1	Total O S 4 3 1	0	0
11	C	1	Total O S 4 3 1	0	0
11	E	1	Total O S 4 3 1	0	0

- Molecule 12 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



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 ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 14 is water.

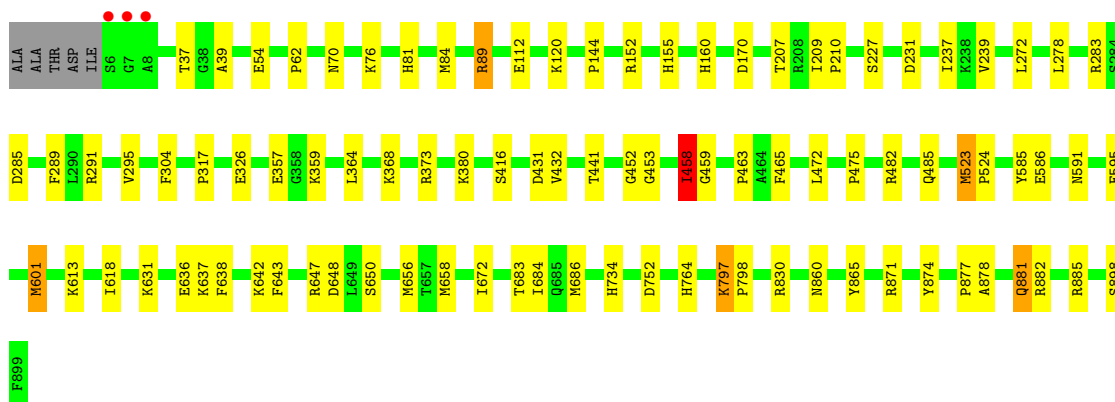
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	531	Total O 531 531	0	0
14	B	273	Total O 273 273	0	0
14	C	362	Total O 362 362	0	0
14	D	92	Total O 92 92	0	0
14	E	520	Total O 520 520	0	0
14	F	198	Total O 198 198	0	0

### 3 Residue-property plots


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.

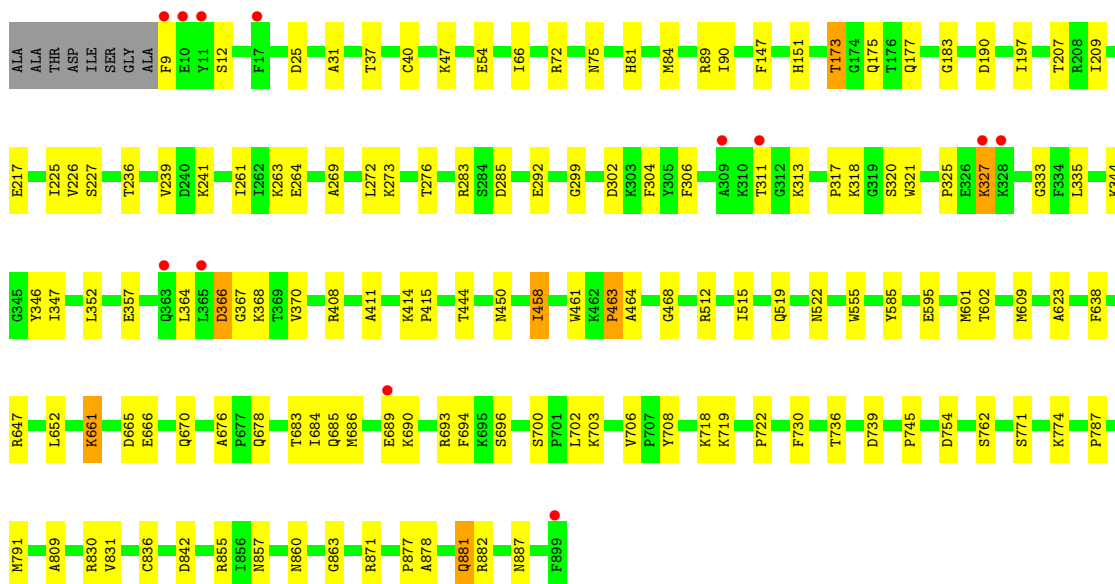
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

Chain A: 



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

Chain C: 



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.178 , 0.233 (Not available) , 0.191	Depositor DCC
$R_{free}$ test set	11303 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.69	0/7399	0.90	5/10039 (0.0%)
1	C	0.62	0/7364	0.88	5/9993 (0.1%)
1	E	0.69	0/7391	0.88	2/10030 (0.0%)
2	B	0.77	0/2632	0.90	1/3567 (0.0%)
2	D	0.55	0/2615	0.91	5/3546 (0.1%)
2	F	0.70	0/2642	0.95	1/3580 (0.0%)
All	All	0.67	0/30043	0.90	19/40755 (0.0%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ILE	CA-C-N	-6.79	112.71	120.04
1	A	209	ILE	C-N-CA	-6.79	112.71	120.04
2	D	161	GLY	N-CA-C	-6.41	106.23	115.27
1	C	857	ASN	CA-C-N	6.22	126.69	119.47
1	C	857	ASN	C-N-CA	6.22	126.69	119.47

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	84	0
1	E	7171	0	6984	79	0
2	B	2564	0	2534	17	0
2	D	2547	0	2513	52	0
2	F	2568	0	2546	29	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	3	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	313	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 313 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:E:860:ASN:HD22	1:E:878:ALA:H	1.32	0.77
2:B:245:PRO:HB2	2:B:254:PRO:HG2	1.69	0.74

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	846/899 (94%)	811 (96%)	33 (4%)	2 (0%)	43	51
1	C	890/899 (99%)	838 (94%)	49 (6%)	3 (0%)	36	42
1	E	893/899 (99%)	850 (95%)	41 (5%)	2 (0%)	43	51
2	B	327/333 (98%)	317 (97%)	9 (3%)	1 (0%)	36	42
2	D	325/333 (98%)	303 (93%)	21 (6%)	1 (0%)	36	42

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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	3609/3696 (98%)	3432 (95%)	168 (5%)	9 (0%)	36	51

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 [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	768/768 (100%)	758 (99%)	10 (1%)	61	76
1	C	765/768 (100%)	751 (98%)	14 (2%)	51	68
1	E	767/768 (100%)	756 (99%)	11 (1%)	59	75
2	B	278/281 (99%)	278 (100%)	0	100	100
2	D	276/281 (98%)	271 (98%)	5 (2%)	51	68
2	F	279/281 (99%)	275 (99%)	4 (1%)	59	75
All	All	3133/3147 (100%)	3089 (99%)	44 (1%)	59	75

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	241	LYS
1	E	398	VAL
1	E	54	GLU
1	E	310	LYS
1	E	458	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	159	GLN
2	D	301	GLN
2	F	215	GLN
1	E	881	GLN
2	F	192	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	F	403	2	0,12,12	-	-	-		
13	ACT	C	1008	-	3,3,3	0.81	0	3,3,3	1.06	0
7	EDO	E	1006	-	3,3,3	0.86	0	2,2,2	0.36	0
11	SO3	C	1010	9	1,3,3	0.80	0	0,3,3	-	-
12	F3S	B	401	2	0,9,9	-	-	-		
7	EDO	A	1007	-	3,3,3	0.53	0	2,2,2	0.21	0
3	SF4	D	403	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MGD	A	1003	4	47,52,52	5.10	23 (48%)	58,81,81	3.29	24 (41%)
3	SF4	F	402	2	0,12,12	-	-	-	-	-
3	SF4	B	403	2	0,12,12	-	-	-	-	-
3	SF4	D	404	2	0,12,12	-	-	-	-	-
3	SF4	D	405	2	0,12,12	-	-	-	-	-
7	EDO	C	1006	-	3,3,3	0.55	0	2,2,2	0.30	0
11	SO3	E	1008	9	1,3,3	1.20	0	0,3,3	-	-
5	MGD	C	1003	4	47,52,52	5.05	24 (51%)	58,81,81	3.03	22 (37%)
7	EDO	B	407	-	3,3,3	0.73	0	2,2,2	0.22	0
7	EDO	B	405	-	3,3,3	0.27	0	2,2,2	0.69	0
3	SF4	E	1001	1	0,12,12	-	-	-	-	-
10	GOL	A	1010	-	5,5,5	0.28	0	5,5,5	0.65	0
12	F3S	F	401	2	0,9,9	-	-	-	-	-
7	EDO	D	401	-	3,3,3	0.69	0	2,2,2	0.18	0
3	SF4	F	404	2	0,12,12	-	-	-	-	-
7	EDO	B	406	-	3,3,3	0.55	0	2,2,2	0.34	0
7	EDO	D	406	-	3,3,3	0.48	0	2,2,2	0.34	0
12	F3S	D	402	2	0,9,9	-	-	-	-	-
7	EDO	A	1005	-	3,3,3	0.76	0	2,2,2	0.37	0
7	EDO	E	1007	-	3,3,3	0.53	0	2,2,2	0.37	0
6	MD1	E	1004	4	47,51,51	2.56	12 (25%)	56,78,78	1.66	14 (25%)
7	EDO	F	406	-	3,3,3	0.48	0	2,2,2	0.53	0
3	SF4	B	404	2	0,12,12	-	-	-	-	-
7	EDO	F	405	-	3,3,3	0.58	0	2,2,2	0.39	0
11	SO3	A	1013	-	1,3,3	0.87	0	0,3,3	-	-
7	EDO	A	1012	-	3,3,3	0.46	0	2,2,2	0.28	0
7	EDO	E	1005	-	3,3,3	0.71	0	2,2,2	0.42	0
7	EDO	C	1005	-	3,3,3	0.74	0	2,2,2	0.28	0
3	SF4	A	1001	1	0,12,12	-	-	-	-	-
11	SO3	A	1011	9	1,3,3	1.04	0	0,3,3	-	-
3	SF4	C	1001	1	0,12,12	-	-	-	-	-
6	MD1	C	1004	4	47,51,51	2.66	12 (25%)	56,78,78	1.74	12 (21%)
11	SO3	C	1009	-	1,3,3	0.77	0	0,3,3	-	-
5	MGD	E	1003	4	47,52,52	4.96	21 (44%)	58,81,81	2.89	20 (34%)
3	SF4	B	402	2	0,12,12	-	-	-	-	-
6	MD1	A	1004	4	47,51,51	2.75	13 (27%)	56,78,78	1.69	13 (23%)
7	EDO	A	1006	-	3,3,3	0.50	0	2,2,2	0.35	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	F	403	2	-	-	0/6/5/5
7	EDO	E	1006	-	-	0/1/1/1	-
12	F3S	B	401	2	-	-	0/3/3/3
7	EDO	A	1007	-	-	1/1/1/1	-
3	SF4	D	403	2	-	-	0/6/5/5
5	MGD	A	1003	4	-	2/22/66/66	0/6/6/6
3	SF4	F	402	2	-	-	0/6/5/5
3	SF4	B	403	2	-	-	0/6/5/5
7	EDO	C	1006	-	-	0/1/1/1	-
3	SF4	D	404	2	-	-	0/6/5/5
3	SF4	D	405	2	-	-	0/6/5/5
5	MGD	C	1003	4	-	1/22/66/66	0/6/6/6
7	EDO	B	407	-	-	0/1/1/1	-
7	EDO	B	405	-	-	0/1/1/1	-
3	SF4	E	1001	1	-	-	0/6/5/5
10	GOL	A	1010	-	-	0/4/4/4	-
12	F3S	F	401	2	-	-	0/3/3/3
7	EDO	D	401	-	-	0/1/1/1	-
7	EDO	B	406	-	-	0/1/1/1	-
7	EDO	D	406	-	-	0/1/1/1	-
3	SF4	F	404	2	-	-	0/6/5/5
12	F3S	D	402	2	-	-	0/3/3/3
7	EDO	A	1005	-	-	0/1/1/1	-
7	EDO	E	1007	-	-	0/1/1/1	-
6	MD1	E	1004	4	-	3/22/59/59	0/5/5/5
7	EDO	F	406	-	-	0/1/1/1	-
7	EDO	F	405	-	-	0/1/1/1	-
3	SF4	B	404	2	-	-	0/6/5/5
7	EDO	A	1012	-	-	0/1/1/1	-
7	EDO	E	1005	-	-	0/1/1/1	-
7	EDO	C	1005	-	-	0/1/1/1	-
3	SF4	A	1001	1	-	-	0/6/5/5
3	SF4	C	1001	1	-	-	0/6/5/5
6	MD1	C	1004	4	-	3/22/59/59	0/5/5/5
5	MGD	E	1003	4	-	4/22/66/66	0/6/6/6
3	SF4	B	402	2	-	-	0/6/5/5
6	MD1	A	1004	4	-	3/22/59/59	0/5/5/5
7	EDO	A	1006	-	-	0/1/1/1	-

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MGD	C23-C14	-19.14	1.38	1.53
5	E	1003	MGD	C23-C14	-19.03	1.38	1.53
5	C	1003	MGD	C23-C14	-18.51	1.38	1.53
5	E	1003	MGD	C16-C21	14.97	1.64	1.38
5	A	1003	MGD	C16-C21	14.72	1.63	1.38

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	MGD	O11-C23-N22	-17.16	93.03	108.61
5	C	1003	MGD	O11-C23-N22	-14.29	95.64	108.61
5	E	1003	MGD	O11-C23-N22	-13.94	95.95	108.61
5	C	1003	MGD	C1'-N9-C8	-7.70	104.86	126.73
5	C	1003	MGD	C1'-N9-C4	7.60	148.95	126.49

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1003	MGD	C5'-O5'-PB-O1B
6	C	1004	MD1	C10-O3A-PB-O1B
6	A	1004	MD1	C10-O3A-PB-O2B
6	C	1004	MD1	C10-O3A-PB-O3B
6	C	1004	MD1	C10-O3A-PB-O2B

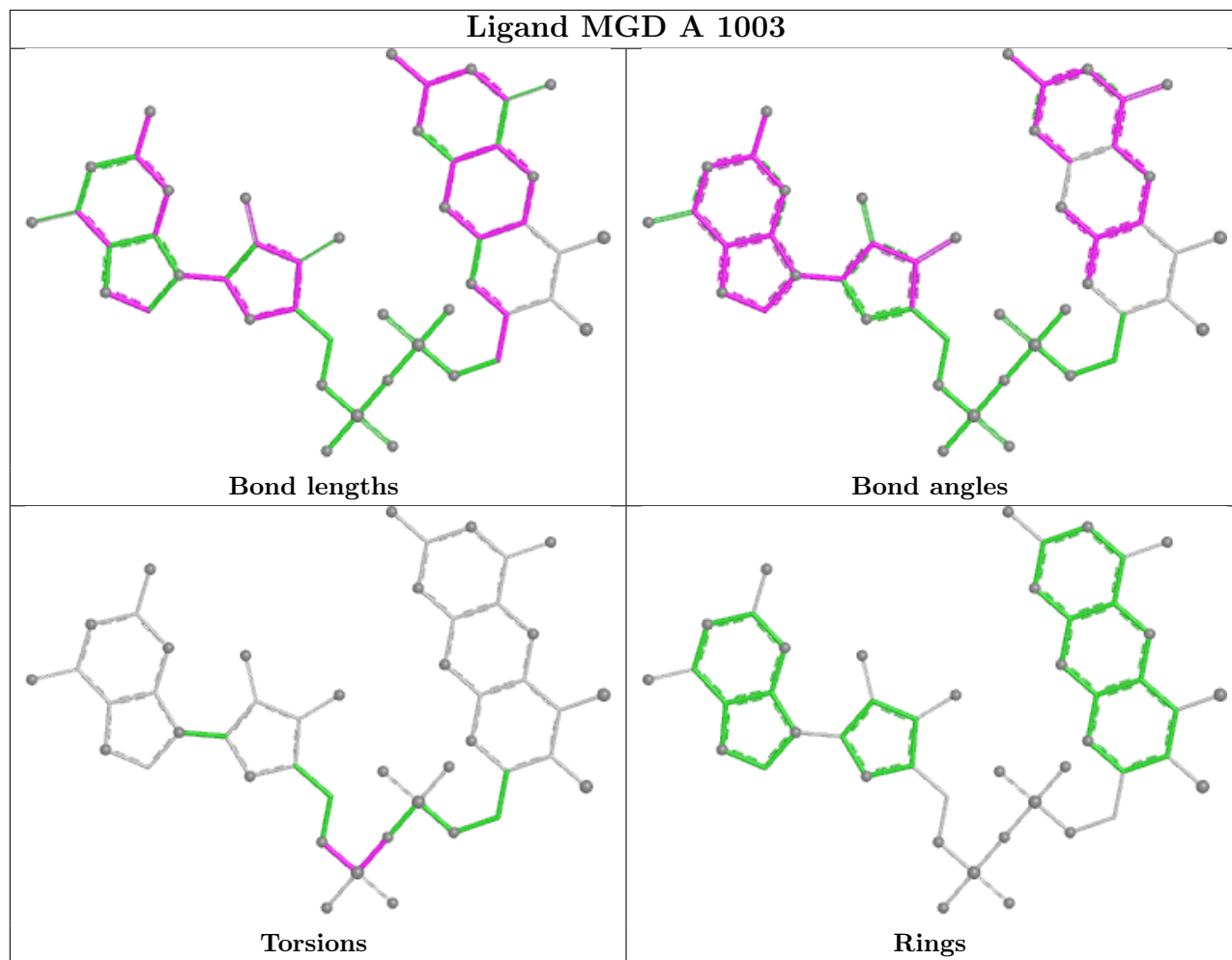
There are no ring outliers.

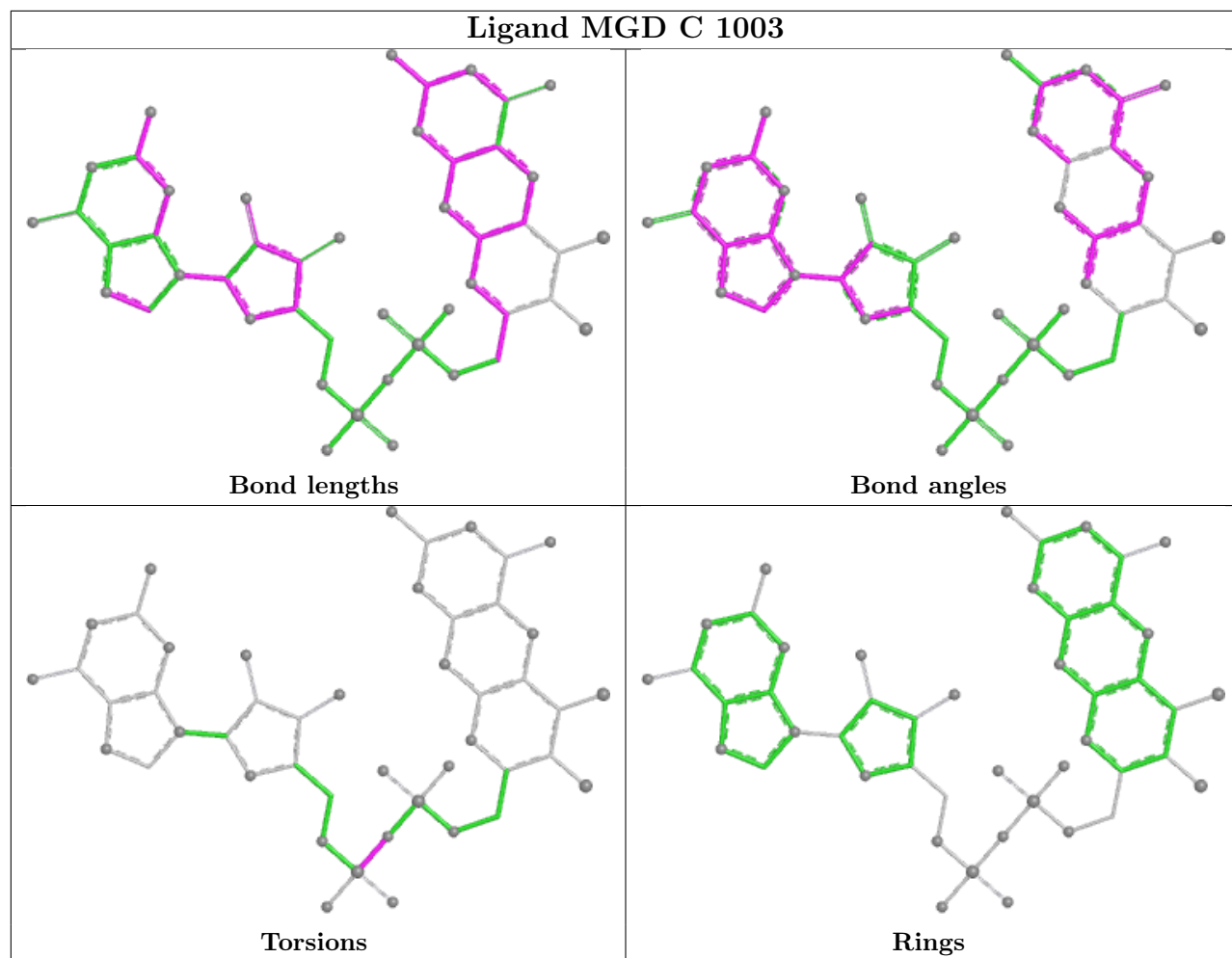
11 monomers are involved in 15 short contacts:

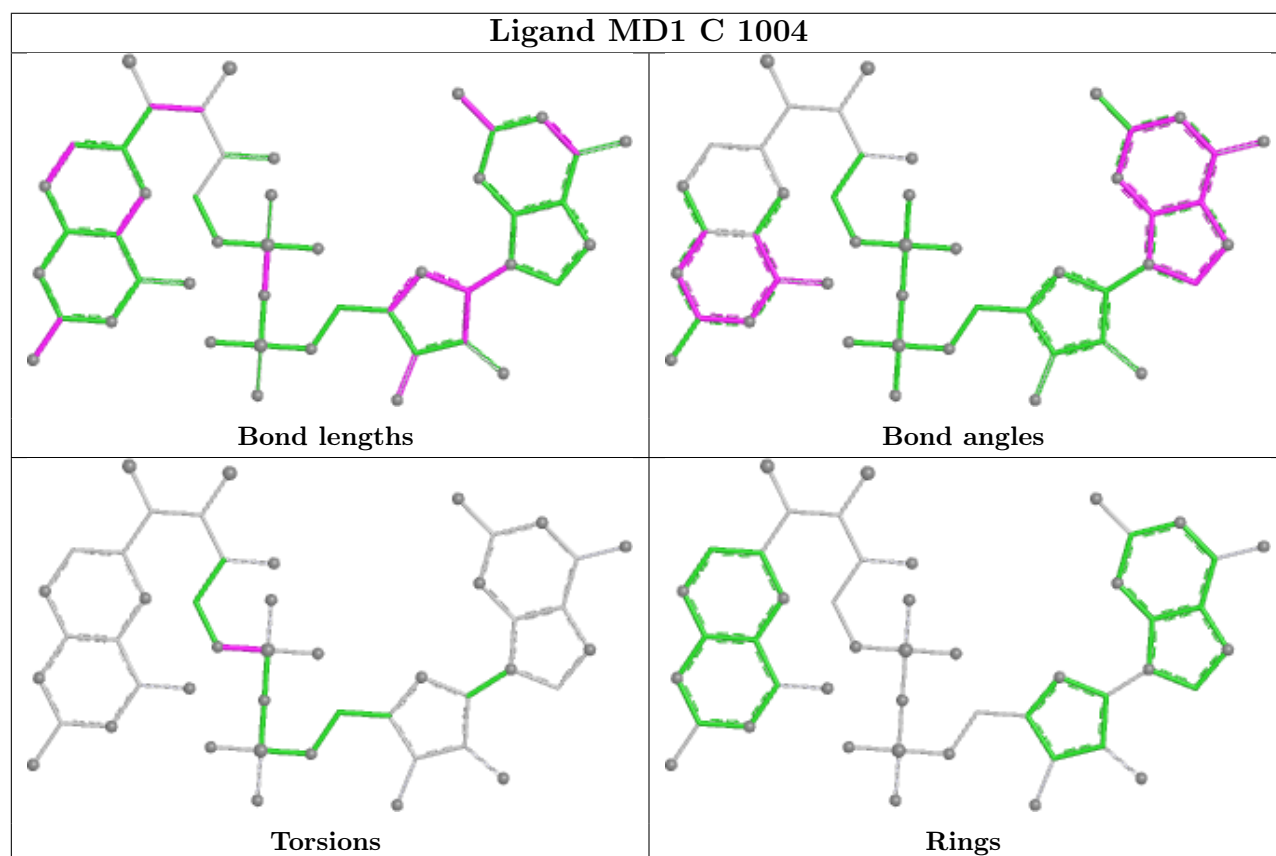
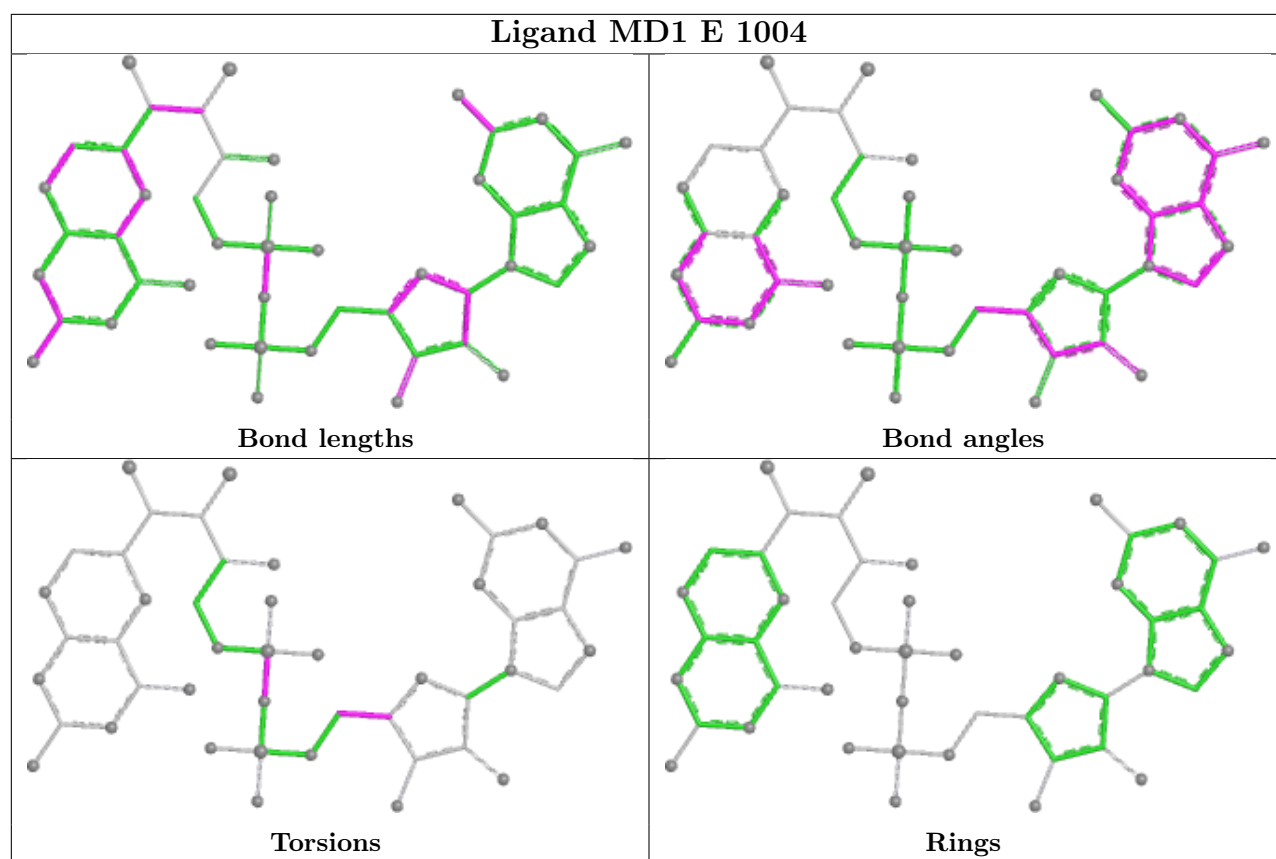
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	1006	EDO	3	0
5	A	1003	MGD	2	0
3	D	405	SF4	1	0
5	C	1003	MGD	2	0
7	B	407	EDO	1	0
10	A	1010	GOL	1	0
3	F	404	SF4	1	0
6	E	1004	MD1	1	0
7	A	1012	EDO	1	0
6	C	1004	MD1	1	0
6	A	1004	MD1	1	0

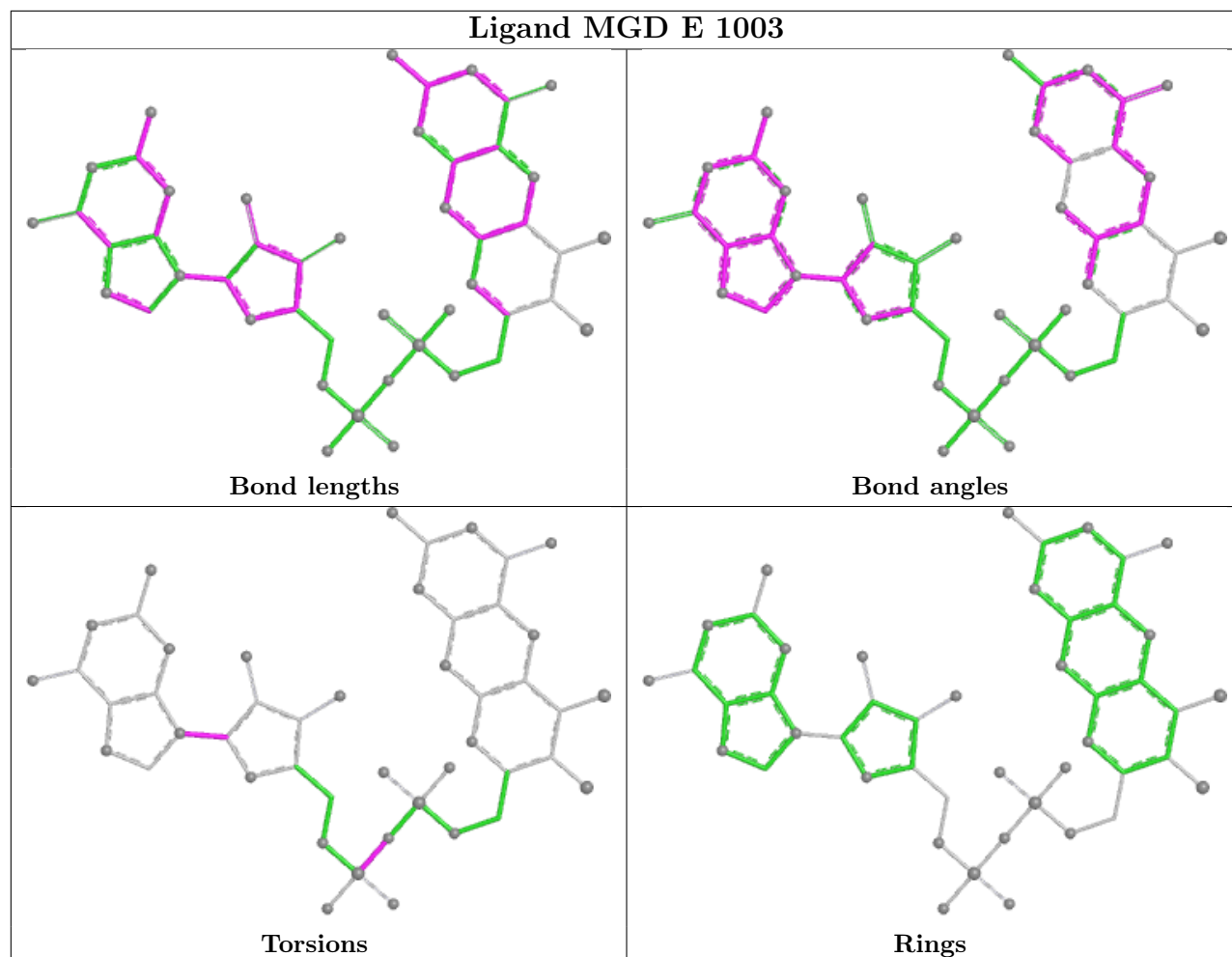
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

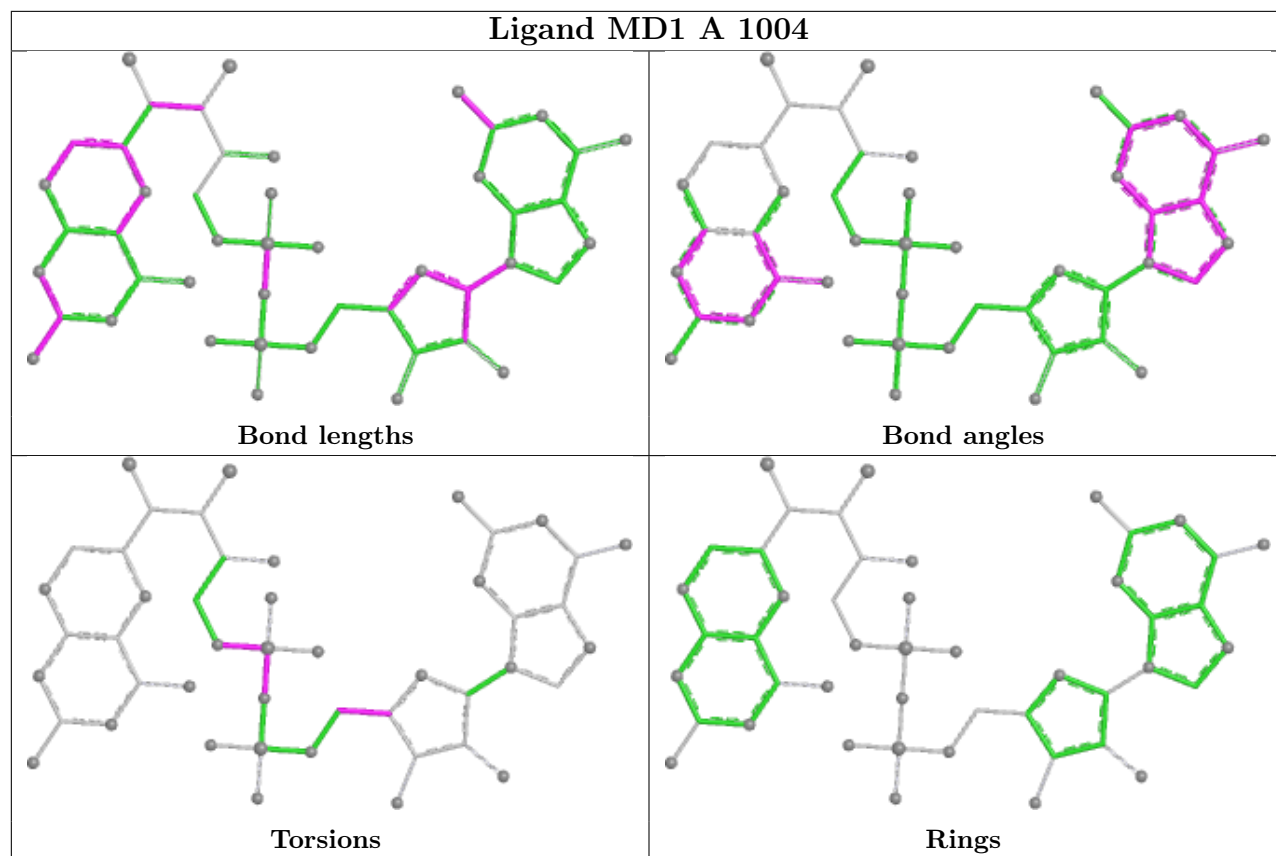
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	894/899 (99%)	-0.31	3 (0%) 90 88	12, 30, 49, 68	3 (0%)
1	C	891/899 (99%)	0.13	12 (1%) 75 73	17, 39, 62, 97	1 (0%)
1	E	892/899 (99%)	-0.23	10 (1%) 78 76	14, 30, 51, 70	3 (0%)
2	B	329/333 (98%)	-0.55	1 (0%) 90 88	17, 24, 38, 64	0
2	D	327/333 (98%)	0.96	35 (10%) 11 8	25, 54, 71, 89	0
2	F	328/333 (98%)	-0.03	2 (0%) 85 83	18, 32, 50, 66	2 (0%)
All	All	3661/3696 (99%)	-0.07	63 (1%) 69 66	12, 32, 59, 97	9 (0%)

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	TYR	5.1
1	C	9	PHE	4.2
2	D	10	ARG	3.8
2	D	7	ALA	3.7
2	D	295	ASP	3.4

### 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 oligosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

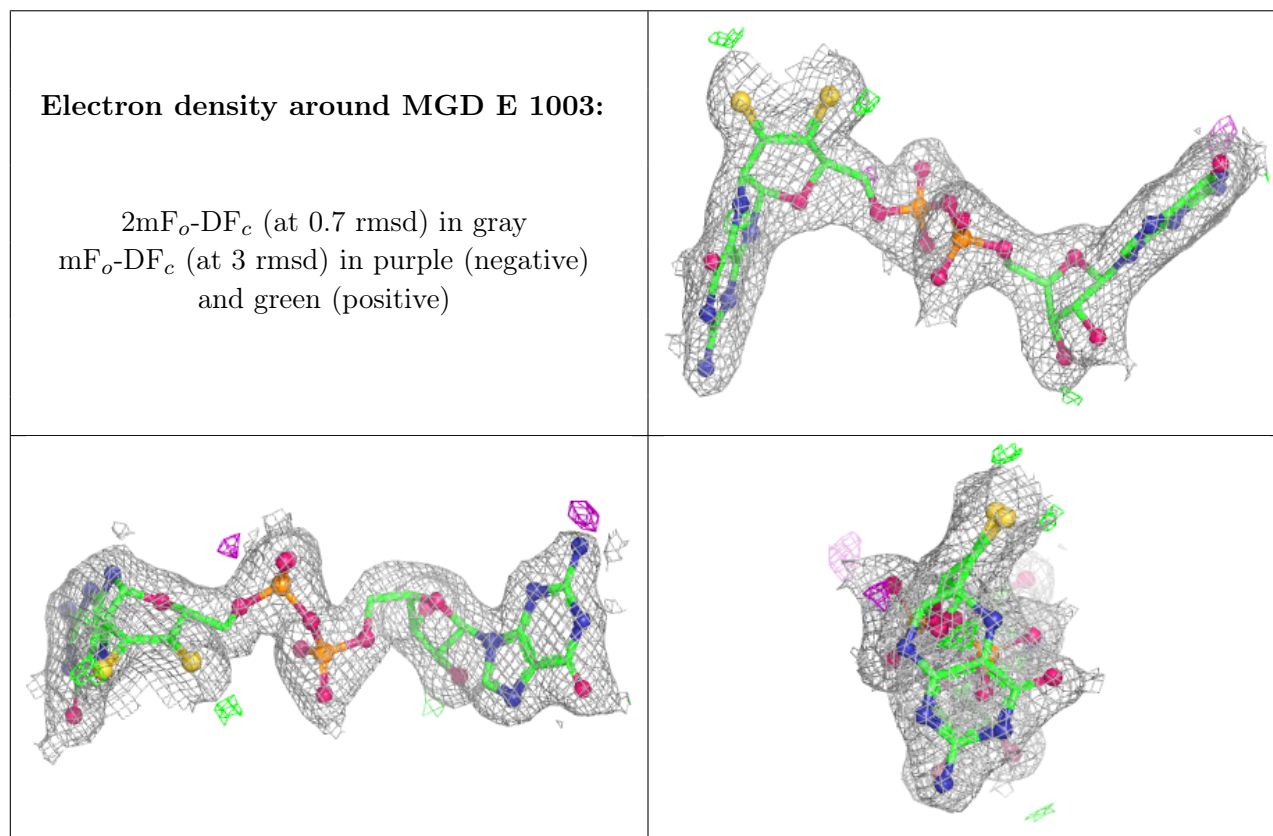
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
11	SO3	E	1008	4/4	0.61	0.20	34,38,48,71	0
11	SO3	C	1010	4/4	0.70	0.14	61,62,70,83	0
10	GOL	A	1010	6/6	0.80	0.17	35,42,48,48	0
7	EDO	E	1006	4/4	0.81	0.17	34,35,38,41	0
7	EDO	C	1005	4/4	0.81	0.15	33,36,45,45	0
7	EDO	B	406	4/4	0.83	0.13	32,34,40,41	0
11	SO3	A	1011	4/4	0.83	0.12	38,39,51,70	0
7	EDO	B	407	4/4	0.84	0.15	34,36,37,42	0
7	EDO	F	406	4/4	0.87	0.12	39,42,43,44	0
11	SO3	A	1013	4/4	0.87	0.29	38,42,42,57	0
7	EDO	E	1007	4/4	0.88	0.10	28,40,44,49	0
11	SO3	C	1009	4/4	0.89	0.25	43,48,50,68	0
7	EDO	A	1005	4/4	0.92	0.12	25,26,31,39	0
7	EDO	A	1007	4/4	0.92	0.09	26,28,29,32	0
8	NA	F	407	1/1	0.92	0.16	41,41,41,41	0
13	ACT	C	1008	4/4	0.92	0.10	31,36,40,44	0
8	NA	C	1007	1/1	0.93	0.10	26,26,26,26	0
7	EDO	A	1012	4/4	0.94	0.19	21,22,27,29	0
3	SF4	D	403	8/8	0.94	0.07	39,45,57,57	0
7	EDO	D	406	4/4	0.94	0.09	30,36,37,38	0
7	EDO	E	1005	4/4	0.94	0.08	16,20,23,23	0
7	EDO	A	1006	4/4	0.95	0.10	32,34,35,37	0
7	EDO	D	401	4/4	0.95	0.07	24,24,28,31	0
3	SF4	D	405	8/8	0.96	0.06	34,48,53,54	0
7	EDO	F	405	4/4	0.96	0.06	23,23,23,25	0
7	EDO	C	1006	4/4	0.96	0.07	20,24,25,27	0
5	MGD	E	1003	47/47	0.97	0.06	16,24,30,31	0
6	MD1	C	1004	47/47	0.97	0.06	20,29,32,35	0
3	SF4	F	402	8/8	0.97	0.05	29,31,35,40	0
8	NA	E	1009	1/1	0.97	0.06	14,14,14,14	0
3	SF4	F	404	8/8	0.97	0.05	26,28,29,29	0
12	F3S	D	402	7/7	0.97	0.06	53,58,64,74	0
5	MGD	C	1003	47/47	0.97	0.06	21,28,32,33	0
3	SF4	E	1001	8/8	0.98	0.04	19,22,25,26	0
9	ZN	C	1011	1/1	0.98	0.04	58,58,58,58	0
3	SF4	D	404	8/8	0.98	0.04	45,49,56,57	0
7	EDO	B	405	4/4	0.98	0.05	22,22,23,23	0

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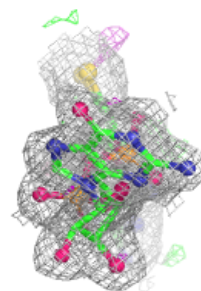
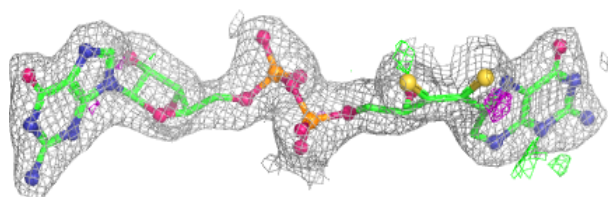
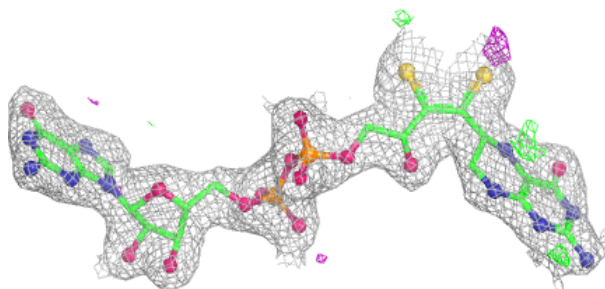
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MD1	A	1004	47/47	0.98	0.05	19,23,28,30	0
3	SF4	F	403	8/8	0.98	0.04	27,31,37,38	0
6	MD1	E	1004	47/47	0.98	0.05	15,22,28,29	0
8	NA	A	1008	1/1	0.98	0.07	18,18,18,18	0
3	SF4	C	1001	8/8	0.98	0.04	34,36,40,42	0
12	F3S	F	401	7/7	0.98	0.04	28,31,33,36	0
5	MGD	A	1003	47/47	0.98	0.05	13,20,25,28	0
3	SF4	A	1001	8/8	0.99	0.03	20,22,26,26	0
3	SF4	B	402	8/8	0.99	0.03	22,24,24,30	0
3	SF4	B	403	8/8	0.99	0.03	19,22,24,28	0
3	SF4	B	404	8/8	0.99	0.02	19,21,22,23	0
4	MO	A	1002	1/1	0.99	0.02	33,33,33,33	0
12	F3S	B	401	7/7	0.99	0.03	26,27,28,31	0
4	MO	C	1002	1/1	0.99	0.02	38,38,38,38	0
9	ZN	E	1010	1/1	0.99	0.02	33,33,33,33	0
4	MO	E	1002	1/1	0.99	0.02	32,32,32,32	0
9	ZN	A	1009	1/1	1.00	0.01	34,34,34,34	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.

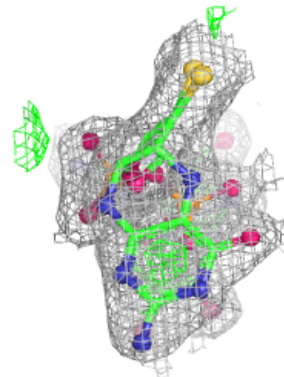
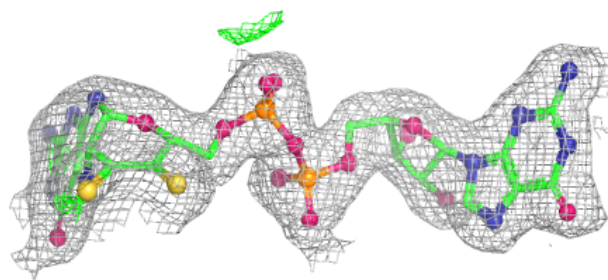
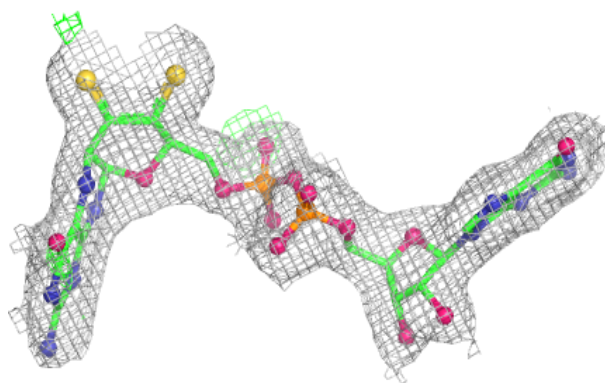


**Electron density around MD1 C 1004:**

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

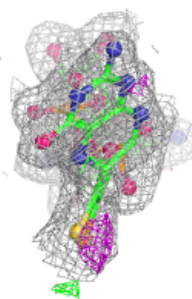
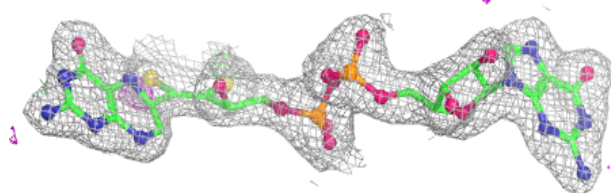
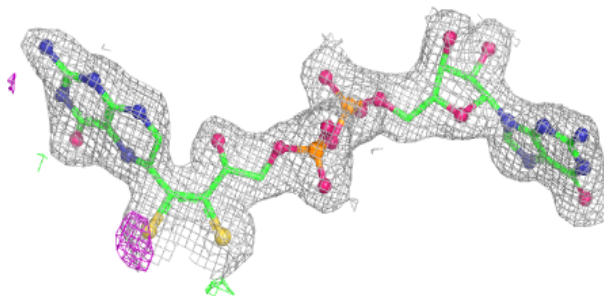
**Electron density around MGD C 1003:**

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

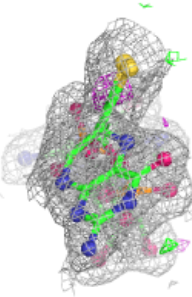
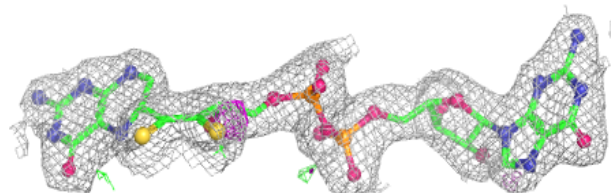
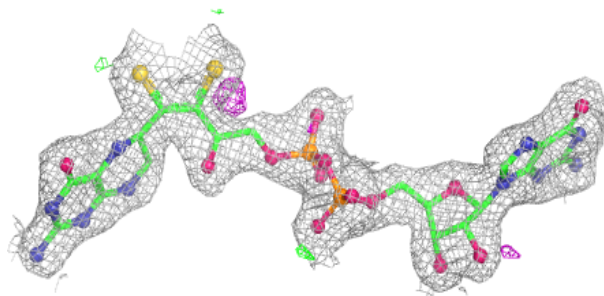


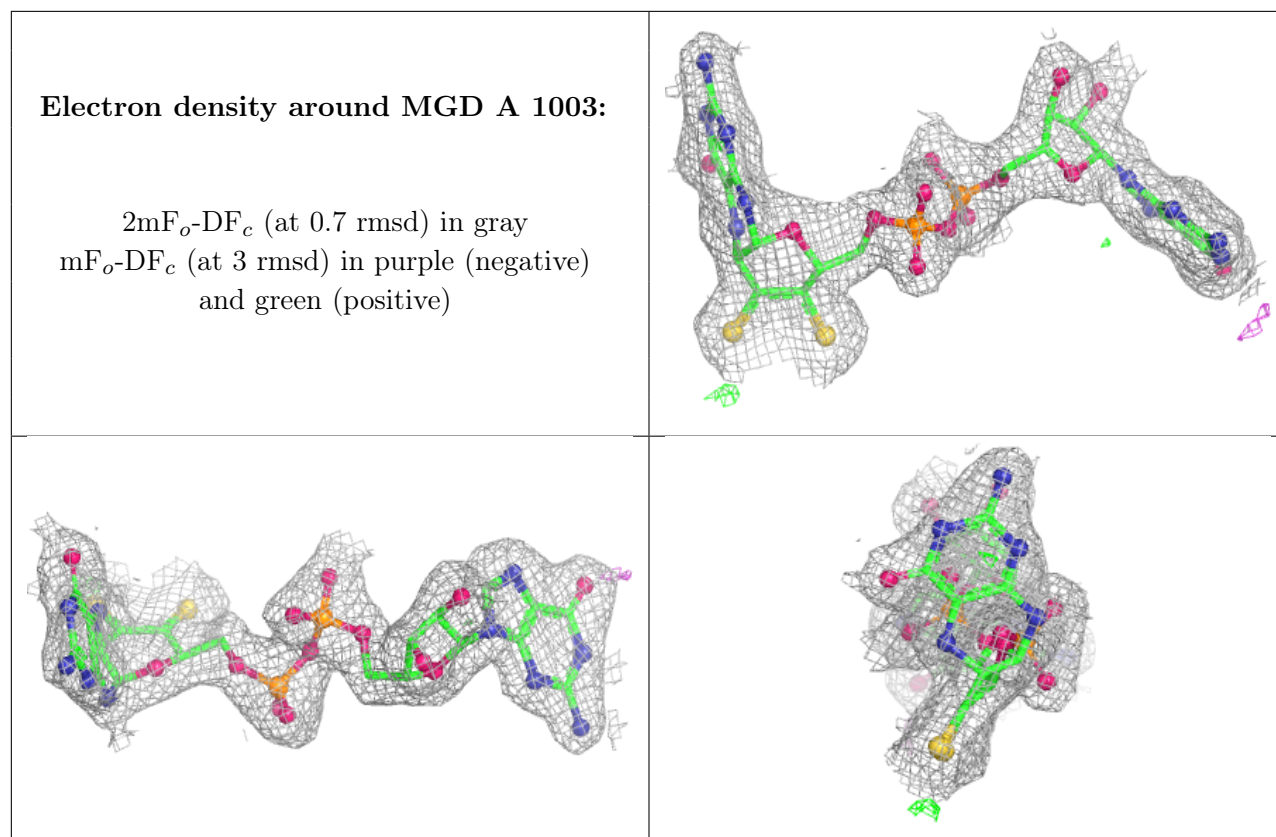
**Electron density around MD1 A 1004:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.