



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2020 – 09:24 AM BST

PDB ID : 4YDD  
Title : Crystal structure of the perchlorate reductase PcrAB from Azospira suillum PS  
Authors : Tsai, C.-L.; Youngblut, M.D.; Tainer, J.A.  
Deposited on : 2015-02-21  
Resolution : 1.86 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

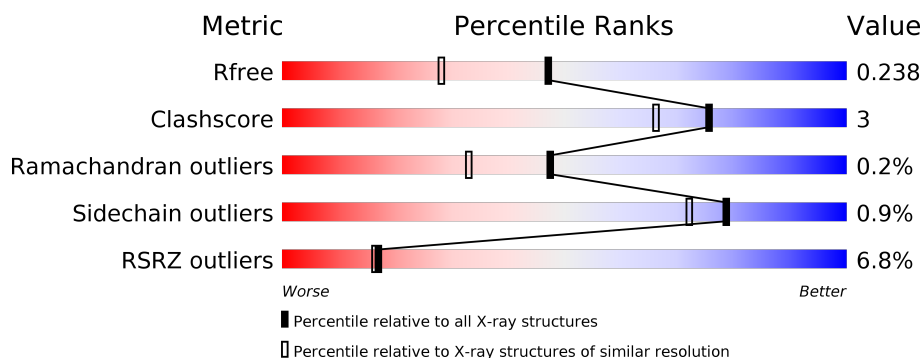
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>5%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	C	899	<div> <div>8%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	E	899	<div> <div>7%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> </div>
2	B	333	<div> <div>0%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
2	D	333	<div> <div>19%</div> <div> <div></div> <div>88%</div> <div>10%</div> </div> </div>
2	F	333	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 61265 atoms, of which 28814 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.

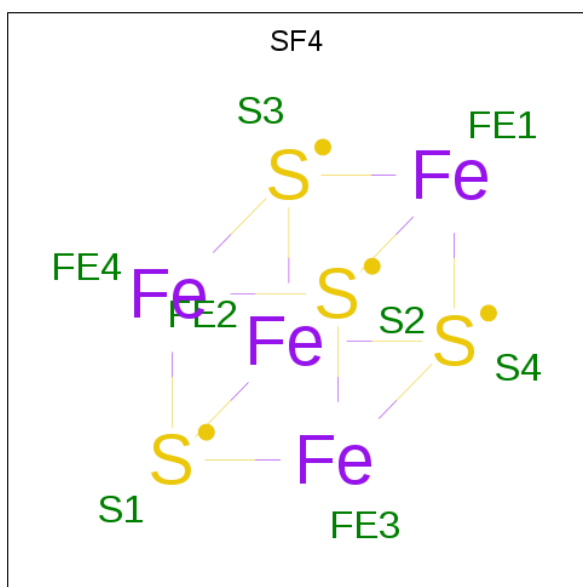
- Molecule 1 is a protein called DMSO reductase family type II enzyme, molybdopterin subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	895	Total	C	H	N	O	S	0	3	0
			14201	4589	7016	1247	1311	38			
1	C	892	Total	C	H	N	O	S	0	0	0
			14110	4563	6962	1240	1307	38			
1	E	892	Total	C	H	N	O	S	0	2	0
			14140	4575	6977	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	H	N	O	S	0	0	0
			5098	1627	2534	447	465	25			
2	D	328	Total	C	H	N	O	S	0	0	0
			5081	1622	2525	446	464	24			
2	F	328	Total	C	H	N	O	S	0	1	0
			5095	1626	2533	447	465	24			

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

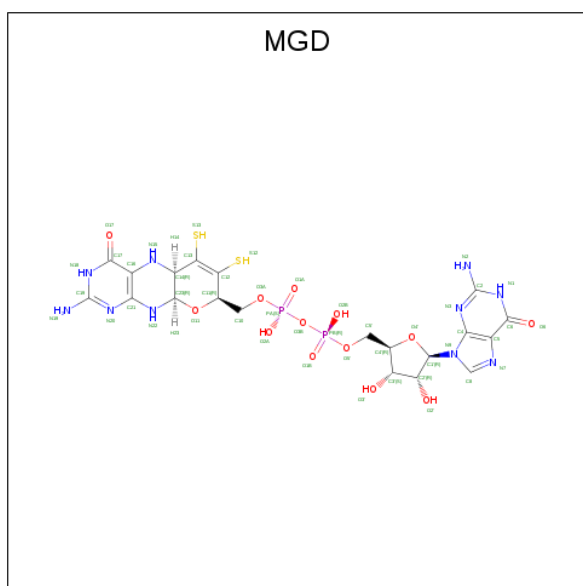


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3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

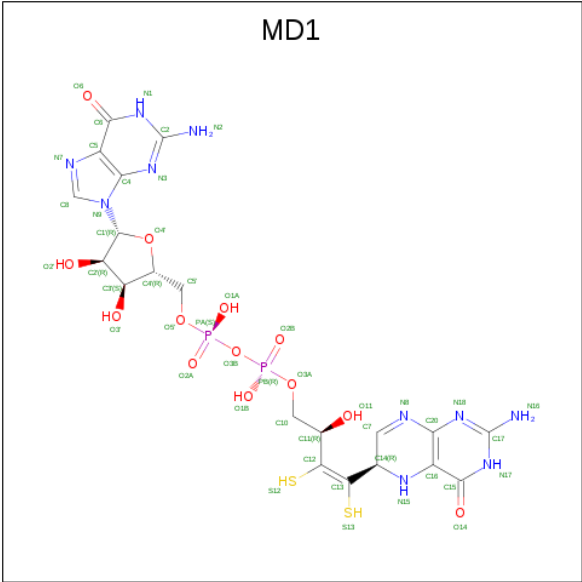
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0

- 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	H	N	O	P	S	0	0
			70	20	23	10	13	2	2		
5	C	1	Total	C	H	N	O	P	S	0	0
			70	20	23	10	13	2	2		
5	E	1	Total	C	H	N	O	P	S	0	0
			70	20	23	10	13	2	2		

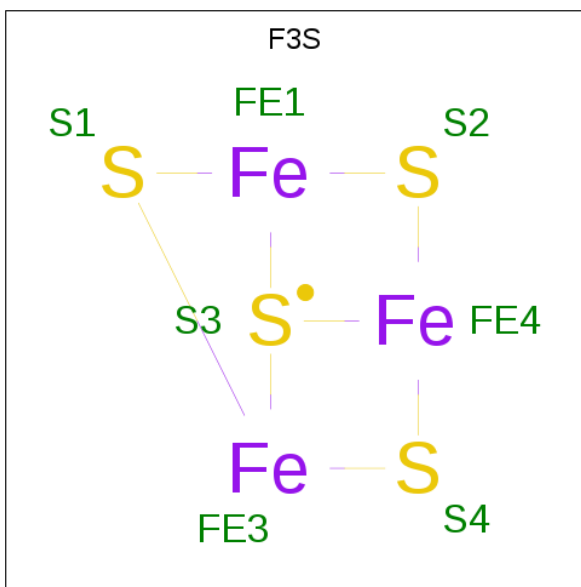
- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula:  $C_{20}H_{26}N_{10}O_{13}P_2S_2$ ).



*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	F	1	Total	C	H	O	0	0
			10	2	6	2		

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

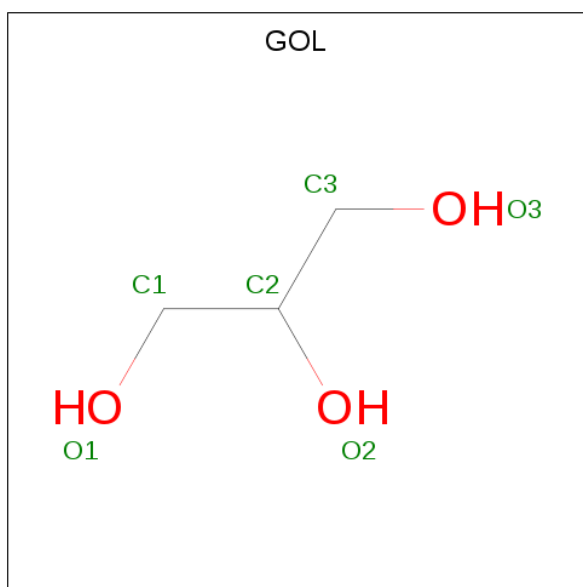


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	D	1	Total	Fe	S	0	0
			7	3	4		
8	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

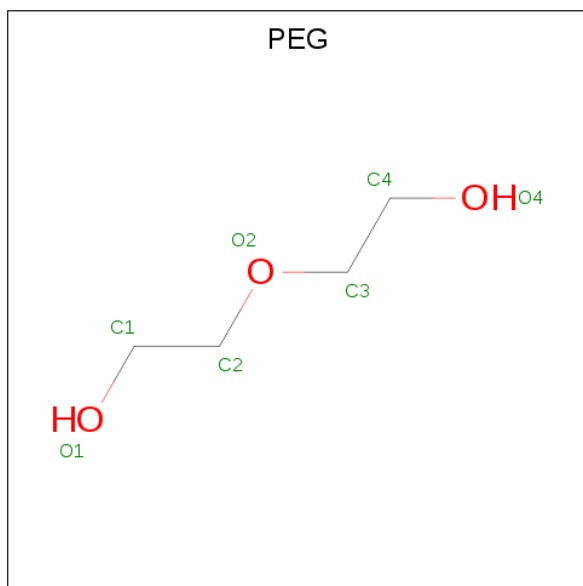
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Na	0	0
			1	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	H	O	0	0
			17	4	10	3		

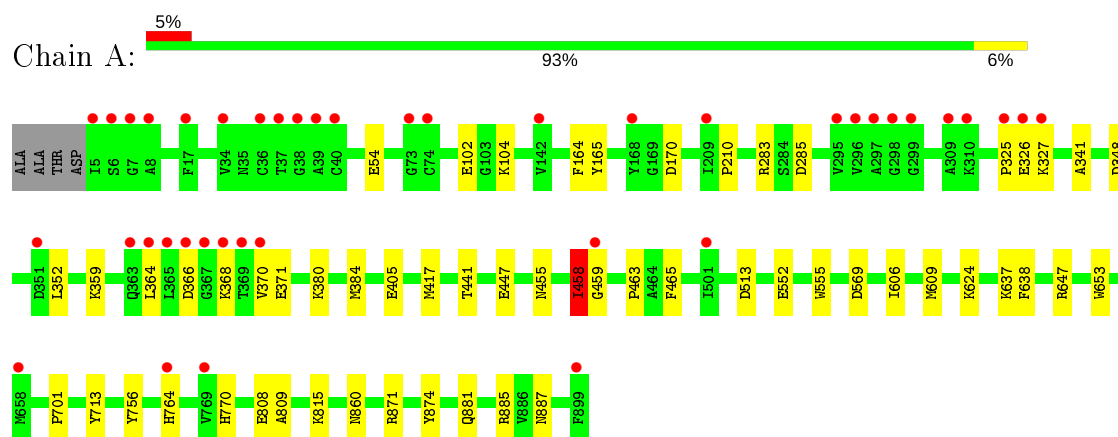
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	738	Total 738	O 738	0	0
12	B	357	Total 358	O 358	0	1
12	C	575	Total 576	O 576	0	1
12	D	140	Total 141	O 141	0	1
12	E	681	Total 681	O 681	0	0
12	F	291	Total 291	O 291	0	0

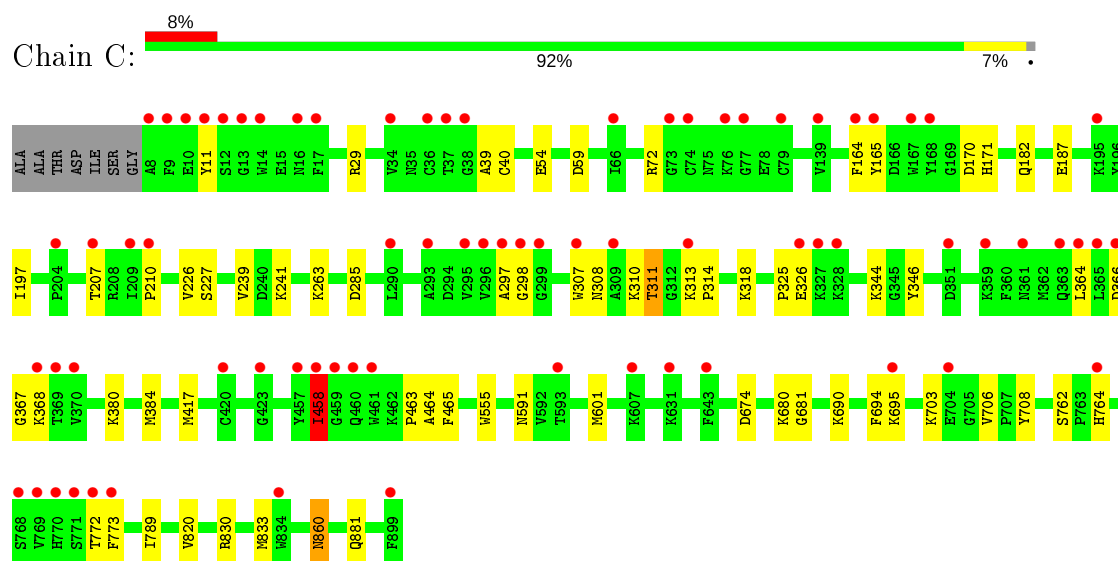
### 3 Residue-property plots [i](#)

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.83Å 175.50Å 193.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 1.86 48.35 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.35-1.86) 98.9 (48.35-1.86)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 1.86Å)	Xtriage
Refinement program	PHENIX dev_2299	Depositor
R, $R_{free}$	0.201 , 0.237 0.202 , 0.238	Depositor DCC
$R_{free}$ test set	18589 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	61265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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: GOL, PEG, MGD, NA, SF4, EDO, 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	0.51	0/7403	0.65	1/10045 (0.0%)
1	C	0.47	0/7357	0.64	0/9984
1	E	0.50	0/7379	0.68	6/10014 (0.1%)
2	B	0.55	0/2632	0.68	1/3567 (0.0%)
2	D	0.42	0/2624	0.61	0/3557
2	F	0.50	0/2633	0.66	0/3569
All	All	0.50	0/30028	0.65	8/40736 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	830	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	E	625	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	E	830	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	B	81	MET	CG-SD-CE	-6.03	90.56	100.20
1	E	625	ARG	NE-CZ-NH1	5.62	123.11	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7185	7016	7016	32	0
1	C	7148	6962	6960	44	0
1	E	7163	6977	6975	53	0
2	B	2564	2534	2534	11	0
2	D	2556	2525	2525	24	0
2	F	2562	2533	2533	10	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	23	21	0	0
5	C	47	23	21	1	0
5	E	47	23	21	1	0
6	A	47	24	22	5	0
6	C	47	24	21	4	0
6	E	47	24	21	4	0
7	A	24	36	36	1	0
7	B	8	12	12	0	0
7	C	8	12	12	0	0
7	D	4	6	6	0	0
7	E	24	36	36	0	0
7	F	4	6	6	0	0
8	B	7	0	0	0	0
8	D	7	0	0	1	0
8	F	7	0	0	0	0
9	B	1	0	0	0	0
10	C	6	8	8	0	0
11	C	7	10	10	1	0
12	A	738	0	0	7	1
12	B	358	0	0	2	2
12	C	576	0	0	3	0
12	D	141	0	0	0	0
12	E	681	0	0	7	2
12	F	291	0	0	2	1
All	All	32451	28814	28796	179	3

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 3.

The worst 5 of 179 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:E:369:THR:O	12:E:1101:HOH:O	2.01	0.78
1:E:231:ASP:OD1	1:E:830:ARG:NH2	2.21	0.74
1:A:405:GLU:OE2	12:A:1101:HOH:O	2.06	0.73
1:E:368:LYS:O	1:E:369:THR:OG1	2.05	0.73
1:C:680:LYS:O	1:C:695:LYS:HE3	1.90	0.72

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:791:HOH:O	12:E:1471:HOH:O[4_477]	2.04	0.16
12:B:808:HOH:O	12:E:1633:HOH:O[4_477]	2.06	0.14
12:A:1703:HOH:O	12:F:578:HOH:O[2_874]	2.08	0.12

## 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	896/899 (100%)	864 (96%)	30 (3%)	2 (0%)	47	33
1	C	890/899 (99%)	851 (96%)	36 (4%)	3 (0%)	41	26
1	E	892/899 (99%)	854 (96%)	34 (4%)	4 (0%)	34	19
2	B	327/333 (98%)	316 (97%)	11 (3%)	0	100	100
2	D	326/333 (98%)	314 (96%)	12 (4%)	0	100	100
2	F	327/333 (98%)	316 (97%)	11 (3%)	0	100	100
All	All	3658/3696 (99%)	3515 (96%)	134 (4%)	9 (0%)	47	33

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	311	THR
1	C	458	ILE
1	E	369	THR
1	A	458	ILE
1	E	368	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	769/768 (100%)	764 (99%)	5 (1%)	84	79
1	C	764/768 (100%)	757 (99%)	7 (1%)	78	72
1	E	766/768 (100%)	756 (99%)	10 (1%)	69	58
2	B	278/281 (99%)	275 (99%)	3 (1%)	73	65
2	D	277/281 (99%)	275 (99%)	2 (1%)	84	79
2	F	278/281 (99%)	276 (99%)	2 (1%)	84	79
All	All	3132/3147 (100%)	3103 (99%)	29 (1%)	78	72

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	860	ASN
2	D	253	GLU
1	E	881	GLN
1	C	881	GLN
1	E	54	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	166	HIS
2	D	178	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 4 are monoatomic - leaving 41 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
7	EDO	C	1007	-	3,3,3	0.52	0	2,2,2	0.50	0
7	EDO	A	1010	-	3,3,3	0.64	0	2,2,2	0.62	0
3	SF4	B	403	2	0,12,12	0.00	-	-		
3	SF4	C	1001	1	0,12,12	0.00	-	-		
8	F3S	B	401	2	0,9,9	0.00	-	-		
7	EDO	E	1005	-	3,3,3	0.75	0	2,2,2	0.48	0
3	SF4	F	404	2	0,12,12	0.00	-	-		
5	MGD	C	1003	4	41,52,52	5.77	26 (63%)	43,81,81	2.72	15 (34%)
6	MD1	C	1004	4	38,51,51	4.07	13 (34%)	35,78,78	1.49	7 (20%)
7	EDO	A	1009	-	3,3,3	0.53	0	2,2,2	0.60	0
7	EDO	A	1007	-	3,3,3	0.48	0	2,2,2	0.37	0
11	PEG	C	1008	-	6,6,6	0.58	0	5,5,5	0.57	0
7	EDO	E	1007	-	3,3,3	0.65	0	2,2,2	0.21	0
3	SF4	A	1001	1	0,12,12	0.00	-	-		
3	SF4	F	402	2	0,12,12	0.00	-	-		
7	EDO	E	1006	-	3,3,3	1.02	0	2,2,2	0.44	0
7	EDO	A	1005	-	3,3,3	0.49	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	F3S	F	401	2	0,9,9	0.00	-	-		
7	EDO	A	1006	-	3,3,3	0.45	0	2,2,2	0.46	0
3	SF4	F	403	2	0,12,12	0.00	-	-		
8	F3S	D	401	2	0,9,9	0.00	-	-		
7	EDO	E	1010	-	3,3,3	0.66	0	2,2,2	0.18	0
7	EDO	D	405	-	3,3,3	0.50	0	2,2,2	0.38	0
7	EDO	B	405	-	3,3,3	0.48	0	2,2,2	0.91	0
3	SF4	D	403	2	0,12,12	0.00	-	-		
3	SF4	D	402	2	0,12,12	0.00	-	-		
7	EDO	E	1009	-	3,3,3	0.57	0	2,2,2	0.42	0
10	GOL	C	1006	-	5,5,5	0.48	0	5,5,5	0.38	0
5	MGD	A	1003	4	41,52,52	5.55	26 (63%)	43,81,81	2.80	15 (34%)
7	EDO	A	1008	-	3,3,3	0.41	0	2,2,2	0.67	0
3	SF4	B	402	2	0,12,12	0.00	-	-		
3	SF4	E	1001	1	0,12,12	0.00	-	-		
7	EDO	F	405	-	3,3,3	0.32	0	2,2,2	0.51	0
7	EDO	C	1005	-	3,3,3	0.89	0	2,2,2	0.68	0
3	SF4	B	404	2	0,12,12	0.00	-	-		
7	EDO	B	406	-	3,3,3	0.75	0	2,2,2	0.27	0
6	MD1	A	1004	4	38,51,51	3.92	13 (34%)	35,78,78	1.55	10 (28%)
3	SF4	D	404	2	0,12,12	0.00	-	-		
5	MGD	E	1003	4	41,52,52	5.82	26 (63%)	43,81,81	2.73	17 (39%)
7	EDO	E	1008	-	3,3,3	0.31	0	2,2,2	0.58	0
6	MD1	E	1004	4	38,51,51	3.87	15 (39%)	35,78,78	1.65	6 (17%)

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
7	EDO	C	1007	-	-	1/1/1/1	-
7	EDO	A	1010	-	-	0/1/1/1	-
3	SF4	B	403	2	-	-	0/6/5/5
7	EDO	A	1006	-	-	0/1/1/1	-
8	F3S	B	401	2	-	-	0/3/3/3
7	EDO	E	1005	-	-	0/1/1/1	-
3	SF4	F	404	2	-	-	0/6/5/5
5	MGD	C	1003	4	-	1/18/66/66	0/6/6/6
6	MD1	C	1004	4	-	7/21/59/59	0/5/5/5
7	EDO	A	1009	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	1007	-	-	1/1/1/1	-
11	PEG	C	1008	-	-	3/4/4/4	-
7	EDO	E	1007	-	-	1/1/1/1	-
3	SF4	A	1001	1	-	-	0/6/5/5
3	SF4	F	402	2	-	-	0/6/5/5
7	EDO	E	1006	-	-	0/1/1/1	-
7	EDO	A	1005	-	-	0/1/1/1	-
8	F3S	F	401	2	-	-	0/3/3/3
3	SF4	C	1001	1	-	-	0/6/5/5
7	EDO	E	1009	-	-	1/1/1/1	-
8	F3S	D	401	2	-	-	0/3/3/3
7	EDO	E	1010	-	-	1/1/1/1	-
7	EDO	D	405	-	-	0/1/1/1	-
7	EDO	B	405	-	-	0/1/1/1	-
3	SF4	D	403	2	-	-	0/6/5/5
3	SF4	D	402	2	-	-	0/6/5/5
3	SF4	F	403	2	-	-	0/6/5/5
10	GOL	C	1006	-	-	2/4/4/4	-
5	MGD	A	1003	4	-	1/18/66/66	0/6/6/6
7	EDO	A	1008	-	-	1/1/1/1	-
3	SF4	B	402	2	-	-	0/6/5/5
3	SF4	E	1001	1	-	-	0/6/5/5
7	EDO	F	405	-	-	0/1/1/1	-
7	EDO	C	1005	-	-	1/1/1/1	-
3	SF4	B	404	2	-	-	0/6/5/5
7	EDO	B	406	-	-	0/1/1/1	-
6	MD1	A	1004	4	-	2/21/59/59	0/5/5/5
3	SF4	D	404	2	-	-	0/6/5/5
5	MGD	E	1003	4	-	0/18/66/66	0/6/6/6
7	EDO	E	1008	-	-	1/1/1/1	-
6	MD1	E	1004	4	-	3/21/59/59	0/5/5/5

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	C2'-C1'	-15.63	1.30	1.53
5	E	1003	MGD	C2'-C1'	-15.51	1.30	1.53
5	A	1003	MGD	C2'-C1'	-14.52	1.31	1.53
6	C	1004	MD1	C7-N8	13.48	1.43	1.27
6	A	1004	MD1	C7-N8	13.18	1.43	1.27

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	MGD	O11-C23-N22	-10.75	97.52	108.57
5	C	1003	MGD	O11-C23-N22	-10.35	97.93	108.57
5	E	1003	MGD	O11-C23-N22	-8.86	99.46	108.57
5	E	1003	MGD	C21-N22-C23	-6.39	111.16	123.67
5	E	1003	MGD	C16-C21-N22	5.86	123.49	118.13

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

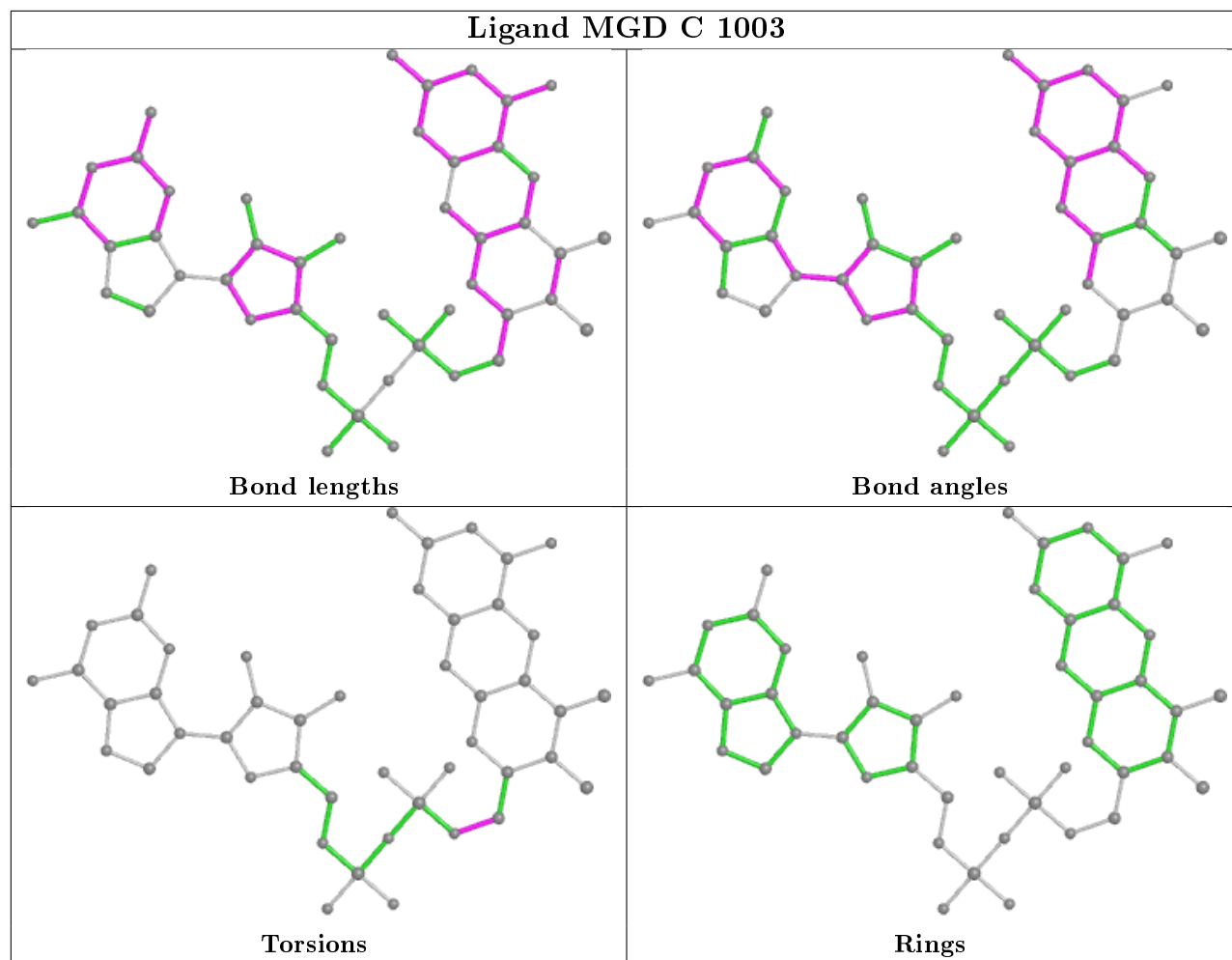
Mol	Chain	Res	Type	Atoms
6	C	1004	MD1	C10-O3A-PB-O1B
6	E	1004	MD1	C2'-C1'-N9-C8
10	C	1006	GOL	C1-C2-C3-O3
11	C	1008	PEG	O2-C3-C4-O4
6	C	1004	MD1	O4'-C4'-C5'-O5'

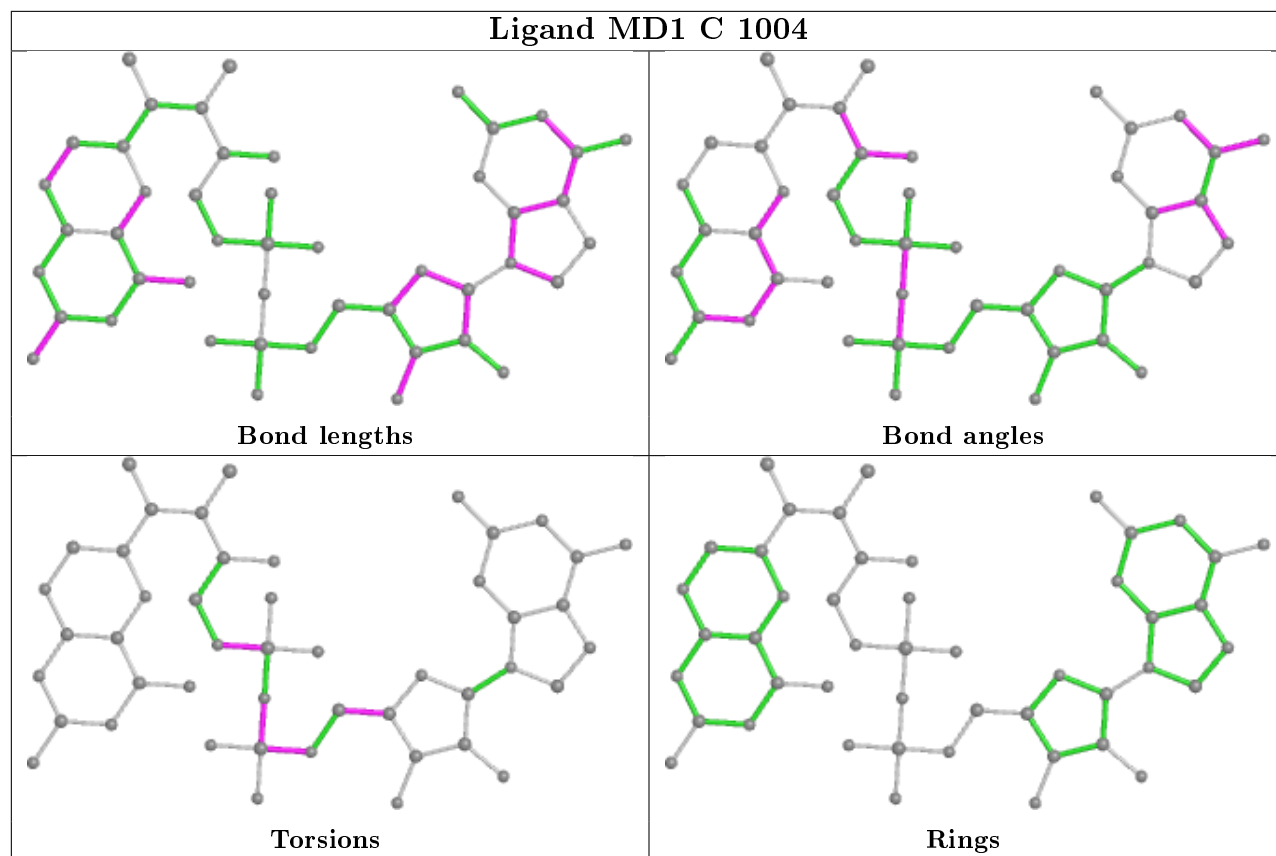
There are no ring outliers.

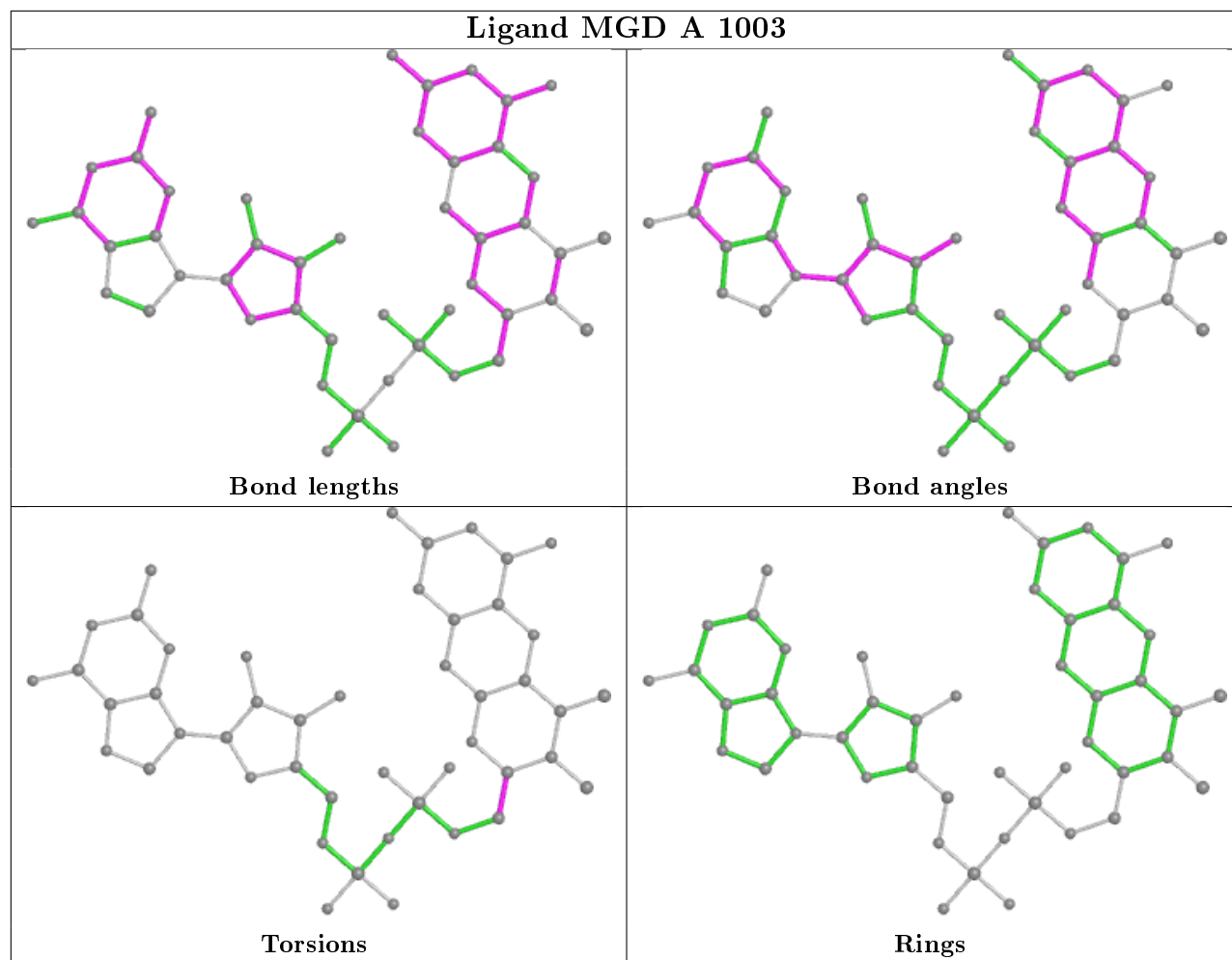
9 monomers are involved in 19 short contacts:

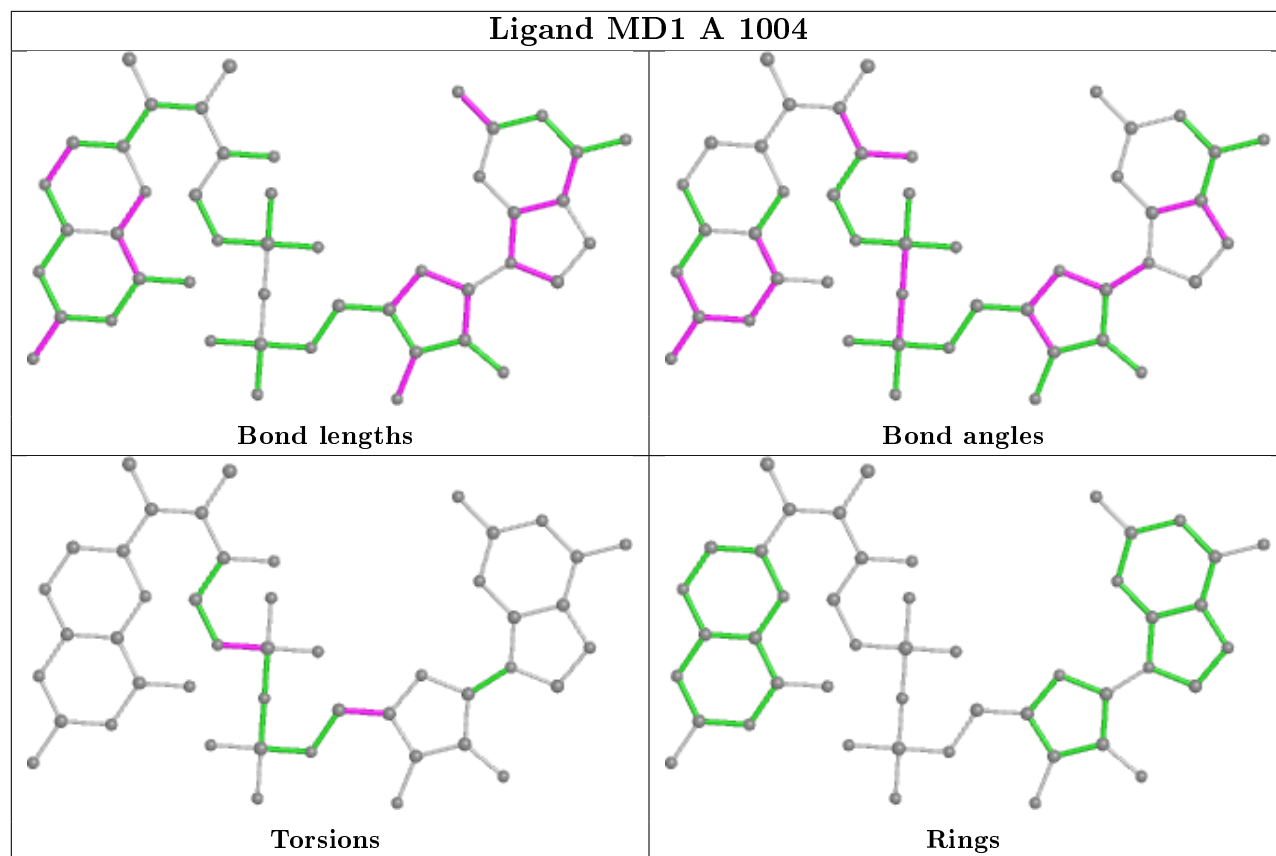
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1010	EDO	1	0
5	C	1003	MGD	1	0
6	C	1004	MD1	4	0
11	C	1008	PEG	1	0
8	D	401	F3S	1	0
3	D	402	SF4	1	0
6	A	1004	MD1	5	0
5	E	1003	MGD	1	0
6	E	1004	MD1	4	0

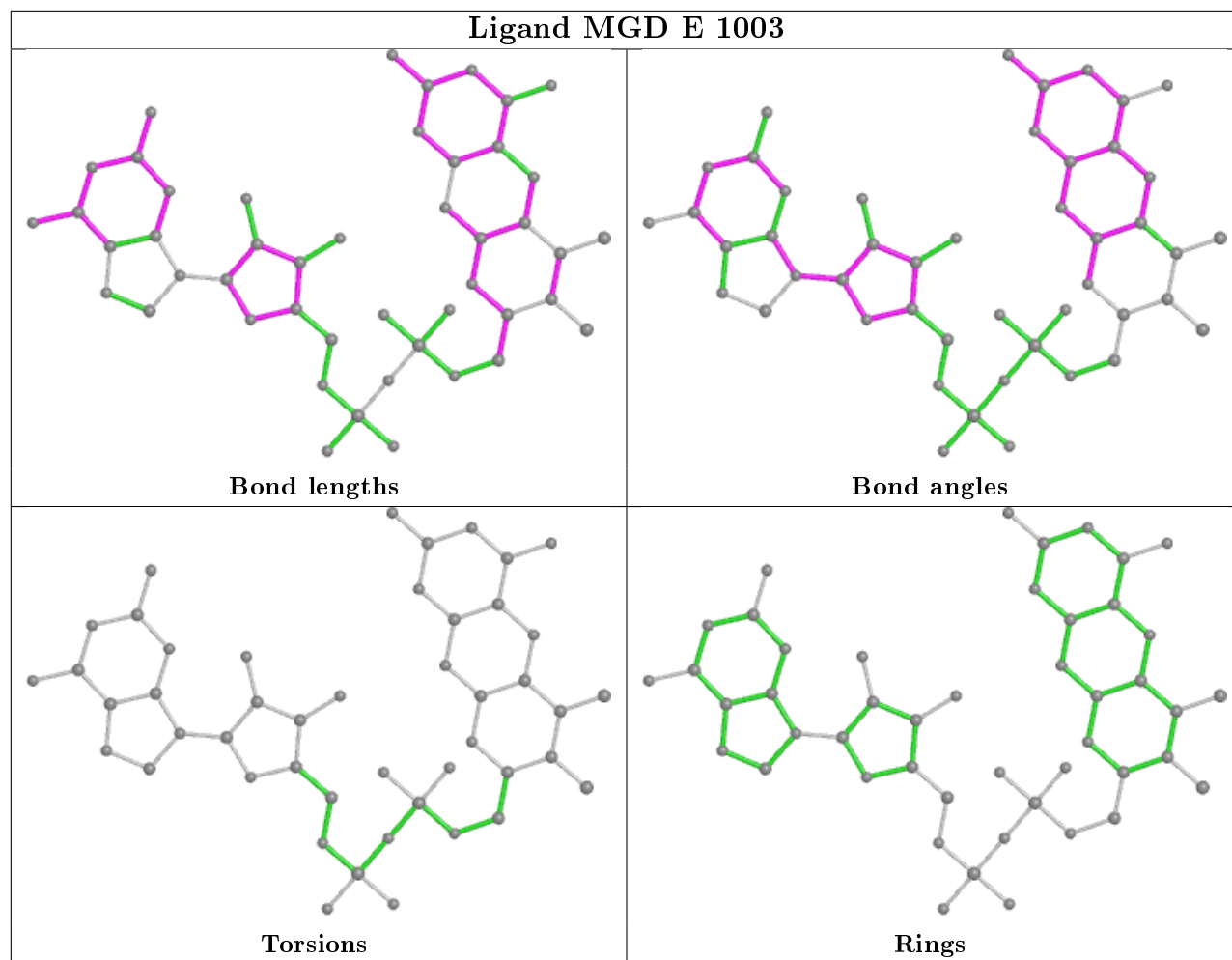
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

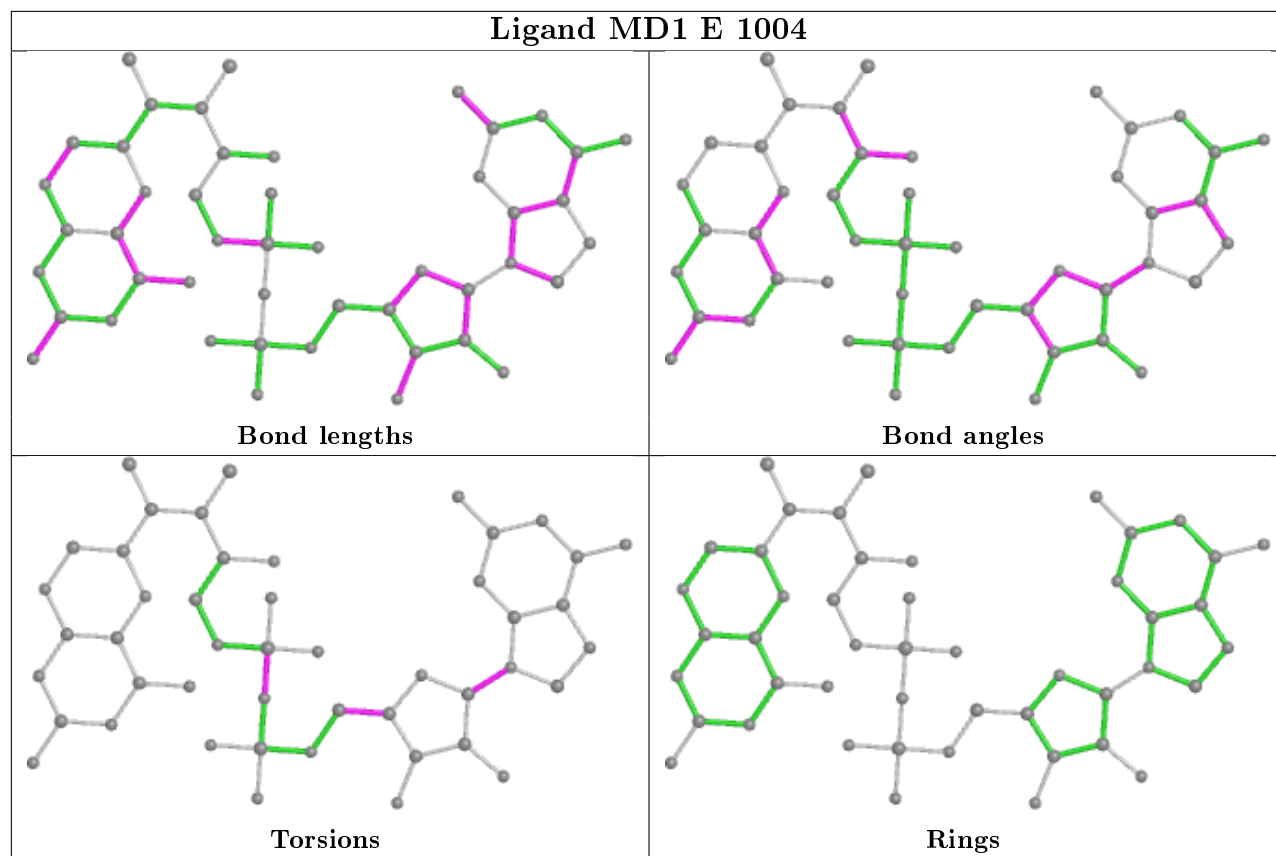












## 5.7 Other polymers [i](#)

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	895/899 (99%)	0.24	41 (4%) 32 31	13, 24, 42, 64	0
1	C	892/899 (99%)	0.56	74 (8%) 11 11	15, 30, 52, 86	0
1	E	892/899 (99%)	0.43	62 (6%) 16 15	13, 25, 55, 76	0
2	B	329/333 (98%)	-0.04	4 (1%) 79 79	14, 20, 32, 55	0
2	D	328/333 (98%)	1.24	62 (18%) 1 1	21, 46, 62, 85	0
2	F	328/333 (98%)	0.27	5 (1%) 73 74	14, 26, 43, 58	0
All	All	3664/3696 (99%)	0.43	248 (6%) 17 16	13, 26, 53, 86	0

The worst 5 of 248 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	ALA	10.3
1	C	9	PHE	7.3
2	D	146	LEU	5.9
1	A	5	ILE	5.6
2	D	250	PHE	5.5

### 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

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
7	EDO	C	1005	4/4	0.60	0.20	27,33,38,42	0
7	EDO	E	1006	4/4	0.68	0.23	25,30,34,36	0
10	GOL	C	1006	6/6	0.74	0.35	37,47,56,57	0
7	EDO	B	406	4/4	0.77	0.26	32,39,40,42	0
11	PEG	C	1008	7/7	0.78	0.22	32,39,42,42	0
7	EDO	E	1010	4/4	0.79	0.27	34,41,43,45	0
7	EDO	E	1007	4/4	0.79	0.19	25,30,35,35	0
7	EDO	E	1009	4/4	0.84	0.38	30,36,40,42	0
7	EDO	A	1010	4/4	0.84	0.28	21,27,30,33	0
7	EDO	A	1008	4/4	0.86	0.20	30,36,41,42	0
9	NA	B	407	1/1	0.87	0.10	35,35,35,35	0
3	SF4	D	402	8/8	0.87	0.09	32,42,49,51	0
3	SF4	D	404	8/8	0.87	0.12	29,38,39,42	0
7	EDO	E	1008	4/4	0.88	0.19	26,31,35,41	0
7	EDO	A	1009	4/4	0.89	0.19	29,35,41,50	0
7	EDO	E	1005	4/4	0.90	0.15	16,20,23,23	0
8	F3S	D	401	7/7	0.91	0.08	45,47,55,57	0
7	EDO	A	1005	4/4	0.92	0.14	18,25,32,32	0
7	EDO	C	1007	4/4	0.94	0.12	17,22,26,27	0
5	MGD	C	1003	47/47	0.94	0.23	20,22,27,30	0
5	MGD	E	1003	47/47	0.94	0.19	15,21,29,31	0
7	EDO	D	405	4/4	0.94	0.11	26,31,35,35	0
7	EDO	A	1007	4/4	0.95	0.13	22,27,28,33	0
3	SF4	D	403	8/8	0.95	0.11	30,35,39,40	0
3	SF4	F	402	8/8	0.95	0.08	19,22,23,25	0
7	EDO	A	1006	4/4	0.96	0.10	24,29,32,32	0
5	MGD	A	1003	47/47	0.96	0.17	13,16,19,23	0
6	MD1	C	1004	47/47	0.96	0.17	17,20,24,26	0
7	EDO	B	405	4/4	0.96	0.08	16,19,19,20	0
6	MD1	E	1004	47/47	0.96	0.15	12,16,21,23	0
3	SF4	F	404	8/8	0.97	0.11	17,18,20,23	0
6	MD1	A	1004	47/47	0.97	0.17	15,17,22,23	0
8	F3S	F	401	7/7	0.97	0.05	21,22,23,24	0
3	SF4	C	1001	8/8	0.98	0.14	24,25,27,27	0
3	SF4	B	404	8/8	0.98	0.09	12,13,14,15	0
8	F3S	B	401	7/7	0.98	0.05	19,20,22,22	0
3	SF4	F	403	8/8	0.98	0.13	18,21,24,25	0

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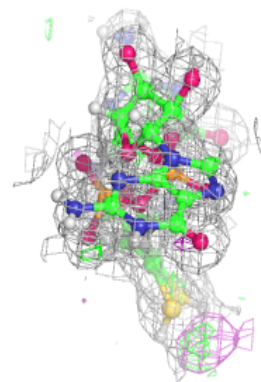
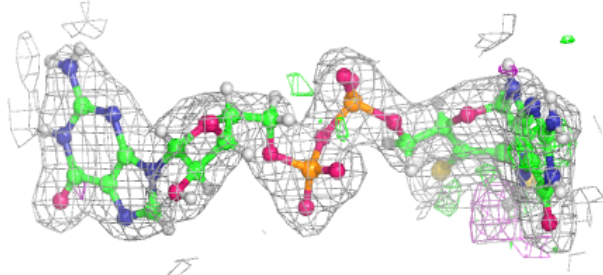
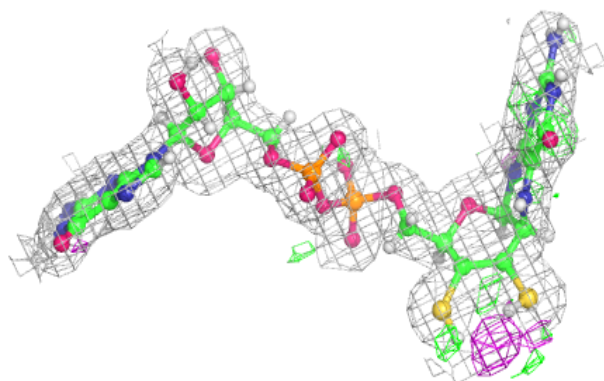
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SF4	B	403	8/8	0.98	0.10	12,14,15,17	0
3	SF4	B	402	8/8	0.98	0.08	15,16,19,20	0
3	SF4	E	1001	8/8	0.98	0.09	13,15,15,15	0
7	EDO	F	405	4/4	0.98	0.09	16,19,21,21	0
4	MO	E	1002	1/1	0.99	0.08	21,21,21,21	0
4	MO	A	1002	1/1	0.99	0.06	20,20,20,20	0
4	MO	C	1002	1/1	0.99	0.08	24,24,24,24	0
3	SF4	A	1001	8/8	0.99	0.13	13,14,17,19	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.

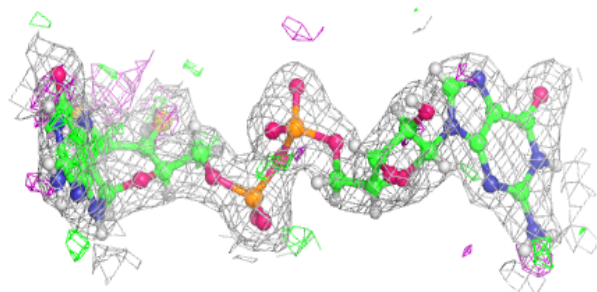
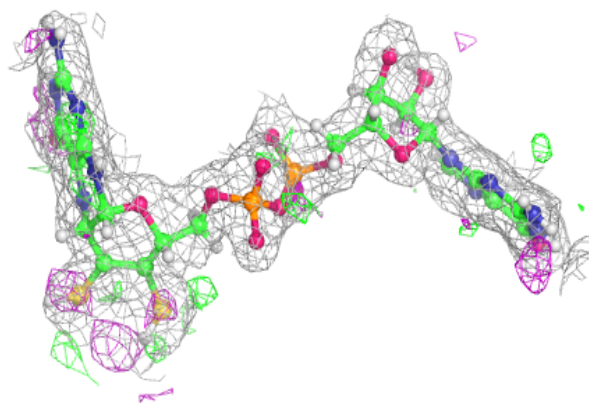
**Electron density around MGD C 1003:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

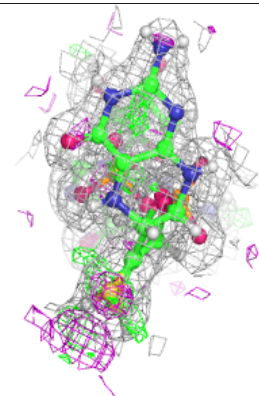
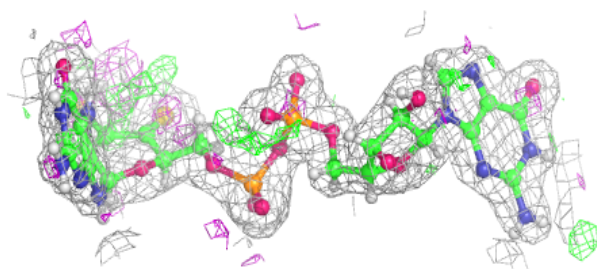
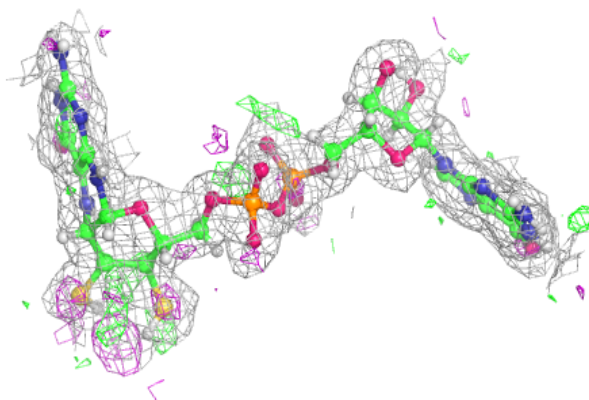


**Electron density around MGD E 1003:**

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

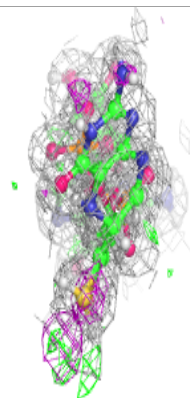
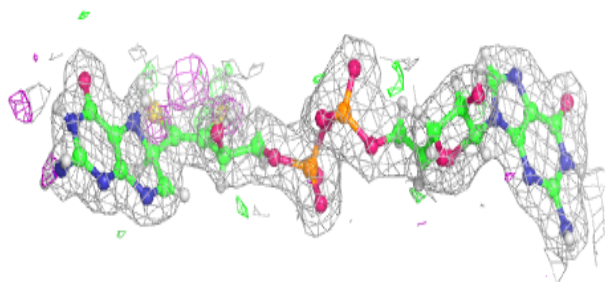
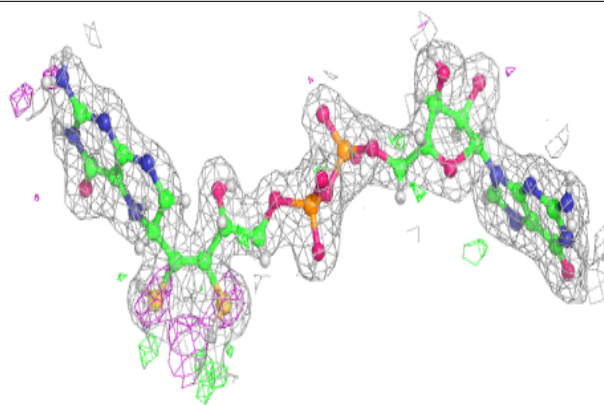
**Electron density around MGD A 1003:**

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and green (positive)

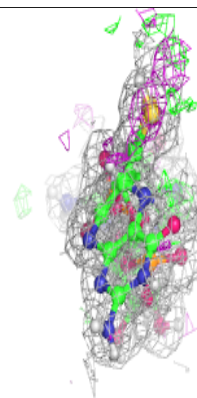
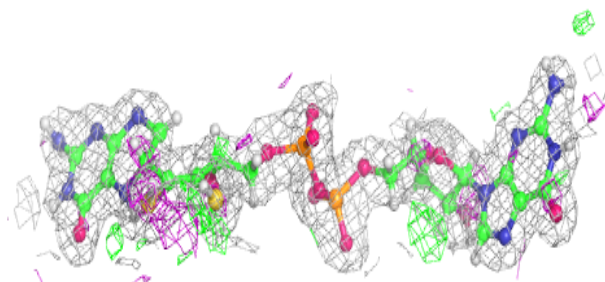
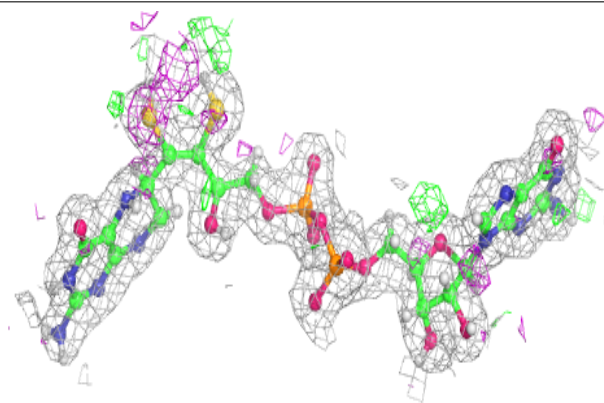


**Electron density around MD1 C 1004:**

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

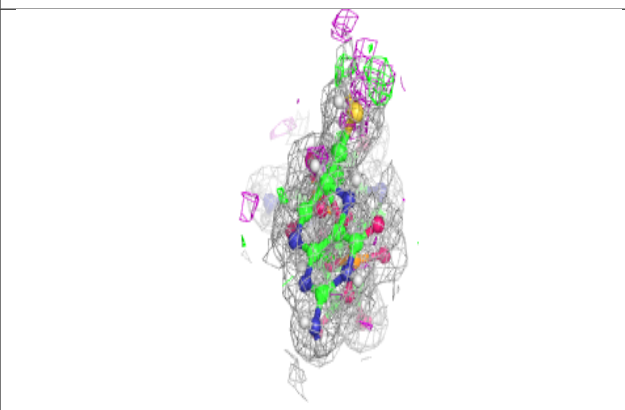
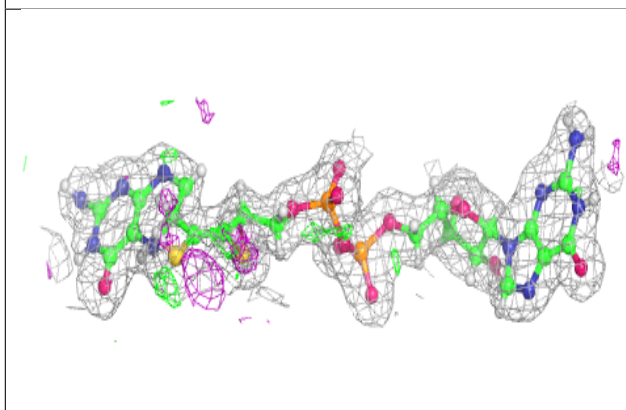
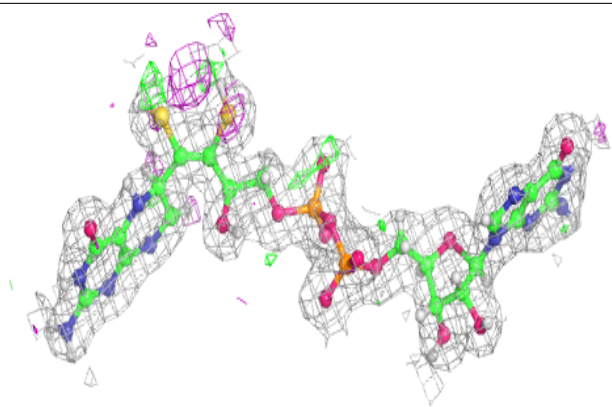
**Electron density around MD1 E 1004:**

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 $mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.