



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 01:30 pm BST

PDB ID : 5E7O  
Title : Crystal structure of the perchlorate reductase PcrAB mutant W461E of PcrA from *Azospira suillum* PS  
Authors : Tsai, C.-L.; Tainer, J.A.  
Deposited on : 2015-10-12  
Resolution : 2.40 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 : 2.11  
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) : 2.11

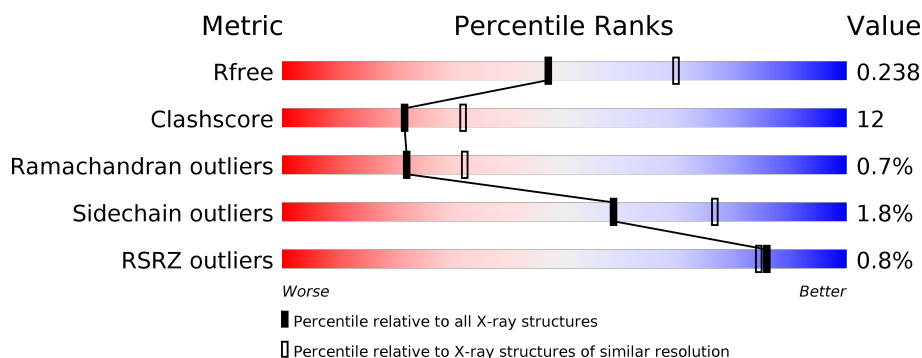
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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>81%</div> <div>18%</div> </div>
1	C	899	<div> <div>82%</div> <div>17%</div> </div>
1	E	899	<div> <div>78%</div> <div>21%</div> </div>
1	G	899	<div> <div>79%</div> <div>20%</div> </div>
1	I	899	<div> <div>68%</div> <div>30%</div> </div>
1	K	899	<div> <div>71%</div> <div>27%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	333	
2	D	333	
2	F	333	
2	H	333	
2	J	333	
2	L	333	

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
3	SF4	I	1001	-	-	X	-
3	SF4	K	1001	-	-	X	-
7	EDO	F	401	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 62374 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	C	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	E	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	G	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	I	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	K	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	GLU	TRP	engineered mutation	UNP G8QM55
C	461	GLU	TRP	engineered mutation	UNP G8QM55
E	461	GLU	TRP	engineered mutation	UNP G8QM55
G	461	GLU	TRP	engineered mutation	UNP G8QM55
I	461	GLU	TRP	engineered mutation	UNP G8QM55
K	461	GLU	TRP	engineered mutation	UNP G8QM55

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

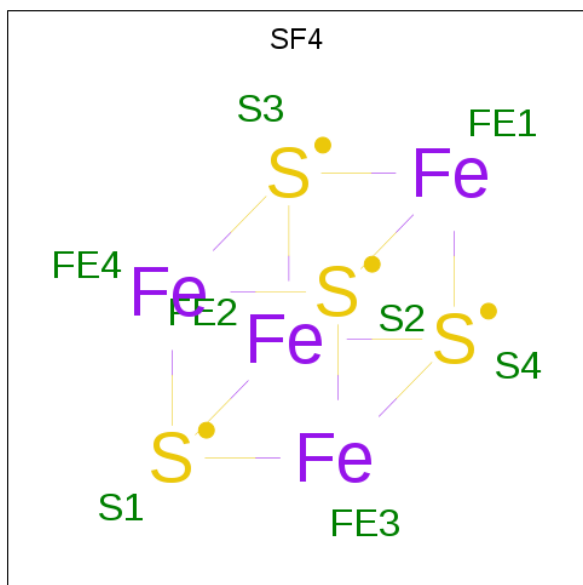
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	D	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	F	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	J	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	L	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			

- 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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total 8	Fe 4	S 4	0	0
3	F	1	Total 8	Fe 4	S 4	0	0
3	F	1	Total 8	Fe 4	S 4	0	0
3	F	1	Total 8	Fe 4	S 4	0	0
3	G	1	Total 8	Fe 4	S 4	0	0
3	H	1	Total 8	Fe 4	S 4	0	0
3	H	1	Total 8	Fe 4	S 4	0	0
3	H	1	Total 8	Fe 4	S 4	0	0
3	I	1	Total 8	Fe 4	S 4	0	0
3	J	1	Total 8	Fe 4	S 4	0	0
3	J	1	Total 8	Fe 4	S 4	0	0
3	J	1	Total 8	Fe 4	S 4	0	0
3	K	1	Total 8	Fe 4	S 4	0	0
3	L	1	Total 8	Fe 4	S 4	0	0
3	L	1	Total 8	Fe 4	S 4	0	0
3	L	1	Total 8	Fe 4	S 4	0	0

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

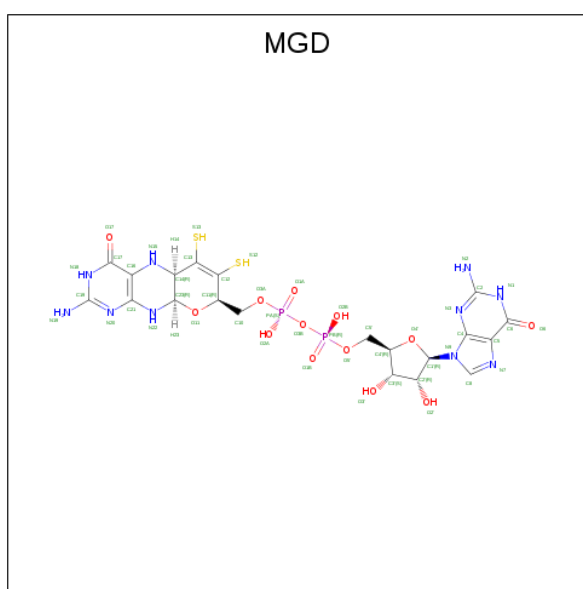
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Mo 1	0	0
4	K	1	Total 1	Mo 1	0	0
4	E	1	Total 1	Mo 1	0	0

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

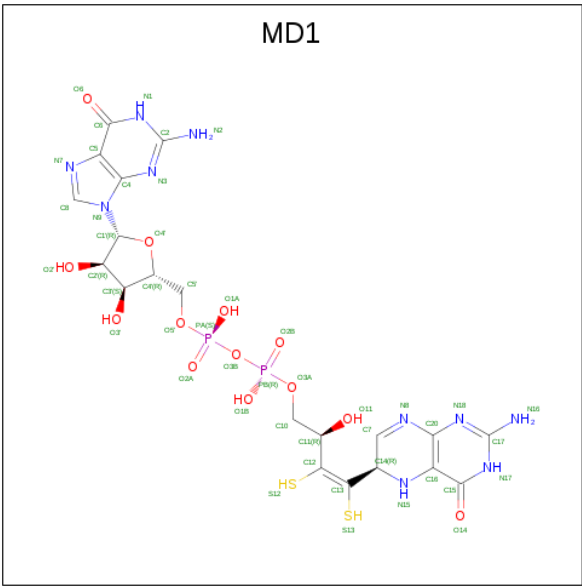
- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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
5	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	I	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	K	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 (three-letter code: 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
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		
6	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





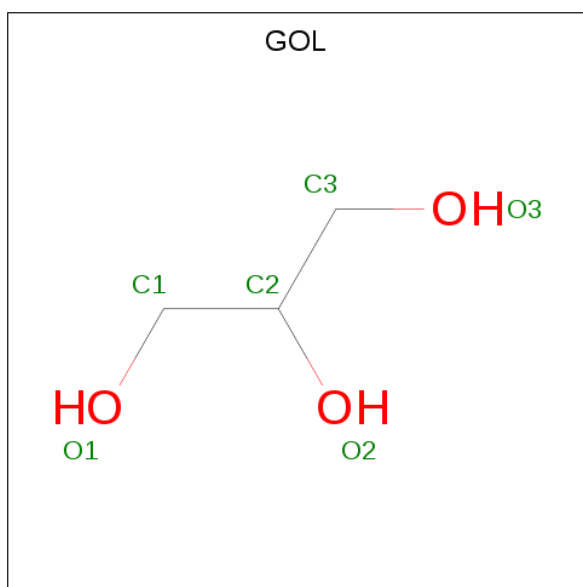
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total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

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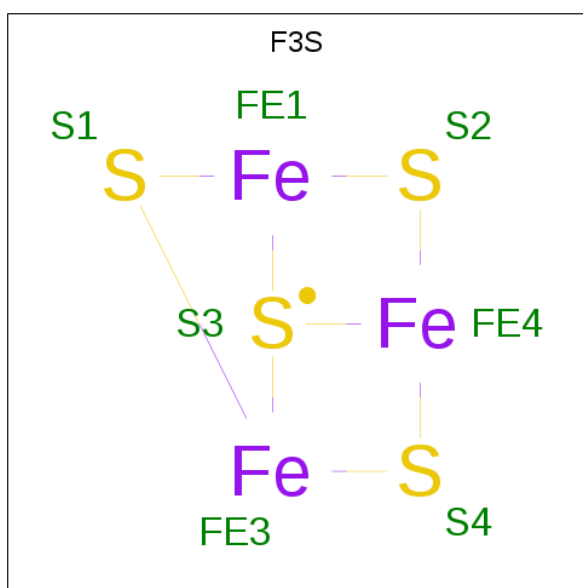
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	H	1	Total 4	C 2	O 2	0	0
7	H	1	Total 4	C 2	O 2	0	0
7	H	1	Total 4	C 2	O 2	0	0
7	I	1	Total 4	C 2	O 2	0	0
7	I	1	Total 4	C 2	O 2	0	0
7	J	1	Total 4	C 2	O 2	0	0
7	K	1	Total 4	C 2	O 2	0	0
7	K	1	Total 4	C 2	O 2	0	0
7	L	1	Total 4	C 2	O 2	0	0
7	L	1	Total 4	C 2	O 2	0	0

- Molecule 8 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
8	A	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total 7	Fe 3	S 4	0	0
9	H	1	Total 7	Fe 3	S 4	0	0
9	J	1	Total 7	Fe 3	S 4	0	0
9	L	1	Total 7	Fe 3	S 4	0	0

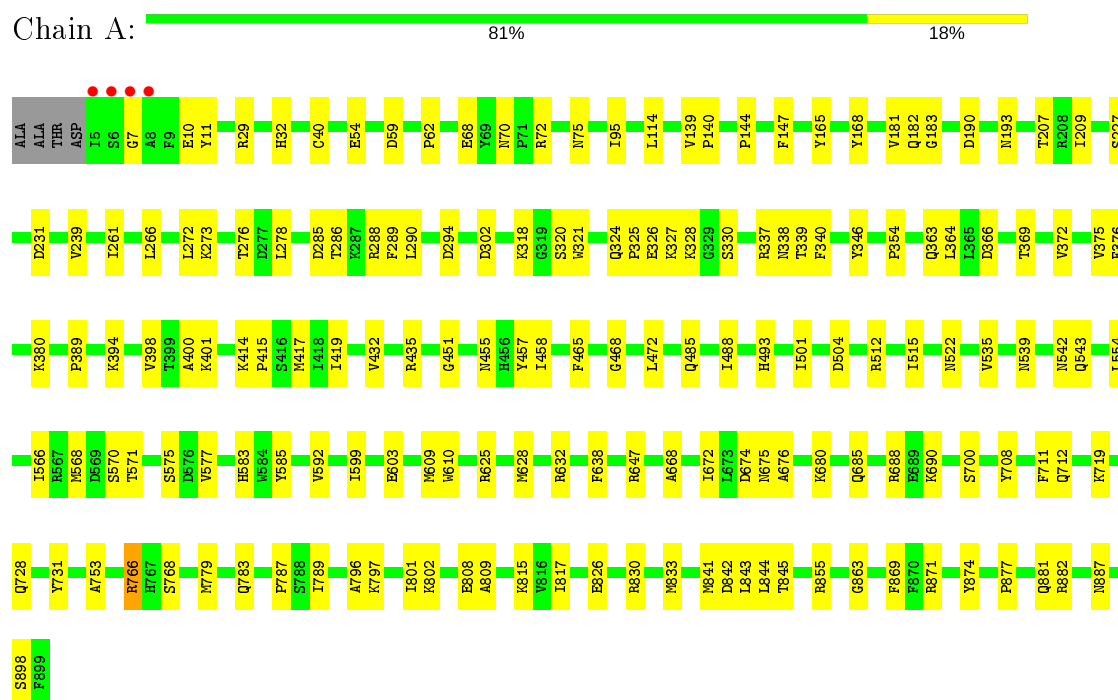
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	399	Total 399	O 399	0	0
10	B	179	Total 179	O 179	0	0
10	C	417	Total 417	O 417	0	0
10	D	176	Total 176	O 176	0	0
10	E	384	Total 384	O 384	0	0
10	F	148	Total 148	O 148	0	0
10	G	348	Total 348	O 348	0	0
10	H	116	Total 116	O 116	0	0
10	I	266	Total 266	O 266	0	0
10	J	127	Total 127	O 127	0	0
10	K	287	Total 287	O 287	0	0
10	L	131	Total 131	O 131	0	0

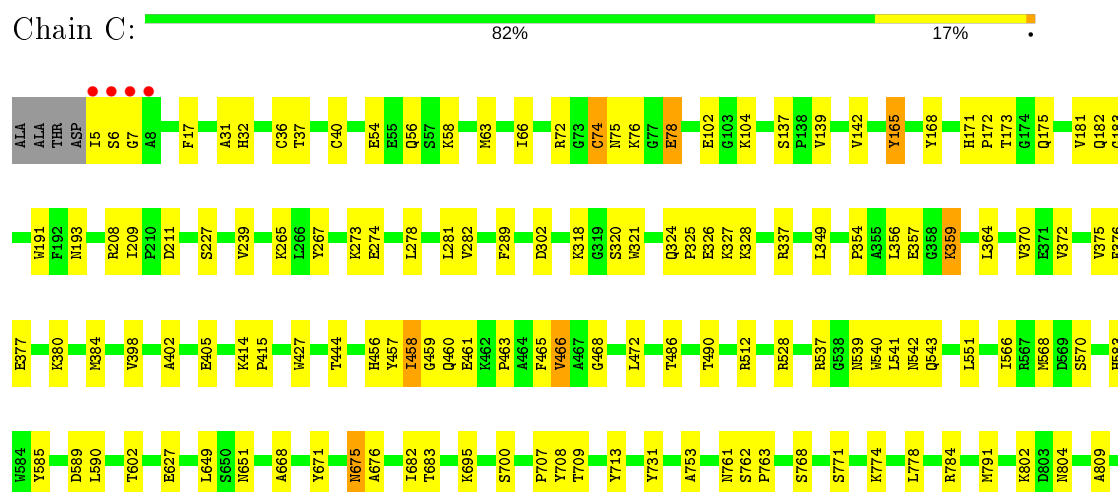
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



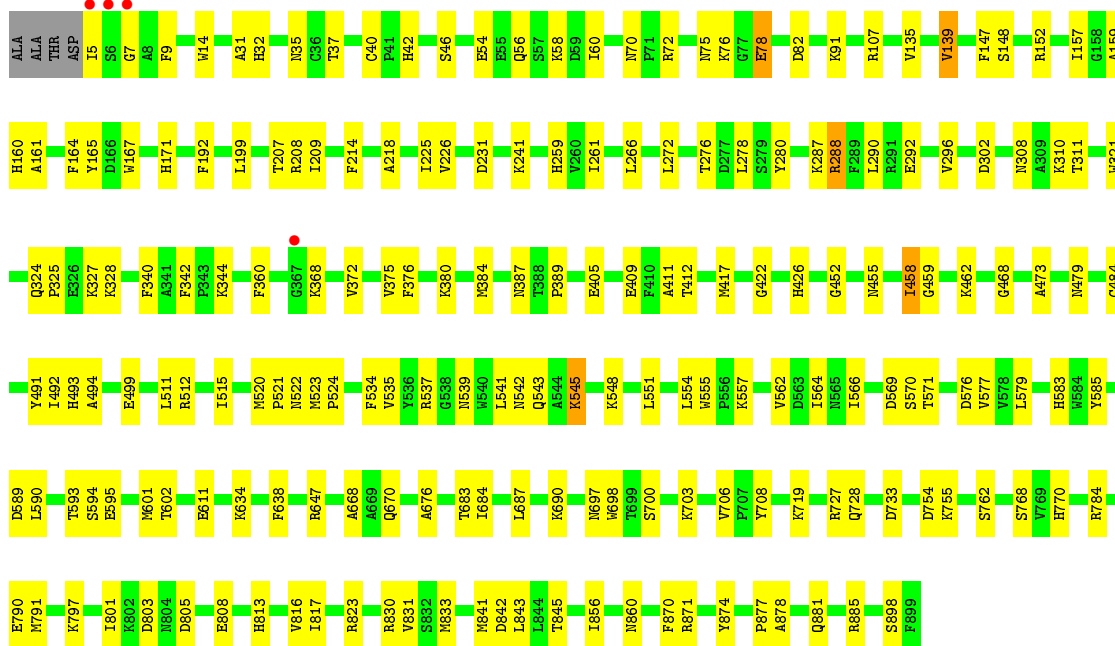
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit





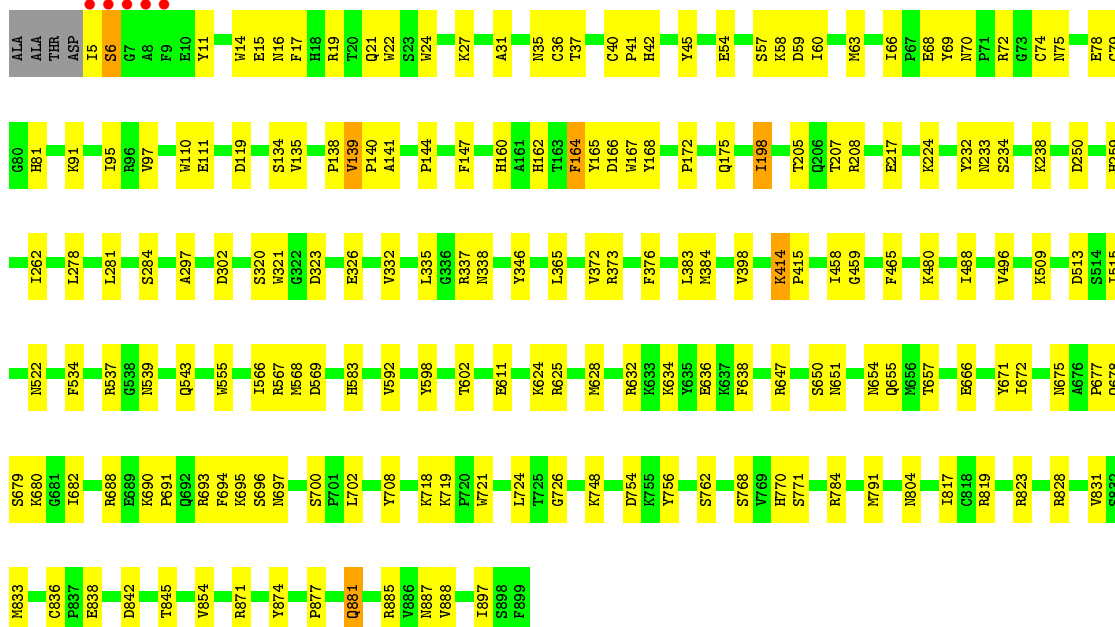
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

Chain E: 78% 21%



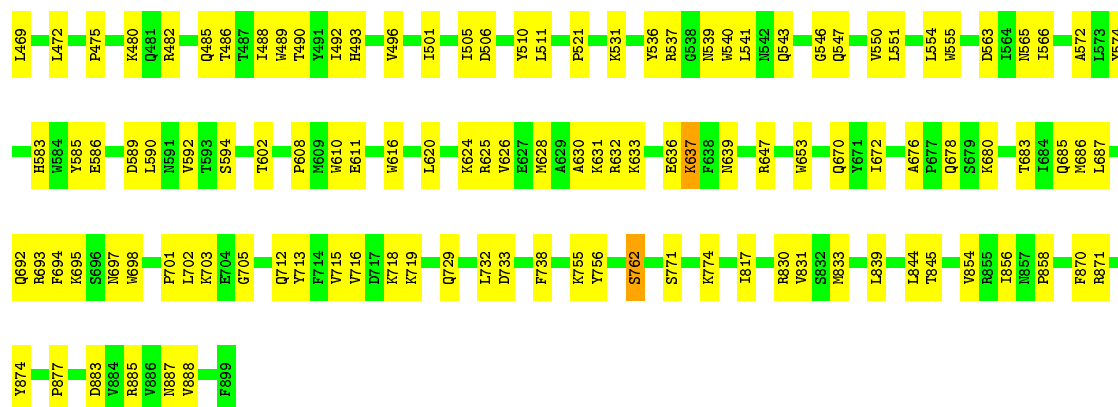
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

Chain G: 79% 20%

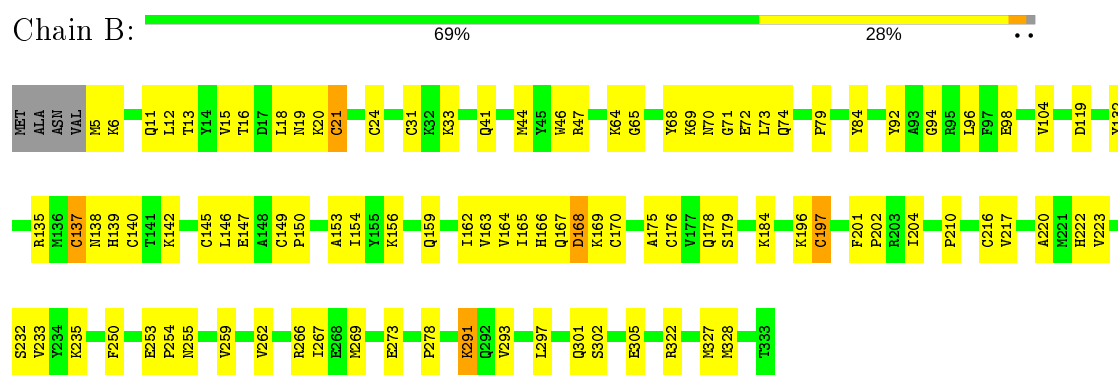


- [illegible]

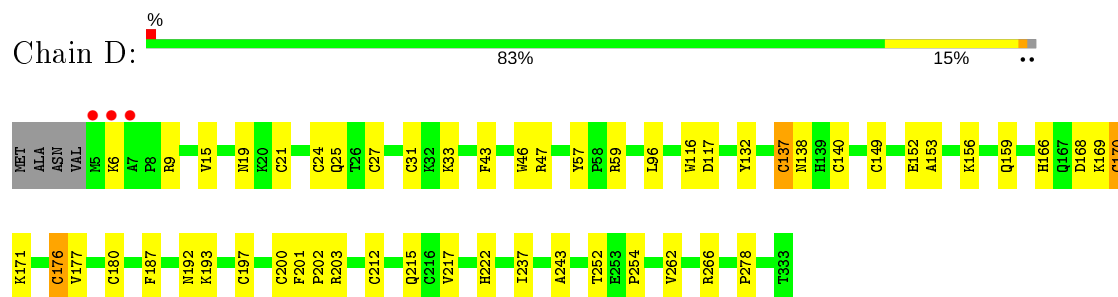
- Chain K:
- 
- 71% 27%
- ALA  
ALA  
THR  
ASP  
T15  
S16  
G17  
A18  
F19  
E10  
G13  
R29  
G30  
A31  
R32  
T37  
Q38  
A39  
Q40  
P41  
H42  
E54  
E55  
Q56  
S57  
R58  
D59  
L60  
A61  
P62  
N63  
P64  
R72  
R73  
G74  
K76  
G77  
E78  
T79  
G80  
R81  
K91  
R91  
E106  
T108  
W110  
E111  
E112  
D115  
T236  
V239  
I243  
P247  
I262  
Y267  
L272  
K273  
E274  
Q275  
T276  
D277  
L278  
S279  
Y280  
L281  
V282  
R283  
S284  
T285  
D286  
K287  
R288  
F289  
L290  
R291  
E292  
A293  
D294  
V295  
G299  
D302  
K303  
F304  
Y305  
F306  
W307  
N308  
A309  
K310  
T311  
P317  
K318  
W321  
G322  
D323  
K324  
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F342  
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I347  
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D366  
G367  
V372  
R373  
R374  
P374  
V375  
F376  
K414  
P415  
S416  
M417  
Y428  
H438  
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L443  
T446  
E447  
G448  
G452  
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E461  
K462  
P463  
A464  
F465  
L468



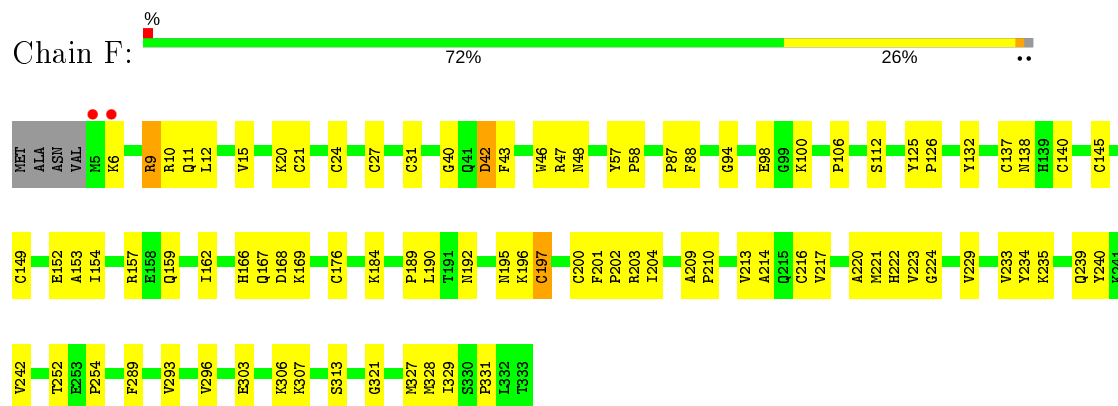
- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



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

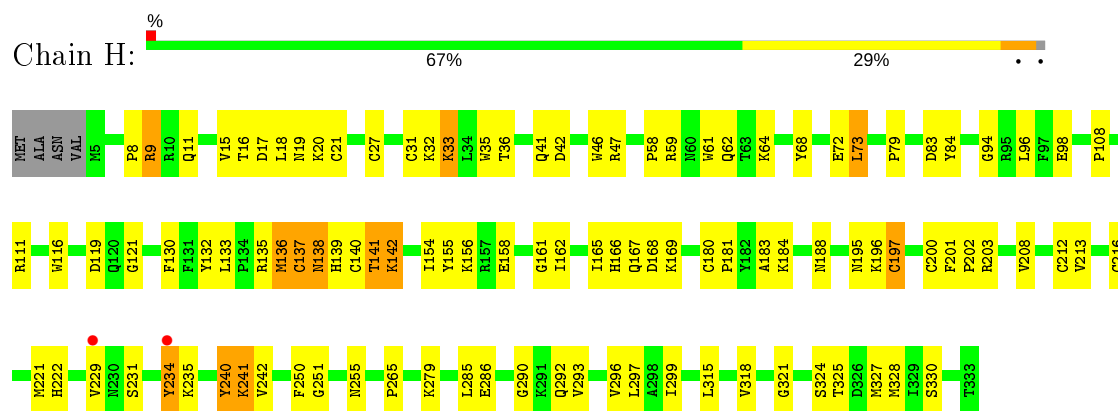


- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit

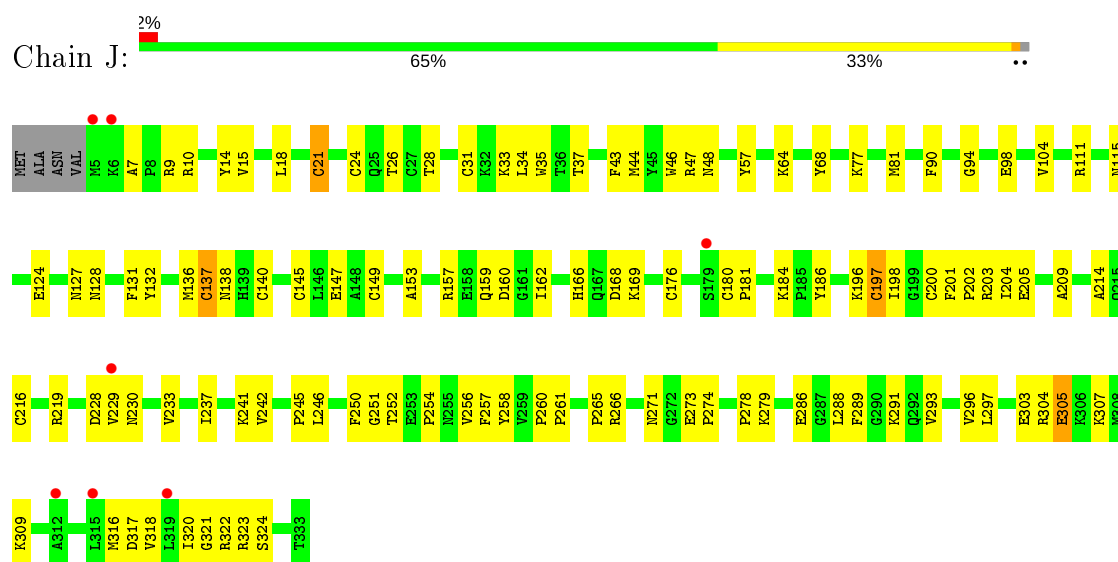




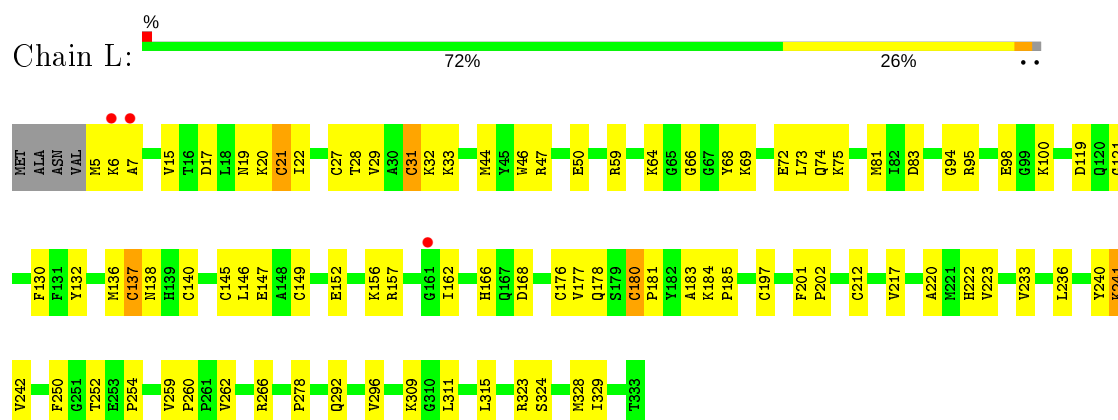
- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.59Å 253.13Å 135.80Å 90.00° 119.77° 90.00°	Depositor
Resolution (Å)	48.32 – 2.40 48.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.32-2.40) 99.2 (48.32-2.40)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.195 , 0.249 0.189 , 0.238	Depositor DCC
$R_{free}$ test set	14935 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 22.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.137 for -h-l,k,h 0.137 for l,k,-h-l 0.186 for h,-k,-h-l 0.135 for -h-l,-k,l 0.127 for l,-k,h	Xtriage
Reported twinning fraction	0.160 for l,k,-h-l	Depositor
Outliers	0 of 306123 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	62374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MGD, 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	0.24	0/7396	0.43	0/10034
1	C	0.25	0/7396	0.44	0/10034
1	E	0.25	0/7396	0.45	0/10034
1	G	0.26	0/7396	0.45	0/10034
1	I	0.30	0/7396	0.50	3/10034 (0.0%)
1	K	0.29	1/7396 (0.0%)	0.48	1/10034 (0.0%)
2	B	0.26	0/2632	0.44	0/3567
2	D	0.26	0/2632	0.45	1/3567 (0.0%)
2	F	0.25	0/2632	0.43	0/3567
2	H	0.30	0/2632	0.50	1/3567 (0.0%)
2	J	0.28	0/2632	0.49	0/3567
2	L	0.28	0/2632	0.46	0/3567
All	All	0.27	1/60168 (0.0%)	0.46	6/81606 (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	I	0	2
1	K	0	1
2	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	324	GLN	C-N	5.12	1.44	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	73	LEU	CA-CB-CG	-7.69	97.61	115.30
1	I	406	LEU	CA-CB-CG	6.90	131.18	115.30
1	K	294	ASP	CB-CG-OD1	-6.26	112.67	118.30
2	D	176	CYS	CA-CB-SG	-5.65	103.83	114.00
1	I	19	ARG	NE-CZ-NH1	5.37	122.98	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	240	TYR	Peptide
1	I	345	GLY	Peptide
1	I	644	LYS	Peptide
1	K	294	ASP	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	7180	0	7012	108	0
1	C	7180	0	7013	113	0
1	E	7180	0	7013	158	0
1	G	7180	0	7014	144	0
1	I	7180	0	7014	265	0
1	K	7180	0	7013	209	0
2	B	2564	0	2545	75	0
2	D	2564	0	2547	39	0
2	F	2564	0	2546	66	0
2	H	2564	0	2549	99	0
2	J	2564	0	2548	98	0
2	L	2564	0	2547	78	0
3	A	8	0	0	0	0
3	B	24	0	0	1	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
3	G	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	24	0	0	0	0
3	I	8	0	0	2	0
3	J	24	0	0	0	0
3	K	8	0	0	2	0
3	L	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
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	A	47	0	22	2	0
5	C	47	0	22	1	0
5	E	47	0	22	4	0
5	G	47	0	22	3	0
5	I	47	0	22	7	0
5	K	47	0	22	1	0
6	A	47	0	21	1	0
6	C	47	0	21	2	0
6	E	47	0	21	1	0
6	G	47	0	22	6	0
6	I	47	0	23	2	0
6	K	47	0	21	3	0
7	A	20	0	30	1	0
7	B	8	0	12	0	0
7	C	12	0	18	2	0
7	D	4	0	6	0	0
7	E	8	0	12	2	0
7	F	8	0	12	1	0
7	G	16	0	24	3	0
7	H	12	0	18	3	0
7	I	8	0	12	3	0
7	J	4	0	6	0	0
7	K	8	0	12	0	0
7	L	8	0	12	0	0
8	A	6	0	8	1	0
8	E	6	0	8	1	0
9	B	7	0	0	0	0
9	D	7	0	0	0	0
9	F	7	0	0	0	0
9	H	7	0	0	0	0
9	J	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	7	0	0	0	0
10	A	399	0	0	19	0
10	B	179	0	0	23	0
10	C	417	0	0	25	0
10	D	176	0	0	5	0
10	E	384	0	0	39	0
10	F	148	0	0	13	0
10	G	348	0	0	23	0
10	H	116	0	0	13	0
10	I	266	0	0	41	0
10	J	127	0	0	18	0
10	K	287	0	0	24	0
10	L	131	0	0	13	0
All	All	62374	0	57812	1396	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 12.

The worst 5 of 1396 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:K:294:ASP:HB3	1:K:364:LEU:HD12	1.48	0.94
1:I:53:ARG:NH2	1:I:55:GLU:OE1	2.04	0.90
1:A:628:MET:SD	1:A:632:ARG:NH1	2.45	0.90
2:J:245:PRO:HB2	2:J:254:PRO:HG2	1.54	0.87
1:A:830:ARG:NH1	10:A:1101:HOH:O	2.08	0.87

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	896/899 (100%)	852 (95%)	40 (4%)	4 (0%)	34	48
1	C	896/899 (100%)	849 (95%)	42 (5%)	5 (1%)	25	36
1	E	896/899 (100%)	845 (94%)	47 (5%)	4 (0%)	34	48
1	G	896/899 (100%)	841 (94%)	49 (6%)	6 (1%)	22	32
1	I	896/899 (100%)	815 (91%)	71 (8%)	10 (1%)	14	20
1	K	896/899 (100%)	822 (92%)	64 (7%)	10 (1%)	14	20
2	B	327/333 (98%)	314 (96%)	11 (3%)	2 (1%)	25	36
2	D	327/333 (98%)	311 (95%)	15 (5%)	1 (0%)	41	55
2	F	327/333 (98%)	312 (95%)	15 (5%)	0	100	100
2	H	327/333 (98%)	306 (94%)	16 (5%)	5 (2%)	10	14
2	J	327/333 (98%)	313 (96%)	13 (4%)	1 (0%)	41	55
2	L	327/333 (98%)	311 (95%)	16 (5%)	0	100	100
All	All	7338/7392 (99%)	6891 (94%)	399 (5%)	48 (1%)	22	32

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	70	ASN
1	G	6	SER
2	H	141	THR
2	H	241	LYS
1	I	317	PRO

### 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%)	761 (99%)	8 (1%)	76	88
1	C	769/768 (100%)	759 (99%)	10 (1%)	69	84
1	E	769/768 (100%)	762 (99%)	7 (1%)	78	90
1	G	769/768 (100%)	759 (99%)	10 (1%)	69	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	769/768 (100%)	752 (98%)	17 (2%)	52	71
1	K	769/768 (100%)	754 (98%)	15 (2%)	55	74
2	B	278/281 (99%)	269 (97%)	9 (3%)	39	59
2	D	278/281 (99%)	273 (98%)	5 (2%)	59	76
2	F	278/281 (99%)	271 (98%)	7 (2%)	47	67
2	H	278/281 (99%)	269 (97%)	9 (3%)	39	59
2	J	278/281 (99%)	270 (97%)	8 (3%)	42	62
2	L	278/281 (99%)	272 (98%)	6 (2%)	52	71
All	All	6282/6294 (100%)	6171 (98%)	111 (2%)	59	76

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	198	ILE
2	H	216	CYS
1	K	465	PHE
1	G	205	THR
2	H	33	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	195	ASN
1	I	363	GLN
2	L	74	GLN
1	I	16	ASN
1	I	21	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 79 ligands modelled in this entry, 6 are monoatomic - leaving 73 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	B	405	2	0,12,12	0.00	-	-		
3	SF4	F	405	-	0,12,12	0.00	-	-		
9	F3S	B	402	-	0,9,9	0.00	-	-		
9	F3S	F	402	-	0,9,9	0.00	-	-		
7	EDO	I	1005	-	3,3,3	0.46	0	2,2,2	0.34	0
7	EDO	C	1006	-	3,3,3	0.44	0	2,2,2	0.34	0
7	EDO	C	1007	-	3,3,3	0.45	0	2,2,2	0.32	0
3	SF4	D	404	2	0,12,12	0.00	-	-		
6	MD1	C	1004	4	38,51,51	4.43	15 (39%)	35,78,78	1.42	5 (14%)
3	SF4	B	403	2	0,12,12	0.00	-	-		
7	EDO	A	1007	-	3,3,3	0.46	0	2,2,2	0.35	0
6	MD1	A	1004	4	38,51,51	4.43	15 (39%)	35,78,78	1.41	5 (14%)
3	SF4	L	404	2	0,12,12	0.00	-	-		
5	MGD	E	1003	4	41,52,52	6.50	27 (65%)	43,81,81	2.40	17 (39%)
8	GOL	A	1008	-	5,5,5	0.36	0	5,5,5	0.27	0
3	SF4	H	403	-	0,12,12	0.00	-	-		
9	F3S	D	401	-	0,9,9	0.00	-	-		
7	EDO	I	1006	-	3,3,3	0.46	0	2,2,2	0.37	0
7	EDO	H	406	-	3,3,3	0.46	0	2,2,2	0.32	0
3	SF4	H	404	-	0,12,12	0.00	-	-		
5	MGD	C	1003	4	41,52,52	6.48	27 (65%)	43,81,81	2.41	16 (37%)
3	SF4	D	402	-	0,12,12	0.00	-	-		
7	EDO	G	1006	-	3,3,3	0.46	0	2,2,2	0.33	0
7	EDO	A	1006	-	3,3,3	0.45	0	2,2,2	0.33	0
7	EDO	G	1007	-	3,3,3	0.45	0	2,2,2	0.33	0
3	SF4	E	1001	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SF4	L	402	-	0,12,12	0.00	-	-		
3	SF4	F	403	2	0,12,12	0.00	-	-		
6	MD1	K	1004	4	38,51,51	4.40	17 (44%)	35,78,78	1.42	5 (14%)
7	EDO	A	1010	-	3,3,3	0.46	0	2,2,2	0.36	0
7	EDO	J	405	-	3,3,3	0.46	0	2,2,2	0.36	0
7	EDO	A	1009	-	3,3,3	0.45	0	2,2,2	0.33	0
9	F3S	L	401	-	0,9,9	0.00	-	-		
7	EDO	F	406	-	3,3,3	0.46	0	2,2,2	0.34	0
6	MD1	G	1004	4	38,51,51	4.42	17 (44%)	35,78,78	1.41	5 (14%)
7	EDO	K	1005	-	3,3,3	0.45	0	2,2,2	0.30	0
3	SF4	K	1001	1	0,12,12	0.00	-	-		
7	EDO	B	401	-	3,3,3	0.46	0	2,2,2	0.31	0
3	SF4	J	402	-	0,12,12	0.00	-	-		
7	EDO	L	406	-	3,3,3	0.47	0	2,2,2	0.34	0
3	SF4	C	1001	1	0,12,12	0.00	-	-		
7	EDO	A	1005	-	3,3,3	0.46	0	2,2,2	0.35	0
8	GOL	E	1006	-	5,5,5	0.37	0	5,5,5	0.34	0
3	SF4	D	403	-	0,12,12	0.00	-	-		
7	EDO	G	1008	-	3,3,3	0.46	0	2,2,2	0.34	0
7	EDO	H	405	-	3,3,3	0.45	0	2,2,2	0.32	0
3	SF4	B	404	-	0,12,12	0.00	-	-		
5	MGD	A	1003	4	41,52,52	6.48	27 (65%)	43,81,81	2.49	17 (39%)
5	MGD	G	1003	4	41,52,52	6.51	27 (65%)	43,81,81	2.41	17 (39%)
7	EDO	E	1005	-	3,3,3	0.45	0	2,2,2	0.34	0
3	SF4	F	404	-	0,12,12	0.00	-	-		
3	SF4	J	404	-	0,12,12	0.00	-	-		
7	EDO	B	406	-	3,3,3	0.46	0	2,2,2	0.37	0
3	SF4	A	1001	1	0,12,12	0.00	-	-		
7	EDO	G	1005	-	3,3,3	0.46	0	2,2,2	0.32	0
7	EDO	H	407	-	3,3,3	0.44	0	2,2,2	0.39	0
7	EDO	C	1005	-	3,3,3	0.45	0	2,2,2	0.35	0
3	SF4	G	1001	1	0,12,12	0.00	-	-		
7	EDO	E	1007	-	3,3,3	0.46	0	2,2,2	0.31	0
7	EDO	D	405	-	3,3,3	0.45	0	2,2,2	0.32	0
9	F3S	J	401	-	0,9,9	0.00	-	-		
7	EDO	K	1006	-	3,3,3	0.45	0	2,2,2	0.32	0
5	MGD	K	1003	4	41,52,52	6.49	27 (65%)	43,81,81	2.49	17 (39%)
6	MD1	I	1004	4	38,51,51	4.39	17 (44%)	35,78,78	1.39	5 (14%)
7	EDO	L	405	-	3,3,3	0.47	0	2,2,2	0.31	0
3	SF4	H	402	-	0,12,12	0.00	-	-		
9	F3S	H	401	-	0,9,9	0.00	-	-		
3	SF4	I	1001	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SF4	L	403	-	0,12,12	0.00	-	-		
6	MD1	E	1004	4	38,51,51	4.41	15 (39%)	35,78,78	1.41	4 (11%)
3	SF4	J	403	-	0,12,12	0.00	-	-		
7	EDO	F	401	-	3,3,3	0.45	0	2,2,2	0.33	0
5	MGD	I	1003	4	41,52,52	6.53	27 (65%)	43,81,81	2.46	17 (39%)

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	B	405	2	-	-	0/6/5/5
3	SF4	F	405	-	-	-	0/6/5/5
9	F3S	B	402	-	-	-	0/3/3/3
3	SF4	L	404	2	-	-	0/6/5/5
7	EDO	I	1005	-	-	0/1/1/1	-
7	EDO	C	1006	-	-	1/1/1/1	-
7	EDO	C	1007	-	-	1/1/1/1	-
3	SF4	D	404	2	-	-	0/6/5/5
7	EDO	E	1007	-	-	0/1/1/1	-
3	SF4	B	403	2	-	-	0/6/5/5
7	EDO	A	1007	-	-	0/1/1/1	-
6	MD1	A	1004	4	-	5/21/59/59	0/5/5/5
6	MD1	C	1004	4	-	8/21/59/59	0/5/5/5
5	MGD	E	1003	4	-	2/18/66/66	0/6/6/6
8	GOL	A	1008	-	-	0/4/4/4	-
3	SF4	H	403	-	-	-	0/6/5/5
9	F3S	D	401	-	-	-	0/3/3/3
7	EDO	I	1006	-	-	0/1/1/1	-
7	EDO	H	406	-	-	0/1/1/1	-
7	EDO	K	1006	-	-	0/1/1/1	-
5	MGD	C	1003	4	-	6/18/66/66	0/6/6/6
3	SF4	D	402	-	-	-	0/6/5/5
7	EDO	G	1006	-	-	0/1/1/1	-
7	EDO	A	1006	-	-	0/1/1/1	-
7	EDO	G	1007	-	-	0/1/1/1	-
3	SF4	E	1001	1	-	-	0/6/5/5
3	SF4	L	402	-	-	-	0/6/5/5
3	SF4	F	403	2	-	-	0/6/5/5
6	MD1	K	1004	4	-	8/21/59/59	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	1010	-	-	0/1/1/1	-
7	EDO	J	405	-	-	0/1/1/1	-
7	EDO	A	1009	-	-	0/1/1/1	-
9	F3S	L	401	-	-	-	0/3/3/3
7	EDO	F	406	-	-	0/1/1/1	-
6	MD1	G	1004	4	-	5/21/59/59	0/5/5/5
7	EDO	K	1005	-	-	0/1/1/1	-
3	SF4	K	1001	1	-	-	0/6/5/5
7	EDO	B	401	-	-	0/1/1/1	-
3	SF4	J	402	-	-	-	0/6/5/5
7	EDO	L	406	-	-	0/1/1/1	-
3	SF4	C	1001	1	-	-	0/6/5/5
3	SF4	H	404	-	-	-	0/6/5/5
8	GOL	E	1006	-	-	0/4/4/4	-
3	SF4	D	403	-	-	-	0/6/5/5
7	EDO	G	1008	-	-	0/1/1/1	-
7	EDO	H	405	-	-	0/1/1/1	-
3	SF4	B	404	-	-	-	0/6/5/5
5	MGD	A	1003	4	-	2/18/66/66	0/6/6/6
5	MGD	G	1003	4	-	2/18/66/66	0/6/6/6
7	EDO	E	1005	-	-	0/1/1/1	-
3	SF4	F	404	-	-	-	0/6/5/5
3	SF4	J	404	-	-	-	0/6/5/5
7	EDO	B	406	-	-	0/1/1/1	-
3	SF4	A	1001	1	-	-	0/6/5/5
7	EDO	G	1005	-	-	0/1/1/1	-
7	EDO	H	407	-	-	0/1/1/1	-
3	SF4	J	403	-	-	-	0/6/5/5
3	SF4	G	1001	1	-	-	0/6/5/5
7	EDO	C	1005	-	-	1/1/1/1	-
9	F3S	F	402	-	-	-	0/3/3/3
7	EDO	D	405	-	-	0/1/1/1	-
9	F3S	J	401	-	-	-	0/3/3/3
5	MGD	K	1003	4	-	1/18/66/66	0/6/6/6
6	MD1	I	1004	4	-	7/21/59/59	0/5/5/5
7	EDO	L	405	-	-	0/1/1/1	-
3	SF4	H	402	-	-	-	0/6/5/5
9	F3S	H	401	-	-	-	0/3/3/3
3	SF4	I	1001	1	-	-	0/6/5/5
3	SF4	L	403	-	-	-	0/6/5/5
6	MD1	E	1004	4	-	3/21/59/59	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	1005	-	-	1/1/1/1	-
7	EDO	F	401	-	-	0/1/1/1	-
5	MGD	I	1003	4	-	1/18/66/66	0/6/6/6

The worst 5 of 258 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1003	MGD	C2'-C1'	-17.21	1.27	1.53
5	G	1003	MGD	C2'-C1'	-17.20	1.27	1.53
5	C	1003	MGD	C2'-C1'	-17.18	1.27	1.53
5	K	1003	MGD	C2'-C1'	-17.16	1.27	1.53
5	A	1003	MGD	C2'-C1'	-17.15	1.27	1.53

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1003	MGD	O11-C23-N22	-7.00	101.38	108.57
5	K	1003	MGD	O11-C23-C14	6.00	112.96	108.96
5	A	1003	MGD	O11-C23-C14	5.86	112.87	108.96
5	K	1003	MGD	C17-C16-C21	5.83	119.75	114.57
5	G	1003	MGD	C17-C16-C21	5.76	119.68	114.57

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1003	MGD	C5'-O5'-PB-O1B
5	E	1003	MGD	O3A-C10-C11-O11
6	C	1004	MD1	PB-O3B-PA-O5'
6	C	1004	MD1	C5'-O5'-PA-O1A
6	C	1004	MD1	O4'-C4'-C5'-O5'

There are no ring outliers.

32 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	405	SF4	1	0
3	F	405	SF4	1	0
7	I	1005	EDO	1	0
7	C	1007	EDO	2	0
3	D	404	SF4	1	0

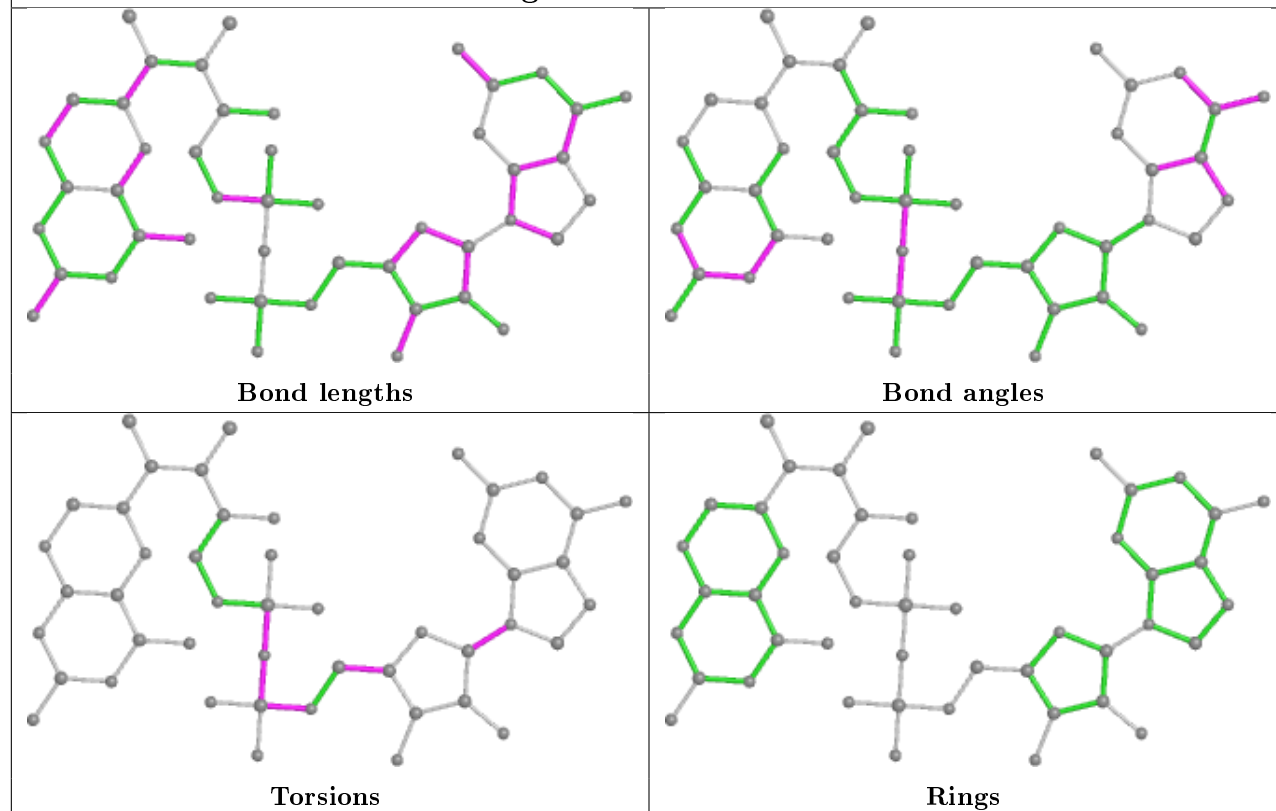
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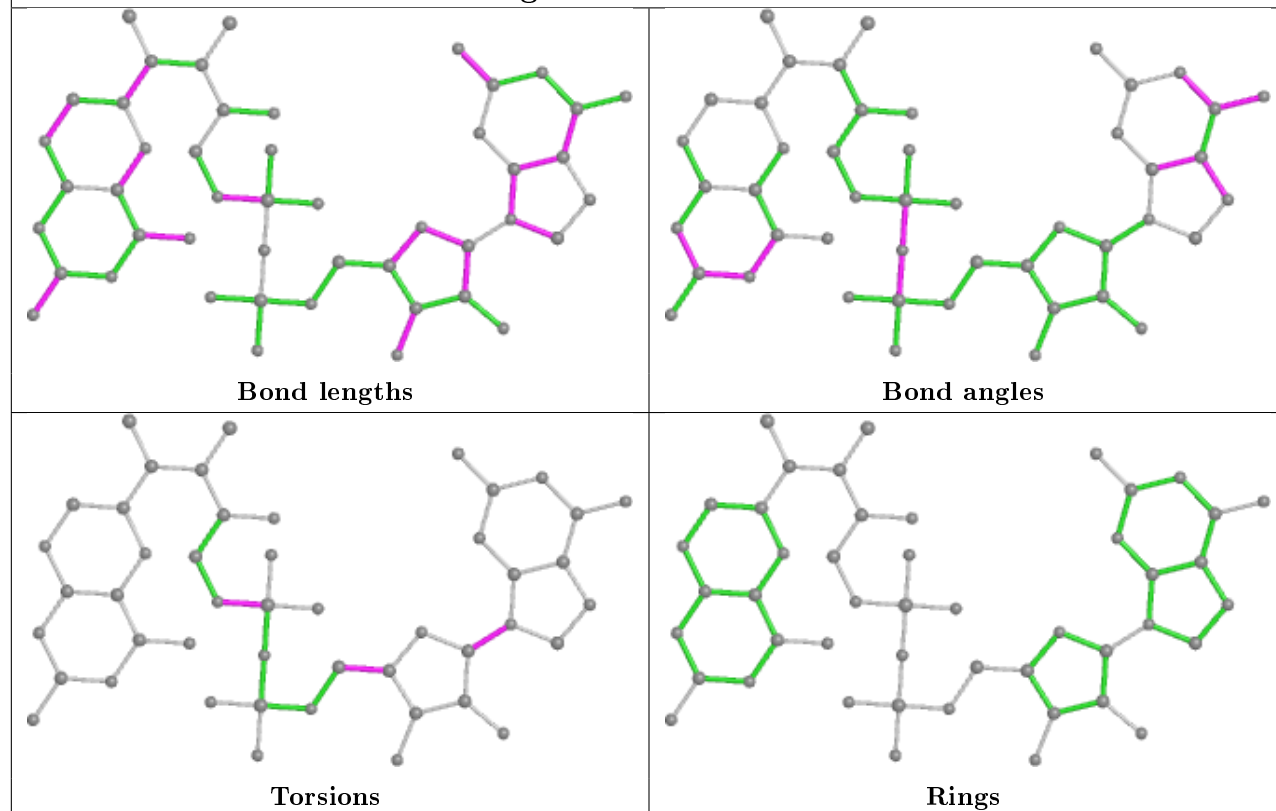
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1004	MD1	2	0
6	A	1004	MD1	1	0
3	L	404	SF4	1	0
5	E	1003	MGD	4	0
8	A	1008	GOL	1	0
7	I	1006	EDO	2	0
7	H	406	EDO	1	0
5	C	1003	MGD	1	0
7	G	1007	EDO	1	0
6	K	1004	MD1	3	0
6	G	1004	MD1	6	0
3	K	1001	SF4	2	0
7	A	1005	EDO	1	0
8	E	1006	GOL	1	0
7	G	1008	EDO	1	0
7	H	405	EDO	2	0
5	A	1003	MGD	2	0
5	G	1003	MGD	3	0
7	E	1005	EDO	1	0
7	G	1005	EDO	1	0
7	E	1007	EDO	1	0
5	K	1003	MGD	1	0
6	I	1004	MD1	2	0
3	I	1001	SF4	2	0
6	E	1004	MD1	1	0
7	F	401	EDO	1	0
5	I	1003	MGD	7	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.

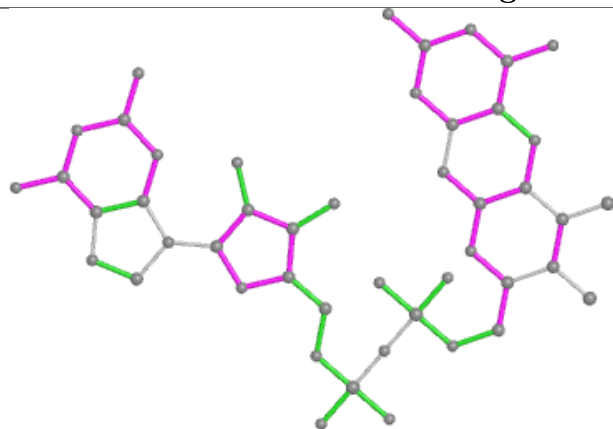
## Ligand MD1 C 1004



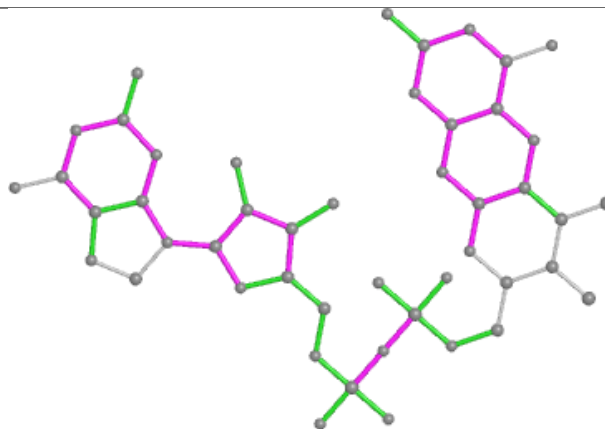
## Ligand MD1 A 1004



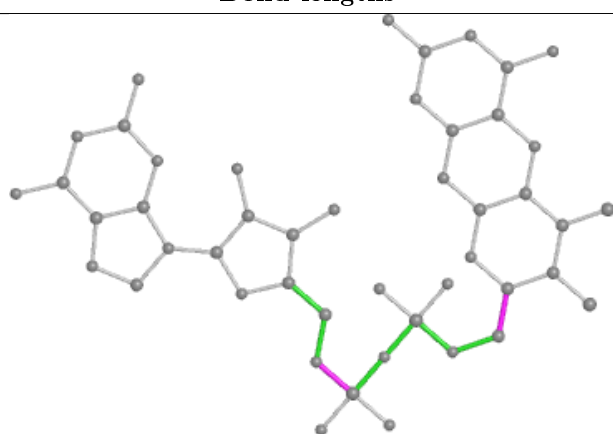
## Ligand MGD E 1003



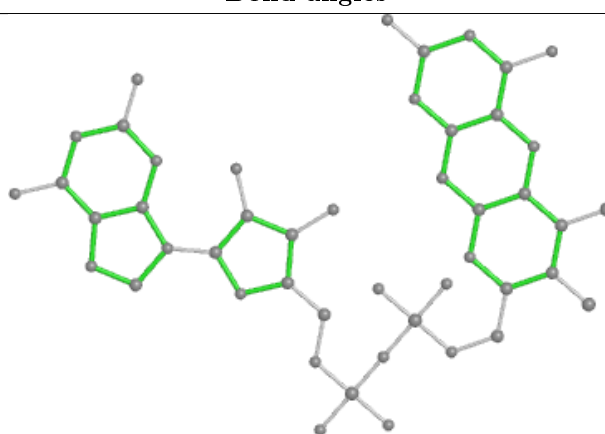
Bond lengths



Bond angles

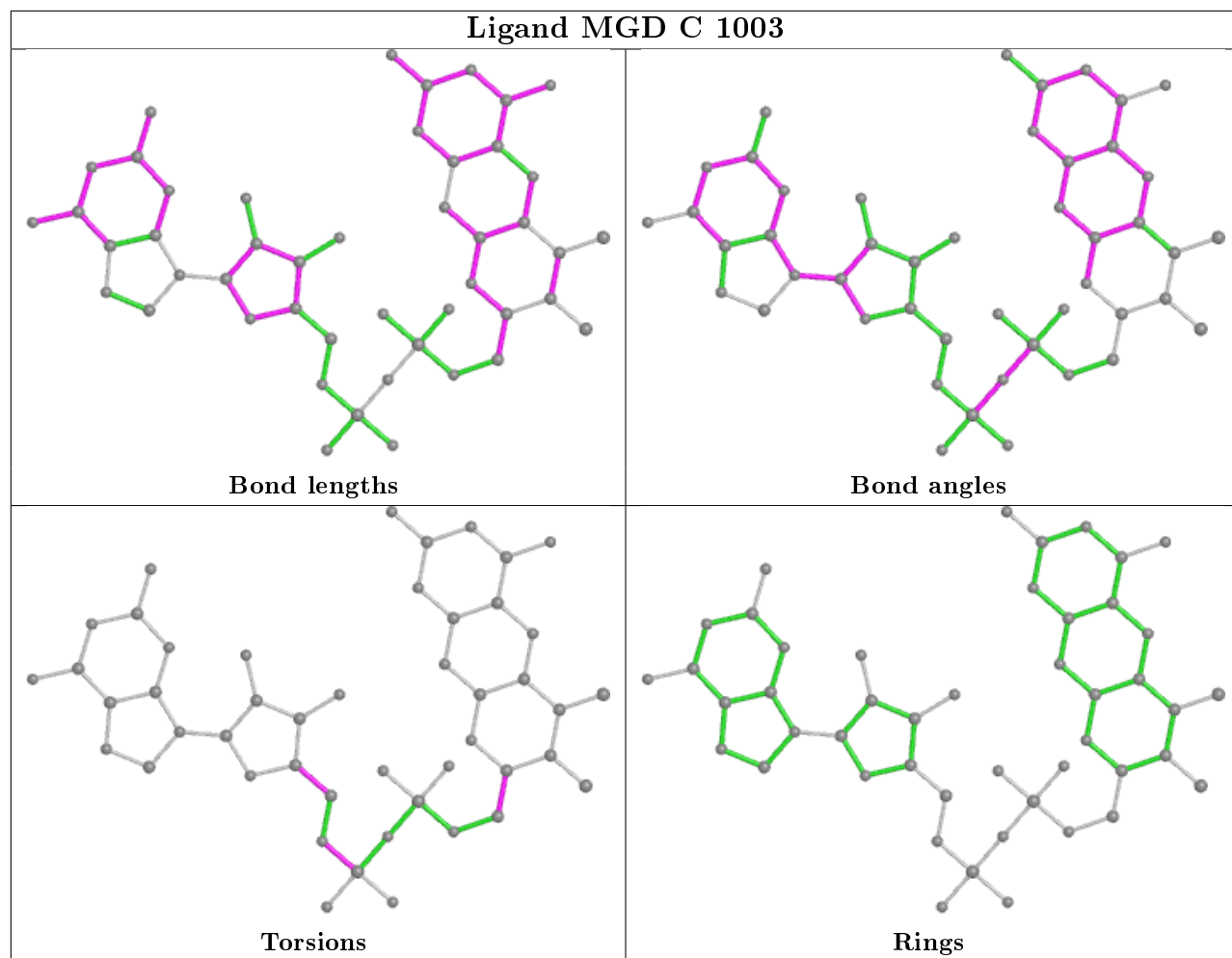


Torsions

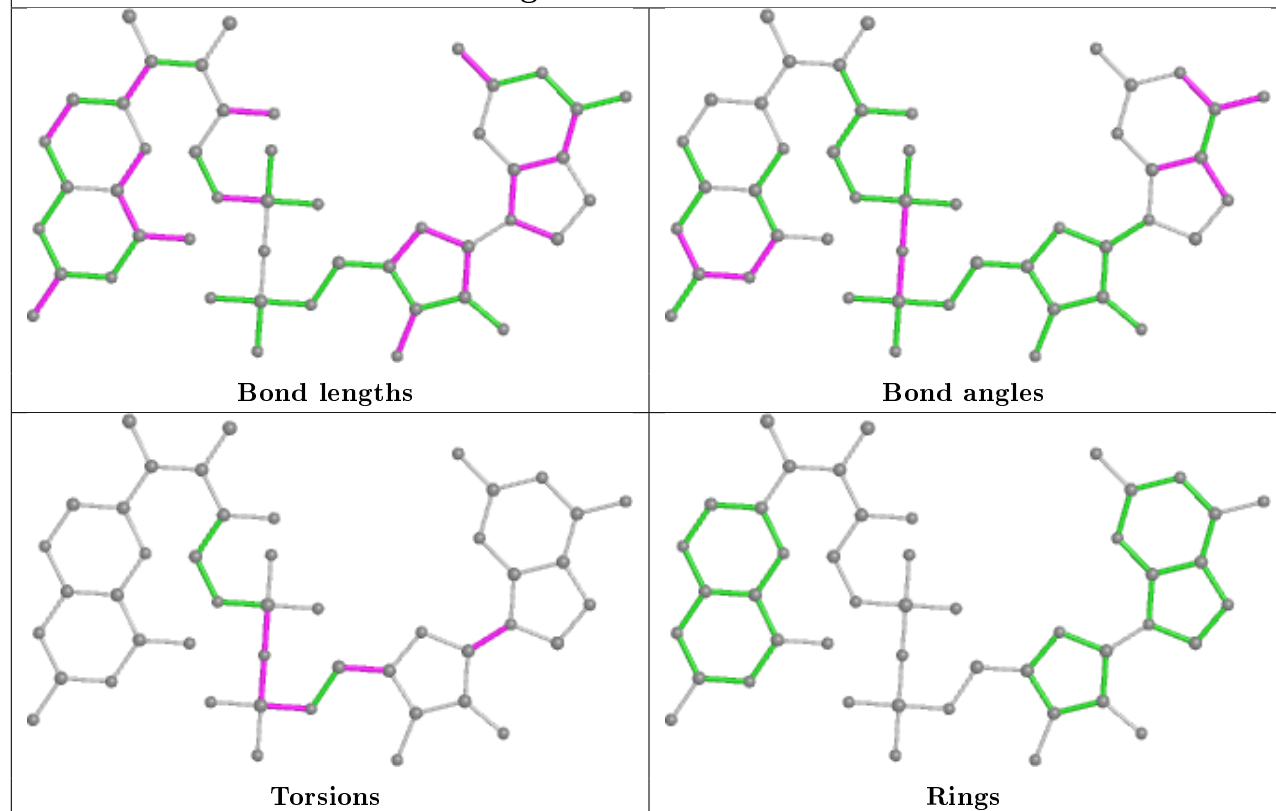


Rings

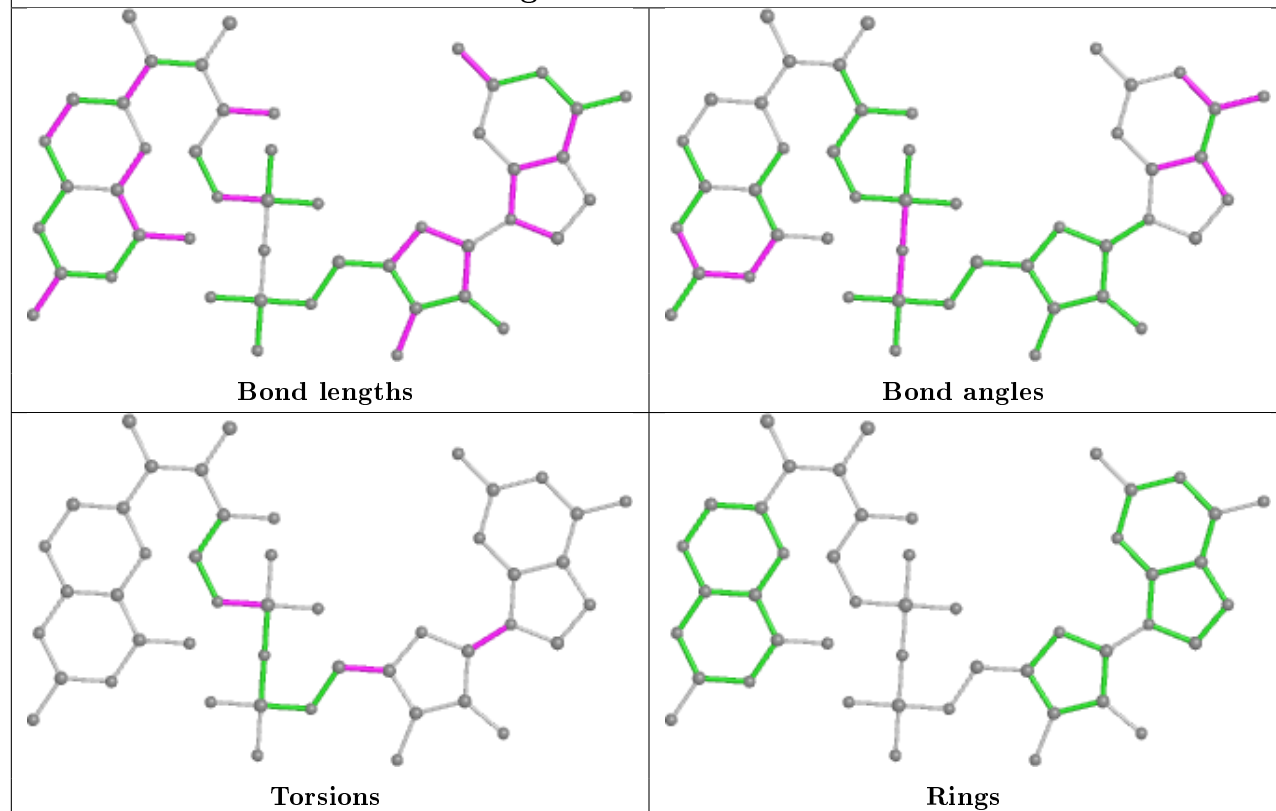




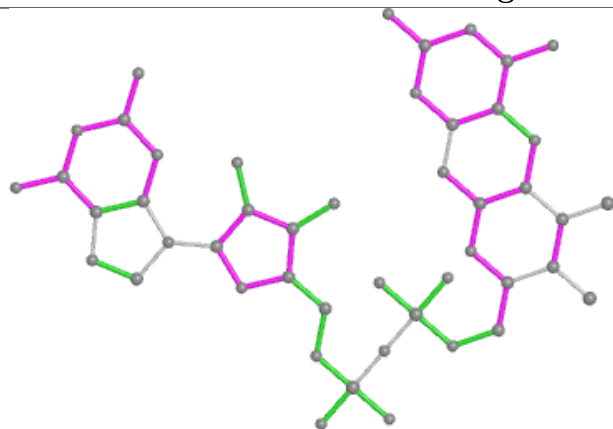
## Ligand MD1 K 1004



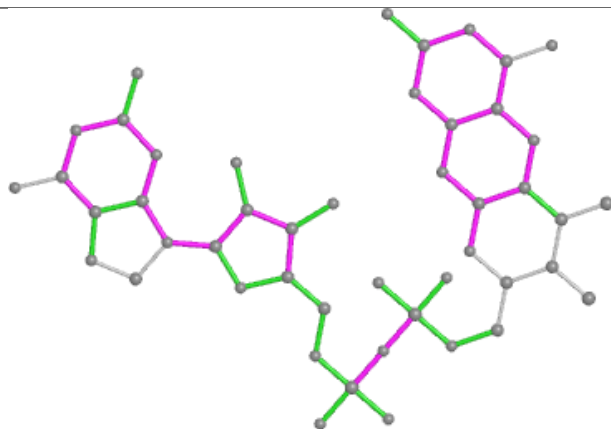
## Ligand MD1 G 1004



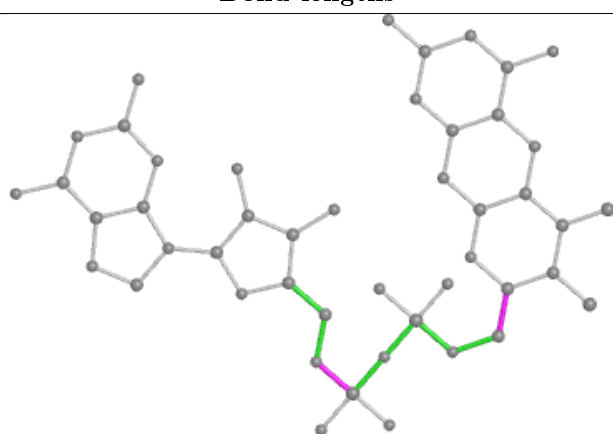
## Ligand MGD A 1003



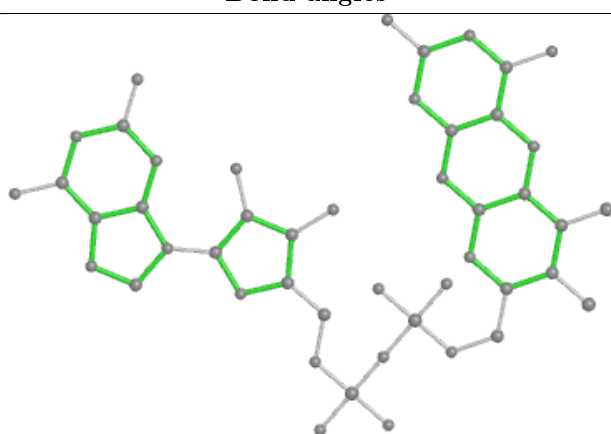
Bond lengths



Bond angles

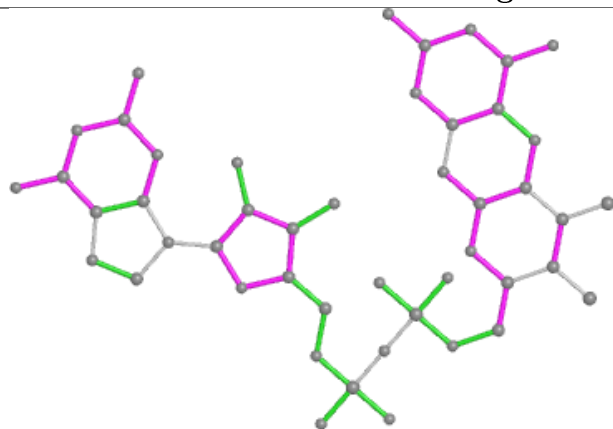


Torsions

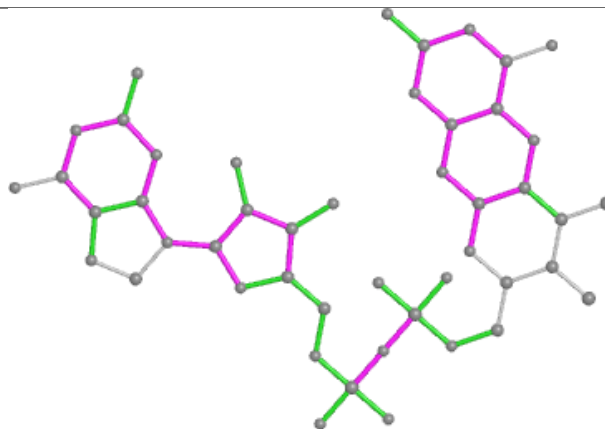


Rings

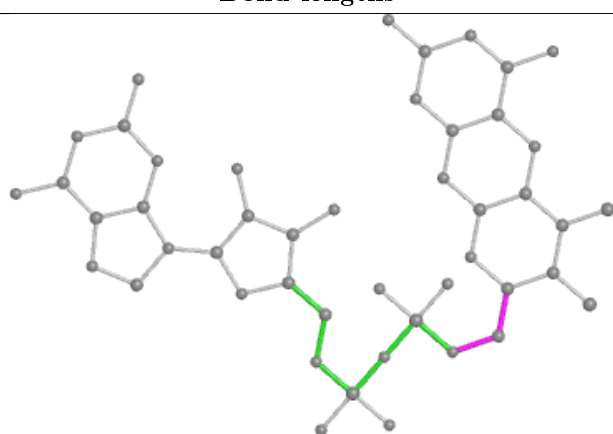
## Ligand MGD G 1003



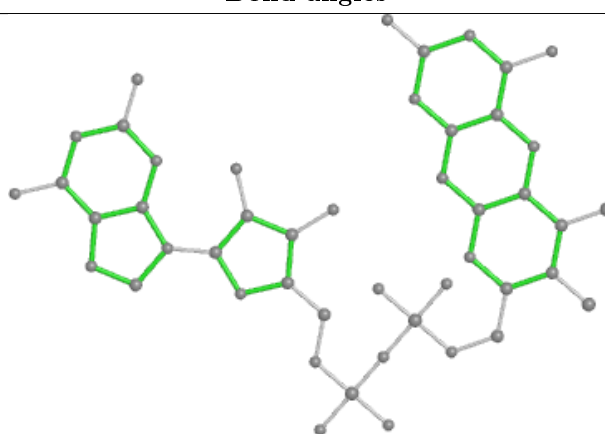
Bond lengths



Bond angles

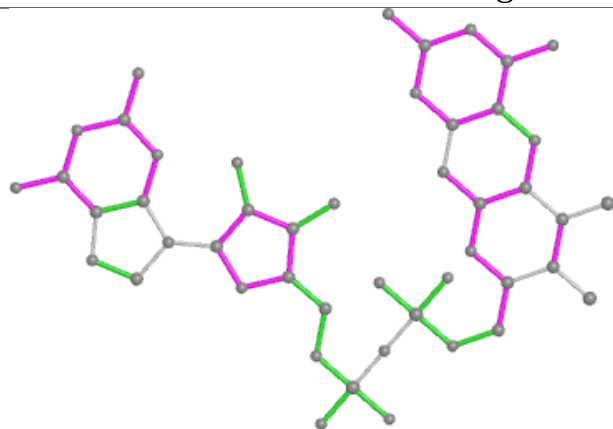


Torsions

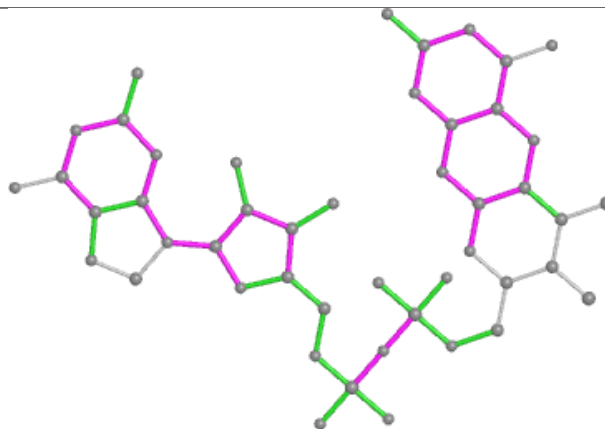


Rings

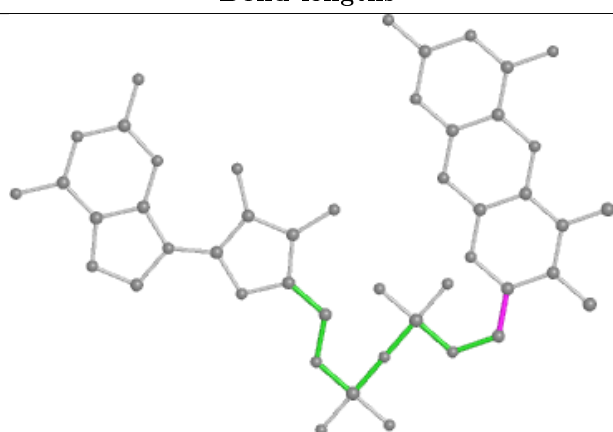
## Ligand MGD K 1003



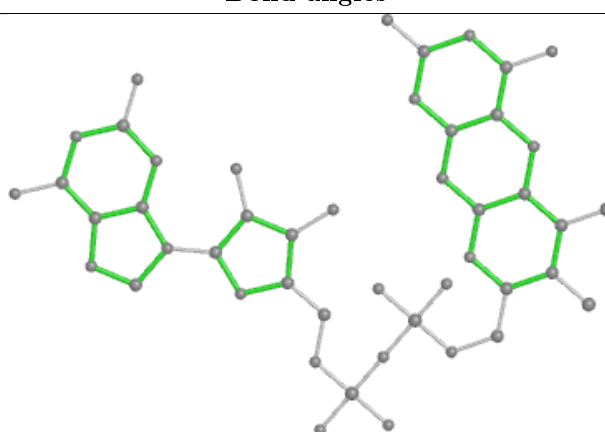
Bond lengths



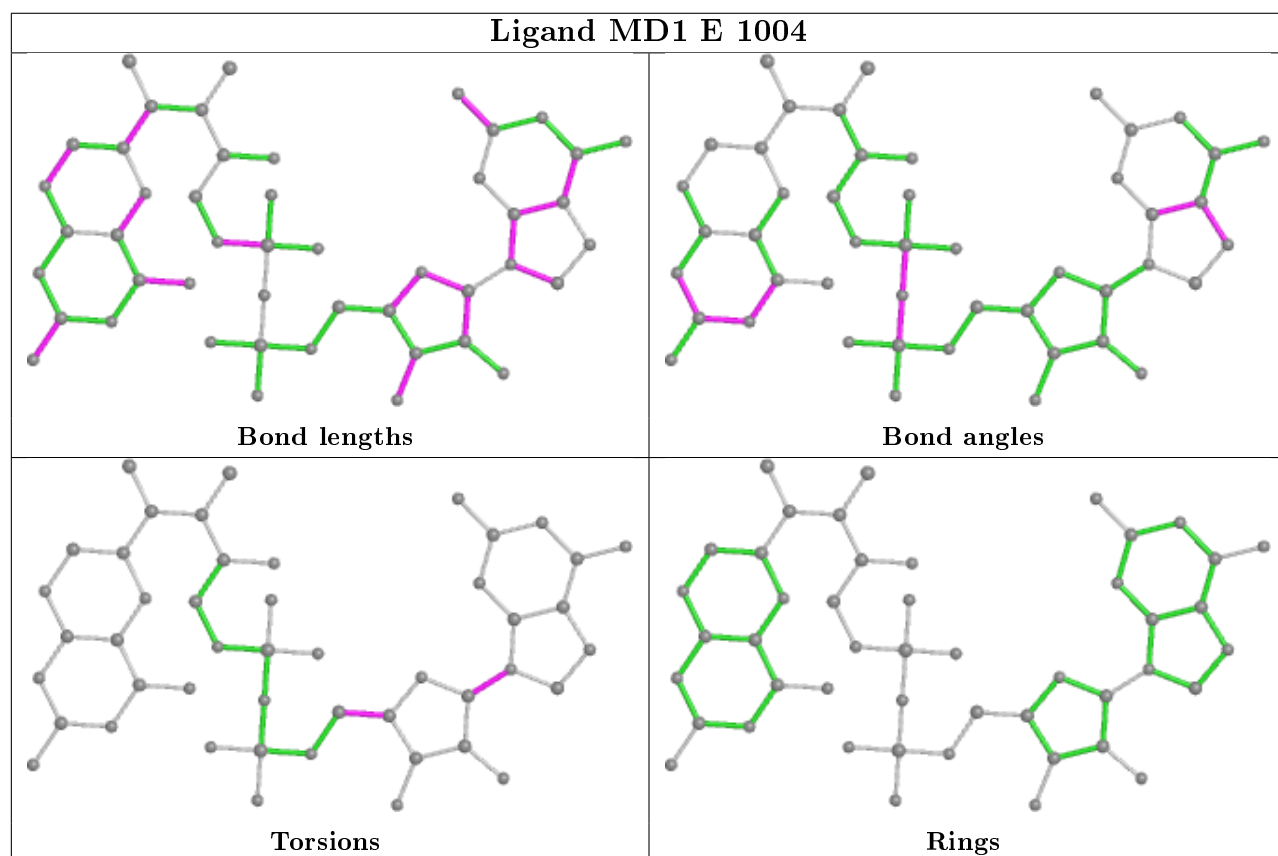
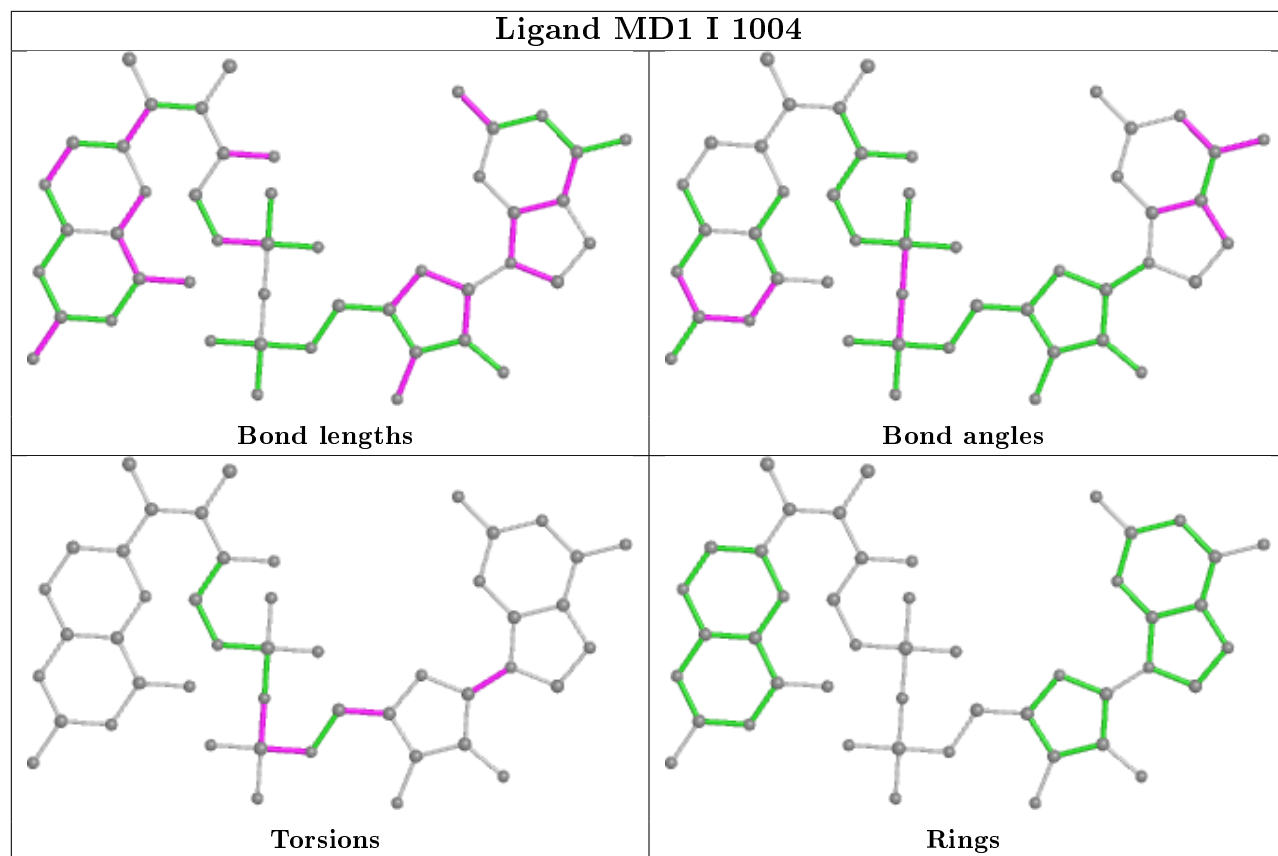
Bond angles

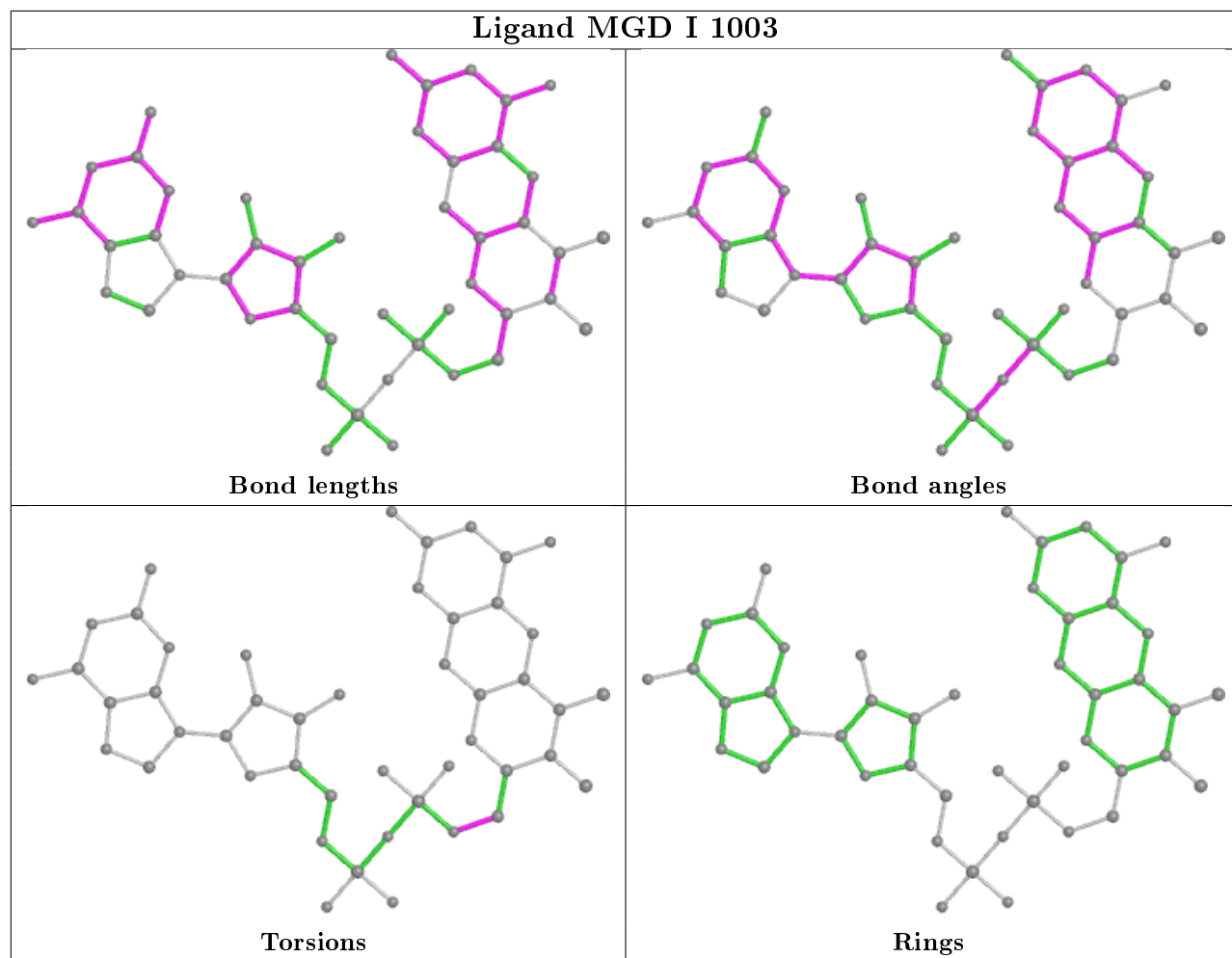


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	-0.58	4 (0%) 92 91	20, 32, 47, 80	0
1	C	895/899 (99%)	-0.62	4 (0%) 92 91	20, 30, 41, 76	0
1	E	895/899 (99%)	-0.57	4 (0%) 92 91	22, 32, 44, 81	0
1	G	895/899 (99%)	-0.44	5 (0%) 89 88	20, 37, 53, 76	0
1	I	895/899 (99%)	-0.16	15 (1%) 70 68	25, 46, 66, 90	0
1	K	895/899 (99%)	-0.28	13 (1%) 73 72	25, 43, 62, 91	0
2	B	329/333 (98%)	-0.51	0 100 100	21, 34, 47, 66	0
2	D	329/333 (98%)	-0.58	3 (0%) 84 82	22, 33, 44, 72	0
2	F	329/333 (98%)	-0.55	2 (0%) 89 88	23, 35, 49, 62	0
2	H	329/333 (98%)	-0.13	2 (0%) 89 88	27, 46, 63, 78	0
2	J	329/333 (98%)	0.02	7 (2%) 63 61	26, 53, 65, 79	0
2	L	329/333 (98%)	-0.33	3 (0%) 84 82	27, 44, 55, 72	0
All	All	7344/7392 (99%)	-0.41	62 (0%) 86 84	20, 36, 58, 91	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	6	SER	7.9
1	E	5	ILE	7.7
1	I	7	GLY	6.6
1	K	367	GLY	6.6
1	A	5	ILE	6.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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( $\text{\AA}^2$ )	Q<0.9
7	EDO	F	401	4/4	0.77	0.50	47,50,55,56	0
7	EDO	K	1005	4/4	0.78	0.25	36,41,42,45	0
7	EDO	H	406	4/4	0.81	0.31	56,57,59,67	0
7	EDO	C	1005	4/4	0.82	0.24	34,38,39,39	0
7	EDO	I	1005	4/4	0.84	0.24	46,50,60,60	0
7	EDO	G	1006	4/4	0.84	0.28	50,51,51,53	0
8	GOL	E	1006	6/6	0.85	0.22	35,36,41,41	0
3	SF4	H	402	8/8	0.87	0.14	47,55,63,69	0
7	EDO	L	406	4/4	0.88	0.17	30,32,33,36	0
7	EDO	G	1005	4/4	0.89	0.15	28,32,34,40	0
7	EDO	H	405	4/4	0.89	0.22	30,33,34,37	0
7	EDO	H	407	4/4	0.89	0.14	23,26,27,30	0
7	EDO	E	1005	4/4	0.90	0.16	36,36,36,39	0
7	EDO	A	1005	4/4	0.92	0.14	23,29,31,33	0
3	SF4	F	405	8/8	0.92	0.15	20,38,44,44	0
7	EDO	G	1007	4/4	0.93	0.15	25,26,34,36	0
3	SF4	K	1001	8/8	0.93	0.13	39,45,53,58	0
7	EDO	E	1007	4/4	0.93	0.24	42,46,46,47	0
7	EDO	D	405	4/4	0.93	0.17	35,43,48,49	0
7	EDO	K	1006	4/4	0.93	0.20	33,33,36,38	0
7	EDO	I	1006	4/4	0.93	0.13	38,40,41,43	0
8	GOL	A	1008	6/6	0.93	0.14	29,35,36,36	0
3	SF4	J	402	8/8	0.93	0.11	52,58,65,65	0
5	MGD	I	1003	47/47	0.93	0.14	37,44,49,54	0
9	F3S	L	401	7/7	0.94	0.08	45,50,52,59	0
7	EDO	A	1007	4/4	0.94	0.17	40,40,44,47	0
3	SF4	L	404	8/8	0.94	0.14	43,48,57,60	0
3	SF4	B	405	8/8	0.94	0.14	25,33,37,38	0
3	SF4	J	403	8/8	0.94	0.14	38,51,56,65	0
3	SF4	G	1001	8/8	0.94	0.14	39,43,48,51	0
7	EDO	G	1008	4/4	0.94	0.27	32,32,36,41	0
7	EDO	A	1010	4/4	0.95	0.09	28,28,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	A	1009	4/4	0.95	0.11	27,28,30,32	0
9	F3S	J	401	7/7	0.95	0.10	47,52,56,62	0
7	EDO	A	1006	4/4	0.95	0.10	32,33,34,39	0
7	EDO	F	406	4/4	0.95	0.15	24,26,27,29	0
7	EDO	B	406	4/4	0.95	0.13	23,24,24,27	0
3	SF4	I	1001	8/8	0.95	0.13	42,53,54,66	0
3	SF4	L	403	8/8	0.95	0.11	38,45,51,55	0
3	SF4	A	1001	8/8	0.95	0.14	24,32,42,44	0
4	MO	I	1002	1/1	0.95	0.09	73,73,73,73	0
7	EDO	C	1007	4/4	0.95	0.12	28,29,30,30	0
3	SF4	F	403	8/8	0.96	0.13	25,34,41,46	0
7	EDO	B	401	4/4	0.96	0.12	25,28,28,31	0
6	MD1	K	1004	47/47	0.96	0.11	27,34,43,46	0
3	SF4	H	404	8/8	0.96	0.14	40,47,58,58	0
7	EDO	J	405	4/4	0.96	0.13	32,39,40,44	0
3	SF4	C	1001	8/8	0.96	0.14	28,36,50,59	0
5	MGD	C	1003	47/47	0.96	0.11	22,29,35,37	0
3	SF4	D	404	8/8	0.96	0.13	23,33,41,41	0
5	MGD	K	1003	47/47	0.96	0.12	27,37,41,42	0
6	MD1	I	1004	47/47	0.96	0.12	25,37,47,49	0
7	EDO	C	1006	4/4	0.96	0.11	21,25,26,28	0
6	MD1	G	1004	47/47	0.96	0.12	20,32,36,38	0
9	F3S	H	401	7/7	0.96	0.08	53,54,62,72	0
6	MD1	A	1004	47/47	0.96	0.12	19,28,35,37	0
5	MGD	A	1003	47/47	0.96	0.12	23,28,33,36	0
5	MGD	G	1003	47/47	0.96	0.12	23,30,34,37	0
3	SF4	L	402	8/8	0.96	0.11	36,44,55,58	0
3	SF4	J	404	8/8	0.96	0.12	47,53,60,63	0
9	F3S	F	402	7/7	0.97	0.11	37,44,50,54	0
3	SF4	D	402	8/8	0.97	0.13	26,30,38,40	0
3	SF4	H	403	8/8	0.97	0.15	39,45,47,53	0
3	SF4	D	403	8/8	0.97	0.14	24,31,35,47	0
9	F3S	D	401	7/7	0.97	0.10	31,34,39,42	0
6	MD1	C	1004	47/47	0.97	0.11	18,27,32,33	0
3	SF4	E	1001	8/8	0.97	0.12	31,33,42,49	0
6	MD1	E	1004	47/47	0.97	0.10	20,26,33,37	0
3	SF4	F	404	8/8	0.97	0.14	26,39,44,47	0
3	SF4	B	403	8/8	0.97	0.14	24,35,40,41	0
5	MGD	E	1003	47/47	0.97	0.13	23,29,35,37	0
4	MO	C	1002	1/1	0.98	0.07	52,52,52,52	0
4	MO	G	1002	1/1	0.98	0.06	50,50,50,50	0
9	F3S	B	402	7/7	0.98	0.12	31,39,45,48	0

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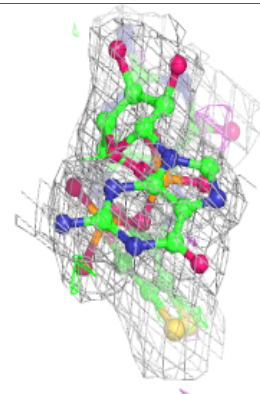
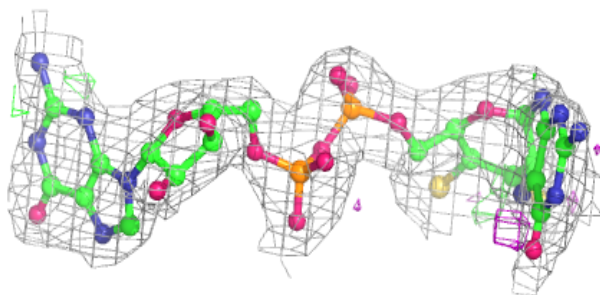
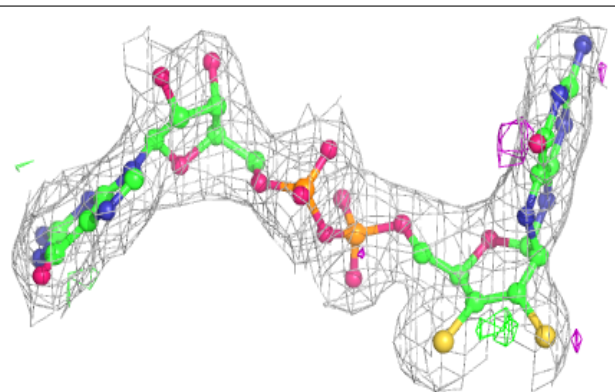
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	L	405	4/4	0.98	0.10	30,32,32,35	0
3	SF4	B	404	8/8	0.98	0.15	29,37,40,43	0
4	MO	A	1002	1/1	0.98	0.07	49,49,49,49	0
4	MO	E	1002	1/1	0.99	0.06	51,51,51,51	0
4	MO	K	1002	1/1	0.99	0.08	53,53,53,53	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.

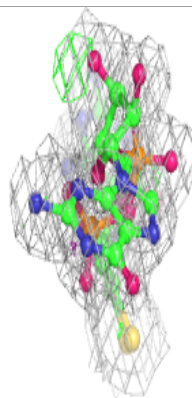
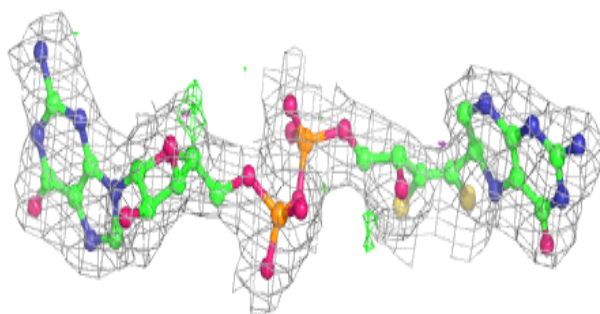
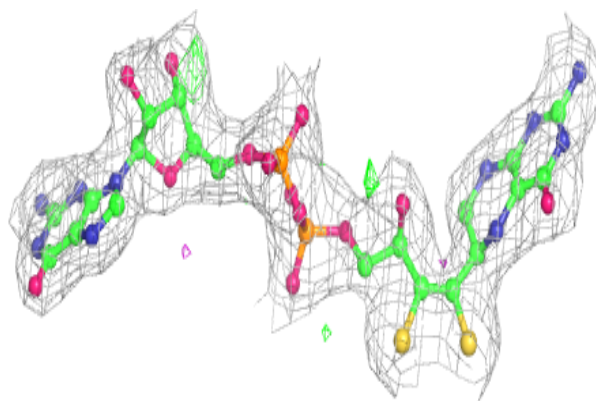
**Electron density around MGD I 1003:**

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)

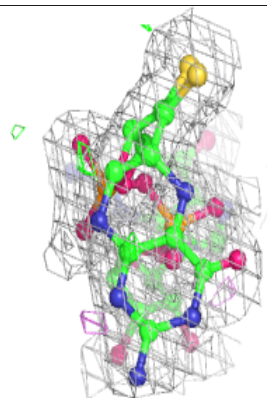
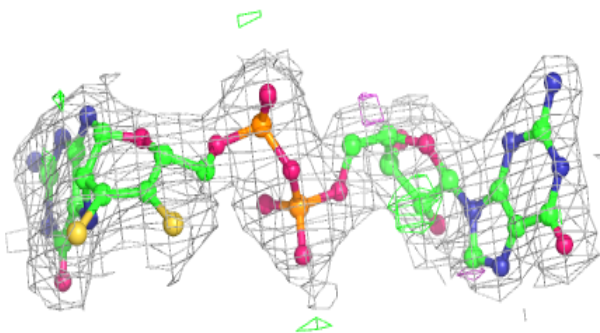
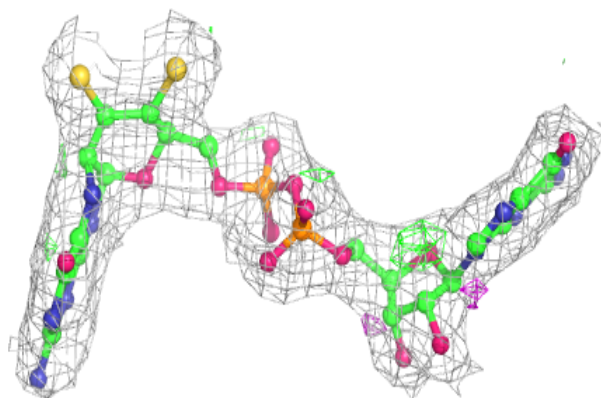


**Electron density around MD1 K 1004:**

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

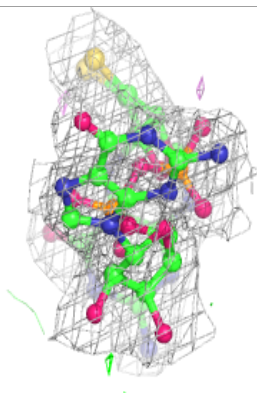
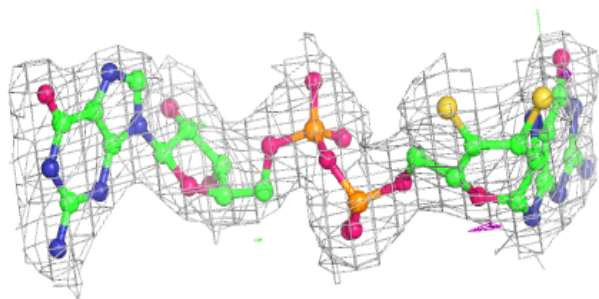
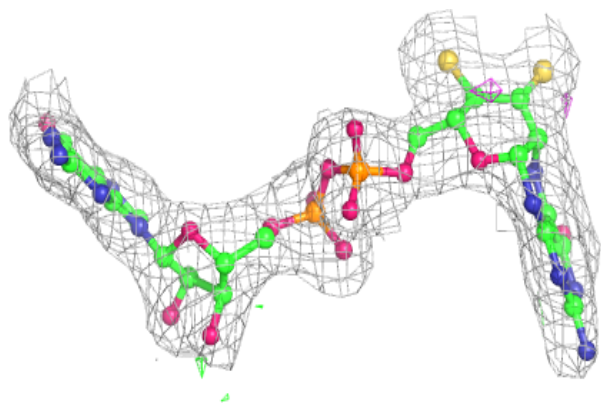
**Electron density around MGD C 1003:**

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

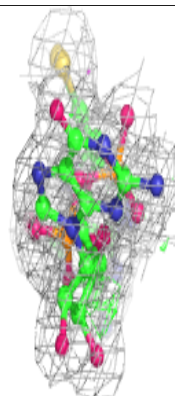
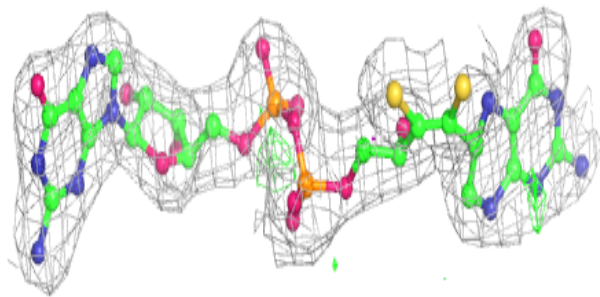
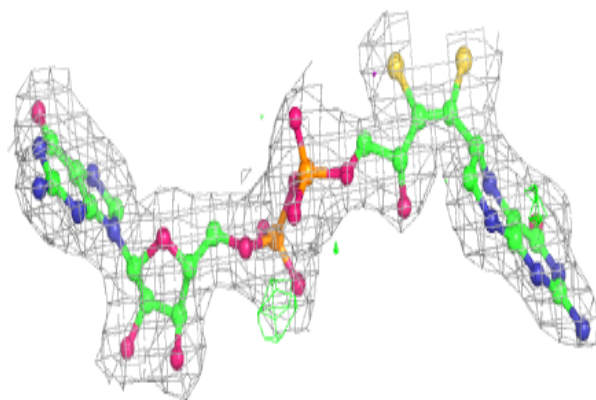


**Electron density around MGD K 1003:**

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

**Electron density around MD1 I 1004:**

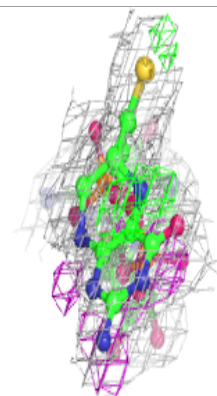
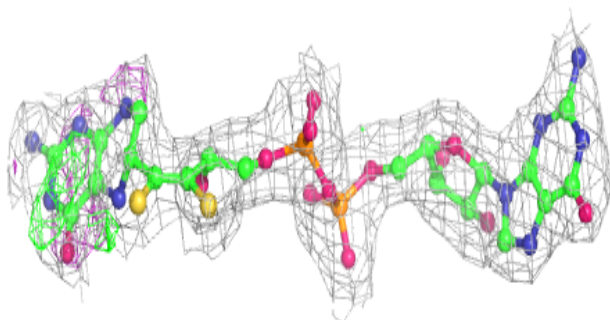
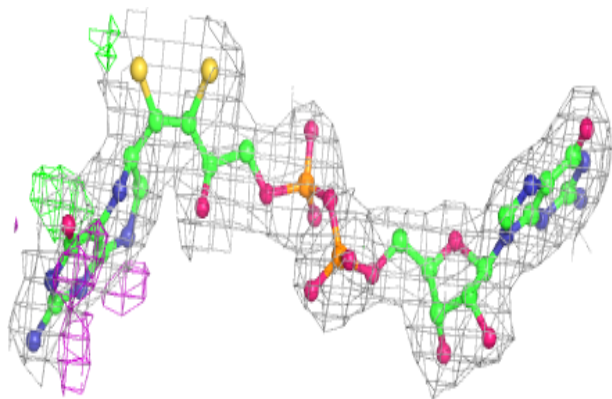
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



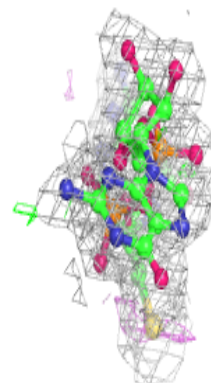
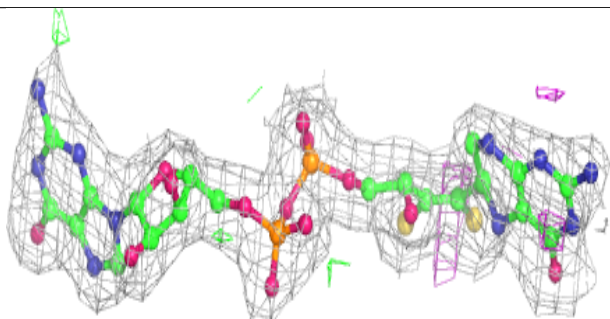


**Electron density around MD1 G 1004:**

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

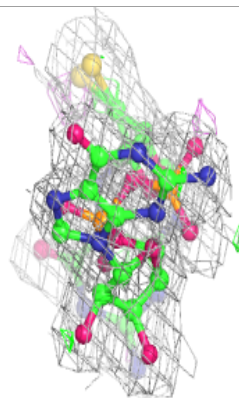
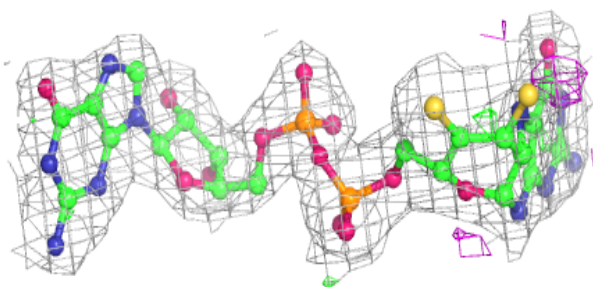
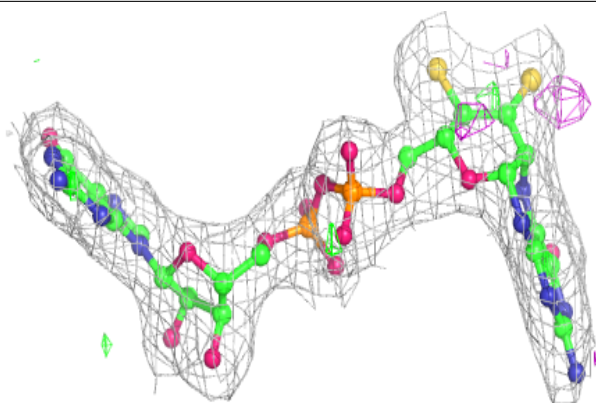
**Electron density around MD1 A 1004:**

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

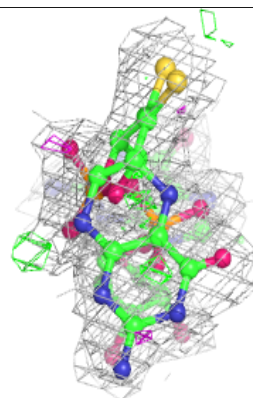
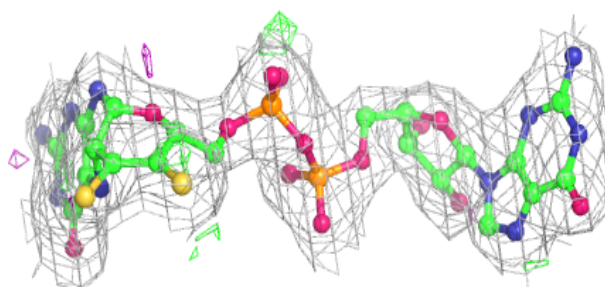
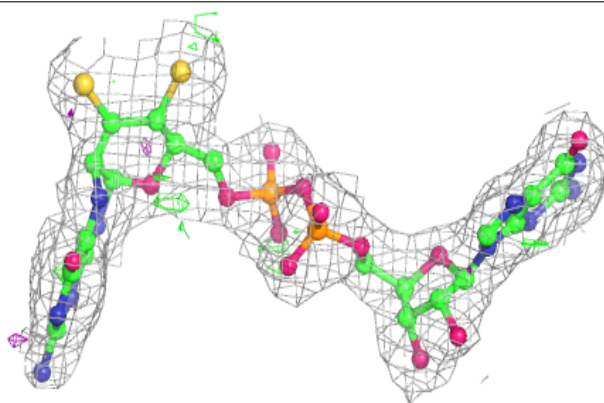


**Electron density around MGD A 1003:**

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

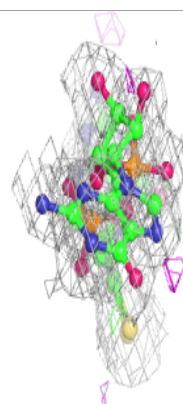
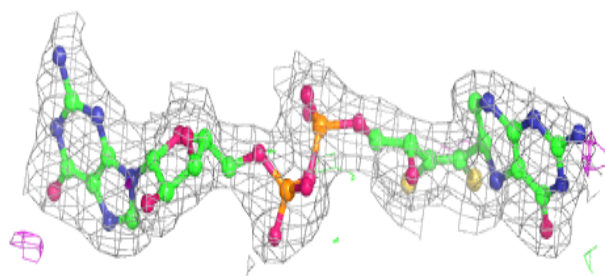
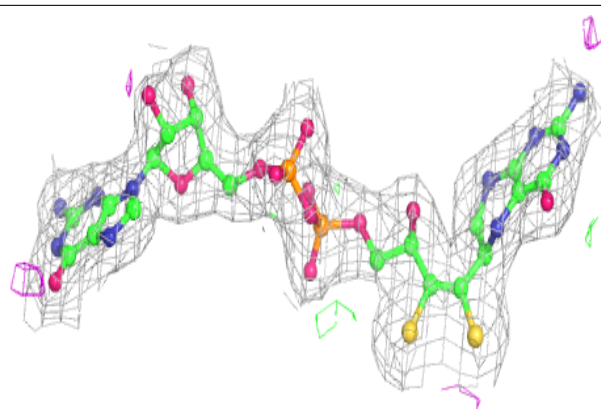
**Electron density around MGD G 1003:**

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

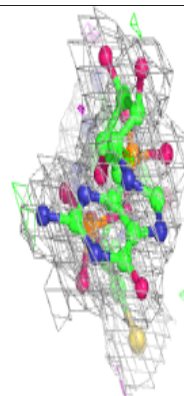
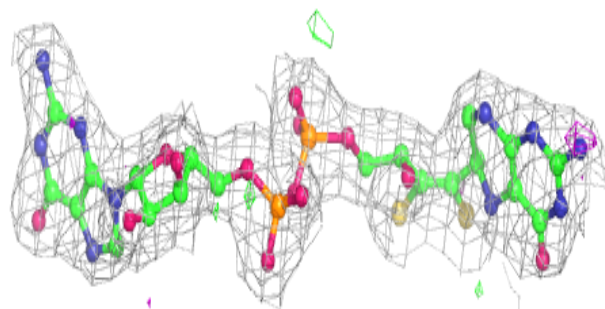
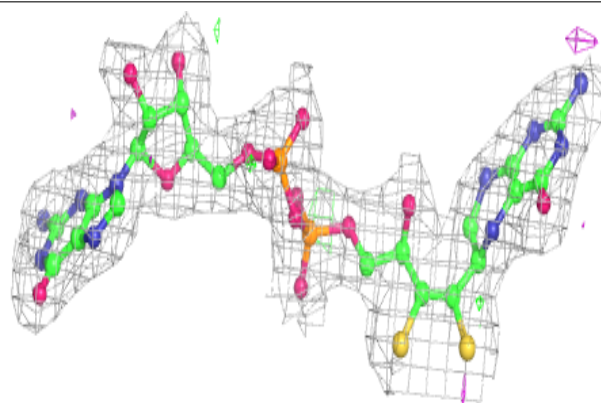


**Electron density around MD1 C 1004:**

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

**Electron density around MD1 E 1004:**

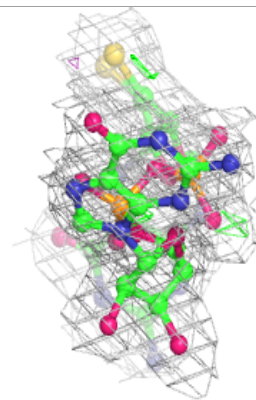
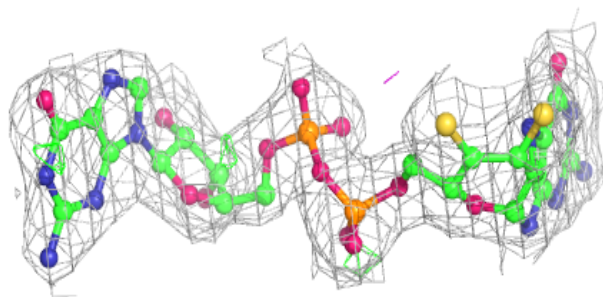
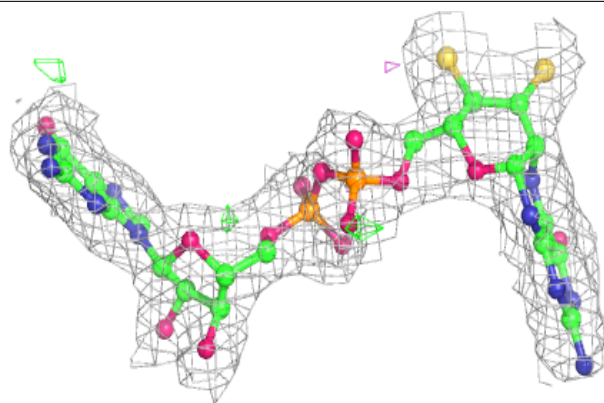
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MGD 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.