



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:04 AM BST

PDB ID : 5CH7  
Title : Crystal structure of the perchlorate reductase PcrAB - Phe164 gate switch intermediate - from Azospira suillum PS  
Authors : Tsai, C.-L.; Tainer, J.A.  
Deposited on : 2015-07-10  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

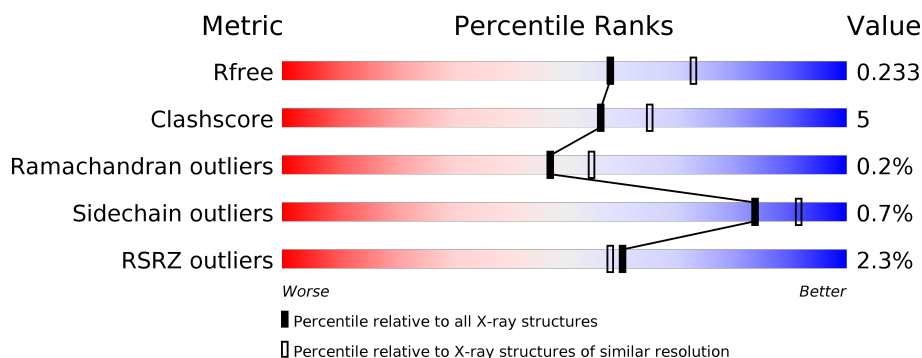
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	C	899	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>..</div> </div> </div>
1	E	899	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
2	B	333	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
2	D	333	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
2	F	333	<div> <div></div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31660 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	894	Total	C	N	O	S	0	3	0
			7180	4586	1246	1310	38			
1	C	891	Total	C	N	O	S	0	1	0
			7151	4568	1239	1306	38			
1	E	892	Total	C	N	O	S	0	3	0
			7171	4583	1240	1310	38			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	D	327	Total	C	N	O	S	0	0	0
			2547	1616	444	463	24			
2	F	328	Total	C	N	O	S	0	2	0
			2568	1631	448	465	24			

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

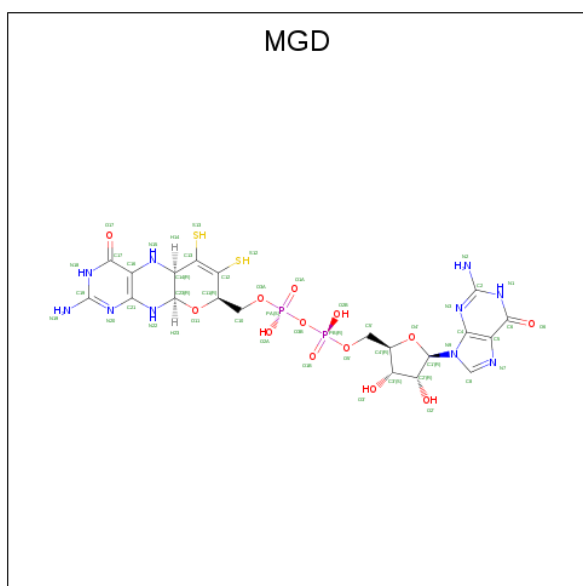


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3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

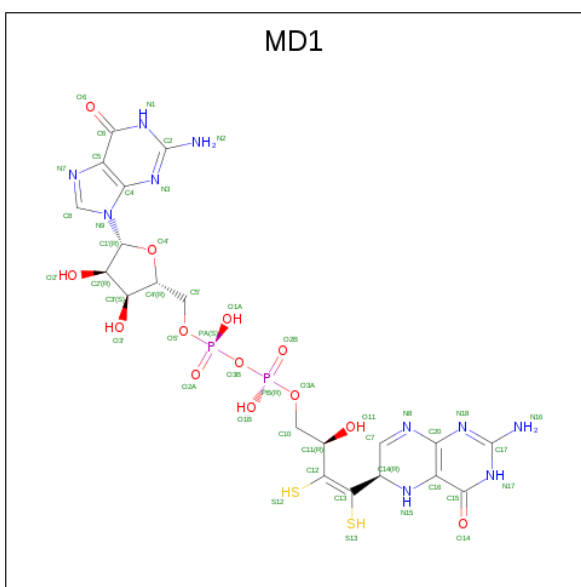
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0

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



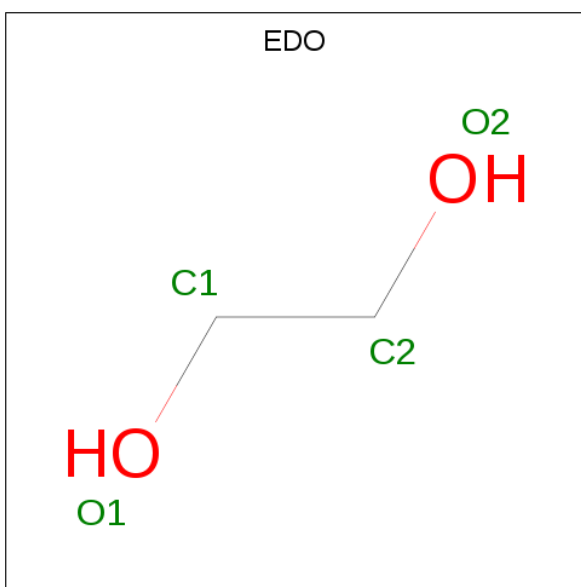
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



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

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

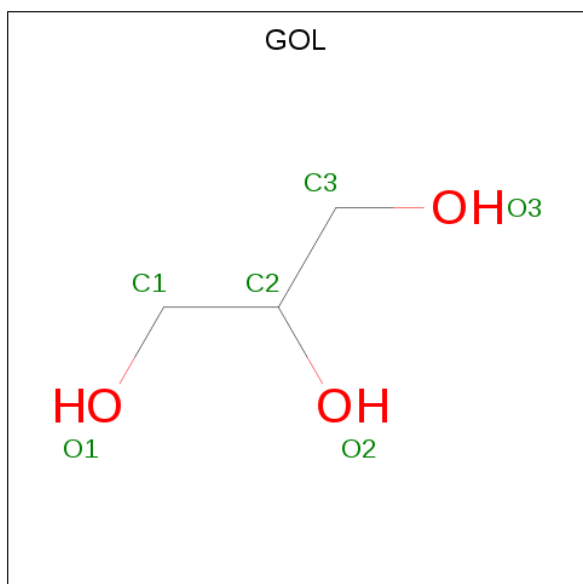
- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

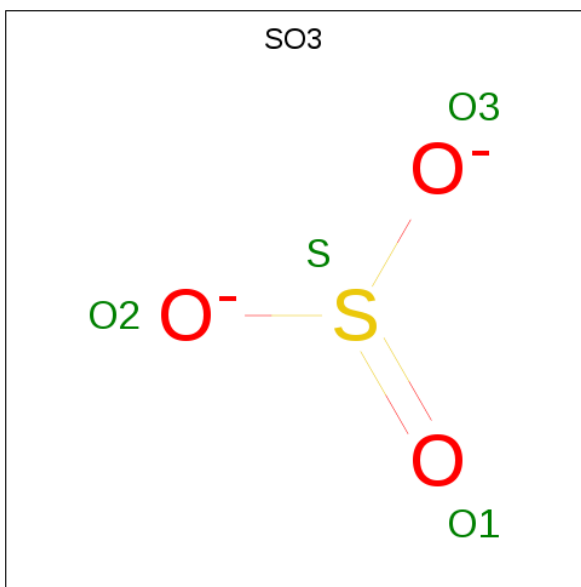
- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

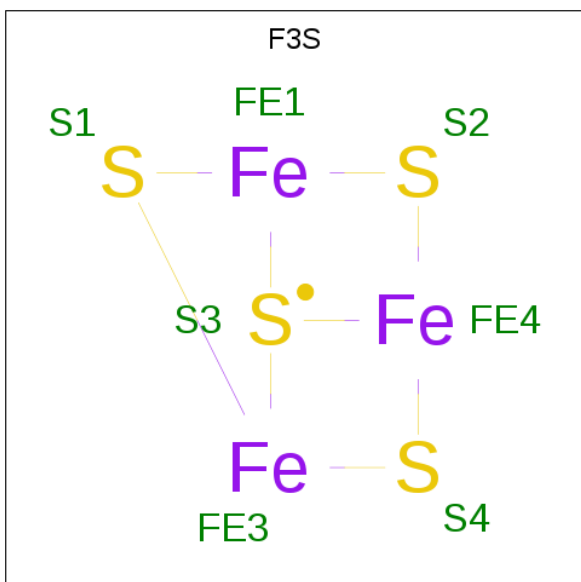
- Molecule 11 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).





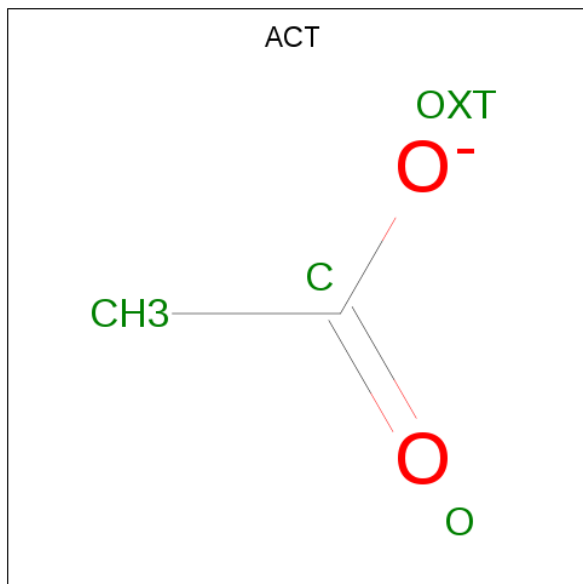
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			4	3	1		
11	A	1	Total	O	S	0	0
			4	3	1		
11	C	1	Total	O	S	0	0
			4	3	1		
11	C	1	Total	O	S	0	0
			4	3	1		
11	E	1	Total	O	S	0	0
			4	3	1		

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



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

- Molecule 13 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



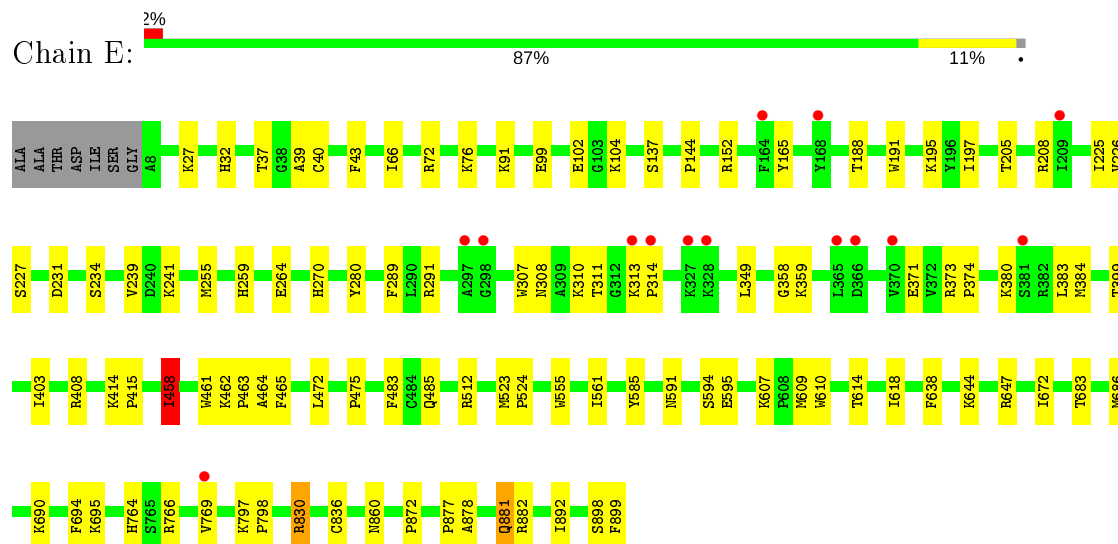
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 14 is water.

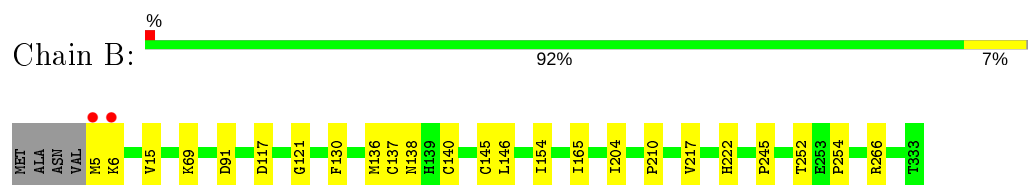
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	531	Total	O	0	0
			531	531		
14	B	273	Total	O	0	0
			273	273		
14	C	362	Total	O	0	0
			362	362		
14	D	92	Total	O	0	0
			92	92		
14	E	520	Total	O	0	0
			520	520		
14	F	198	Total	O	0	0
			198	198		



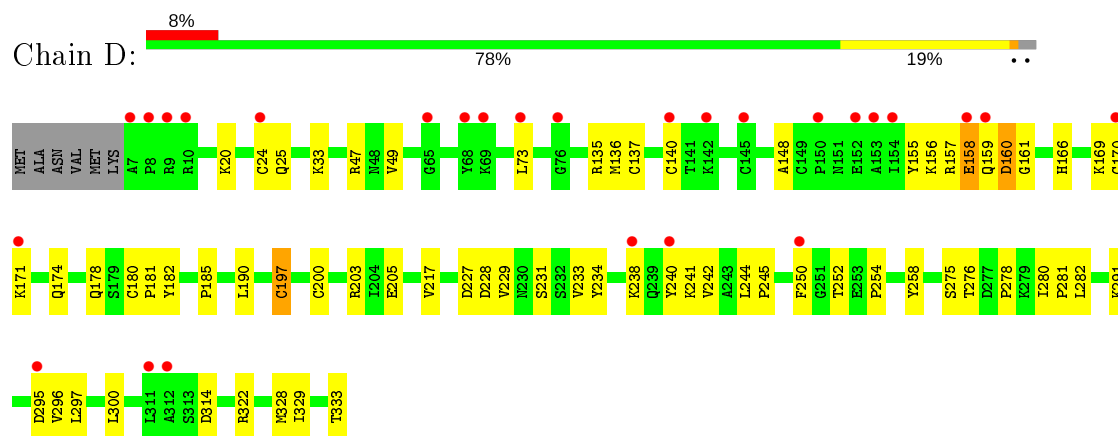
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



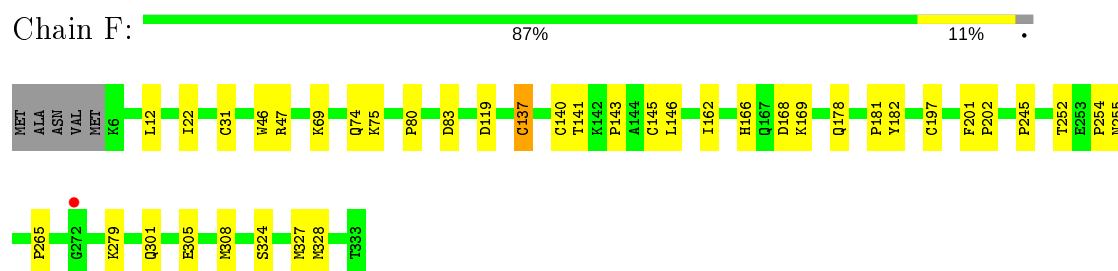
- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.88Å 175.67Å 193.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 2.20 48.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.38-2.20) 99.9 (48.38-2.20)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.178 , 0.233 0.179 , 0.233	Depositor DCC
$R_{free}$ test set	11303 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, MGD, NA, SF4, EDO, SO3, F3S, ACT, 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	0.56	0/7399	0.65	2/10039 (0.0%)
1	C	0.50	0/7364	0.61	1/9993 (0.0%)
1	E	0.56	0/7391	0.64	2/10030 (0.0%)
2	B	0.60	0/2632	0.67	1/3567 (0.0%)
2	D	0.43	0/2615	0.59	0/3546
2	F	0.55	0/2642	0.65	0/3580
All	All	0.54	0/30043	0.63	6/40755 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	830	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	E	830	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	830	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	B	117	ASP	CB-CG-OD1	5.62	123.36	118.30
1	E	830	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	830	ARG	NE-CZ-NH2	-5.15	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	7003	61	0
1	C	7151	0	6964	80	0
1	E	7171	0	6984	73	0
2	B	2564	0	2534	14	0
2	D	2547	0	2513	45	0
2	F	2568	0	2546	27	0
3	A	8	0	0	0	0
3	B	24	0	0	0	0
3	C	8	0	0	0	0
3	D	24	0	0	1	0
3	E	8	0	0	0	0
3	F	24	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	47	0	21	2	0
5	C	47	0	20	2	0
5	E	47	0	20	0	0
6	A	47	0	22	1	0
6	C	47	0	22	1	0
6	E	47	0	22	1	0
7	A	16	0	24	1	0
7	B	12	0	18	1	0
7	C	8	0	12	0	0
7	D	8	0	12	0	0
7	E	12	0	18	2	0
7	F	8	0	12	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
9	E	1	0	0	0	0
10	A	6	0	8	1	0
11	A	8	0	0	0	0
11	C	8	0	0	0	0
11	E	4	0	0	0	0
12	B	7	0	0	0	0
12	D	7	0	0	0	0
12	F	7	0	0	0	0
13	C	4	0	3	0	0
14	A	531	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	273	0	0	1	0
14	C	362	0	0	7	0
14	D	92	0	0	1	0
14	E	520	0	0	12	0
14	F	198	0	0	2	0
All	All	31660	0	28778	291	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:NH1	14:A:1101:HOH:O	1.94	1.01
1:E:226:VAL:HG22	1:E:241:LYS:HB3	1.56	0.87
1:E:308:ASN:HB3	1:E:311:THR:HG22	1.59	0.83
1:A:482:ARG:HB3	1:A:523:MET:HE3	1.65	0.79
1:E:860:ASN:HD22	1:E:878:ALA:H	1.32	0.77
2:B:245:PRO:HB2	2:B:254:PRO:HG2	1.69	0.74
1:C:881:GLN:HE22	1:C:882:ARG:HE	1.35	0.73
1:A:54:GLU:HG2	1:A:585:TYR:OH	1.90	0.72
1:E:695:LYS:NZ	14:E:1102:HOH:O	2.14	0.70
2:D:166:HIS:HB3	2:D:169:LYS:HB2	1.71	0.70
1:A:898:SER:O	1:E:512:ARG:NH1	2.23	0.70
1:C:197:ILE:HB	1:C:225:ILE:HG12	1.74	0.68
1:C:665:ASP:OD2	14:C:1101:HOH:O	2.11	0.68
1:E:358:GLY:O	14:E:1101:HOH:O	2.12	0.68
2:D:245:PRO:HB2	2:D:254:PRO:HG2	1.74	0.68
1:E:195:LYS:HD2	1:E:414:LYS:O	1.94	0.67
2:F:245:PRO:HB2	2:F:254:PRO:HG2	1.76	0.67
1:A:881:GLN:NE2	1:A:882:ARG:HE	1.93	0.67
1:A:62:PRO:HD3	10:A:1010:GOL:H11	1.76	0.66
1:C:860:ASN:HD22	1:C:878:ALA:H	1.41	0.66
1:C:512:ARG:NH1	1:E:898:SER:O	2.28	0.66
1:E:462:LYS:NZ	7:E:1006:EDO:H21	2.11	0.65
1:A:357:GLU:OE2	1:A:380:LYS:HE2	1.96	0.65
1:E:881:GLN:HE22	1:E:882:ARG:HE	1.44	0.65
1:A:860:ASN:HD22	1:A:878:ALA:H	1.44	0.65
1:A:89:ARG:HH11	1:A:89:ARG:HG2	1.61	0.65
2:D:140:CYS:HB3	2:D:252:THR:O	1.97	0.65
1:E:373:ARG:HA	14:E:1101:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:ASP:OD1	1:E:830:ARG:NH2	2.30	0.63
2:D:227:ASP:OD1	2:D:228:ASP:N	2.31	0.63
2:D:135:ARG:NH2	2:D:182:TYR:O	2.31	0.63
2:D:231:SER:HB3	2:D:233:VAL:HG22	1.81	0.63
1:A:601:MET:HE1	1:A:684:ILE:HG23	1.80	0.62
2:F:166:HIS:CE1	2:F:168:ASP:HB2	2.34	0.62
2:D:295:ASP:OD1	2:D:296:VAL:N	2.33	0.62
1:A:89:ARG:NH2	1:A:586:GLU:OE1	2.32	0.61
1:C:464:ALA:HB3	1:C:694:PHE:CE1	2.34	0.61
1:C:54:GLU:HG2	1:C:585:TYR:OH	2.01	0.61
2:D:240:TYR:OH	2:D:314:ASP:OD2	2.19	0.61
1:C:791:MET:HG2	1:C:831:VAL:HG12	1.83	0.60
1:A:881:GLN:HE22	1:A:882:ARG:HE	1.50	0.60
1:E:359:LYS:HA	14:E:1101:HOH:O	2.00	0.60
2:F:301:GLN:O	2:F:305:GLU:HG3	2.01	0.60
1:A:231:ASP:OD1	1:A:830:ARG:NH2	2.35	0.60
1:A:89:ARG:CG	1:A:89:ARG:HH11	2.15	0.60
2:F:69:LYS:HE3	2:F:74:GLN:HG3	1.84	0.59
1:C:690:LYS:NZ	14:C:1108:HOH:O	2.35	0.59
1:C:306:PHE:HZ	1:C:352:LEU:HD13	1.68	0.59
1:C:693:ARG:HH12	1:C:702:LEU:HG	1.67	0.59
2:D:238:LYS:NZ	2:D:241:LYS:HE3	2.18	0.59
1:E:462:LYS:HZ3	7:E:1006:EDO:H21	1.66	0.59
1:C:480:LYS:NZ	14:C:1110:HOH:O	2.37	0.58
1:C:366:ASP:HB3	1:C:368:LYS:H	1.67	0.58
1:E:264:GLU:OE2	1:E:408:ARG:NH2	2.29	0.57
1:C:226:VAL:HG22	1:C:241:LYS:HB3	1.87	0.56
2:F:137:CYS:HB3	2:F:197:CYS:HB3	1.85	0.56
1:E:227:SER:HB2	1:E:239:VAL:HG11	1.87	0.56
1:C:683:THR:HG23	1:C:686:MET:H	1.70	0.56
1:C:685:GLN:NE2	1:C:689:GLU:OE2	2.38	0.56
2:D:73:LEU:HD21	2:D:148:ALA:HB2	1.87	0.56
2:B:140:CYS:HB3	2:B:252:THR:O	2.06	0.56
1:E:860:ASN:HB3	1:E:877:PRO:HA	1.88	0.56
2:F:166:HIS:HE1	2:F:168:ASP:HB2	1.70	0.56
1:A:170:ASP:HB3	1:A:458:ILE:HD13	1.88	0.56
1:C:683:THR:HG22	1:C:686:MET:HG3	1.87	0.56
1:E:259:HIS:CE1	1:E:384:MET:HA	2.41	0.56
1:E:27:LYS:HE3	1:E:43:PHE:CD2	2.41	0.56
1:A:631:LYS:NZ	1:A:636:GLU:OE1	2.40	0.55
1:E:644:LYS:NZ	14:E:1116:HOH:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:LYS:NZ	2:D:161:GLY:O	2.40	0.55
1:C:89:ARG:NH1	14:C:1115:HOH:O	2.41	0.54
1:E:270:HIS:NE2	1:E:349:LEU:HD23	2.22	0.54
1:C:9:PHE:N	1:C:12:SER:HG	2.05	0.54
2:D:275:SER:OG	2:D:276:THR:N	2.41	0.54
1:E:76:LYS:HE3	1:E:766:ARG:O	2.07	0.54
1:A:683:THR:OG1	1:A:686:MET:HG3	2.08	0.54
1:C:703:LYS:HB2	1:C:706:VAL:HB	1.90	0.53
2:D:229:VAL:HG13	2:D:234:TYR:CE1	2.44	0.53
1:A:373:ARG:NH1	14:A:1102:HOH:O	2.10	0.53
1:A:144:PRO:HB2	1:A:672:ILE:HD13	1.90	0.53
2:B:266:ARG:N	2:B:266:ARG:HD2	2.23	0.53
1:C:335:LEU:HD22	1:C:722:PRO:HG3	1.90	0.53
1:C:468:GLY:H	1:C:676:ALA:HB2	1.73	0.53
1:A:871:ARG:HB3	1:A:874:TYR:HB3	1.91	0.52
2:B:91:ASP:HB3	7:B:407:EDO:H21	1.90	0.52
1:C:366:ASP:HB3	1:C:368:LYS:N	2.25	0.52
1:E:40:CYS:SG	1:E:72:ARG:HB3	2.49	0.52
1:C:40:CYS:SG	1:C:72:ARG:HB3	2.49	0.52
1:A:112:GLU:OE1	14:A:1105:HOH:O	2.19	0.52
1:E:289:PHE:HB2	1:E:291:ARG:NH1	2.25	0.52
1:E:462:LYS:HB3	1:E:594:SER:HB3	1.92	0.52
1:C:512:ARG:HG3	1:E:899:PHE:HB3	1.92	0.52
2:D:322:ARG:HH11	2:D:322:ARG:HG3	1.75	0.52
2:F:141:THR:HG23	2:F:255:ASN:OD1	2.10	0.52
1:C:207:THR:HA	5:C:1003:MGD:N20	2.25	0.51
1:C:304:PHE:O	1:C:317:PRO:HD2	2.10	0.51
1:E:76:LYS:HD2	1:E:769:VAL:HG23	1.91	0.51
2:B:136:MET:HG3	2:B:137:CYS:O	2.10	0.51
2:B:15:VAL:HB	2:B:222:HIS:HB2	1.92	0.51
2:D:181:PRO:HB2	2:D:250:PHE:CD2	2.46	0.51
1:A:752:ASP:HB3	1:A:885[A]:ARG:NH2	2.26	0.51
1:C:347:ILE:HG12	1:C:718:LYS:O	2.10	0.51
2:D:180:CYS:SG	2:D:185:PRO:HD3	2.51	0.51
2:F:75[B]:LYS:HG2	14:F:501:HOH:O	2.10	0.51
1:E:380:LYS:O	1:E:384:MET:HG2	2.10	0.50
1:E:764:HIS:HE2	6:E:1004:MD1:H15	1.59	0.50
1:C:89:ARG:HH21	1:C:609:MET:HB2	1.75	0.50
2:B:145:CYS:SG	2:B:146:LEU:N	2.85	0.50
1:C:217:GLU:HG3	2:D:20:LYS:HE3	1.93	0.50
1:A:658:MET:HE2	1:A:661:LYS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:HB	1:A:595:GLU:OE1	2.12	0.49
1:C:693:ARG:NH1	1:C:702:LEU:HG	2.28	0.49
1:C:366:ASP:N	1:C:367:GLY:HA2	2.28	0.49
2:D:137:CYS:HB3	2:D:197:CYS:SG	2.53	0.49
1:E:270:HIS:CD2	1:E:349:LEU:HD23	2.48	0.49
1:E:892:ILE:HG12	14:E:1220:HOH:O	2.13	0.49
1:A:283:ARG:HB3	1:A:285:ASP:OD1	2.13	0.49
1:E:234:SER:OG	2:F:119:ASP:OD2	2.31	0.48
1:E:280:TYR:O	1:E:374:PRO:HA	2.12	0.48
1:E:313:LYS:CG	1:E:314:PRO:HD2	2.42	0.48
1:C:364:LEU:HD21	1:C:370:VAL:HG11	1.95	0.48
1:E:860:ASN:CB	1:E:877:PRO:HA	2.44	0.48
1:C:787:PRO:HD2	1:C:842:ASP:HB3	1.95	0.48
1:C:81:HIS:HE2	2:D:33:LYS:HE3	1.79	0.48
1:C:700:SER:HB2	1:C:708:TYR:CE1	2.49	0.48
1:A:237:ILE:HG13	7:A:1012:EDO:H11	1.96	0.48
1:A:227:SER:HB2	1:A:239:VAL:HG11	1.96	0.48
1:C:638:PHE:CZ	1:C:647:ARG:HD2	2.49	0.48
1:C:678:GLN:HG3	1:C:696:SER:OG	2.14	0.48
2:F:12:LEU:HD22	2:F:162:ILE:HD11	1.95	0.48
1:C:306:PHE:CZ	1:C:352:LEU:HD13	2.48	0.47
2:D:242:VAL:HA	2:D:296:VAL:HG13	1.96	0.47
1:A:152:ARG:HD2	1:A:472:LEU:O	2.15	0.47
1:C:173:THR:O	1:C:177:GLN:HG3	2.14	0.47
1:E:144:PRO:HB2	1:E:672:ILE:HD13	1.96	0.47
2:D:282:LEU:N	14:D:505:HOH:O	2.39	0.47
1:E:797:LYS:HB3	1:E:798:PRO:HD3	1.96	0.47
1:E:32:HIS:NE2	1:E:585:TYR:OH	2.46	0.47
1:C:261:ILE:HG12	1:C:411:ALA:HB2	1.96	0.47
1:A:84:MET:O	1:A:89:ARG:HD2	2.15	0.47
2:F:201:PHE:CG	2:F:202:PRO:HD3	2.49	0.47
2:B:69:LYS:HE3	2:B:69:LYS:HB2	1.74	0.46
2:D:322:ARG:NH1	2:D:322:ARG:HG3	2.28	0.46
2:B:138:ASN:HB3	2:B:254:PRO:HB3	1.98	0.46
2:D:170:CYS:O	2:D:171:LYS:HG3	2.15	0.46
2:D:157:ARG:NE	2:D:160:ASP:OD2	2.46	0.46
2:D:238:LYS:HZ1	2:D:241:LYS:HE3	1.79	0.46
1:E:464:ALA:HB3	1:E:694:PHE:CE1	2.50	0.46
1:A:272:LEU:HD22	1:A:278:LEU:HD12	1.96	0.46
2:F:145:CYS:SG	2:F:146:LEU:N	2.88	0.46
1:C:344:LYS:HE2	1:C:344:LYS:HB3	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:458:ILE:HD11	1:E:461:TRP:CD1	2.51	0.46
1:E:609:MET:HE2	1:E:610:TRP:NE1	2.31	0.46
1:A:416:SER:O	1:A:452:GLY:HA2	2.15	0.46
1:E:37:THR:HG21	1:E:208:ARG:NH1	2.31	0.46
1:E:555:TRP:CE2	1:E:561:ILE:HD13	2.51	0.46
1:C:860:ASN:HB3	1:C:877:PRO:HA	1.97	0.46
2:D:155:TYR:HE1	2:D:157:ARG:HG2	1.81	0.46
1:E:307:TRP:CZ3	1:E:314:PRO:HD3	2.52	0.45
1:E:374:PRO:HD3	14:E:1101:HOH:O	2.16	0.45
1:C:269:ALA:O	1:C:273:LYS:HG3	2.16	0.45
1:C:37:THR:HB	1:C:595:GLU:OE1	2.17	0.45
1:C:836:CYS:HB2	14:C:1229:HOH:O	2.16	0.45
1:A:881:GLN:HE22	1:A:882:ARG:NE	2.13	0.45
1:E:483:PHE:CD2	1:E:872:PRO:HG3	2.51	0.45
2:F:255:ASN:ND2	14:F:507:HOH:O	2.41	0.45
2:F:305:GLU:HA	2:F:308:MET:HB2	1.98	0.45
1:A:431:ASP:OD1	1:A:432:VAL:N	2.48	0.45
1:A:631:LYS:HZ3	1:A:636:GLU:CD	2.20	0.45
1:C:623:ALA:HA	1:C:652:LEU:HD23	1.98	0.45
2:D:200:CYS:SG	2:D:203:ARG:HD3	2.56	0.45
1:A:155:HIS:CD2	1:A:475:PRO:HD2	2.52	0.45
2:D:136:MET:HG3	2:D:137:CYS:O	2.17	0.45
1:C:661:LYS:HE3	1:C:661:LYS:HB3	1.60	0.45
1:C:719:LYS:NZ	14:C:1127:HOH:O	2.49	0.45
2:F:324:SER:O	2:F:328:MET:HG2	2.17	0.45
1:A:76:LYS:HD3	1:A:76:LYS:H	1.82	0.44
1:C:175:GLN:OE1	1:C:183:GLY:HA2	2.17	0.44
1:E:152:ARG:HD2	1:E:472:LEU:O	2.17	0.44
1:C:227:SER:HB2	1:C:239:VAL:HG11	1.98	0.44
1:E:607:LYS:HB2	1:E:607:LYS:HE2	1.68	0.44
2:B:204:ILE:HD11	2:B:210:PRO:HD3	1.99	0.44
1:C:75:ASN:HB3	2:D:24:CYS:O	2.18	0.44
1:A:638:PHE:CZ	1:A:647:ARG:HD2	2.52	0.44
5:C:1003:MGD:H2'	5:C:1003:MGD:H8	1.70	0.44
1:A:601:MET:HG3	1:A:602:THR:N	2.29	0.44
1:C:809:ALA:HA	1:C:887:ASN:O	2.18	0.44
2:D:158:GLU:H	2:D:158:GLU:HG2	1.53	0.44
2:D:244:LEU:O	2:D:258:TYR:N	2.35	0.44
2:F:140:CYS:HB3	2:F:252:THR:O	2.17	0.44
1:A:317:PRO:O	14:A:1106:HOH:O	2.21	0.44
2:D:278:PRO:HG2	2:D:280:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ARG:HB2	3:D:405:SF4:S4	2.58	0.44
2:F:245:PRO:CB	2:F:254:PRO:HG2	2.45	0.44
2:B:121:GLY:HA3	2:B:130:PHE:HB3	2.00	0.43
1:E:37:THR:HB	1:E:595:GLU:OE1	2.18	0.43
1:C:685:GLN:O	1:C:689:GLU:HG2	2.18	0.43
2:F:75[A]:LYS:HE3	2:F:178:GLN:NE2	2.33	0.43
2:D:159:GLN:CD	2:D:159:GLN:H	2.22	0.43
1:C:302:ASP:HB3	1:C:321:TRP:HB3	2.00	0.43
1:A:764:HIS:HE2	6:A:1004:MD1:H15	1.67	0.43
1:E:99[A]:GLU:OE1	14:E:1103:HOH:O	2.21	0.43
2:F:80:PRO:HD2	2:F:83:ASP:OD2	2.18	0.43
1:E:683:THR:OG1	1:E:686:MET:HG3	2.18	0.43
1:C:325:PRO:O	1:C:327:LYS:N	2.52	0.43
1:C:414:LYS:HA	1:C:415:PRO:HA	1.67	0.43
1:C:771:SER:HA	1:C:774:LYS:HG3	2.01	0.43
2:B:154:ILE:HG12	2:B:165:ILE:HG12	2.01	0.43
1:C:264:GLU:OE1	1:C:408:ARG:NE	2.45	0.43
1:C:515:ILE:HD13	1:C:522:ASN:HB2	2.01	0.43
2:D:328:MET:HG3	2:D:329:ILE:O	2.18	0.43
1:E:91:LYS:HE2	1:E:610:TRP:CZ2	2.54	0.43
1:A:441:THR:HG21	1:A:453:GLY:HA2	2.01	0.43
1:A:797:LYS:HB3	1:A:798:PRO:HD3	2.01	0.43
1:A:207:THR:HA	5:A:1003:MGD:N20	2.34	0.43
1:E:359:LYS:HD2	1:E:371:GLU:OE2	2.18	0.43
1:E:205:THR:HG23	2:F:22:ILE:HB	2.01	0.43
1:A:54:GLU:OE2	1:A:81:HIS:N	2.50	0.42
1:C:318:LYS:HE2	1:C:346:TYR:O	2.19	0.42
1:C:666:GLU:HG3	1:C:684:ILE:HG13	2.00	0.42
1:E:152:ARG:CZ	1:E:475:PRO:HG3	2.48	0.42
2:F:181:PRO:HG2	2:F:182:TYR:CD2	2.54	0.42
1:C:283:ARG:HB3	1:C:285:ASP:OD1	2.20	0.42
1:C:333:GLY:O	1:C:871:ARG:NH1	2.41	0.42
1:C:464:ALA:HB3	1:C:694:PHE:CZ	2.54	0.42
1:A:523:MET:HG3	1:A:524:PRO:HA	2.00	0.42
1:C:670:GLN:HE22	1:C:683:THR:HA	1.84	0.42
1:C:830:ARG:NH1	14:C:1134:HOH:O	2.51	0.42
1:E:310:LYS:HA	1:E:310:LYS:HD2	1.78	0.42
1:A:885[B]:ARG:NH2	14:A:1104:HOH:O	2.17	0.42
6:C:1004:MD1:C11	6:C:1004:MD1:H7	2.50	0.42
1:C:414:LYS:NZ	1:C:444:THR:O	2.53	0.42
1:E:66:ILE:HD11	14:E:1453:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:836:CYS:HB2	14:E:1286:HOH:O	2.19	0.42
2:F:31:CYS:SG	2:F:46:TRP:HB2	2.60	0.42
1:C:81:HIS:NE2	2:D:33:LYS:HE3	2.35	0.42
1:E:614:THR:O	1:E:618:ILE:HG13	2.20	0.42
1:A:210:PRO:HA	2:B:217:VAL:CG1	2.50	0.42
1:C:190:ASP:OD1	1:C:450:ASN:ND2	2.48	0.42
2:D:174:GLN:O	2:D:178:GLN:HG3	2.20	0.42
2:D:333:THR:O	2:D:333:THR:OG1	2.34	0.42
2:F:47:ARG:HB2	3:F:404:SF4:S4	2.60	0.42
1:C:519:GLN:HB3	1:C:863:GLY:HA3	2.01	0.42
1:C:209:ILE:HG22	2:D:217:VAL:HG11	2.01	0.42
1:A:642:LYS:HD3	1:A:643:PHE:CZ	2.55	0.41
1:A:39:ALA:HA	1:A:591:ASN:OD1	2.20	0.41
2:D:190:LEU:HD23	2:D:190:LEU:HA	1.91	0.41
1:E:259:HIS:ND1	1:E:383:LEU:O	2.50	0.41
1:A:881:GLN:NE2	1:A:882:ARG:NE	2.65	0.41
2:B:5:MET:N	14:B:514:HOH:O	2.53	0.41
1:C:730:PHE:O	1:C:745:PRO:HD3	2.20	0.41
1:E:197:ILE:HB	1:E:225:ILE:HG12	2.02	0.41
2:F:265:PRO:HG2	2:F:279:LYS:HE2	2.02	0.41
1:C:736:THR:O	1:C:739:ASP:HB2	2.20	0.41
1:E:690:LYS:HE2	14:E:1591:HOH:O	2.20	0.41
1:A:54:GLU:HG2	1:A:585:TYR:HH	1.84	0.41
1:A:364:LEU:HD12	1:A:368:LYS:HB3	2.02	0.41
1:A:613:LYS:HB2	1:A:618:ILE:HG13	2.02	0.41
2:D:297:LEU:HA	2:D:300:LEU:HD12	2.01	0.41
1:E:359:LYS:N	14:E:1110:HOH:O	2.34	0.41
1:E:797:LYS:HE3	1:E:797:LYS:HB2	1.76	0.41
1:E:485:GLN:CD	1:E:877:PRO:HD2	2.41	0.41
1:C:236:THR:O	1:C:239:VAL:HG22	2.20	0.41
1:E:188:THR:HG22	1:E:191:TRP:CZ2	2.55	0.41
1:C:292:GLU:HG2	1:C:299:GLY:HA3	2.02	0.41
1:C:311:THR:O	1:C:313:LYS:HG3	2.21	0.41
1:E:399:THR:O	1:E:403:ILE:HG13	2.21	0.41
1:C:31:ALA:HB3	1:C:602:THR:HB	2.03	0.41
2:D:280:ILE:HA	2:D:281:PRO:HD3	1.84	0.41
2:F:166:HIS:ND1	2:F:169:LYS:HG3	2.35	0.41
1:E:414:LYS:HA	1:E:415:PRO:HA	1.85	0.41
1:E:523:MET:HA	1:E:524:PRO:C	2.42	0.41
1:E:638:PHE:CZ	1:E:647:ARG:HD2	2.56	0.40
1:A:120:LYS:HD3	1:A:120:LYS:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLU:OE1	1:E:104:LYS:HE2	2.21	0.40
1:E:255:MET:HE3	1:E:383:LEU:HD21	2.03	0.40
2:F:140:CYS:O	2:F:143:PRO:HD3	2.20	0.40
1:A:289:PHE:HB2	1:A:291:ARG:NH1	2.37	0.40
1:A:160:HIS:CD2	1:A:523:MET:HG2	2.57	0.40
1:A:734:HIS:HD2	1:A:865:TYR:HB2	1.86	0.40
1:C:147:PHE:CE2	1:C:151:HIS:CE1	3.10	0.40
2:D:25:GLN:NE2	2:D:49:VAL:HB	2.36	0.40
2:D:291:LYS:N	2:D:291:LYS:HD2	2.37	0.40
2:D:33:LYS:HD2	2:D:33:LYS:HA	1.76	0.40
1:A:304:PHE:O	1:A:317:PRO:HD2	2.20	0.40
1:A:459:GLY:HA2	5:A:1003:MGD:S13	2.61	0.40
1:A:485:GLN:CD	1:A:877:PRO:HD2	2.42	0.40
1:A:152:ARG:NE	1:A:656:MET:O	2.54	0.40
1:C:461:TRP:O	1:C:463:PRO:HD3	2.21	0.40
1:E:39:ALA:HA	1:E:591:ASN:OD1	2.22	0.40
2:F:327:MET:HB3	2:F:327:MET:HE2	1.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	895/899 (100%)	860 (96%)	33 (4%)	2 (0%)	47	55
1	C	890/899 (99%)	838 (94%)	49 (6%)	3 (0%)	41	46
1	E	893/899 (99%)	850 (95%)	41 (5%)	2 (0%)	47	55
2	B	327/333 (98%)	317 (97%)	9 (3%)	1 (0%)	41	46
2	D	325/333 (98%)	303 (93%)	21 (6%)	1 (0%)	41	46
2	F	328/333 (98%)	313 (95%)	15 (5%)	0	100	100
All	All	3658/3696 (99%)	3481 (95%)	168 (5%)	9 (0%)	47	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	ILE
1	C	458	ILE
2	D	205	GLU
1	E	458	ILE
2	B	6	LYS
1	C	463	PRO
1	E	463	PRO
1	C	47	LYS
1	A	463	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	768/768 (100%)	762 (99%)	6 (1%)	81	90
1	C	765/768 (100%)	758 (99%)	7 (1%)	78	88
1	E	767/768 (100%)	762 (99%)	5 (1%)	84	91
2	B	278/281 (99%)	278 (100%)	0	100	100
2	D	276/281 (98%)	273 (99%)	3 (1%)	73	85
2	F	279/281 (99%)	278 (100%)	1 (0%)	91	96
All	All	3133/3147 (100%)	3111 (99%)	22 (1%)	84	91

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	ILE
1	A	465	PHE
1	A	555	TRP
1	A	601	MET
1	A	637	LYS
1	A	881	GLN
1	C	11	TYR
1	C	276	THR

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Mol	Chain	Res	Type
1	C	327	LYS
1	C	458	ILE
1	C	465	PHE
1	C	555	TRP
1	C	881	GLN
2	D	158	GLU
2	D	160	ASP
2	D	197	CYS
1	E	137	SER
1	E	165	TYR
1	E	458	ILE
1	E	465	PHE
1	E	881	GLN
2	F	137	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	860	ASN
1	A	881	GLN
1	C	860	ASN
1	C	881	GLN
1	E	860	ASN
1	E	881	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 54 ligands modelled in this entry, 10 are monoatomic - leaving 44 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	A	1007	-	3,3,3	0.57	0	2,2,2	0.22	0
7	EDO	A	1006	-	3,3,3	0.54	0	2,2,2	0.31	0
3	SF4	F	402	2	0,12,12	0.00	-	-		
3	SF4	C	1001	1	0,12,12	0.00	-	-		
10	GOL	A	1010	-	5,5,5	0.27	0	5,5,5	0.62	0
3	SF4	A	1001	1	0,12,12	0.00	-	-		
7	EDO	D	401	-	3,3,3	0.71	0	2,2,2	0.12	0
7	EDO	F	406	-	3,3,3	0.52	0	2,2,2	0.49	0
12	F3S	F	401	2	0,9,9	0.00	-	-		
3	SF4	B	404	2	0,12,12	0.00	-	-		
12	F3S	B	401	2	0,9,9	0.00	-	-		
3	SF4	F	404	2	0,12,12	0.00	-	-		
3	SF4	D	404	2	0,12,12	0.00	-	-		
11	SO3	C	1009	-	1,3,3	0.77	0	0,3,3	0.00	-
3	SF4	D	403	2	0,12,12	0.00	-	-		
7	EDO	B	405	-	3,3,3	0.30	0	2,2,2	0.67	0
3	SF4	E	1001	1	0,12,12	0.00	-	-		
7	EDO	B	406	-	3,3,3	0.57	0	2,2,2	0.31	0
11	SO3	E	1008	9	1,3,3	1.21	0	0,3,3	0.00	-
6	MD1	C	1004	4	38,51,51	3.52	12 (31%)	35,78,78	1.64	8 (22%)
11	SO3	C	1010	9	1,3,3	0.81	0	0,3,3	0.00	-
6	MD1	A	1004	4	38,51,51	3.58	14 (36%)	35,78,78	1.82	9 (25%)
6	MD1	E	1004	4	38,51,51	3.46	13 (34%)	35,78,78	1.68	9 (25%)
7	EDO	B	407	-	3,3,3	0.76	0	2,2,2	0.23	0
3	SF4	B	403	2	0,12,12	0.00	-	-		
7	EDO	E	1006	-	3,3,3	0.89	0	2,2,2	0.43	0
13	ACT	C	1008	-	1,3,3	1.71	0	0,3,3	0.00	-
7	EDO	E	1005	-	3,3,3	0.74	0	2,2,2	0.47	0
7	EDO	C	1006	-	3,3,3	0.57	0	2,2,2	0.26	0
7	EDO	D	406	-	3,3,3	0.50	0	2,2,2	0.37	0
7	EDO	A	1005	-	3,3,3	0.80	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MGD	A	1003	4	41,52,52	5.84	25 (60%)	43,81,81	3.87	19 (44%)
5	MGD	C	1003	4	41,52,52	5.81	27 (65%)	43,81,81	3.71	18 (41%)
11	SO3	A	1013	-	1,3,3	0.88	0	0,3,3	0.00	-
7	EDO	E	1007	-	3,3,3	0.55	0	2,2,2	0.32	0
7	EDO	F	405	-	3,3,3	0.62	0	2,2,2	0.36	0
3	SF4	B	402	2	0,12,12	0.00	-	-	-	-
7	EDO	A	1012	-	3,3,3	0.51	0	2,2,2	0.24	0
11	SO3	A	1011	9	1,3,3	1.05	0	0,3,3	0.00	-
3	SF4	D	405	2	0,12,12	0.00	-	-	-	-
7	EDO	C	1005	-	3,3,3	0.77	0	2,2,2	0.36	0
12	F3S	D	402	2	0,9,9	0.00	-	-	-	-
5	MGD	E	1003	4	41,52,52	5.79	25 (60%)	43,81,81	3.42	17 (39%)
3	SF4	F	403	2	0,12,12	0.00	-	-	-	-

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	A	1007	-	-	1/1/1/1	-
7	EDO	A	1006	-	-	0/1/1/1	-
3	SF4	F	402	2	-	-	0/6/5/5
3	SF4	C	1001	1	-	-	0/6/5/5
10	GOL	A	1010	-	-	0/4/4/4	-
7	EDO	C	1006	-	-	0/1/1/1	-
3	SF4	B	402	2	-	-	0/6/5/5
7	EDO	F	406	-	-	0/1/1/1	-
3	SF4	B	404	2	-	-	0/6/5/5
12	F3S	B	401	2	-	-	0/3/3/3
3	SF4	F	404	2	-	-	0/6/5/5
6	MD1	C	1004	4	-	5/21/59/59	0/5/5/5
3	SF4	D	403	2	-	-	0/6/5/5
7	EDO	B	405	-	-	0/1/1/1	-
3	SF4	E	1001	1	-	-	0/6/5/5
3	SF4	D	405	2	-	-	0/6/5/5
3	SF4	D	404	2	-	-	0/6/5/5
6	MD1	A	1004	4	-	5/21/59/59	0/5/5/5
6	MD1	E	1004	4	-	3/21/59/59	0/5/5/5
7	EDO	B	407	-	-	0/1/1/1	-
3	SF4	B	403	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	E	1006	-	-	0/1/1/1	-
7	EDO	E	1005	-	-	0/1/1/1	-
3	SF4	A	1001	1	-	-	0/6/5/5
7	EDO	D	406	-	-	0/1/1/1	-
7	EDO	A	1005	-	-	0/1/1/1	-
5	MGD	A	1003	4	-	2/18/66/66	0/6/6/6
5	MGD	C	1003	4	-	0/18/66/66	0/6/6/6
7	EDO	E	1007	-	-	0/1/1/1	-
7	EDO	F	405	-	-	0/1/1/1	-
7	EDO	D	401	-	-	0/1/1/1	-
7	EDO	A	1012	-	-	0/1/1/1	-
7	EDO	B	406	-	-	0/1/1/1	-
7	EDO	C	1005	-	-	0/1/1/1	-
12	F3S	D	402	2	-	-	0/3/3/3
5	MGD	E	1003	4	-	2/18/66/66	0/6/6/6
3	SF4	F	403	2	-	-	0/6/5/5
12	F3S	F	401	2	-	-	0/3/3/3

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MGD	C23-C14	-19.14	1.38	1.53
5	E	1003	MGD	C23-C14	-19.03	1.38	1.53
5	C	1003	MGD	C23-C14	-18.51	1.38	1.53
5	A	1003	MGD	O11-C11	12.58	1.60	1.43
5	E	1003	MGD	O11-C11	12.50	1.60	1.43
5	C	1003	MGD	O11-C11	12.34	1.60	1.43
5	E	1003	MGD	C16-C21	12.04	1.64	1.41
5	A	1003	MGD	C16-C21	11.82	1.63	1.41
6	A	1004	MD1	C7-N8	11.66	1.41	1.27
5	C	1003	MGD	C16-C21	11.39	1.62	1.41
5	E	1003	MGD	C19-N18	11.28	1.55	1.35
6	C	1004	MD1	C7-N8	10.98	1.40	1.27
5	C	1003	MGD	C19-N18	10.92	1.54	1.35
6	E	1004	MD1	C7-N8	10.52	1.40	1.27
5	A	1003	MGD	C19-N18	10.25	1.53	1.35
5	C	1003	MGD	C2'-C3'	-10.03	1.25	1.53
5	E	1003	MGD	C2'-C3'	-9.65	1.26	1.53
5	A	1003	MGD	C2'-C3'	-9.35	1.27	1.53
6	E	1004	MD1	C5-C6	-9.08	1.37	1.52
6	C	1004	MD1	C5-C6	-8.59	1.38	1.52
6	E	1004	MD1	C4-N9	-8.37	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1004	MD1	C4-N9	-8.33	1.36	1.47
6	C	1004	MD1	C4-N9	-8.18	1.36	1.47
6	A	1004	MD1	C5-C6	-8.00	1.39	1.52
6	C	1004	MD1	O4'-C1'	7.96	1.60	1.42
6	A	1004	MD1	O4'-C1'	7.76	1.60	1.42
5	A	1003	MGD	C19-N20	7.59	1.48	1.35
5	C	1003	MGD	C19-N20	7.43	1.48	1.35
5	C	1003	MGD	C17-N18	7.42	1.46	1.33
5	E	1003	MGD	C17-N18	7.42	1.46	1.33
5	A	1003	MGD	C17-N18	7.33	1.45	1.33
5	E	1003	MGD	C19-N20	7.28	1.48	1.35
5	C	1003	MGD	O4'-C1'	7.17	1.51	1.41
5	E	1003	MGD	O4'-C1'	7.07	1.50	1.41
5	A	1003	MGD	O4'-C1'	6.93	1.50	1.41
5	C	1003	MGD	O4'-C4'	-6.90	1.29	1.45
5	A	1003	MGD	O4'-C4'	-6.83	1.29	1.45
5	A	1003	MGD	C14-N15	6.72	1.54	1.45
6	E	1004	MD1	O4'-C1'	6.64	1.57	1.42
5	E	1003	MGD	O4'-C4'	-6.56	1.30	1.45
5	E	1003	MGD	C6-C5	6.33	1.52	1.41
5	A	1003	MGD	C6-C5	6.23	1.52	1.41
5	C	1003	MGD	C14-N15	6.18	1.54	1.45
5	E	1003	MGD	C4-N3	6.18	1.45	1.35
5	C	1003	MGD	C6-C5	6.11	1.51	1.41
6	C	1004	MD1	C2'-C1'	-6.01	1.34	1.53
6	A	1004	MD1	C2'-C1'	-5.87	1.34	1.53
6	E	1004	MD1	C2'-C1'	-5.83	1.34	1.53
5	C	1003	MGD	C4-N3	5.80	1.44	1.35
5	A	1003	MGD	C4-N3	5.68	1.44	1.35
5	A	1003	MGD	C6-N1	5.48	1.42	1.33
5	E	1003	MGD	C6-N1	5.35	1.42	1.33
5	C	1003	MGD	C6-N1	5.35	1.42	1.33
5	A	1003	MGD	C3'-C4'	5.29	1.66	1.53
5	E	1003	MGD	C14-N15	5.27	1.52	1.45
5	C	1003	MGD	C3'-C4'	5.21	1.66	1.53
6	E	1004	MD1	O4'-C4'	-5.10	1.33	1.45
5	E	1003	MGD	C3'-C4'	4.98	1.65	1.53
6	C	1004	MD1	O4'-C4'	-4.91	1.34	1.45
5	C	1003	MGD	C23-N22	4.87	1.54	1.44
5	A	1003	MGD	C19-N19	4.80	1.43	1.33
5	C	1003	MGD	C2-N2	4.74	1.43	1.33
6	A	1004	MD1	C16-N15	4.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	C19-N19	4.51	1.42	1.33
5	E	1003	MGD	C23-N22	4.49	1.53	1.44
6	A	1004	MD1	O4'-C4'	-4.48	1.35	1.45
6	C	1004	MD1	C16-N15	4.43	1.47	1.38
6	A	1004	MD1	C17-N16	4.42	1.42	1.33
5	E	1003	MGD	C2-N2	4.26	1.42	1.33
5	A	1003	MGD	C2-N2	4.20	1.42	1.33
5	A	1003	MGD	C23-N22	4.19	1.52	1.44
6	E	1004	MD1	C16-N15	4.16	1.46	1.38
5	A	1003	MGD	O2'-C2'	4.15	1.52	1.43
5	E	1003	MGD	C19-N19	3.98	1.41	1.33
5	E	1003	MGD	C2-N1	3.80	1.42	1.35
6	E	1004	MD1	C17-N16	3.75	1.41	1.33
5	C	1003	MGD	O2'-C2'	3.69	1.51	1.43
5	A	1003	MGD	C17-C16	3.63	1.46	1.41
5	C	1003	MGD	O11-C23	-3.55	1.38	1.43
5	C	1003	MGD	C2-N1	3.35	1.41	1.35
6	C	1004	MD1	C17-N16	3.28	1.40	1.33
5	A	1003	MGD	C2-N1	3.25	1.41	1.35
5	C	1003	MGD	C16-N15	3.23	1.44	1.38
5	A	1003	MGD	C2'-C1'	3.18	1.58	1.53
5	A	1003	MGD	C16-N15	3.01	1.44	1.38
5	A	1003	MGD	C13-C12	2.90	1.54	1.35
5	E	1003	MGD	C8-N7	2.85	1.39	1.34
5	C	1003	MGD	C13-C12	2.82	1.53	1.35
5	E	1003	MGD	C17-C16	2.78	1.45	1.41
5	E	1003	MGD	C13-C12	2.78	1.53	1.35
5	C	1003	MGD	C2'-C1'	2.71	1.57	1.53
5	C	1003	MGD	C21-N20	2.65	1.39	1.34
6	A	1004	MD1	C8-N9	-2.64	1.36	1.45
6	C	1004	MD1	C5-C4	-2.61	1.36	1.53
6	E	1004	MD1	C5-C4	-2.60	1.37	1.53
5	E	1003	MGD	C2'-C1'	2.60	1.57	1.53
5	C	1003	MGD	C17-C16	2.59	1.45	1.41
6	A	1004	MD1	C15-C16	-2.56	1.38	1.41
6	E	1004	MD1	C15-C16	-2.56	1.38	1.41
6	A	1004	MD1	C5-C4	-2.56	1.37	1.53
6	C	1004	MD1	C13-C12	2.53	1.42	1.34
6	E	1004	MD1	C8-N9	-2.48	1.37	1.45
6	A	1004	MD1	C13-C12	2.48	1.42	1.34
5	A	1003	MGD	C10-C11	2.46	1.55	1.52
5	C	1003	MGD	C8-N7	2.43	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MGD	C8-N7	2.42	1.39	1.34
6	C	1004	MD1	O3'-C3'	-2.34	1.37	1.43
6	A	1004	MD1	C14-C7	2.31	1.56	1.50
6	E	1004	MD1	O3'-C3'	-2.28	1.37	1.43
6	C	1004	MD1	C8-N9	-2.27	1.37	1.45
6	E	1004	MD1	C13-C12	2.21	1.41	1.34
5	E	1003	MGD	O2'-C2'	2.17	1.48	1.43
6	A	1004	MD1	O3'-C3'	-2.10	1.38	1.43
5	E	1003	MGD	O11-C23	-2.05	1.40	1.43
5	C	1003	MGD	C10-C11	2.03	1.54	1.52
5	E	1003	MGD	C16-N15	2.02	1.42	1.38

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	MGD	O11-C23-N22	-15.12	93.03	108.57
5	C	1003	MGD	C1'-N9-C4	12.70	148.95	126.64
5	C	1003	MGD	O11-C23-N22	-12.58	95.64	108.57
5	E	1003	MGD	O11-C23-N22	-12.27	95.95	108.57
5	E	1003	MGD	C1'-N9-C4	11.33	146.54	126.64
5	A	1003	MGD	C1'-N9-C4	11.12	146.19	126.64
5	C	1003	MGD	N3-C2-N1	-6.91	118.00	127.22
5	A	1003	MGD	C17-C16-N15	6.88	124.90	119.12
5	A	1003	MGD	N3-C2-N1	-6.68	118.31	127.22
5	C	1003	MGD	C17-C16-N15	6.20	124.32	119.12
5	E	1003	MGD	C17-C16-C21	6.18	120.06	114.57
5	E	1003	MGD	N3-C2-N1	-5.54	119.83	127.22
5	C	1003	MGD	C17-C16-C21	5.33	119.30	114.57
6	C	1004	MD1	O11-C11-C12	-5.20	101.68	111.05
5	A	1003	MGD	C6-C5-C4	-4.92	116.10	120.80
5	E	1003	MGD	C17-C16-N15	4.86	123.20	119.12
5	C	1003	MGD	C6-C5-C4	-4.43	116.57	120.80
5	A	1003	MGD	N2-C2-N1	4.38	124.07	117.25
5	C	1003	MGD	C6-N1-C2	4.27	122.72	115.93
5	A	1003	MGD	C17-C16-C21	4.09	118.21	114.57
6	E	1004	MD1	C4-C5-N7	4.02	107.78	102.46
5	A	1003	MGD	C6-N1-C2	3.99	122.27	115.93
5	A	1003	MGD	N18-C19-N20	-3.96	119.21	125.42
6	C	1004	MD1	C4-C5-N7	3.92	107.65	102.46
6	A	1004	MD1	C15-C16-N15	-3.91	115.84	119.12
6	A	1004	MD1	O11-C11-C12	-3.91	104.02	111.05
5	C	1003	MGD	C2-N3-C4	3.86	119.76	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1003	MGD	N2-C2-N1	3.84	123.23	117.25
6	A	1004	MD1	N17-C17-N18	-3.82	119.42	125.42
5	A	1003	MGD	C21-N22-C23	-3.72	116.38	123.67
5	E	1003	MGD	N2-C2-N1	3.71	123.02	117.25
5	E	1003	MGD	O4'-C1'-C2'	-3.70	101.52	106.93
6	A	1004	MD1	C15-N17-C17	3.63	121.70	115.93
6	E	1004	MD1	O11-C11-C12	-3.63	104.51	111.05
5	E	1003	MGD	C5-C6-N1	-3.63	118.47	123.43
5	E	1003	MGD	C6-N1-C2	3.63	121.69	115.93
5	A	1003	MGD	C2-N3-C4	3.60	119.47	115.36
5	A	1003	MGD	C17-N18-C19	3.57	121.60	115.93
5	C	1003	MGD	O4'-C1'-C2'	-3.44	101.90	106.93
6	A	1004	MD1	C4-C5-N7	3.42	106.99	102.46
5	E	1003	MGD	C6-C5-C4	-3.36	117.59	120.80
5	C	1003	MGD	C5-C6-N1	-3.25	118.98	123.43
6	E	1004	MD1	N17-C17-N18	-3.23	120.35	125.42
5	A	1003	MGD	C2'-C3'-C4'	3.19	108.84	102.64
5	C	1003	MGD	N18-C19-N20	-3.18	120.43	125.42
5	C	1003	MGD	C17-N18-C19	3.17	120.97	115.93
5	E	1003	MGD	C17-N18-C19	3.07	120.80	115.93
5	A	1003	MGD	C19-N20-C21	3.01	121.28	114.54
5	A	1003	MGD	C5-C6-N1	-2.96	119.38	123.43
6	C	1004	MD1	N17-C17-N18	-2.95	120.79	125.42
5	E	1003	MGD	C4-C5-N7	-2.92	106.36	109.40
6	E	1004	MD1	C15-N17-C17	2.88	120.51	115.93
6	A	1004	MD1	N16-C17-N18	2.82	121.64	117.25
5	E	1003	MGD	C21-N22-C23	-2.71	118.36	123.67
6	E	1004	MD1	PA-O3B-PB	-2.66	123.70	132.83
5	A	1003	MGD	N19-C19-N18	2.64	121.37	117.25
6	A	1004	MD1	PA-O3B-PB	-2.63	123.81	132.83
5	A	1003	MGD	O3'-C3'-C4'	-2.59	103.56	111.05
5	C	1003	MGD	C16-C21-N22	-2.53	115.82	118.13
6	C	1004	MD1	C15-N17-C17	2.51	119.92	115.93
5	E	1003	MGD	C2-N3-C4	2.49	118.20	115.36
6	E	1004	MD1	C5'-C4'-C3'	-2.48	105.88	115.18
5	A	1003	MGD	C4-C5-N7	-2.40	106.90	109.40
6	C	1004	MD1	O6-C6-N1	-2.38	119.49	122.69
6	E	1004	MD1	C15-C16-N15	-2.33	117.17	119.12
5	E	1003	MGD	C16-C17-N18	-2.31	117.45	124.01
6	A	1004	MD1	O4'-C1'-N9	-2.30	105.61	109.04
6	E	1004	MD1	O2'-C2'-C3'	-2.28	104.44	111.82
6	E	1004	MD1	O4'-C1'-N9	-2.24	105.71	109.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1003	MGD	C19-N20-C21	2.23	119.54	114.54
6	C	1004	MD1	N16-C17-N17	2.23	120.72	117.25
5	C	1003	MGD	O11-C23-C14	2.23	110.45	108.96
5	C	1003	MGD	C4-C5-N7	-2.21	107.10	109.40
6	C	1004	MD1	O4'-C1'-N9	-2.20	105.77	109.04
5	A	1003	MGD	O11-C23-C14	-2.18	107.51	108.96
5	E	1003	MGD	N18-C19-N20	-2.12	122.09	125.42
6	A	1004	MD1	O6-C6-N1	-2.11	119.86	122.69
5	C	1003	MGD	N19-C19-N18	2.10	120.52	117.25
6	C	1004	MD1	PA-O3B-PB	-2.05	125.79	132.83
5	E	1003	MGD	N19-C19-N18	2.02	120.40	117.25

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1004	MD1	C10-O3A-PB-O1B
6	C	1004	MD1	C2'-C1'-N9-C8
6	A	1004	MD1	C2'-C1'-N9-C8
6	E	1004	MD1	C2'-C1'-N9-C8
5	A	1003	MGD	C5'-O5'-PB-O1B
6	C	1004	MD1	C10-O3A-PB-O3B
5	A	1003	MGD	C5'-O5'-PB-O3B
6	C	1004	MD1	C10-O3A-PB-O2B
6	A	1004	MD1	C10-O3A-PB-O2B
6	E	1004	MD1	O4'-C4'-C5'-O5'
6	A	1004	MD1	O4'-C4'-C5'-O5'
6	E	1004	MD1	C3'-C4'-C5'-O5'
7	A	1007	EDO	O1-C1-C2-O2
6	A	1004	MD1	C10-O3A-PB-O3B
6	A	1004	MD1	PA-O3B-PB-O1B
5	E	1003	MGD	PA-O3B-PB-O1B
5	E	1003	MGD	PA-O3B-PB-O2B
6	C	1004	MD1	O4'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1010	GOL	1	0
3	F	404	SF4	1	0

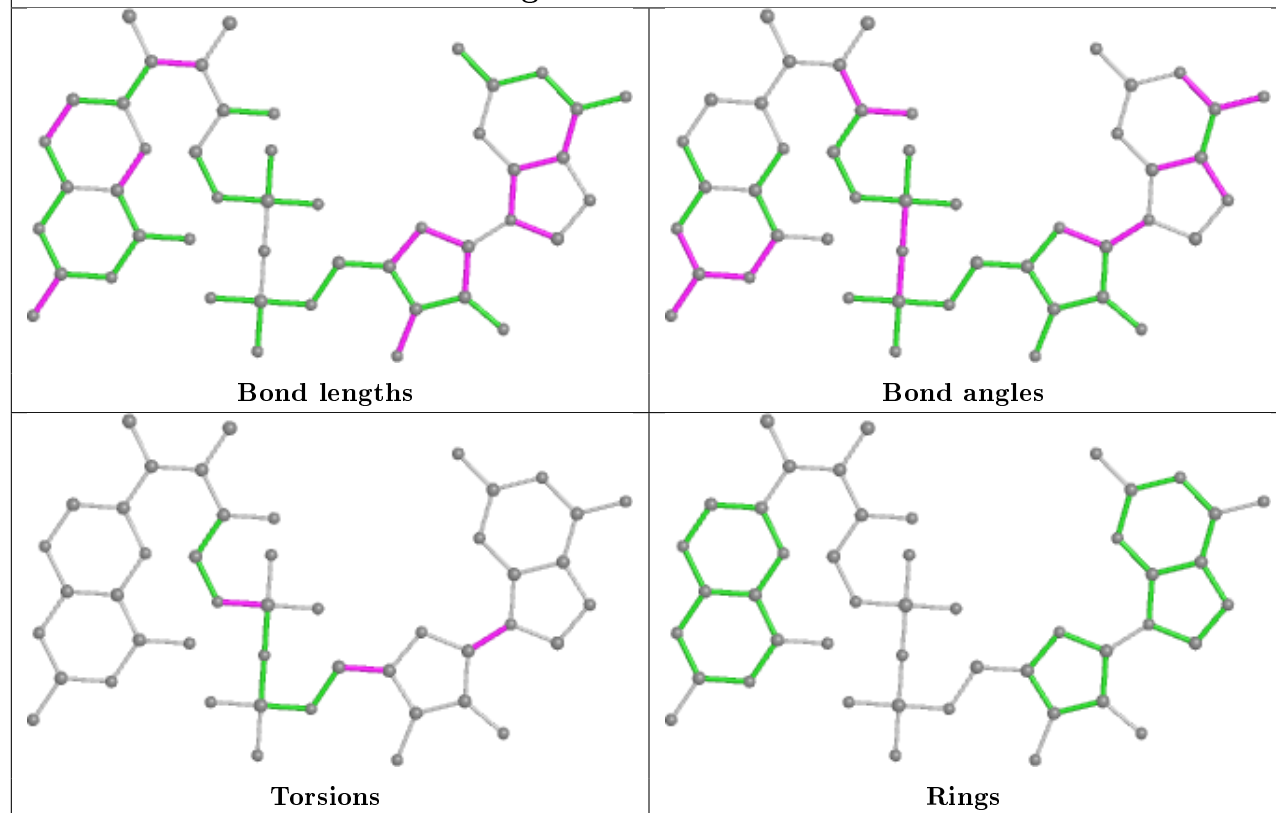
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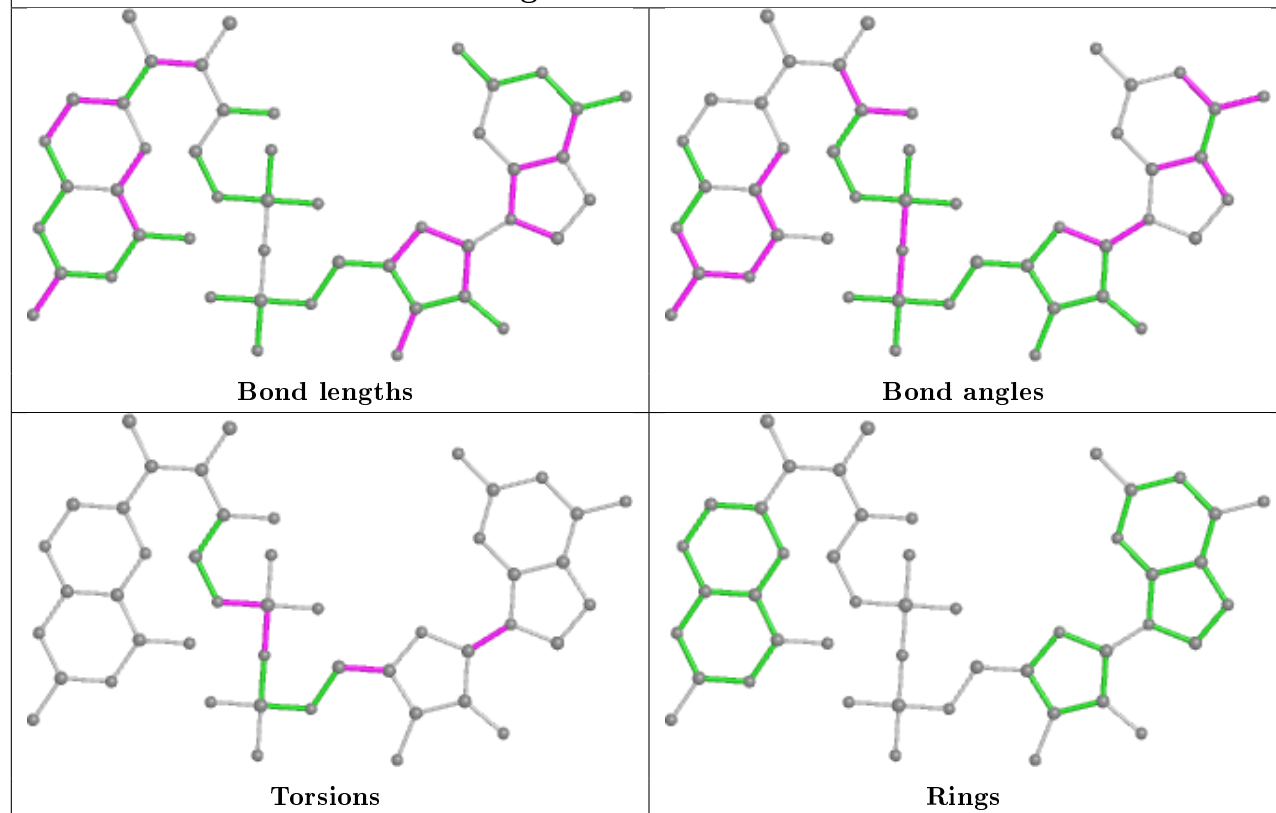
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1004	MD1	1	0
6	A	1004	MD1	1	0
6	E	1004	MD1	1	0
7	B	407	EDO	1	0
7	E	1006	EDO	2	0
5	A	1003	MGD	2	0
5	C	1003	MGD	2	0
7	A	1012	EDO	1	0
3	D	405	SF4	1	0

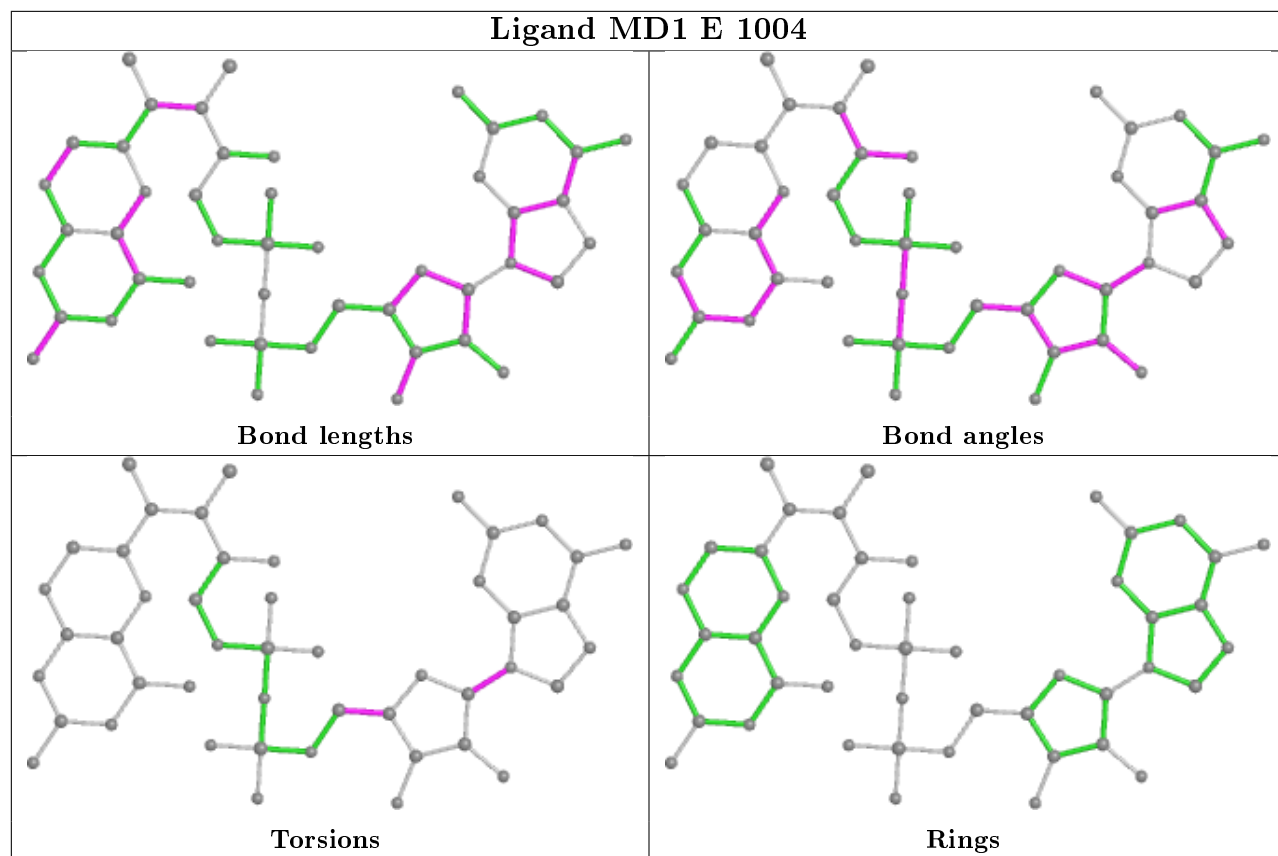
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand MD1 C 1004

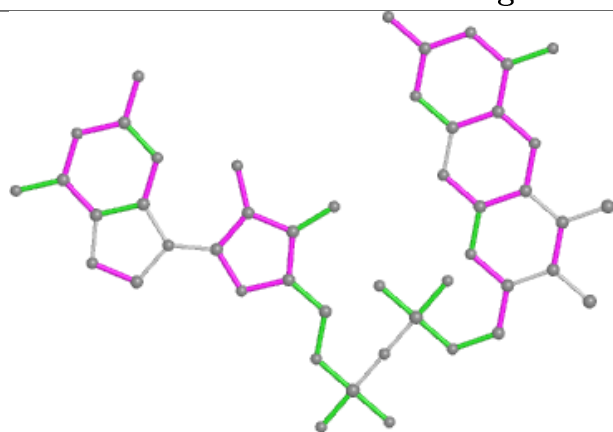


## Ligand MD1 A 1004

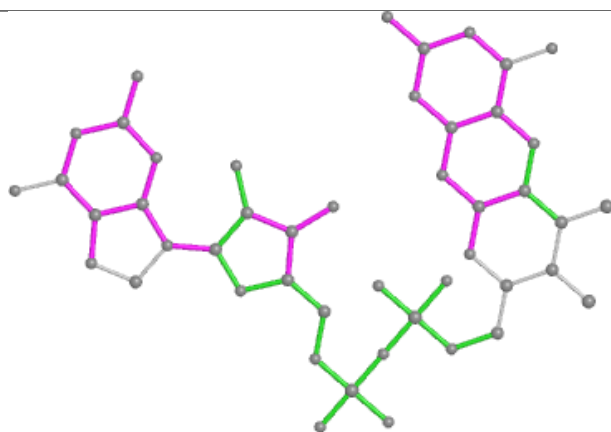




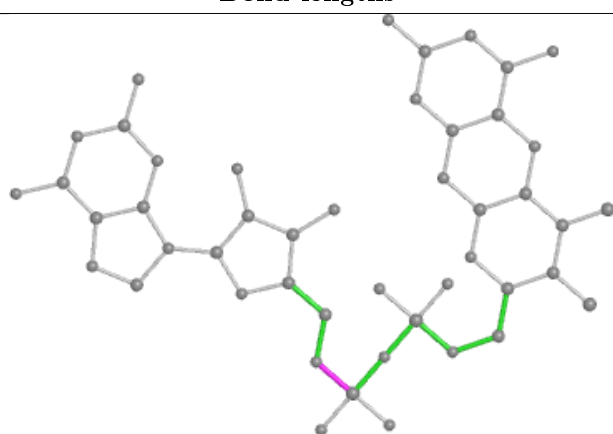
## Ligand MGD A 1003



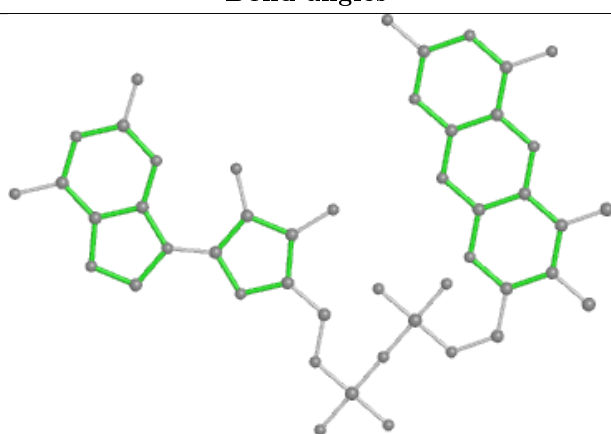
Bond lengths



Bond angles

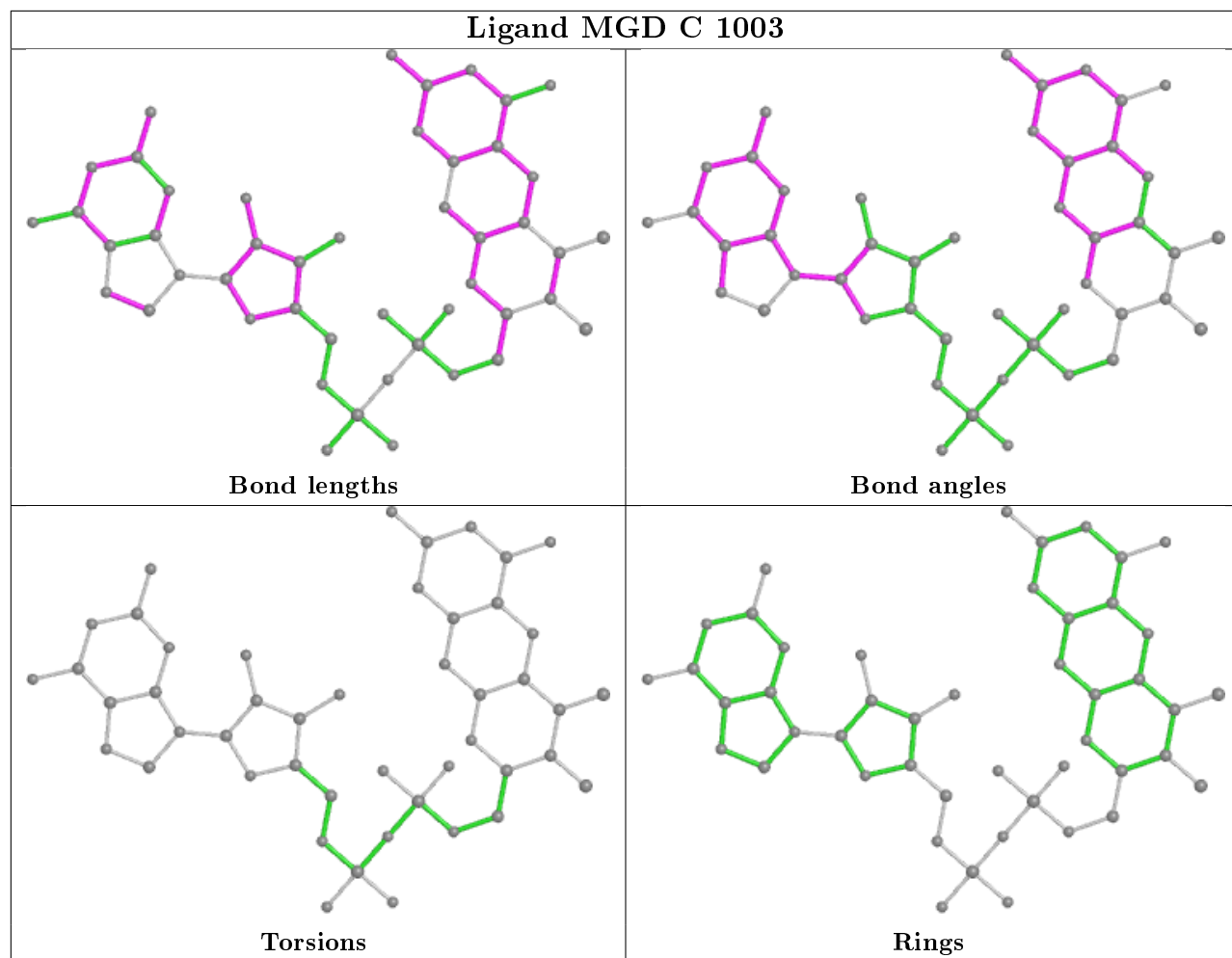


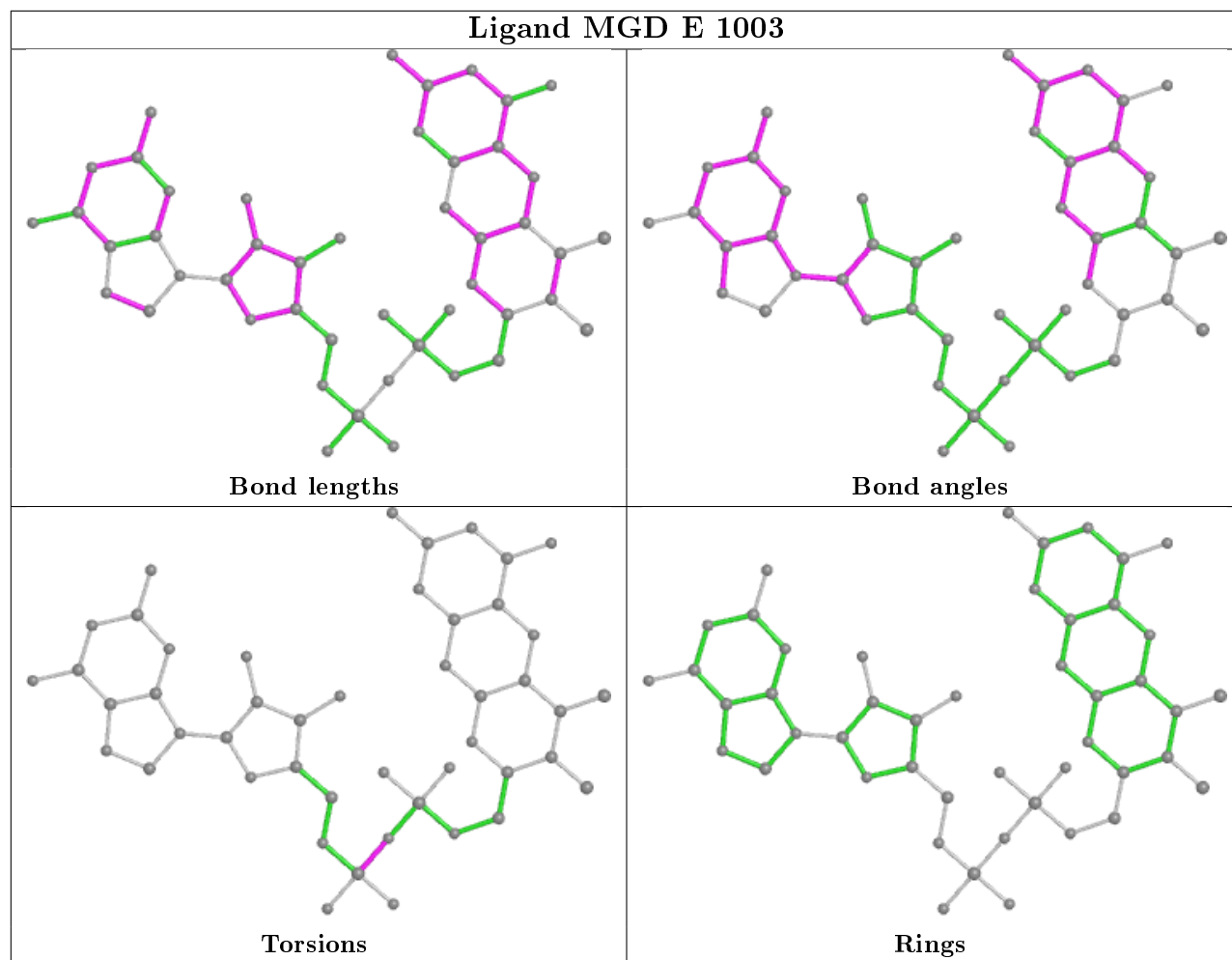
Torsions



Rings

## Ligand MGD C 1003





## 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	894/899 (99%)	-0.36	10 (1%) 80 79	16, 30, 49, 68	0
1	C	891/899 (99%)	-0.04	29 (3%) 46 44	19, 39, 62, 97	0
1	E	892/899 (99%)	-0.34	14 (1%) 72 70	17, 30, 51, 70	0
2	B	329/333 (98%)	-0.62	2 (0%) 89 88	17, 24, 38, 64	0
2	D	327/333 (98%)	0.43	27 (8%) 11 10	25, 54, 71, 89	0
2	F	328/333 (98%)	-0.36	1 (0%) 94 93	18, 32, 50, 66	0
All	All	3661/3696 (99%)	-0.23	83 (2%) 60 58	16, 32, 59, 97	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	TYR	5.5
1	A	8	ALA	5.2
1	C	9	PHE	4.7
1	C	164[A]	PHE	4.6
1	E	164[A]	PHE	4.2
1	C	298	GLY	4.2
1	A	164[A]	PHE	4.1
2	D	7	ALA	3.7
2	D	295	ASP	3.7
2	B	5	MET	3.7
1	C	368	LYS	3.4
1	C	366	ASP	3.2
1	A	7	GLY	3.2
2	D	170	CYS	3.2
2	D	69	LYS	3.1
2	B	6	LYS	3.1
1	A	297	ALA	3.0
1	C	458	ILE	3.0
2	D	250	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	10	ARG	2.9
2	D	171	LYS	2.8
1	E	298	GLY	2.8
2	D	154	ILE	2.8
2	D	8	PRO	2.7
1	C	207	THR	2.7
1	C	365	LEU	2.7
1	A	328	LYS	2.7
2	D	9	ARG	2.6
1	A	769	VAL	2.6
1	C	363	GLN	2.6
2	D	152	GLU	2.6
1	C	689	GLU	2.6
2	D	65	GLY	2.5
1	C	168	TYR	2.5
1	E	314	PRO	2.5
1	C	769	VAL	2.5
2	D	145	CYS	2.5
1	A	6	SER	2.4
1	E	366	ASP	2.4
2	D	150	PRO	2.4
1	C	770	HIS	2.4
2	D	240	TYR	2.4
2	D	153	ALA	2.4
1	C	139	VAL	2.4
1	C	209	ILE	2.4
1	E	328	LYS	2.4
2	D	312	ALA	2.4
1	C	309	ALA	2.3
1	E	365	LEU	2.3
2	D	311	LEU	2.3
1	E	370	VAL	2.3
1	C	299	GLY	2.3
1	A	168	TYR	2.3
2	D	142	LYS	2.3
2	D	24	CYS	2.3
1	C	768	SER	2.3
2	D	159	GLN	2.3
2	D	76	GLY	2.2
2	D	68	TYR	2.2
1	E	313	LYS	2.2
2	D	158	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	36	CYS	2.2
1	C	420	CYS	2.2
1	C	297	ALA	2.2
1	C	327	LYS	2.2
1	E	327	LYS	2.2
1	C	704	GLU	2.2
1	C	313	LYS	2.2
1	C	74	CYS	2.2
1	E	209	ILE	2.2
2	D	140	CYS	2.1
1	E	381	SER	2.1
1	A	351	ASP	2.1
2	D	73	LEU	2.1
1	C	35	ASN	2.1
1	C	17	PHE	2.1
1	E	168	TYR	2.1
2	F	272	GLY	2.1
1	E	769	VAL	2.0
1	E	297	ALA	2.0
1	A	327	LYS	2.0
1	C	361	ASN	2.0
2	D	238	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
11	SO3	E	1008	4/4	0.44	0.25	34,38,48,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	E	1006	4/4	0.71	0.23	34,35,38,41	0
7	EDO	C	1005	4/4	0.80	0.27	33,36,45,45	0
11	SO3	A	1011	4/4	0.83	0.14	38,39,51,70	0
11	SO3	C	1010	4/4	0.83	0.17	61,62,70,83	0
10	GOL	A	1010	6/6	0.84	0.21	35,42,48,48	0
7	EDO	B	407	4/4	0.85	0.23	34,36,37,42	0
7	EDO	F	406	4/4	0.88	0.23	39,42,43,44	0
13	ACT	C	1008	4/4	0.89	0.14	31,36,40,44	0
7	EDO	E	1007	4/4	0.89	0.16	28,40,44,49	0
7	EDO	A	1005	4/4	0.90	0.20	25,26,31,39	0
3	SF4	D	403	8/8	0.90	0.06	39,45,57,57	0
11	SO3	C	1009	4/4	0.91	0.29	43,48,50,68	0
7	EDO	B	406	4/4	0.91	0.14	32,34,40,41	0
7	EDO	A	1006	4/4	0.92	0.15	32,34,35,37	0
11	SO3	A	1013	4/4	0.93	0.35	38,42,42,57	0
7	EDO	E	1005	4/4	0.94	0.11	16,20,23,23	0
3	SF4	D	405	8/8	0.94	0.10	34,48,53,54	0
7	EDO	A	1012	4/4	0.94	0.18	21,22,27,29	0
7	EDO	A	1007	4/4	0.95	0.11	26,28,29,32	0
8	NA	C	1007	1/1	0.95	0.21	26,26,26,26	0
12	F3S	D	402	7/7	0.95	0.05	53,58,64,74	0
7	EDO	C	1006	4/4	0.96	0.08	20,24,25,27	0
7	EDO	D	406	4/4	0.96	0.15	30,36,37,38	0
3	SF4	F	402	8/8	0.96	0.07	29,31,35,40	0
5	MGD	C	1003	47/47	0.96	0.21	21,28,32,33	0
3	SF4	F	404	8/8	0.96	0.10	26,28,29,29	0
3	SF4	C	1001	8/8	0.97	0.14	34,36,40,42	0
8	NA	A	1008	1/1	0.97	0.17	18,18,18,18	0
6	MD1	C	1004	47/47	0.97	0.16	20,29,32,35	0
8	NA	F	407	1/1	0.97	0.09	41,41,41,41	0
6	MD1	A	1004	47/47	0.97	0.15	19,23,28,30	0
7	EDO	D	401	4/4	0.97	0.12	24,24,28,31	0
5	MGD	A	1003	47/47	0.97	0.17	13,20,25,28	0
5	MGD	E	1003	47/47	0.97	0.18	16,24,30,31	0
9	ZN	E	1010	1/1	0.97	0.07	33,33,33,33	0
3	SF4	B	402	8/8	0.98	0.08	22,24,24,30	0
12	F3S	F	401	7/7	0.98	0.04	28,31,33,36	0
3	SF4	D	404	8/8	0.98	0.13	45,49,56,57	0
9	ZN	C	1011	1/1	0.98	0.07	58,58,58,58	0
6	MD1	E	1004	47/47	0.98	0.14	15,22,28,29	0
8	NA	E	1009	1/1	0.98	0.17	14,14,14,14	0
3	SF4	E	1001	8/8	0.98	0.12	19,22,25,26	0

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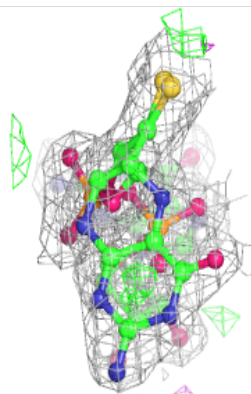
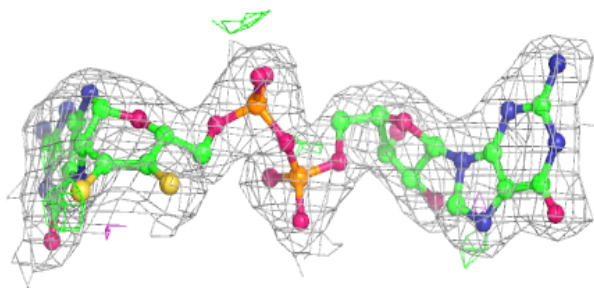
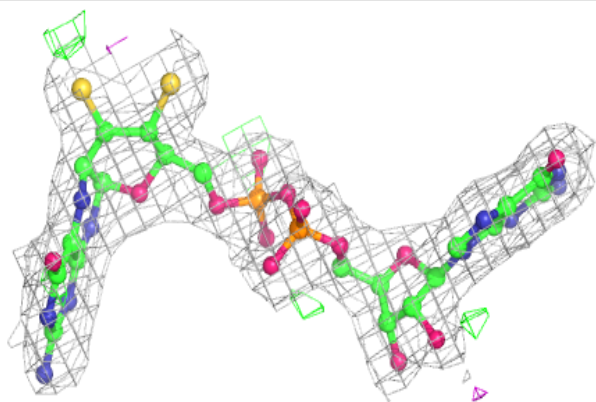
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SF4	F	403	8/8	0.98	0.13	27,31,37,38	0
7	EDO	F	405	4/4	0.98	0.12	23,23,23,25	0
7	EDO	B	405	4/4	0.99	0.09	22,22,23,23	0
4	MO	A	1002	1/1	0.99	0.08	33,33,33,33	0
3	SF4	B	404	8/8	0.99	0.09	19,21,22,23	0
12	F3S	B	401	7/7	0.99	0.04	26,27,28,31	0
3	SF4	A	1001	8/8	0.99	0.13	20,22,26,26	0
3	SF4	B	403	8/8	0.99	0.10	19,22,24,28	0
4	MO	E	1002	1/1	0.99	0.11	32,32,32,32	0
4	MO	C	1002	1/1	0.99	0.10	38,38,38,38	0
9	ZN	A	1009	1/1	0.99	0.08	34,34,34,34	0

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

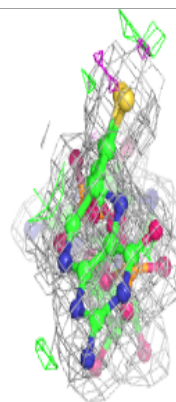
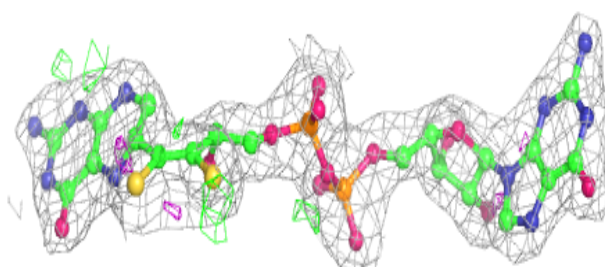
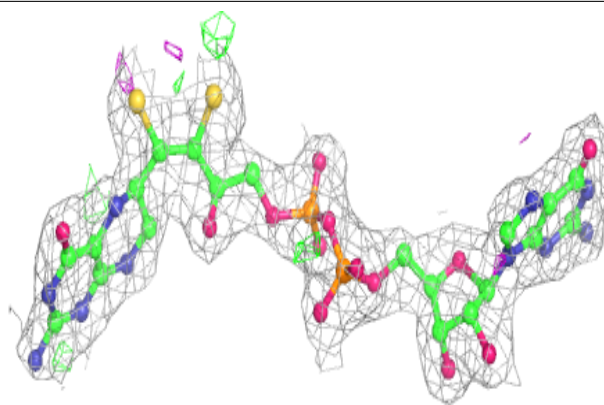
**Electron density around MGD C 1003:**

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)

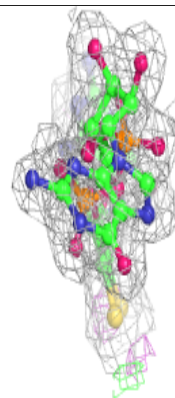
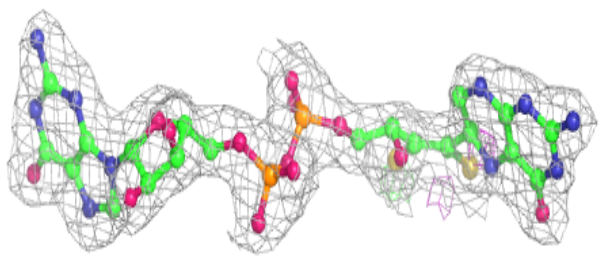
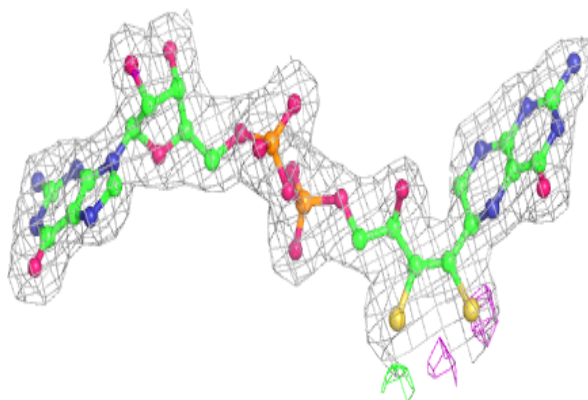


**Electron density around MD1 C 1004:**

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

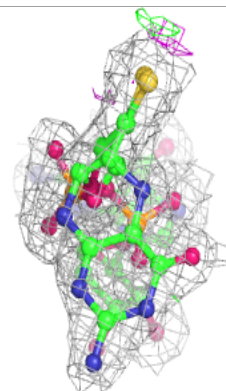
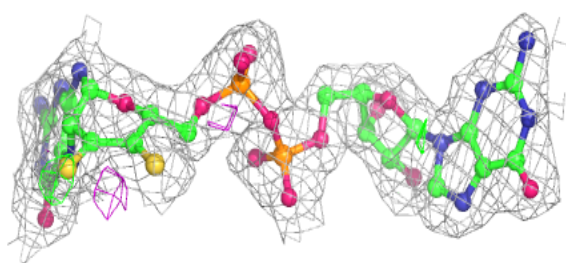
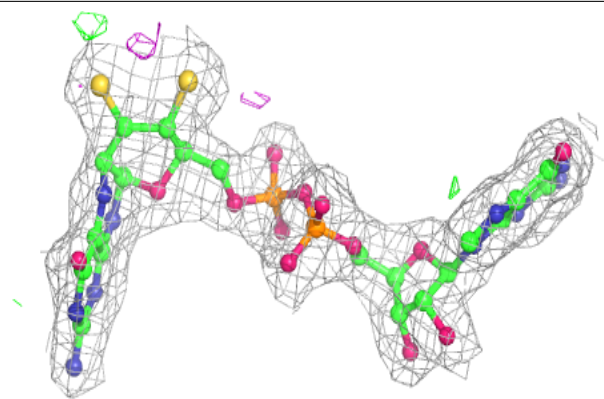
**Electron density around MD1 A 1004:**

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

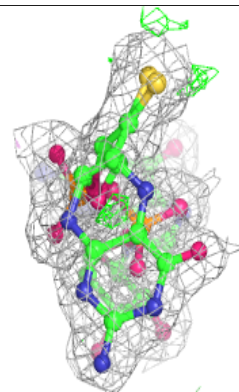
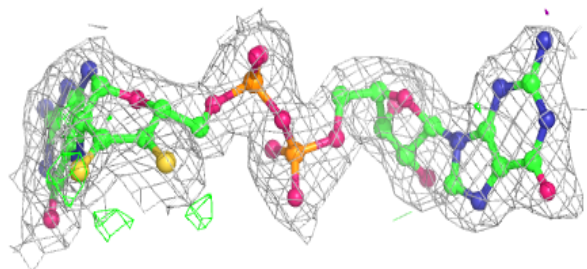
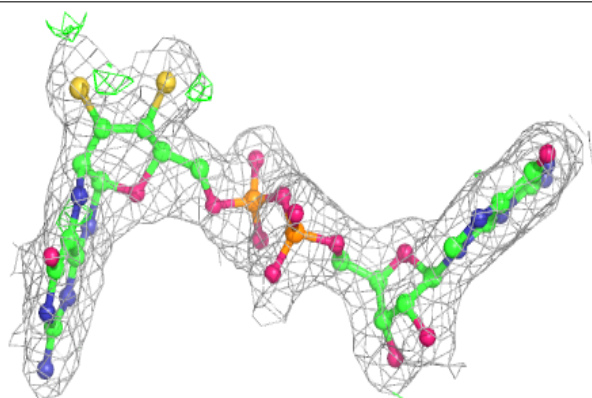


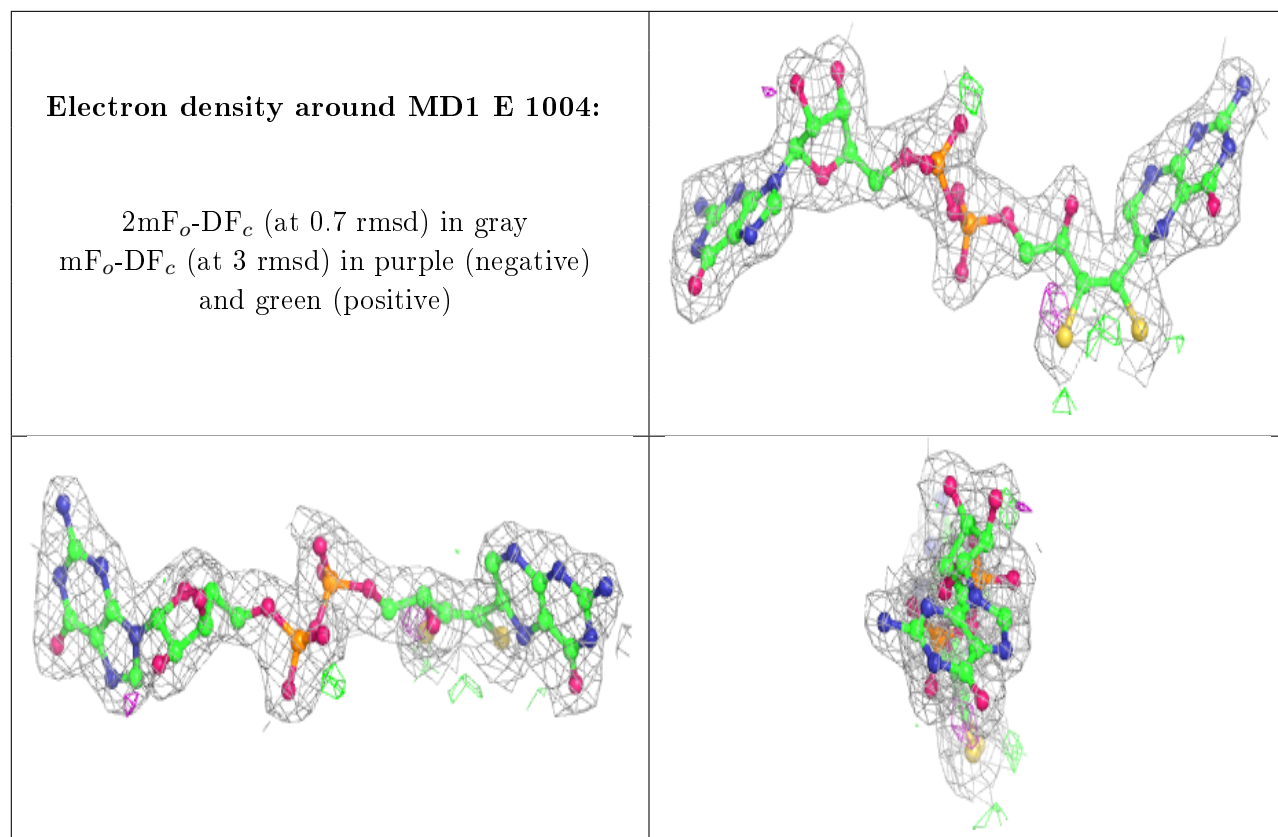
**Electron density around MGD A 1003:**

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

**Electron density around MGD 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.