



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:07 AM EDT

PDB ID : 4YDD / pdb_00004ydd
Title : Crystal structure of the perchlorate reductase PcrAB from *Azospira suillum* PS
Authors : Tsai, C.-L.; Youngblut, M.D.; Tainer, J.A.
Deposited on : 2015-02-21
Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

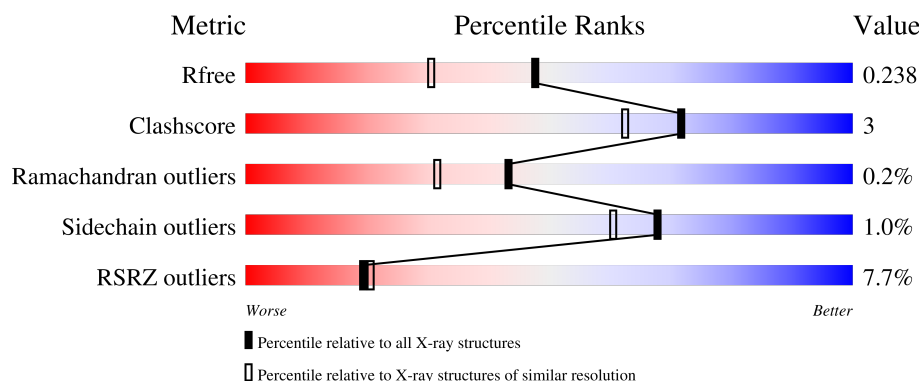
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	899	
1	C	899	
1	E	899	
2	B	333	
2	D	333	

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Mol	Chain	Length	Quality of chain
2	F	333	% 92% 7%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 61265 atoms, of which 28814 are hydrogens and 0 are deuteriums.

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

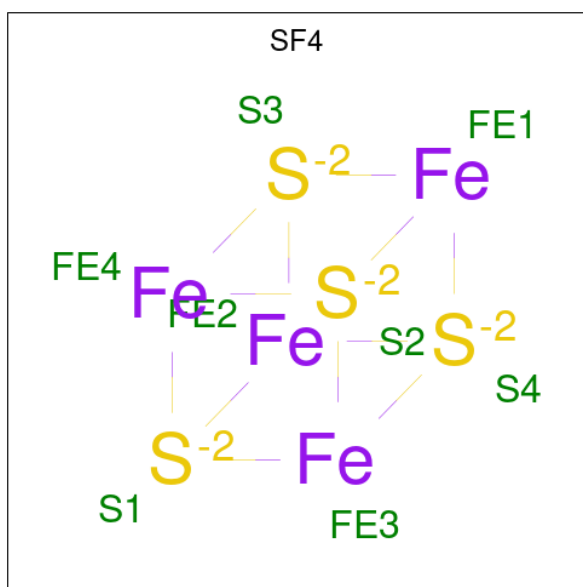
- Molecule 1 is a protein called DMSO reductase family type II enzyme, molybdopterin subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	895	Total	C	H	N	O	S	0	3	0
			14201	4589	7016	1247	1311	38			
1	C	892	Total	C	H	N	O	S	0	0	0
			14110	4563	6962	1240	1307	38			
1	E	892	Total	C	H	N	O	S	0	2	0
			14140	4575	6977	1240	1310	38			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	329	Total	C	H	N	O	S	0	0	0
			5098	1627	2534	447	465	25			
2	D	328	Total	C	H	N	O	S	0	0	0
			5081	1622	2525	446	464	24			
2	F	328	Total	C	H	N	O	S	0	1	0
			5095	1626	2533	447	465	24			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

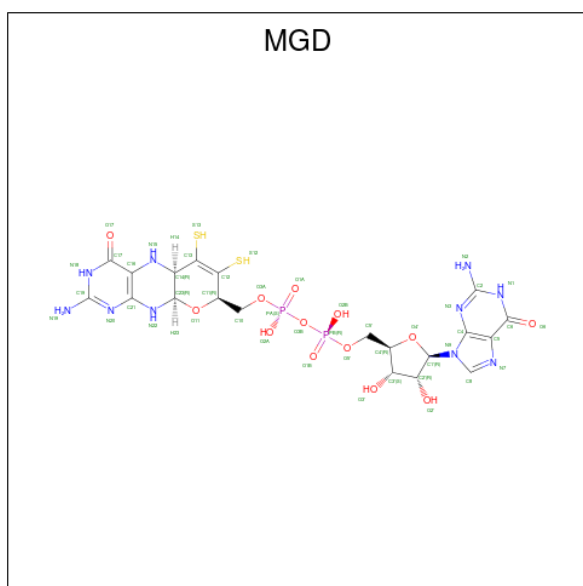


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3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

- Molecule 4 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

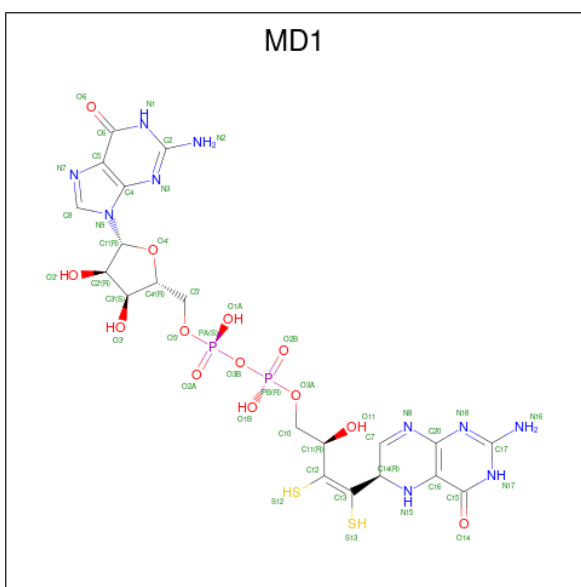
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



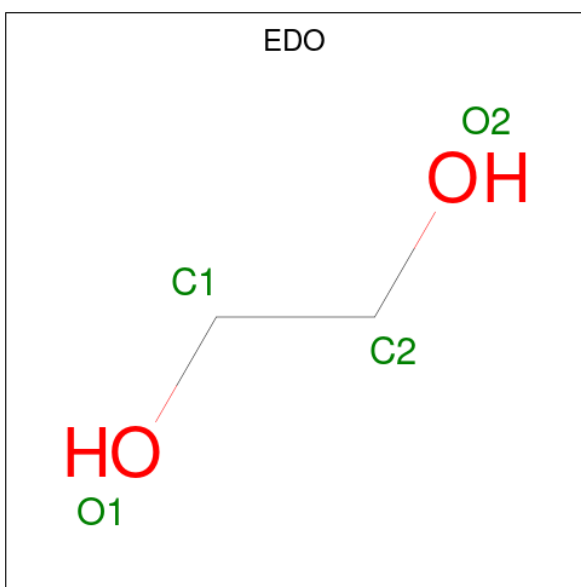
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	S	0	0
			70	20	23	10	13	2	2		
5	C	1	Total	C	H	N	O	P	S	0	0
			70	20	23	10	13	2	2		
5	E	1	Total	C	H	N	O	P	S	0	0
			70	20	23	10	13	2	2		

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



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	A	1	Total 71	C 20	H 24	N 10	O 13	P 2	S 2	0	0
6	C	1	Total 71	C 20	H 24	N 10	O 13	P 2	S 2	0	0
6	E	1	Total 71	C 20	H 24	N 10	O 13	P 2	S 2	0	0

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



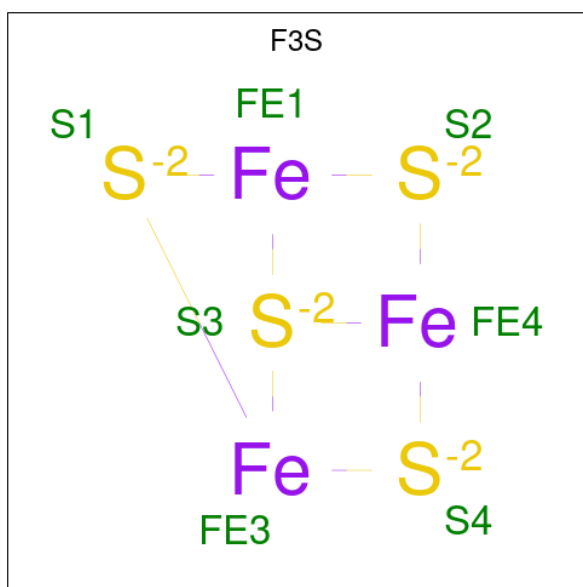
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		

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

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).

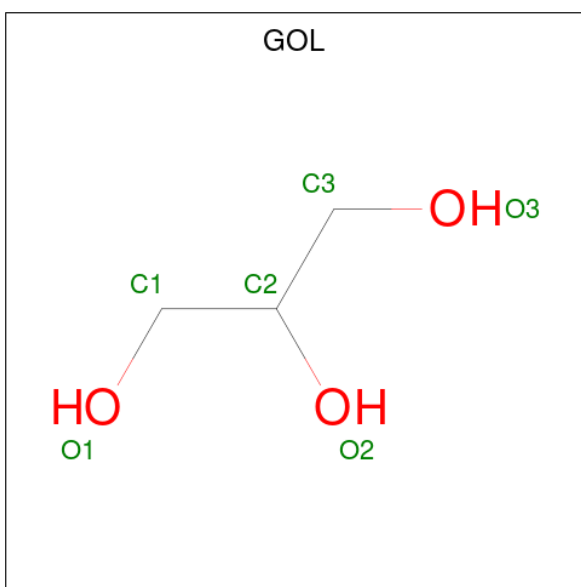


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	D	1	Total	Fe	S	0	0
			7	3	4		
8	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

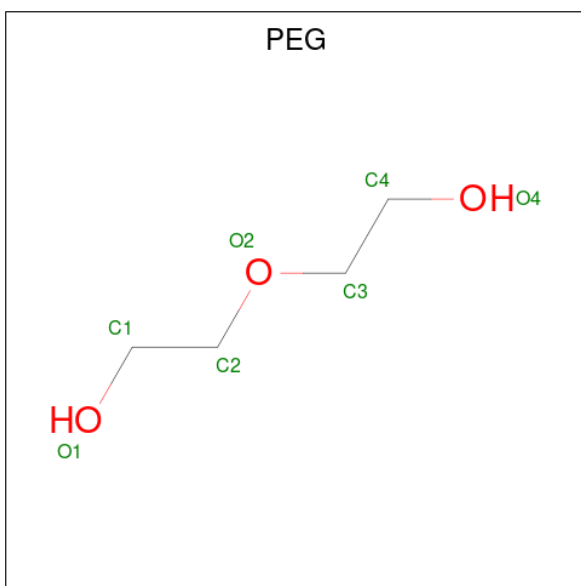
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Na	0	0
			1	1		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

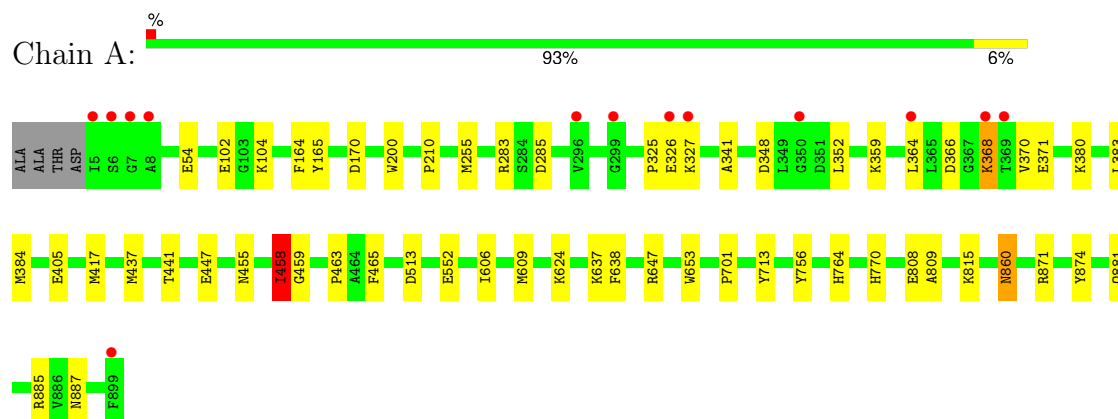
- Molecule 12 is water.

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

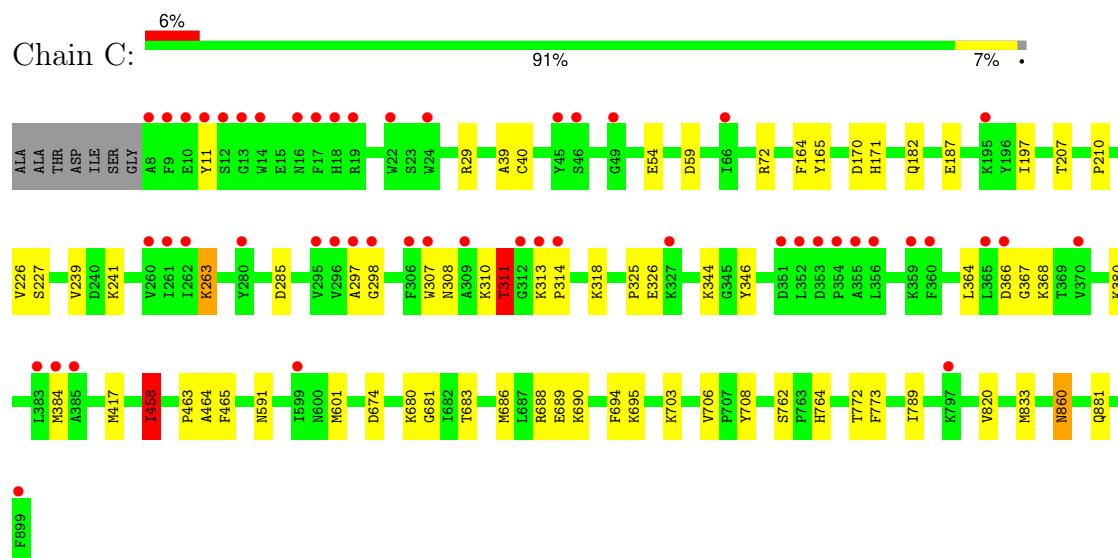
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

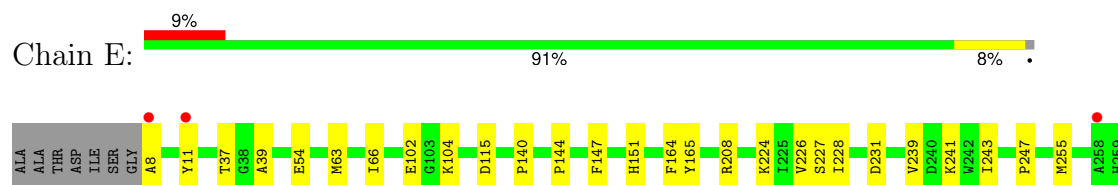
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

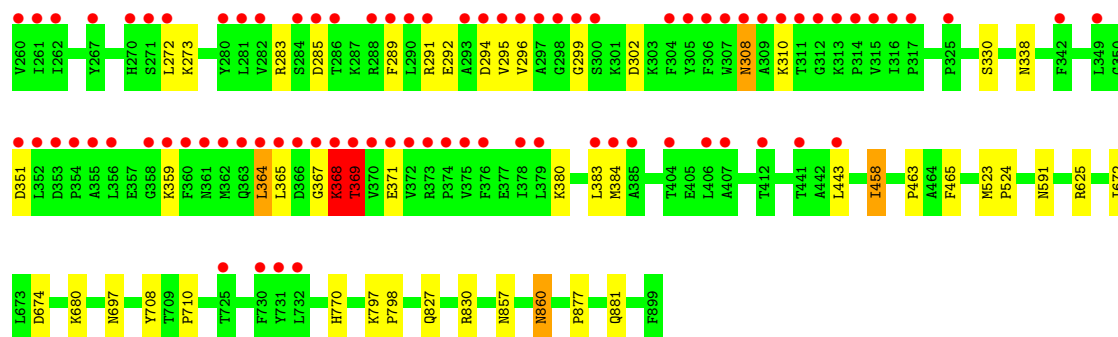


- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



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

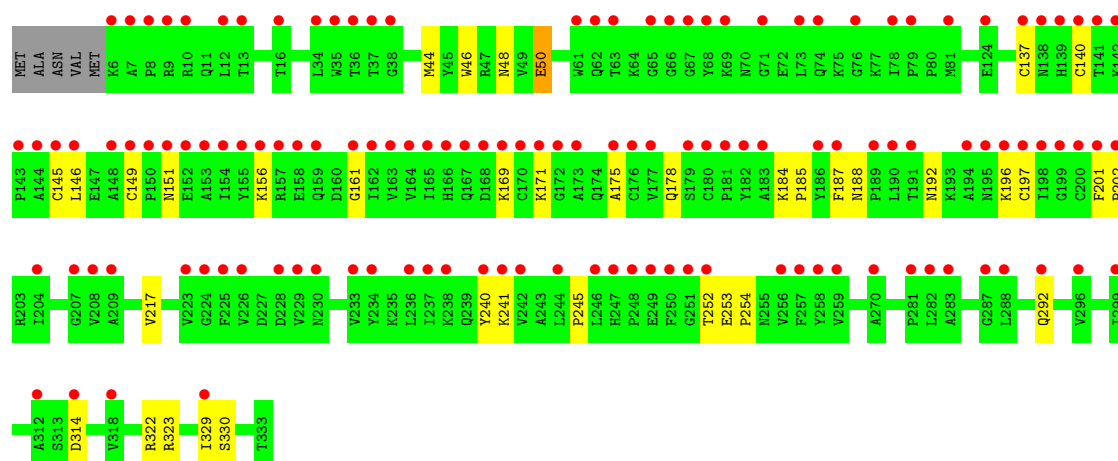
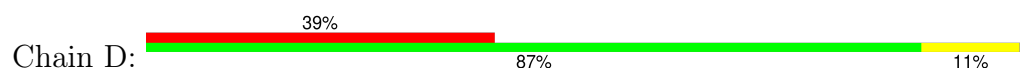




- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.83Å 175.50Å 193.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 1.86 48.35 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.35-1.86) 98.9 (48.35-1.86)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.86Å)	Xtriage
Refinement program	PHENIX dev_2299	Depositor
R, R_{free}	0.201 , 0.237 0.203 , 0.238	Depositor DCC
R_{free} test set	18608 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	61265	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/7403	0.61	0/10045
1	C	0.41	0/7357	0.59	0/9984
1	E	0.45	0/7379	0.63	0/10014
2	B	0.51	0/2632	0.65	0/3567
2	D	0.34	0/2624	0.59	0/3557
2	F	0.45	0/2633	0.62	0/3569
All	All	0.44	0/30028	0.61	0/40736

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7185	7016	7016	34	0
1	C	7148	6962	6960	45	0
1	E	7163	6977	6975	53	0
2	B	2564	2534	2534	14	0
2	D	2556	2525	2525	27	0
2	F	2562	2533	2533	14	0
3	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	0	0	0
3	C	8	0	0	0	0
3	D	24	0	0	1	0
3	E	8	0	0	0	0
3	F	24	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	47	23	21	0	0
5	C	47	23	21	1	0
5	E	47	23	21	1	0
6	A	47	24	22	5	0
6	C	47	24	21	4	0
6	E	47	24	21	4	0
7	A	24	36	36	1	0
7	B	8	12	12	0	0
7	C	8	12	12	0	0
7	D	4	6	6	0	0
7	E	24	36	36	0	0
7	F	4	6	6	0	0
8	B	7	0	0	0	0
8	D	7	0	0	1	0
8	F	7	0	0	0	0
9	B	1	0	0	0	0
10	C	6	8	8	0	0
11	C	7	10	10	1	0
12	A	738	0	0	7	1
12	B	358	0	0	2	2
12	C	576	0	0	3	0
12	D	141	0	0	0	0
12	E	681	0	0	7	2
12	F	291	0	0	2	1
All	All	32451	28814	28796	192	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:THR:O	12:E:1101:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:ASP:OD1	1:E:830:ARG:NH2	2.21	0.74
1:A:405:GLU:OE2	12:A:1101:HOH:O	2.06	0.73
1:E:368:LYS:O	1:E:369:THR:OG1	2.05	0.73
1:C:680:LYS:O	1:C:695:LYS:HE3	1.90	0.72
2:B:42:ASP:OD1	12:B:501:HOH:O	2.08	0.71
1:E:710:PRO:O	12:E:1102:HOH:O	2.11	0.69
2:F:168:ASP:OD1	12:F:501:HOH:O	2.12	0.67
6:E:1004:MD1:C11	6:E:1004:MD1:H7	2.25	0.67
1:E:273:LYS:O	12:E:1103:HOH:O	2.14	0.66
1:E:310:LYS:NZ	1:E:351:ASP:OD1	2.29	0.65
1:C:364:LEU:O	12:C:1101:HOH:O	2.15	0.63
1:C:366:ASP:N	1:C:367:GLY:HA2	2.13	0.63
1:C:11:TYR:CE1	2:D:169:LYS:HE3	2.33	0.62
6:A:1004:MD1:C11	6:A:1004:MD1:H7	2.31	0.61
6:A:1004:MD1:H7	6:A:1004:MD1:H11	1.84	0.60
1:C:308:ASN:O	1:C:310:LYS:N	2.32	0.59
1:E:380:LYS:O	1:E:384:MET:HG2	2.03	0.59
1:E:294:ASP:HB3	1:E:364:LEU:HD21	1.85	0.59
2:D:46:TRP:O	2:D:184:LYS:NZ	2.36	0.58
1:A:325:PRO:O	1:A:326:GLU:HB3	2.03	0.58
2:B:43:PHE:CG	2:B:81:MET:HE1	2.39	0.57
1:E:797:LYS:HB3	1:E:798:PRO:HD3	1.87	0.57
1:A:359:LYS:CE	1:A:371:GLU:OE2	2.53	0.57
2:D:44:MET:HE1	2:D:188:ASN:HB2	1.87	0.56
2:D:196:LYS:HD2	3:D:402:SF4:S3	2.46	0.56
6:C:1004:MD1:H7	6:C:1004:MD1:H11	1.88	0.56
1:C:325:PRO:O	1:C:326:GLU:HB2	2.06	0.56
6:E:1004:MD1:H7	6:E:1004:MD1:H11	1.88	0.55
1:A:756:TYR:O	1:A:885[B]:ARG:HD3	2.07	0.55
2:D:175:ALA:HA	2:D:178:GLN:HE21	1.72	0.55
1:A:170:ASP:HB3	1:A:458:ILE:HD13	1.87	0.54
1:E:63:MET:HB2	1:E:66:ILE:HD11	1.88	0.53
1:A:352:LEU:O	12:A:1102:HOH:O	2.18	0.53
1:E:368:LYS:CG	1:E:369:THR:H	2.22	0.53
1:E:224:LYS:NZ	12:E:1106:HOH:O	2.30	0.52
1:E:308:ASN:HD22	1:E:308:ASN:C	2.17	0.52
2:B:140:CYS:HB3	2:B:252:THR:O	2.10	0.52
1:E:255:MET:HE3	1:E:383:LEU:HD21	1.91	0.52
2:D:187:PHE:CZ	2:D:192:ASN:HA	2.45	0.51
2:D:240:TYR:OH	2:D:314:ASP:OD2	2.23	0.51
1:C:366:ASP:OD1	1:C:368:LYS:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:860:ASN:HD22	1:E:860:ASN:N	2.07	0.51
2:D:175:ALA:HA	2:D:178:GLN:NE2	2.26	0.51
1:C:674:ASP:O	1:C:680:LYS:HD3	2.11	0.50
1:C:170:ASP:HB3	1:C:458:ILE:HD13	1.92	0.50
1:E:115:ASP:OD1	1:E:625:ARG:HD2	2.12	0.50
1:E:860:ASN:HB3	1:E:877:PRO:HA	1.94	0.50
1:A:770:HIS:CE1	6:A:1004:MD1:S12	3.04	0.50
1:A:283:ARG:HB3	1:A:285:ASP:OD1	2.11	0.50
1:C:307:TRP:CZ3	1:C:314:PRO:HG3	2.46	0.49
1:E:368:LYS:C	1:E:369:THR:OG1	2.55	0.49
2:D:140:CYS:HB3	2:D:252:THR:O	2.12	0.49
1:A:764:HIS:HE2	6:A:1004:MD1:H15	1.59	0.49
1:C:681:GLY:HA3	1:C:695:LYS:HE3	1.95	0.49
1:C:680:LYS:O	1:C:695:LYS:CE	2.59	0.49
2:F:305:GLU:HA	2:F:308:MET:HE3	1.95	0.49
1:A:327:LYS:O	1:A:341:ALA:HB1	2.13	0.48
6:C:1004:MD1:H7	6:C:1004:MD1:C11	2.42	0.48
1:A:364:LEU:HD11	1:A:370:VAL:CG1	2.43	0.48
1:A:380:LYS:O	1:A:384:MET:HG2	2.13	0.48
1:E:359:LYS:HE2	1:E:371:GLU:OE2	2.13	0.48
1:A:441:THR:HG21	1:A:447:GLU:OE2	2.14	0.47
2:D:292:GLN:H	2:D:292:GLN:CD	2.22	0.47
2:D:48:ASN:ND2	2:D:50:GLU:HG2	2.28	0.47
2:F:141:THR:HG22	12:F:526:HOH:O	2.13	0.47
1:E:302:ASP:OD1	12:E:1104:HOH:O	2.20	0.47
1:E:292:GLU:HG2	1:E:299:GLY:HA3	1.96	0.47
1:E:294:ASP:O	1:E:364:LEU:HD22	2.13	0.47
1:A:102:GLU:OE2	1:A:104:LYS:NZ	2.48	0.47
1:A:348:ASP:OD1	12:A:1103:HOH:O	2.20	0.47
1:C:860:ASN:N	1:C:860:ASN:HD22	2.13	0.47
1:C:464:ALA:HB3	1:C:694:PHE:CE1	2.49	0.46
1:C:683:THR:HG23	1:C:686:MET:HE3	1.96	0.46
1:E:115:ASP:OD1	1:E:625:ARG:CD	2.63	0.46
1:C:210:PRO:HA	2:D:217:VAL:CG1	2.45	0.46
2:D:329:ILE:O	2:D:330:SER:C	2.58	0.46
1:C:311:THR:O	1:C:313:LYS:HG3	2.15	0.46
1:A:210:PRO:HA	2:B:217:VAL:CG1	2.46	0.46
6:E:1004:MD1:C11	6:E:1004:MD1:C7	2.94	0.46
1:C:366:ASP:OD1	1:C:368:LYS:HG3	2.16	0.46
1:E:226:VAL:HG22	1:E:241:LYS:HG2	1.98	0.46
1:C:764:HIS:HE2	6:C:1004:MD1:H15	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ASP:N	1:C:367:GLY:CA	2.79	0.45
1:A:606:ILE:HD11	1:A:609:MET:CE	2.47	0.45
1:A:808:GLU:OE2	1:A:815:LYS:HD2	2.17	0.45
1:E:147:PHE:CE2	1:E:151:HIS:CE1	3.05	0.45
1:E:857:ASN:OD1	1:E:857:ASN:C	2.60	0.45
1:E:294:ASP:O	1:E:365:LEU:HB2	2.17	0.45
1:A:255:MET:HE3	1:A:383:LEU:HD21	1.99	0.45
2:D:145:CYS:SG	2:D:146:LEU:N	2.89	0.45
1:C:197:ILE:HG12	1:C:417:MET:HG2	1.99	0.44
7:A:1010:EDO:H22	2:B:111:ARG:HG2	2.00	0.44
1:C:170:ASP:HB3	1:C:458:ILE:CD1	2.47	0.44
2:D:184:LYS:N	2:D:185:PRO:CD	2.81	0.44
1:C:171:HIS:HB3	12:C:1193:HOH:O	2.18	0.44
1:C:187:GLU:HG3	1:C:708:TYR:HB3	1.99	0.44
1:C:285:ASP:OD1	1:C:285:ASP:N	2.51	0.44
2:D:156:LYS:NZ	2:D:161:GLY:O	2.46	0.43
1:E:39:ALA:HA	1:E:591:ASN:OD1	2.18	0.43
1:E:308:ASN:O	1:E:310:LYS:N	2.50	0.43
1:E:368:LYS:HG2	1:E:369:THR:H	1.82	0.43
2:F:201:PHE:CG	2:F:202:PRO:HD3	2.53	0.43
1:C:59:ASP:HB2	1:C:690:LYS:HE2	1.99	0.43
1:E:285:ASP:OD1	1:E:285:ASP:N	2.52	0.43
1:A:459:GLY:HA3	12:A:1110:HOH:O	2.17	0.43
1:A:164:PHE:CD1	1:A:165:TYR:N	2.87	0.43
2:B:81:MET:HE2	12:E:1736:HOH:O	2.18	0.43
1:E:283:ARG:HB3	1:E:285:ASP:OD1	2.18	0.43
1:E:289:PHE:HB2	1:E:291:ARG:NH1	2.33	0.43
1:E:674:ASP:O	1:E:680:LYS:HD3	2.18	0.43
6:A:1004:MD1:C11	6:A:1004:MD1:C7	2.95	0.43
1:E:368:LYS:CG	1:E:369:THR:N	2.81	0.43
1:E:697:ASN:HB3	1:E:708:TYR:CE1	2.53	0.43
2:F:266:ARG:N	2:F:266:ARG:HD2	2.34	0.43
2:B:166:HIS:CE1	2:B:168:ASP:HB2	2.54	0.43
2:D:137:CYS:CB	2:D:197:CYS:HB3	2.49	0.43
2:F:14:TYR:CE2	2:F:136:MET:HE1	2.53	0.43
1:E:102:GLU:OE1	1:E:104:LYS:HE2	2.18	0.43
1:A:624:LYS:HE3	1:A:653:TRP:CD1	2.54	0.42
1:A:860:ASN:N	1:A:860:ASN:HD22	2.17	0.42
6:C:1004:MD1:C11	6:C:1004:MD1:C7	2.97	0.42
1:A:637:LYS:HA	1:A:647:ARG:O	2.19	0.42
2:D:149:CYS:HA	8:D:401:F3S:S4	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:ASN:O	2:F:139:HIS:C	2.62	0.42
1:C:11:TYR:HE1	2:D:169:LYS:HE3	1.82	0.42
1:C:29:ARG:HG2	1:C:601:MET:HG3	2.01	0.42
1:C:318:LYS:HB3	1:C:346:TYR:CE2	2.55	0.42
1:E:247:PRO:HD3	1:E:827:GLN:OE1	2.19	0.42
2:D:196:LYS:HG2	2:D:197:CYS:N	2.34	0.42
1:E:295:VAL:HG12	1:E:296:VAL:HG23	2.00	0.42
1:A:701:PRO:HD3	1:A:713:TYR:CE1	2.55	0.42
1:C:40:CYS:SG	1:C:72:ARG:HB3	2.60	0.42
2:F:140:CYS:HB3	2:F:252:THR:O	2.20	0.42
1:A:417:MET:HG3	1:A:455:ASN:HD22	1.85	0.42
1:A:552:GLU:OE2	12:A:1105:HOH:O	2.22	0.42
2:D:240:TYR:O	2:D:241:LYS:HB3	2.19	0.42
1:E:227:SER:HB2	1:E:239:VAL:HG11	2.01	0.42
2:B:92:TYR:CD1	2:B:104:VAL:HG11	2.55	0.41
1:C:39:ALA:HA	1:C:591:ASN:OD1	2.19	0.41
2:D:151:ASN:CG	2:D:171:LYS:NZ	2.79	0.41
2:D:322:ARG:O	2:D:323:ARG:NH1	2.51	0.41
1:A:359:LYS:HE3	1:A:371:GLU:OE2	2.20	0.41
2:B:138:ASN:O	2:B:139:HIS:C	2.63	0.41
2:D:137:CYS:HB3	2:D:197:CYS:HB3	2.02	0.41
1:E:8:ALA:N	12:E:1145:HOH:O	2.53	0.41
1:E:272:LEU:HD21	1:E:443:LEU:HA	2.03	0.41
2:F:14:TYR:CZ	2:F:136:MET:HE1	2.55	0.41
1:E:11[A]:TYR:CZ	2:F:169:LYS:HE3	2.56	0.41
1:E:37:THR:HG21	1:E:208:ARG:NH1	2.35	0.41
6:E:1004:MD1:H7	6:E:1004:MD1:O11	2.20	0.41
1:C:164:PHE:CD1	1:C:165:TYR:N	2.88	0.41
1:C:297:ALA:HA	1:C:298:GLY:HA2	1.83	0.41
1:E:330:SER:O	1:E:338:ASN:ND2	2.50	0.41
12:A:1568:HOH:O	2:B:42:ASP:HB3	2.20	0.41
2:B:15:VAL:HB	2:B:222:HIS:HB2	2.02	0.41
1:C:344:LYS:HB3	1:C:344:LYS:HE2	1.90	0.41
2:F:242:VAL:HA	2:F:296:VAL:HG13	2.03	0.41
2:F:141:THR:HG23	2:F:255:ASN:OD1	2.21	0.41
1:A:200:TRP:CD2	1:A:437:MET:HE2	2.56	0.41
1:A:366:ASP:O	1:A:368:LYS:N	2.49	0.41
2:B:136:MET:HG2	2:B:137:CYS:O	2.20	0.41
1:C:789:ILE:O	1:C:820:VAL:HA	2.21	0.41
1:E:523:MET:HA	1:E:524:PRO:C	2.45	0.41
2:D:146:LEU:C	2:D:146:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:PHE:CG	2:D:202:PRO:HD3	2.55	0.41
1:E:228:ILE:HA	1:E:243:ILE:O	2.21	0.41
1:E:367:GLY:O	1:E:368:LYS:CB	2.68	0.41
1:E:770:HIS:CE1	5:E:1003:MGD:S13	3.14	0.41
1:A:513:ASP:OD1	12:A:1104:HOH:O	2.22	0.41
2:B:138:ASN:HB3	2:B:254:PRO:HB3	2.02	0.41
1:C:226:VAL:HG22	1:C:241:LYS:HG2	2.03	0.41
1:C:772:THR:HG22	1:C:773:PHE:CD2	2.56	0.41
1:C:464:ALA:HB3	1:C:694:PHE:CZ	2.56	0.40
1:C:703:LYS:HB2	1:C:706:VAL:HB	2.02	0.40
1:C:762:SER:HA	1:C:833:MET:O	2.21	0.40
1:A:809:ALA:HA	1:A:887:ASN:O	2.21	0.40
1:C:182:GLN:OE1	11:C:1008:PEG:H22	2.21	0.40
2:D:245:PRO:HB2	2:D:254:PRO:HG2	2.03	0.40
1:E:164:PHE:CD1	1:E:165:TYR:N	2.90	0.40
2:F:328:MET:HG3	2:F:329:ILE:O	2.21	0.40
1:A:638:PHE:CZ	1:A:647:ARG:HD2	2.56	0.40
1:A:871:ARG:HB3	1:A:874:TYR:HB3	2.03	0.40
1:E:140:PRO:HB3	1:E:147:PHE:CD1	2.56	0.40
1:E:226:VAL:HG22	1:E:241:LYS:CG	2.52	0.40
2:B:75:LYS:HE2	12:B:555:HOH:O	2.21	0.40
1:C:207:THR:HA	5:C:1003:MGD:N20	2.36	0.40
1:C:227:SER:HB2	1:C:239:VAL:HG11	2.04	0.40
1:C:263:LYS:HE3	12:C:1129:HOH:O	2.20	0.40
1:C:380:LYS:O	1:C:384:MET:HG2	2.22	0.40
1:E:144:PRO:HB2	1:E:672:ILE:HD13	2.03	0.40
2:F:292[B]:GLN:H	2:F:292[B]:GLN:CD	2.30	0.40

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

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	896/899 (100%)	864 (96%)	30 (3%)	2 (0%)	43	31
1	C	890/899 (99%)	851 (96%)	36 (4%)	3 (0%)	36	25
1	E	892/899 (99%)	854 (96%)	34 (4%)	4 (0%)	30	17
2	B	327/333 (98%)	316 (97%)	11 (3%)	0	100	100
2	D	326/333 (98%)	314 (96%)	12 (4%)	0	100	100
2	F	327/333 (98%)	316 (97%)	11 (3%)	0	100	100
All	All	3658/3696 (99%)	3515 (96%)	134 (4%)	9 (0%)	43	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	311	THR
1	C	458	ILE
1	E	369	THR
1	A	458	ILE
1	E	368	LYS
1	E	458	ILE
1	C	463	PRO
1	A	463	PRO
1	E	463	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	769/768 (100%)	763 (99%)	6 (1%)	73	67
1	C	764/768 (100%)	755 (99%)	9 (1%)	63	55
1	E	766/768 (100%)	757 (99%)	9 (1%)	63	55
2	B	278/281 (99%)	275 (99%)	3 (1%)	65	57
2	D	277/281 (99%)	275 (99%)	2 (1%)	76	70
2	F	278/281 (99%)	275 (99%)	3 (1%)	65	57
All	All	3132/3147 (100%)	3100 (99%)	32 (1%)	68	60

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	368	LYS
1	A	458	ILE
1	A	465	PHE
1	A	860	ASN
1	A	881	GLN
2	B	50	GLU
2	B	136	MET
2	B	192	ASN
1	C	54	GLU
1	C	263	LYS
1	C	311	THR
1	C	458	ILE
1	C	465	PHE
1	C	688	ARG
1	C	689	GLU
1	C	860	ASN
1	C	881	GLN
2	D	50	GLU
2	D	253	GLU
1	E	54	GLU
1	E	308	ASN
1	E	364	LEU
1	E	368	LYS
1	E	369	THR
1	E	458	ILE
1	E	465	PHE
1	E	860	ASN
1	E	881	GLN
2	F	50	GLU

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Mol	Chain	Res	Type
2	F	72	GLU
2	F	171	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	783	GLN
2	B	292	GLN
1	C	88	HIS
1	C	553	ASN
2	D	60	ASN
2	D	178	GLN
1	E	522	ASN
1	E	617	GLN
1	E	654	ASN
2	F	151	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 4 are monoatomic - leaving 41 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EDO	C	1005	-	3,3,3	0.85	0	2,2,2	0.58	0
6	MD1	E	1004	4	47,51,51	3.08	17 (36%)	56,78,78	1.67	12 (21%)
10	GOL	C	1006	-	5,5,5	0.49	0	5,5,5	0.42	0
7	EDO	A	1010	-	3,3,3	0.63	0	2,2,2	0.62	0
5	MGD	A	1003	4	47,52,52	4.44	28 (59%)	58,81,81	2.33	14 (24%)
5	MGD	E	1003	4	47,52,52	4.63	27 (57%)	58,81,81	2.27	19 (32%)
3	SF4	B	402	2	0,12,12	-	-	-	-	-
7	EDO	A	1007	-	3,3,3	0.46	0	2,2,2	0.40	0
7	EDO	E	1010	-	3,3,3	0.64	0	2,2,2	0.11	0
7	EDO	E	1005	-	3,3,3	0.72	0	2,2,2	0.50	0
7	EDO	E	1008	-	3,3,3	0.29	0	2,2,2	0.61	0
7	EDO	A	1006	-	3,3,3	0.41	0	2,2,2	0.50	0
3	SF4	E	1001	1	0,12,12	-	-	-	-	-
7	EDO	D	405	-	3,3,3	0.47	0	2,2,2	0.42	0
3	SF4	F	402	2	0,12,12	-	-	-	-	-
7	EDO	A	1005	-	3,3,3	0.46	0	2,2,2	0.14	0
6	MD1	C	1004	4	47,51,51	3.25	17 (36%)	56,78,78	1.58	11 (19%)
8	F3S	F	401	2	0,9,9	-	-	-	-	-
7	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.93	0
7	EDO	A	1008	-	3,3,3	0.39	0	2,2,2	0.69	0
3	SF4	D	404	2	0,12,12	-	-	-	-	-
11	PEG	C	1008	-	6,6,6	0.59	0	5,5,5	0.57	0
3	SF4	C	1001	1	0,12,12	-	-	-	-	-
7	EDO	A	1009	-	3,3,3	0.50	0	2,2,2	0.63	0
3	SF4	F	403	2	0,12,12	-	-	-	-	-
7	EDO	E	1006	-	3,3,3	0.99	0	2,2,2	0.37	0
7	EDO	F	405	-	3,3,3	0.30	0	2,2,2	0.55	0
8	F3S	B	401	2	0,9,9	-	-	-	-	-
5	MGD	C	1003	4	47,52,52	4.64	28 (59%)	58,81,81	2.43	19 (32%)
7	EDO	C	1007	-	3,3,3	0.49	0	2,2,2	0.41	0
3	SF4	B	404	2	0,12,12	-	-	-	-	-
3	SF4	D	403	2	0,12,12	-	-	-	-	-
6	MD1	A	1004	4	47,51,51	3.16	16 (34%)	56,78,78	1.61	13 (23%)
3	SF4	F	404	2	0,12,12	-	-	-	-	-
3	SF4	D	402	2	0,12,12	-	-	-	-	-
7	EDO	B	406	-	3,3,3	0.72	0	2,2,2	0.32	0
7	EDO	E	1007	-	3,3,3	0.63	0	2,2,2	0.25	0
8	F3S	D	401	2	0,9,9	-	-	-	-	-
3	SF4	B	403	2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	E	1009	-	3,3,3	0.55	0	2,2,2	0.46	0
3	SF4	A	1001	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	C	1005	-	-	1/1/1/1	-
6	MD1	E	1004	4	-	1/22/59/59	0/5/5/5
10	GOL	C	1006	-	-	2/4/4/4	-
7	EDO	A	1010	-	-	0/1/1/1	-
5	MGD	A	1003	4	-	2/22/66/66	0/6/6/6
5	MGD	E	1003	4	-	2/22/66/66	0/6/6/6
3	SF4	B	402	2	-	-	0/6/5/5
7	EDO	A	1007	-	-	1/1/1/1	-
7	EDO	E	1010	-	-	1/1/1/1	-
7	EDO	E	1005	-	-	0/1/1/1	-
7	EDO	E	1008	-	-	1/1/1/1	-
7	EDO	A	1006	-	-	0/1/1/1	-
3	SF4	A	1001	1	-	-	0/6/5/5
3	SF4	E	1001	1	-	-	0/6/5/5
7	EDO	D	405	-	-	0/1/1/1	-
3	SF4	F	402	2	-	-	0/6/5/5
7	EDO	A	1005	-	-	0/1/1/1	-
6	MD1	C	1004	4	-	6/22/59/59	0/5/5/5
8	F3S	F	401	2	-	-	0/3/3/3
7	EDO	B	405	-	-	0/1/1/1	-
7	EDO	A	1008	-	-	1/1/1/1	-
3	SF4	D	404	2	-	-	0/6/5/5
11	PEG	C	1008	-	-	3/4/4/4	-
3	SF4	C	1001	1	-	-	0/6/5/5
7	EDO	A	1009	-	-	0/1/1/1	-
3	SF4	F	403	2	-	-	0/6/5/5
7	EDO	E	1006	-	-	0/1/1/1	-
7	EDO	F	405	-	-	0/1/1/1	-
8	F3S	B	401	2	-	-	0/3/3/3
7	EDO	C	1007	-	-	1/1/1/1	-
5	MGD	C	1003	4	-	2/22/66/66	0/6/6/6
3	SF4	B	404	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	D	403	2	-	-	0/6/5/5
6	MD1	A	1004	4	-	2/22/59/59	0/5/5/5
7	EDO	B	406	-	-	0/1/1/1	-
3	SF4	D	402	2	-	-	0/6/5/5
3	SF4	F	404	2	-	-	0/6/5/5
8	F3S	D	401	2	-	-	0/3/3/3
3	SF4	B	403	2	-	-	0/6/5/5
7	EDO	E	1009	-	-	1/1/1/1	-
7	EDO	E	1007	-	-	1/1/1/1	-

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MGD	C16-C21	13.16	1.61	1.38
5	E	1003	MGD	C16-C21	12.33	1.59	1.38
6	C	1004	MD1	C7-N8	12.30	1.43	1.28
5	C	1003	MGD	C16-C21	12.12	1.59	1.38
6	A	1004	MD1	C7-N8	12.03	1.43	1.28
6	E	1004	MD1	C7-N8	11.04	1.42	1.28
5	C	1003	MGD	C14-N15	10.46	1.58	1.46
5	A	1003	MGD	C14-N15	9.92	1.57	1.46
5	E	1003	MGD	C23-C14	-9.69	1.45	1.53
5	C	1003	MGD	C23-C14	-9.36	1.46	1.53
5	E	1003	MGD	C14-N15	9.26	1.56	1.46
5	A	1003	MGD	C3'-C4'	-9.19	1.29	1.53
5	E	1003	MGD	C3'-C4'	-9.03	1.30	1.53
5	C	1003	MGD	C3'-C4'	-8.99	1.30	1.53
6	C	1004	MD1	O4'-C1'	8.80	1.62	1.42
5	C	1003	MGD	O11-C11	8.15	1.59	1.43
5	E	1003	MGD	O11-C11	8.14	1.59	1.43
5	A	1003	MGD	C23-C14	-7.69	1.47	1.53
6	A	1004	MD1	O4'-C1'	7.61	1.59	1.42
5	C	1003	MGD	C2'-C1'	-7.46	1.30	1.53
5	E	1003	MGD	C2'-C1'	-7.40	1.30	1.53
5	A	1003	MGD	O11-C11	7.38	1.57	1.43
5	A	1003	MGD	C2'-C1'	-6.92	1.31	1.53
6	E	1004	MD1	PB-O3B	6.86	1.66	1.59
6	E	1004	MD1	O4'-C1'	6.52	1.57	1.42
5	E	1003	MGD	C19-N18	6.47	1.53	1.37
5	C	1003	MGD	C23-N22	6.45	1.55	1.45
5	E	1003	MGD	C23-N22	6.39	1.55	1.45
5	A	1003	MGD	C19-N18	6.33	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	C19-N20	6.31	1.48	1.33
6	E	1004	MD1	C20-N8	6.30	1.46	1.36
6	C	1004	MD1	C20-N8	6.27	1.46	1.36
6	A	1004	MD1	C2-N2	6.21	1.48	1.34
5	E	1003	MGD	C4-N3	6.16	1.48	1.34
6	A	1004	MD1	C20-N8	6.07	1.45	1.36
5	C	1003	MGD	O11-C23	-6.03	1.34	1.43
5	E	1003	MGD	PA-O3B	5.89	1.65	1.59
5	E	1003	MGD	C19-N20	5.89	1.47	1.33
5	C	1003	MGD	C4-N3	5.82	1.47	1.34
6	C	1004	MD1	C2'-C1'	-5.76	1.35	1.53
5	C	1003	MGD	PA-O3B	5.62	1.65	1.59
5	C	1003	MGD	C19-N18	5.54	1.51	1.37
6	E	1004	MD1	C2-N2	5.52	1.47	1.34
5	A	1003	MGD	C4-N3	5.51	1.46	1.34
5	E	1003	MGD	PB-O3B	5.49	1.65	1.59
5	A	1003	MGD	O11-C23	-5.47	1.35	1.43
6	A	1004	MD1	C2'-C1'	-5.43	1.36	1.53
5	E	1003	MGD	C2-N3	5.26	1.45	1.33
5	A	1003	MGD	C19-N20	5.23	1.45	1.33
5	A	1003	MGD	C23-N22	5.21	1.53	1.45
6	A	1004	MD1	O4'-C4'	-5.15	1.33	1.45
5	E	1003	MGD	O4'-C4'	5.11	1.56	1.45
5	E	1003	MGD	O11-C23	-5.10	1.36	1.43
6	C	1004	MD1	O4'-C4'	-5.07	1.33	1.45
6	C	1004	MD1	C6-N1	-5.07	1.29	1.38
6	E	1004	MD1	C2'-C1'	-5.05	1.37	1.53
5	A	1003	MGD	O4'-C4'	5.01	1.56	1.45
5	A	1003	MGD	C2-N3	5.00	1.45	1.33
6	C	1004	MD1	C2-N2	5.00	1.45	1.34
5	C	1003	MGD	C2-N3	4.96	1.45	1.33
5	E	1003	MGD	O4'-C1'	4.78	1.53	1.42
5	C	1003	MGD	O4'-C1'	4.73	1.52	1.42
6	E	1004	MD1	C16-N15	4.69	1.48	1.37
5	C	1003	MGD	O4'-C4'	4.68	1.55	1.45
5	E	1003	MGD	C17-N18	4.63	1.47	1.38
5	C	1003	MGD	PB-O3B	4.62	1.64	1.59
5	A	1003	MGD	C21-N20	4.57	1.43	1.36
6	A	1004	MD1	PA-O3B	4.57	1.64	1.59
5	C	1003	MGD	C17-N18	4.50	1.47	1.38
5	A	1003	MGD	O4'-C1'	4.44	1.52	1.42
5	E	1003	MGD	C2-N2	4.36	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MGD	PA-O3B	4.33	1.64	1.59
5	C	1003	MGD	C19-N19	4.28	1.44	1.34
5	A	1003	MGD	C17-N18	4.20	1.46	1.38
6	E	1004	MD1	O4'-C4'	-4.18	1.35	1.45
5	C	1003	MGD	C2'-C3'	4.14	1.64	1.53
5	E	1003	MGD	C19-N19	4.08	1.43	1.34
6	A	1004	MD1	C16-N15	4.07	1.47	1.37
5	A	1003	MGD	C2'-C3'	4.02	1.64	1.53
6	C	1004	MD1	C16-N15	3.99	1.47	1.37
5	E	1003	MGD	C2'-C3'	3.99	1.64	1.53
6	C	1004	MD1	C17-N16	3.95	1.43	1.34
6	A	1004	MD1	C17-N16	3.84	1.43	1.34
5	A	1003	MGD	C2-N2	3.83	1.43	1.34
6	C	1004	MD1	PB-O3B	3.80	1.63	1.59
6	E	1004	MD1	C6-N1	-3.77	1.31	1.38
5	A	1003	MGD	C19-N19	3.63	1.42	1.34
5	C	1003	MGD	C5-N7	-3.54	1.32	1.39
5	C	1003	MGD	C2-N2	3.50	1.42	1.34
5	A	1003	MGD	PB-O3B	3.46	1.63	1.59
6	A	1004	MD1	PB-O3B	3.37	1.63	1.59
5	C	1003	MGD	C21-N20	3.32	1.41	1.36
6	A	1004	MD1	C15-N17	-3.29	1.32	1.38
5	C	1003	MGD	C10-C11	3.25	1.56	1.51
6	E	1004	MD1	C17-N16	3.24	1.41	1.34
5	A	1003	MGD	C5-N7	-3.23	1.32	1.39
6	C	1004	MD1	O3'-C3'	-3.14	1.35	1.43
5	E	1003	MGD	C21-N20	3.01	1.40	1.36
6	C	1004	MD1	C5-N7	-2.97	1.33	1.39
5	E	1003	MGD	C10-C11	2.96	1.56	1.51
6	E	1004	MD1	O3'-C3'	-2.89	1.35	1.43
5	E	1003	MGD	C5-N7	-2.87	1.33	1.39
6	E	1004	MD1	C5-N7	-2.87	1.33	1.39
5	E	1003	MGD	C2-N1	2.86	1.44	1.37
6	A	1004	MD1	C6-N1	-2.84	1.33	1.38
5	C	1003	MGD	C21-N22	2.78	1.38	1.35
5	A	1003	MGD	C10-C11	2.76	1.55	1.51
6	C	1004	MD1	C16-C20	-2.74	1.32	1.39
6	E	1004	MD1	C4-N9	-2.68	1.31	1.38
5	C	1003	MGD	O17-C17	-2.65	1.18	1.23
6	A	1004	MD1	C16-C20	-2.55	1.33	1.39
6	E	1004	MD1	C16-C20	-2.55	1.33	1.39
5	A	1003	MGD	C2-N1	2.50	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1004	MD1	C15-N17	-2.48	1.34	1.38
6	C	1004	MD1	PA-O3B	2.44	1.62	1.59
6	A	1004	MD1	C5-N7	-2.39	1.34	1.39
5	A	1003	MGD	O17-C17	-2.37	1.19	1.23
6	A	1004	MD1	C4-N9	-2.36	1.32	1.38
5	C	1003	MGD	C2-N1	2.35	1.43	1.37
5	E	1003	MGD	O6-C6	-2.34	1.19	1.23
6	C	1004	MD1	C4-N9	-2.33	1.32	1.38
5	C	1003	MGD	C4-N9	-2.33	1.32	1.38
5	E	1003	MGD	C4-N9	-2.29	1.32	1.38
5	A	1003	MGD	C6-N1	2.26	1.43	1.38
6	E	1004	MD1	PA-O3B	2.24	1.61	1.59
6	C	1004	MD1	O14-C15	-2.23	1.19	1.23
6	E	1004	MD1	O14-C15	-2.21	1.19	1.23
6	E	1004	MD1	PB-O3A	2.14	1.67	1.59
5	E	1003	MGD	C5-C6	2.13	1.52	1.44
5	A	1003	MGD	C21-N22	2.12	1.37	1.35
6	A	1004	MD1	O3'-C3'	-2.08	1.37	1.43
5	C	1003	MGD	O6-C6	-2.05	1.19	1.23
5	A	1003	MGD	C16-C17	2.01	1.47	1.41

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	MGD	O11-C23-N22	-12.22	97.52	108.61
5	C	1003	MGD	O11-C23-N22	-11.76	97.93	108.61
5	E	1003	MGD	O11-C23-N22	-10.08	99.46	108.61
6	C	1004	MD1	C5-C4-N3	-5.15	120.20	128.39
5	C	1003	MGD	C23-C14-N15	5.13	112.91	107.87
5	E	1003	MGD	C23-C14-N15	4.85	112.63	107.87
6	E	1004	MD1	C5-C4-N3	-4.85	120.68	128.39
5	A	1003	MGD	C23-C14-N15	4.79	112.58	107.87
6	A	1004	MD1	C5-C4-N3	-4.76	120.81	128.39
5	C	1003	MGD	C4'-O4'-C1'	-4.51	99.51	109.47
5	C	1003	MGD	C5-C4-N3	-4.40	121.39	128.39
6	A	1004	MD1	C2-N3-C4	4.32	119.75	112.30
5	A	1003	MGD	C5-C4-N3	-4.15	121.78	128.39
5	E	1003	MGD	C5-C4-N3	-4.13	121.81	128.39
5	C	1003	MGD	C19-N20-C21	4.08	120.55	113.36
5	E	1003	MGD	C4'-O4'-C1'	-3.82	101.04	109.47
6	E	1004	MD1	C17-N17-C15	-3.78	118.26	125.11
5	E	1003	MGD	C19-N20-C21	3.75	119.98	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1004	MD1	C2-N3-C4	3.35	118.07	112.30
5	E	1003	MGD	N9-C8-N7	-3.20	107.46	113.40
6	C	1004	MD1	N9-C8-N7	-3.15	107.56	113.40
6	E	1004	MD1	O14-C15-C16	-3.14	119.70	127.26
6	C	1004	MD1	C17-N17-C15	-3.13	119.43	125.11
5	A	1003	MGD	C2-N3-C4	3.07	117.59	112.30
5	A	1003	MGD	C19-N20-C21	2.98	118.62	113.36
6	C	1004	MD1	O14-C15-C16	-2.96	120.11	127.26
5	E	1003	MGD	C2-N3-C4	2.91	117.31	112.30
5	C	1003	MGD	C2-N3-C4	2.90	117.30	112.30
5	C	1003	MGD	N9-C8-N7	-2.82	108.18	113.40
5	A	1003	MGD	C4'-O4'-C1'	-2.81	103.27	109.47
5	C	1003	MGD	C2-N1-C6	-2.80	120.03	125.11
6	A	1004	MD1	N9-C8-N7	-2.80	108.20	113.40
6	C	1004	MD1	N9-C4-N3	2.77	131.50	125.95
6	E	1004	MD1	C2-N3-C4	2.73	117.01	112.30
5	E	1003	MGD	N9-C4-N3	2.72	131.40	125.95
6	C	1004	MD1	C2-N1-C6	-2.72	120.18	125.11
6	A	1004	MD1	C4-C5-N7	-2.70	106.40	110.67
5	A	1003	MGD	O6-C6-C5	-2.68	119.46	126.53
6	C	1004	MD1	C17-N18-C20	2.67	117.89	114.20
5	E	1003	MGD	O11-C23-C14	-2.64	107.20	108.96
6	A	1004	MD1	C8-N7-C5	2.64	108.96	104.26
5	C	1003	MGD	N9-C4-N3	2.59	131.14	125.95
5	C	1003	MGD	C16-C17-N18	2.58	119.22	112.13
5	E	1003	MGD	C16-C17-N18	2.55	119.13	112.13
6	E	1004	MD1	C2-N1-C6	-2.53	120.53	125.11
6	A	1004	MD1	C17-N18-C20	2.51	117.68	114.20
6	E	1004	MD1	C17-N18-C20	2.51	117.67	114.20
5	C	1003	MGD	O4'-C1'-N9	2.47	113.96	108.36
6	A	1004	MD1	O14-C15-C16	-2.46	121.32	127.26
6	E	1004	MD1	N16-C17-N18	-2.44	114.90	119.67
6	C	1004	MD1	C8-N7-C5	2.40	108.54	104.26
6	E	1004	MD1	N9-C4-N3	2.37	130.69	125.95
5	E	1003	MGD	N19-C19-N18	2.37	121.76	116.76
5	E	1003	MGD	C2-N1-C6	-2.35	120.84	125.11
5	C	1003	MGD	O17-C17-C16	-2.35	121.59	127.26
5	A	1003	MGD	C2-N1-C6	-2.35	120.85	125.11
5	A	1003	MGD	N9-C8-N7	-2.35	109.05	113.40
6	A	1004	MD1	C2-N1-C6	-2.31	120.91	125.11
6	E	1004	MD1	C16-C15-N17	2.29	118.42	112.13
5	A	1003	MGD	O4'-C1'-C2'	-2.25	101.79	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1003	MGD	O4'-C1'-N9	2.23	113.42	108.36
5	A	1003	MGD	C16-C17-N18	2.22	118.22	112.13
6	E	1004	MD1	N16-C17-N17	2.21	121.43	116.76
6	A	1004	MD1	C4'-O4'-C1'	-2.21	104.58	109.47
6	E	1004	MD1	N9-C8-N7	-2.21	109.30	113.40
5	E	1003	MGD	O17-C17-C16	-2.21	121.94	127.26
5	C	1003	MGD	O6-C6-C5	-2.20	120.71	126.53
6	C	1004	MD1	C5-C6-N1	2.19	118.83	113.25
6	A	1004	MD1	N9-C4-N3	2.17	130.29	125.95
5	C	1003	MGD	O4'-C4'-C3'	2.15	109.43	105.15
6	A	1004	MD1	O1A-PA-O3B	-2.15	101.45	107.27
5	A	1003	MGD	N9-C4-N3	2.14	130.23	125.95
5	E	1003	MGD	O2A-PA-O3B	-2.13	101.51	107.27
6	E	1004	MD1	O4'-C4'-C3'	2.12	109.36	105.15
6	C	1004	MD1	C16-C15-N17	2.11	117.94	112.13
5	C	1003	MGD	O4'-C1'-C2'	-2.11	102.10	106.62
5	E	1003	MGD	O4'-C4'-C3'	2.10	109.33	105.15
5	E	1003	MGD	C8-N7-C5	2.10	108.01	104.26
5	E	1003	MGD	N18-C19-N20	-2.06	119.56	123.32
6	A	1004	MD1	N2-C2-N1	2.04	121.07	116.76
5	E	1003	MGD	C1'-N9-C4	-2.03	120.48	126.49
5	C	1003	MGD	O4'-C4'-C5'	-2.02	102.85	109.33
5	C	1003	MGD	C8-N7-C5	2.02	107.86	104.26
5	A	1003	MGD	O3'-C3'-C2'	-2.02	105.35	111.82
5	A	1003	MGD	C1'-N9-C4	-2.01	120.56	126.49
5	C	1003	MGD	N18-C19-N20	-2.01	119.65	123.32
6	A	1004	MD1	O4'-C4'-C3'	2.01	109.13	105.15
5	C	1003	MGD	C19-N18-C17	-2.00	121.48	125.11

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1004	MD1	C10-O3A-PB-O1B
10	C	1006	GOL	C1-C2-C3-O3
11	C	1008	PEG	O2-C3-C4-O4
7	E	1008	EDO	O1-C1-C2-O2
11	C	1008	PEG	O1-C1-C2-O2
7	E	1010	EDO	O1-C1-C2-O2
10	C	1006	GOL	O2-C2-C3-O3
5	A	1003	MGD	O3A-C10-C11-O11
6	C	1004	MD1	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	C	1004	MD1	O4'-C4'-C5'-O5'
11	C	1008	PEG	C4-C3-O2-C2
6	C	1004	MD1	C10-O3A-PB-O2B
5	A	1003	MGD	C2'-C1'-N9-C8
6	A	1004	MD1	O4'-C4'-C5'-O5'
6	C	1004	MD1	PB-O3B-PA-O5'
7	A	1007	EDO	O1-C1-C2-O2
7	A	1008	EDO	O1-C1-C2-O2
7	C	1007	EDO	O1-C1-C2-O2
7	E	1007	EDO	O1-C1-C2-O2
7	E	1009	EDO	O1-C1-C2-O2
6	E	1004	MD1	PA-O3B-PB-O1B
5	E	1003	MGD	C2'-C1'-N9-C8
7	C	1005	EDO	O1-C1-C2-O2
5	C	1003	MGD	C11-C10-O3A-PA
5	C	1003	MGD	PA-O3B-PB-O2B
5	E	1003	MGD	PA-O3B-PB-O2B
6	A	1004	MD1	PA-O3B-PB-O1B
6	C	1004	MD1	PA-O3B-PB-O1B

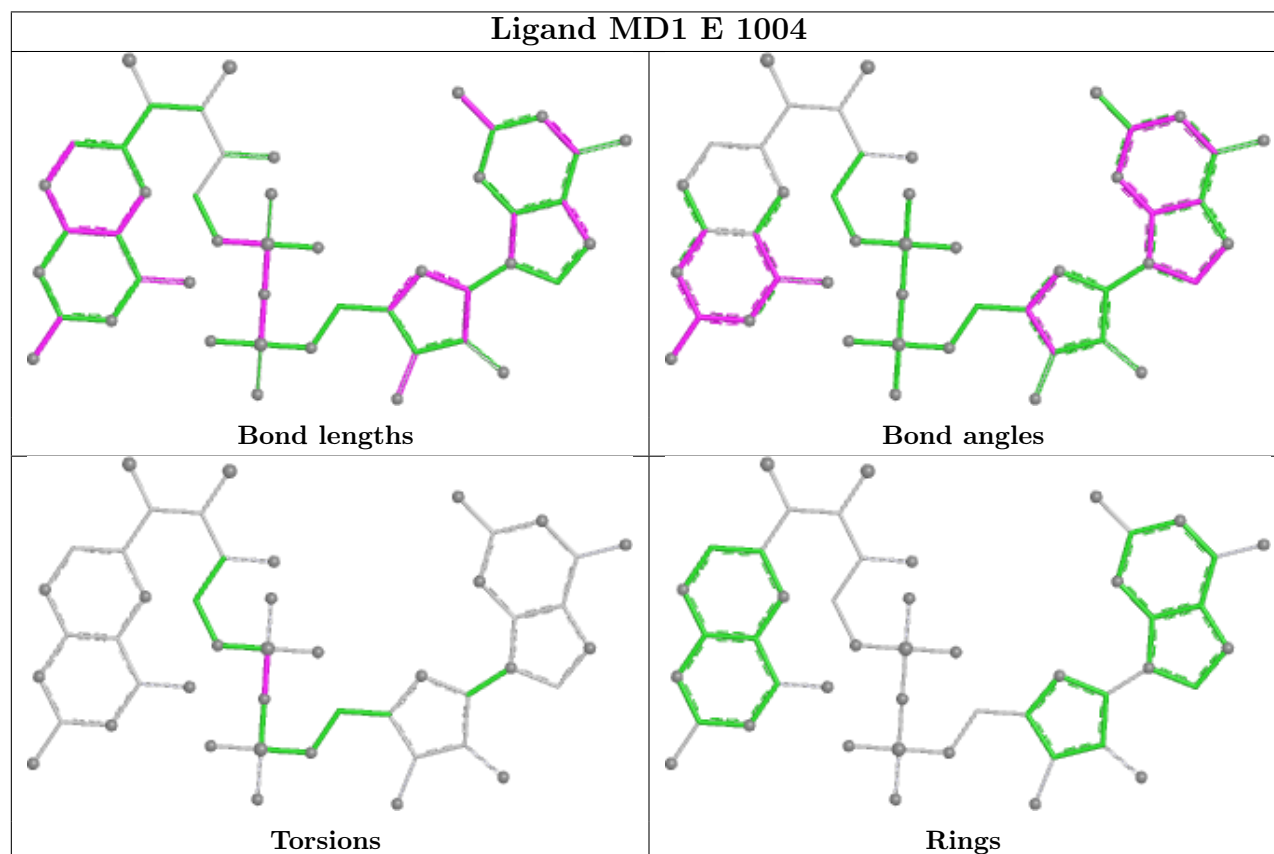
There are no ring outliers.

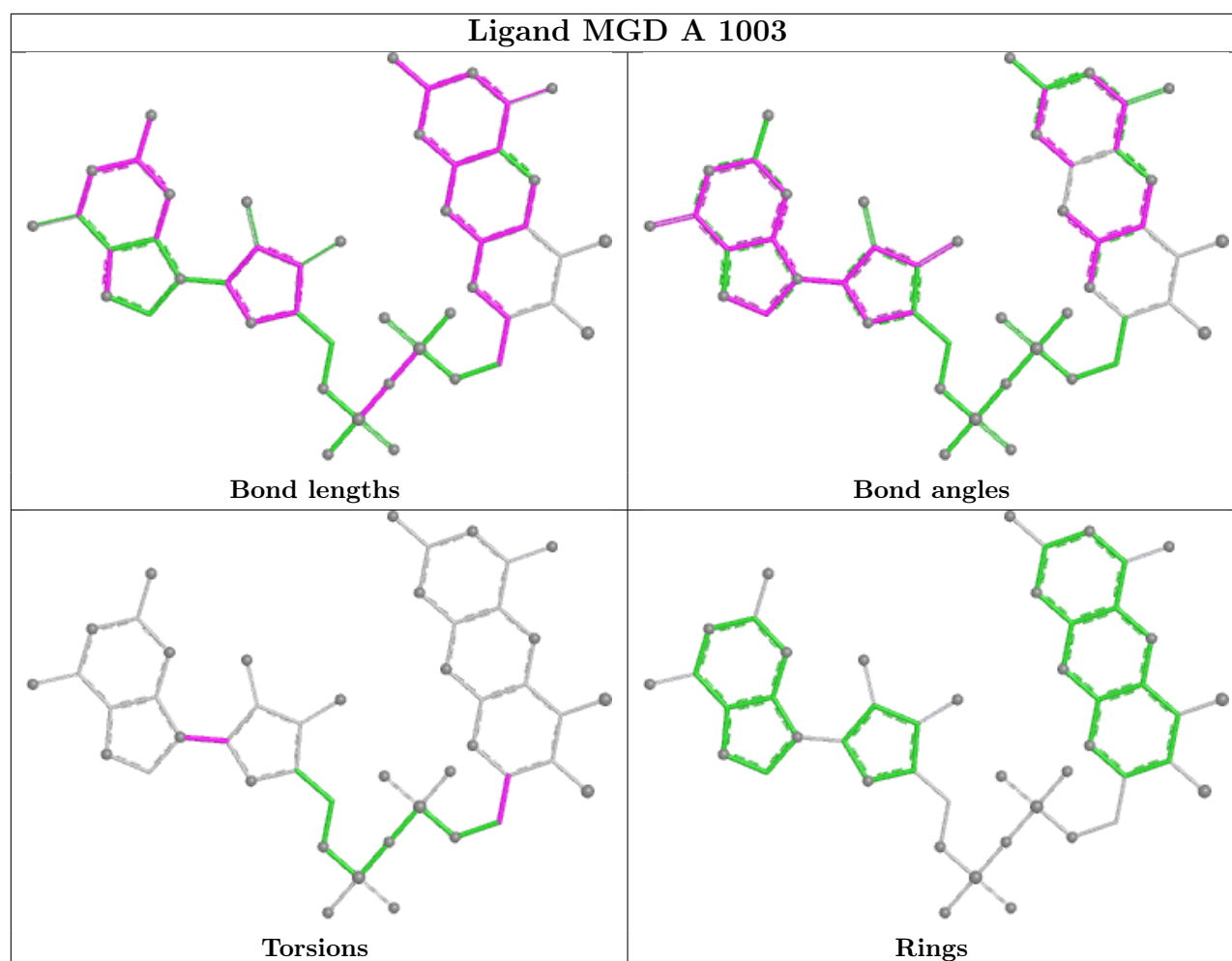
9 monomers are involved in 19 short contacts:

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

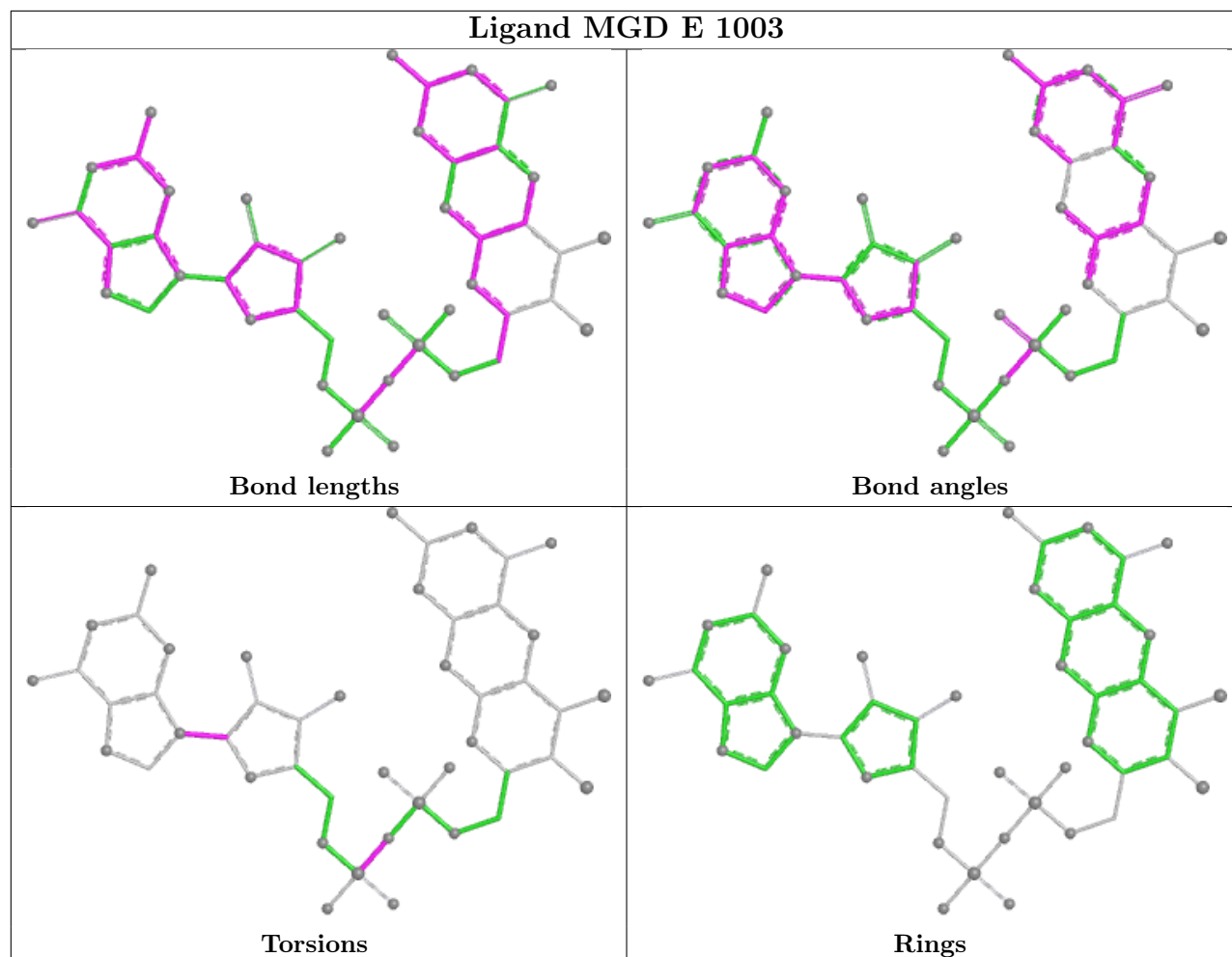
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

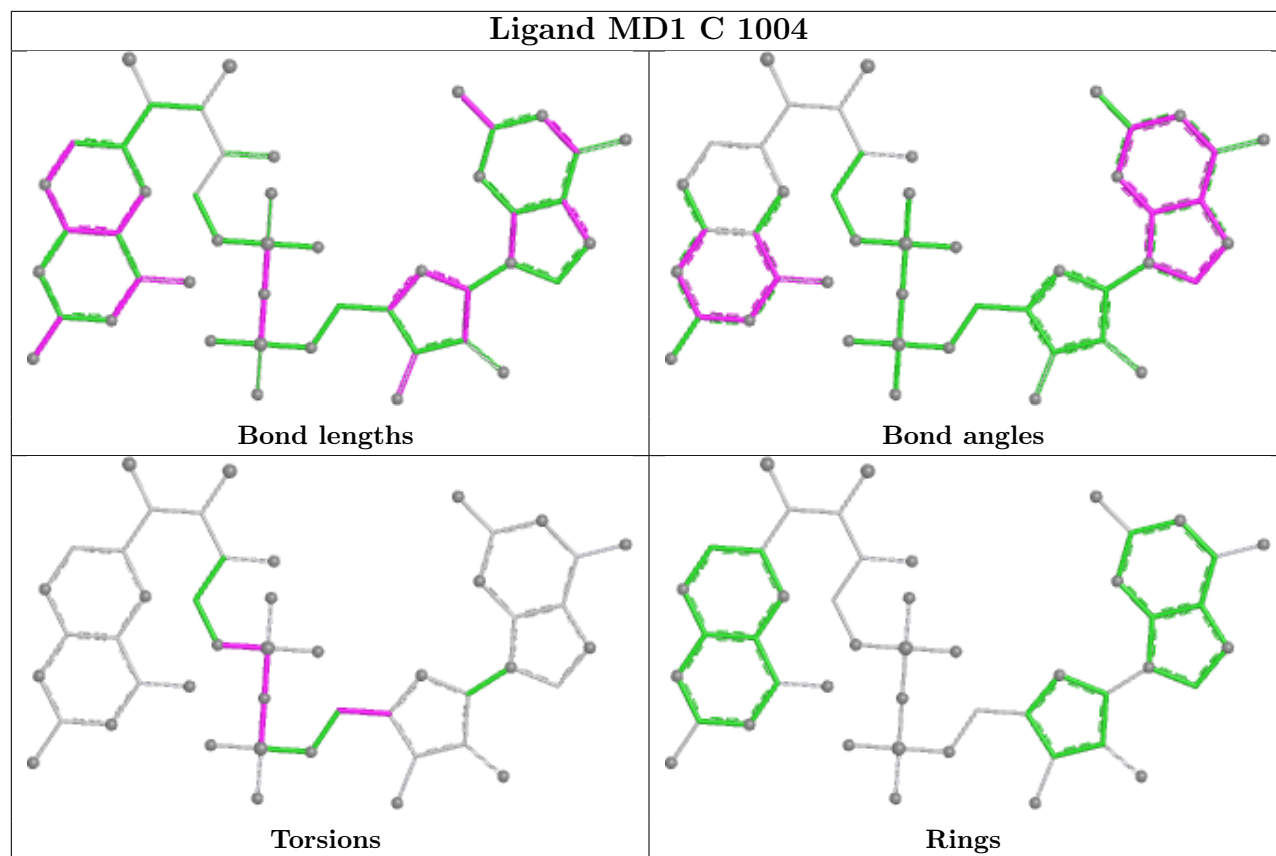
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



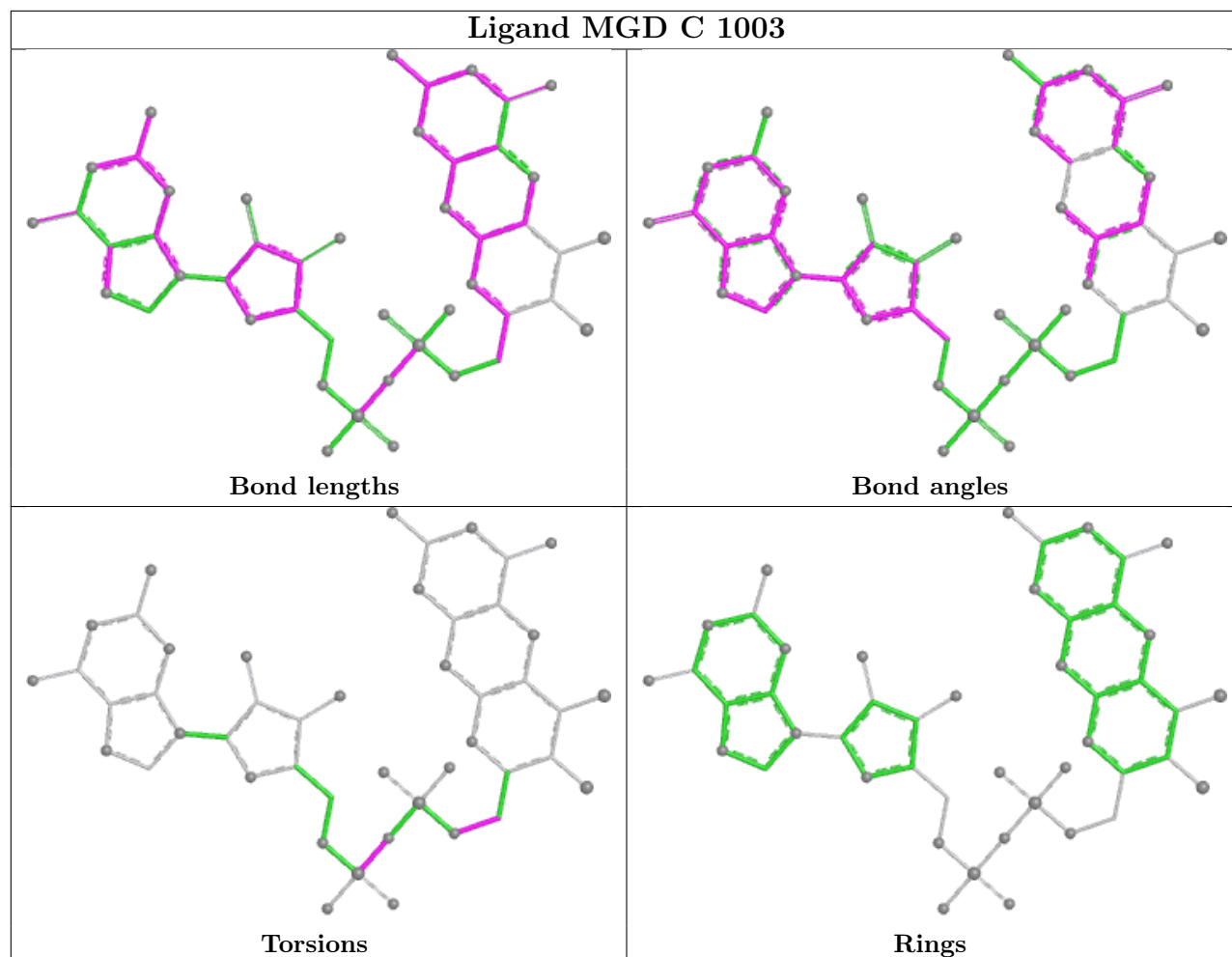


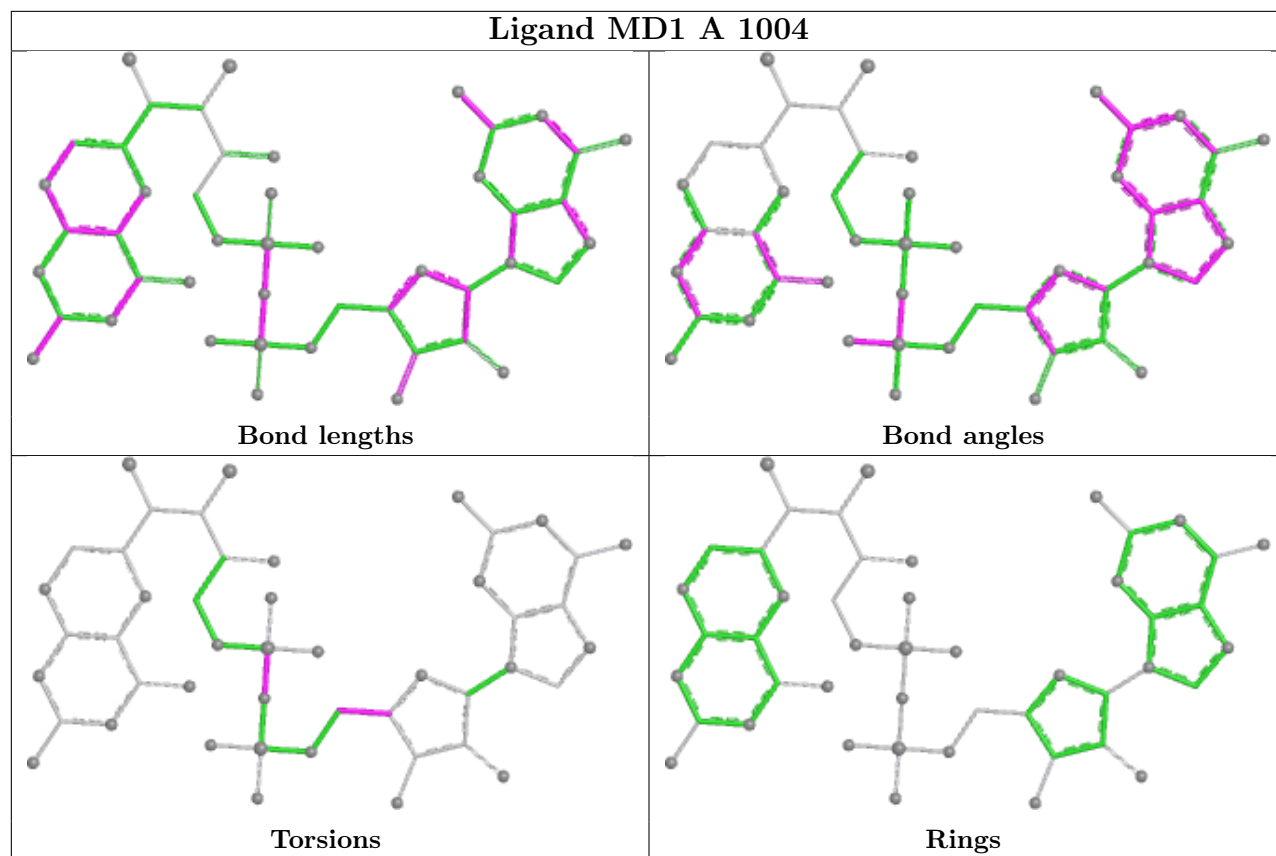
Ligand MGD E 1003





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	895/899 (99%)	0.02	13 (1%)	72 76	11, 26, 46, 73	3 (0%)
1	C	892/899 (99%)	0.48	50 (5%)	30 33	16, 33, 56, 92	0
1	E	892/899 (99%)	0.37	85 (9%)	14 14	14, 27, 60, 84	2 (0%)
2	B	329/333 (98%)	-0.24	2 (0%)	85 88	15, 22, 36, 63	0
2	D	328/333 (98%)	1.69	130 (39%)	1 0	23, 50, 68, 94	0
2	F	328/333 (98%)	0.27	3 (0%)	81 84	15, 29, 47, 67	1 (0%)
All	All	3664/3696 (99%)	0.37	283 (7%)	19 20	11, 29, 58, 94	6 (0%)

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	282	VAL	6.7
1	A	5	ILE	6.0
1	E	11[A]	TYR	5.9
1	E	360	PHE	5.6
2	D	145	CYS	5.3
1	E	370	VAL	5.3
1	E	364	LEU	5.3
2	D	154	ILE	5.1
1	C	8	ALA	5.0
1	C	9	PHE	5.0
2	D	146	LEU	4.9
1	E	366	ASP	4.9
1	E	365	LEU	4.8
1	E	314	PRO	4.8
2	D	7	ALA	4.6
1	E	296	VAL	4.5
2	D	73	LEU	4.5
1	E	369	THR	4.5
2	D	250	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	899	PHE	4.3
2	D	144	ALA	4.3
1	C	14	TRP	4.0
1	E	293	ALA	3.9
1	C	22	TRP	3.9
1	E	312	GLY	3.9
2	D	225	PHE	3.9
1	E	372	VAL	3.9
2	D	177	VAL	3.9
1	C	12	SER	3.8
2	D	175	ALA	3.8
2	D	6	LYS	3.8
1	E	367	GLY	3.8
1	E	355	ALA	3.7
2	D	226	VAL	3.7
1	C	17	PHE	3.7
1	E	313	LYS	3.7
1	C	11	TYR	3.6
1	E	311	THR	3.6
2	D	170	CYS	3.6
2	D	176	CYS	3.6
2	D	150	PRO	3.5
2	D	165	ILE	3.5
1	E	304	PHE	3.5
2	B	5	MET	3.5
1	E	295	VAL	3.5
1	E	297	ALA	3.4
1	E	307	TRP	3.4
1	E	285	ASP	3.4
1	C	309	ALA	3.4
1	E	315	VAL	3.4
2	D	173	ALA	3.4
1	E	286	THR	3.4
2	D	140	CYS	3.3
2	D	155	TYR	3.3
2	D	153	ALA	3.3
1	E	305	TYR	3.3
2	D	163	VAL	3.3
1	E	310	LYS	3.3
1	C	351	ASP	3.3
1	C	297	ALA	3.3
2	D	164	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	10	ARG	3.2
2	D	68	TYR	3.2
1	E	309	ALA	3.2
1	E	290	LEU	3.2
1	E	404	THR	3.2
2	D	208	VAL	3.2
1	C	360	PHE	3.2
2	D	37	THR	3.1
2	D	78	ILE	3.1
2	D	158	GLU	3.1
2	D	149	CYS	3.1
2	D	299	ILE	3.1
1	E	306	PHE	3.1
2	D	224	GLY	3.1
1	E	368	LYS	3.0
2	D	223	VAL	3.0
2	D	138	ASN	3.0
2	D	234	TYR	3.0
2	D	189	PRO	3.0
2	D	151	ASN	3.0
1	A	364	LEU	3.0
2	D	233	VAL	3.0
1	E	379	LEU	2.9
1	C	370	VAL	2.9
1	E	731	TYR	2.9
2	D	8	PRO	2.9
2	D	187	PHE	2.9
2	D	12	LEU	2.9
2	D	124	GLU	2.9
2	D	199	GLY	2.9
1	A	7	GLY	2.9
2	D	251	GLY	2.9
2	D	256	VAL	2.9
2	D	182	TYR	2.9
1	E	378	ILE	2.9
2	D	204	ILE	2.9
2	D	143	PRO	2.8
2	D	35	TRP	2.8
1	E	262	ILE	2.8
1	E	358	GLY	2.8
2	D	76	GLY	2.8
2	D	63	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	362	MET	2.8
2	D	237	ILE	2.8
1	A	327	LYS	2.8
2	D	156	LYS	2.8
2	D	252	THR	2.8
1	A	6	SER	2.8
1	E	289	PHE	2.8
2	D	61	TRP	2.8
2	D	318	VAL	2.8
2	D	240	TYR	2.7
2	D	159	GLN	2.7
1	C	313	LYS	2.7
2	D	38	GLY	2.7
1	C	66	ILE	2.7
1	E	354	PRO	2.7
2	D	296	VAL	2.7
1	C	307	TRP	2.7
1	E	267	TYR	2.7
1	C	49	GLY	2.7
1	E	383	LEU	2.7
1	C	359	LYS	2.7
2	D	139	HIS	2.7
2	D	148	ALA	2.7
2	D	283	ALA	2.7
2	D	137	CYS	2.7
1	E	281	LEU	2.7
1	E	317	PRO	2.7
1	E	298	GLY	2.6
2	D	67	GLY	2.6
2	D	257	PHE	2.6
2	D	248	PRO	2.6
2	D	162	ILE	2.6
1	E	299	GLY	2.6
1	E	407	ALA	2.6
2	D	66	GLY	2.6
1	E	8	ALA	2.6
1	E	375	VAL	2.6
2	D	230	ASN	2.6
1	A	899	PHE	2.6
1	C	306	PHE	2.6
2	D	9	ARG	2.6
2	D	282	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	62	GLN	2.6
1	A	8	ALA	2.6
1	E	385	ALA	2.6
1	C	45	TYR	2.5
1	C	10	GLU	2.5
2	D	190	LEU	2.5
2	D	71	GLY	2.5
2	D	198	ILE	2.5
2	D	241	LYS	2.5
1	E	308	ASN	2.5
1	A	369	THR	2.5
1	E	363	GLN	2.5
1	E	359	LYS	2.5
2	F	6	LYS	2.5
1	E	258	ALA	2.5
2	D	65	GLY	2.5
1	C	16	ASN	2.5
2	D	229	VAL	2.5
1	C	354	PRO	2.5
1	A	299	GLY	2.4
1	E	352	LEU	2.4
1	E	316	ILE	2.4
2	D	171	LYS	2.4
1	A	296	VAL	2.4
2	D	180	CYS	2.4
2	D	197	CYS	2.4
1	E	353	ASP	2.4
2	D	157	ARG	2.4
1	E	260	VAL	2.4
2	D	166	HIS	2.4
2	D	207	GLY	2.4
2	D	179	SER	2.4
1	E	280	TYR	2.4
2	D	168	ASP	2.4
1	E	288	ARG	2.4
1	C	24	TRP	2.4
1	C	327	LYS	2.4
2	B	6	LYS	2.4
2	D	196	LYS	2.4
2	F	291	LYS	2.4
1	C	352	LEU	2.3
1	C	356	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	291	ARG	2.3
1	E	730	PHE	2.3
1	E	441	THR	2.3
1	E	270	HIS	2.3
1	C	13	GLY	2.3
2	D	69	LYS	2.3
1	E	294	ASP	2.3
2	D	236	LEU	2.3
2	D	244	LEU	2.3
2	D	36	THR	2.3
1	E	342	PHE	2.3
2	D	183	ALA	2.3
2	D	249	GLU	2.3
1	E	356	LEU	2.3
1	C	355	ALA	2.3
1	C	19	ARG	2.3
2	D	161	GLY	2.3
2	D	292	GLN	2.3
1	E	349	LEU	2.3
1	E	725	THR	2.3
1	E	374	PRO	2.2
1	E	261	ILE	2.2
1	C	296	VAL	2.2
1	C	384	MET	2.2
1	E	373	ARG	2.2
1	C	298	GLY	2.2
1	E	284	SER	2.2
1	E	325	PRO	2.2
2	D	181	PRO	2.2
2	D	201	PHE	2.2
1	C	195	LYS	2.2
1	E	361	ASN	2.2
2	D	238	LYS	2.2
2	D	242	VAL	2.2
1	E	371	GLU	2.2
1	E	412	THR	2.2
1	E	732	LEU	2.2
2	D	258	TYR	2.2
1	C	599	ILE	2.2
2	D	81	MET	2.2
2	D	142	LYS	2.2
2	D	247	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	353	ASP	2.2
1	C	312	GLY	2.2
1	E	272	LEU	2.2
2	D	288	LEU	2.2
1	C	314	PRO	2.2
2	D	312	ALA	2.2
2	D	169	LYS	2.2
1	C	18	HIS	2.1
1	E	384	MET	2.1
2	D	329	ILE	2.1
1	C	295	VAL	2.1
2	D	13	THR	2.1
2	D	259	VAL	2.1
1	A	350	GLY	2.1
1	C	365	LEU	2.1
2	D	194	ALA	2.1
2	D	209	ALA	2.1
2	D	270	ALA	2.1
2	D	314	ASP	2.1
1	C	46	SER	2.1
1	E	271	SER	2.1
2	D	287	GLY	2.1
1	C	383	LEU	2.1
2	D	34	LEU	2.1
2	D	79	PRO	2.1
1	C	385	ALA	2.1
1	C	261	ILE	2.1
1	C	262	ILE	2.1
1	E	351	ASP	2.1
2	D	191	THR	2.1
2	D	195	ASN	2.1
2	D	74	GLN	2.1
2	D	167	GLN	2.1
1	E	406	LEU	2.1
2	D	200	CYS	2.1
2	D	246	LEU	2.1
1	C	366	ASP	2.1
2	D	228	ASP	2.1
2	D	141	THR	2.0
1	C	260	VAL	2.0
2	D	202	PRO	2.0
1	E	443	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	326	GLU	2.0
2	D	152	GLU	2.0
1	A	368	LYS	2.0
1	C	797	LYS	2.0
1	E	300	SER	2.0
1	E	376	PHE	2.0
2	D	16	THR	2.0
2	D	172	GLY	2.0
1	C	280	TYR	2.0
2	D	186	TYR	2.0
2	D	281	PRO	2.0
2	F	293	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	GOL	C	1006	6/6	0.69	0.18	37,47,56,57	0
7	EDO	E	1006	4/4	0.72	0.20	25,30,34,36	0
7	EDO	E	1007	4/4	0.74	0.18	25,30,35,35	0
7	EDO	C	1005	4/4	0.80	0.15	27,33,38,42	0
7	EDO	B	406	4/4	0.80	0.17	32,39,40,42	0
7	EDO	E	1008	4/4	0.81	0.15	26,31,35,41	0
7	EDO	E	1009	4/4	0.82	0.18	30,36,40,42	0
11	PEG	C	1008	7/7	0.82	0.15	32,39,42,42	0
7	EDO	A	1010	4/4	0.83	0.20	21,27,30,33	0
7	EDO	A	1008	4/4	0.84	0.14	30,36,41,42	0
7	EDO	E	1010	4/4	0.84	0.14	34,41,43,45	0

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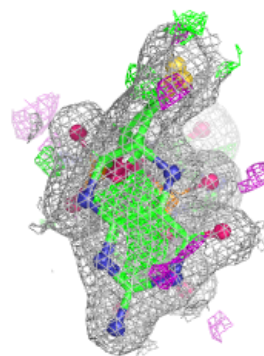
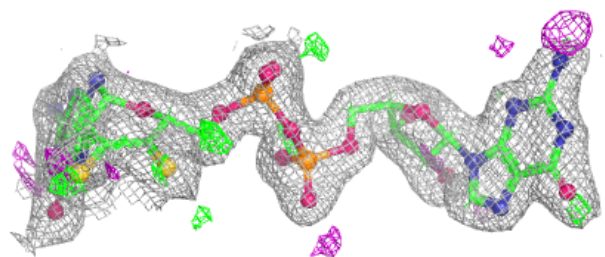
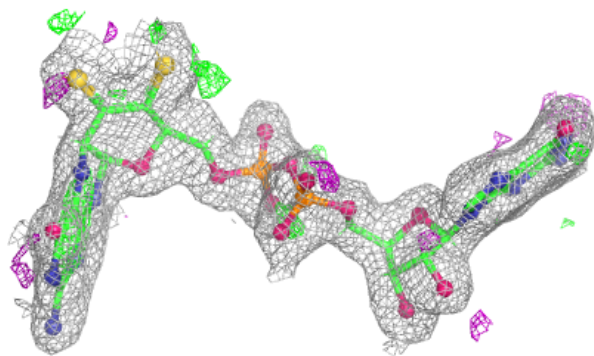
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	1009	4/4	0.86	0.13	29,35,41,50	0
9	NA	B	407	1/1	0.87	0.11	35,35,35,35	0
7	EDO	E	1005	4/4	0.90	0.11	16,20,23,23	0
3	SF4	D	404	8/8	0.91	0.09	29,38,39,42	0
7	EDO	C	1007	4/4	0.92	0.09	17,22,26,27	0
7	EDO	A	1007	4/4	0.92	0.09	22,27,28,33	0
3	SF4	D	402	8/8	0.93	0.08	32,42,49,51	0
7	EDO	A	1005	4/4	0.94	0.09	18,25,32,32	0
7	EDO	D	405	4/4	0.94	0.07	26,31,35,35	0
8	F3S	D	401	7/7	0.94	0.08	45,47,55,57	0
5	MGD	E	1003	47/47	0.95	0.08	15,21,29,31	0
3	SF4	F	402	8/8	0.95	0.06	19,22,23,25	0
7	EDO	A	1006	4/4	0.95	0.10	24,29,32,32	0
7	EDO	B	405	4/4	0.96	0.06	16,19,19,20	0
5	MGD	C	1003	47/47	0.96	0.07	20,22,27,30	0
3	SF4	F	404	8/8	0.96	0.06	17,18,20,23	0
5	MGD	A	1003	47/47	0.97	0.06	13,16,19,23	0
7	EDO	F	405	4/4	0.97	0.05	16,19,21,21	0
6	MD1	A	1004	47/47	0.97	0.05	15,17,22,23	0
8	F3S	F	401	7/7	0.97	0.04	21,22,23,24	0
6	MD1	C	1004	47/47	0.97	0.06	17,20,24,26	0
6	MD1	E	1004	47/47	0.97	0.05	12,16,21,23	0
3	SF4	D	403	8/8	0.97	0.06	30,35,39,40	0
3	SF4	B	403	8/8	0.98	0.04	12,14,15,17	0
3	SF4	C	1001	8/8	0.98	0.05	24,25,27,27	0
3	SF4	E	1001	8/8	0.98	0.04	13,15,15,15	0
3	SF4	B	402	8/8	0.98	0.04	15,16,19,20	0
3	SF4	F	403	8/8	0.98	0.05	18,21,24,25	0
8	F3S	B	401	7/7	0.99	0.03	19,20,22,22	0
4	MO	E	1002	1/1	0.99	0.02	21,21,21,21	0
3	SF4	A	1001	8/8	0.99	0.04	13,14,17,19	0
3	SF4	B	404	8/8	0.99	0.03	12,13,14,15	0
4	MO	A	1002	1/1	0.99	0.03	20,20,20,20	0
4	MO	C	1002	1/1	0.99	0.02	24,24,24,24	0

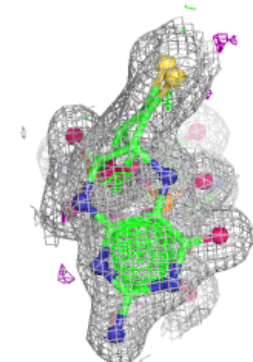
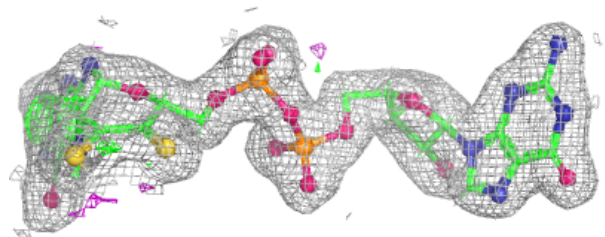
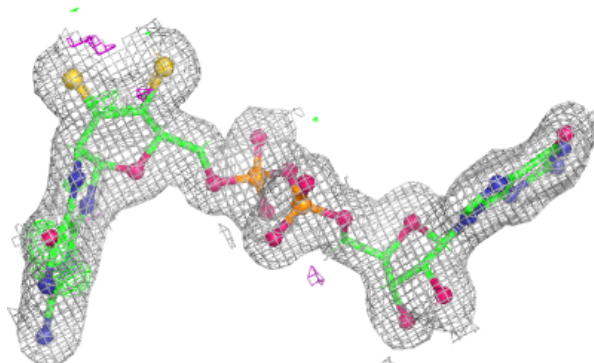
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGD E 1003:

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

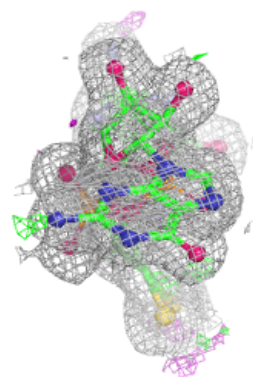
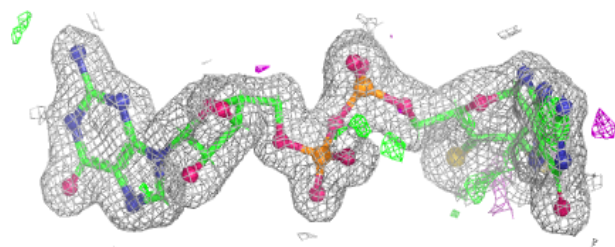
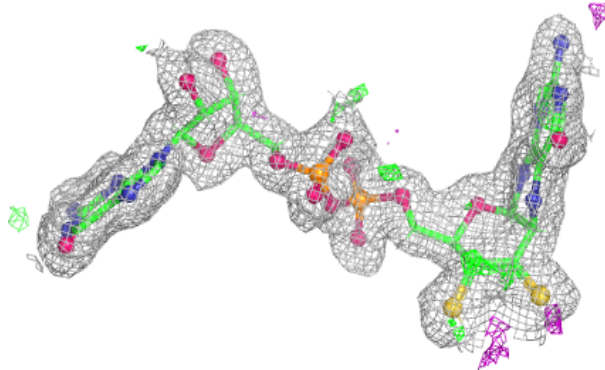
**Electron density around MGD C 1003:**

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

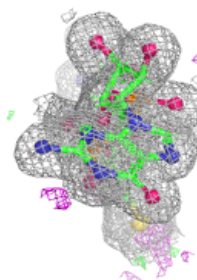
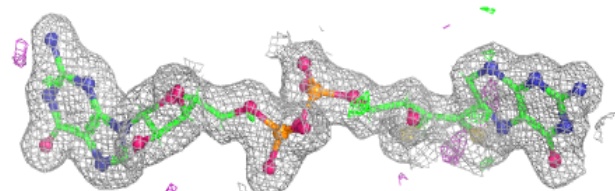
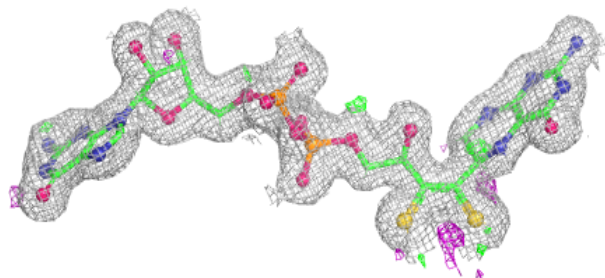


Electron density around MGD A 1003:

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

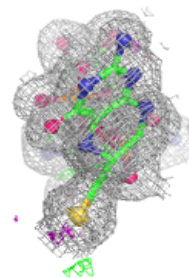
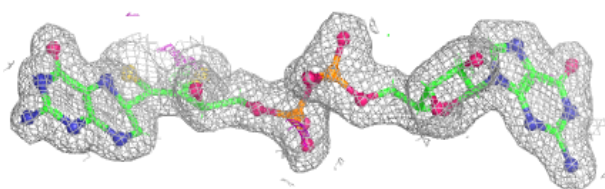
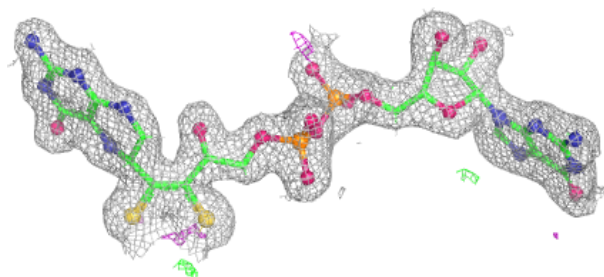
**Electron density around MD1 A 1004:**

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

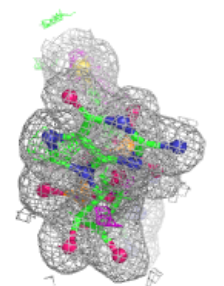
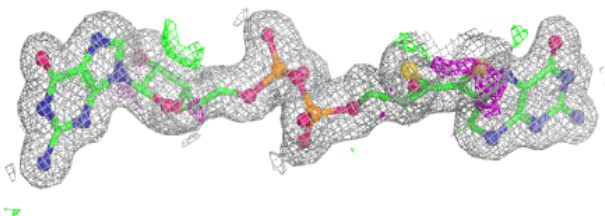
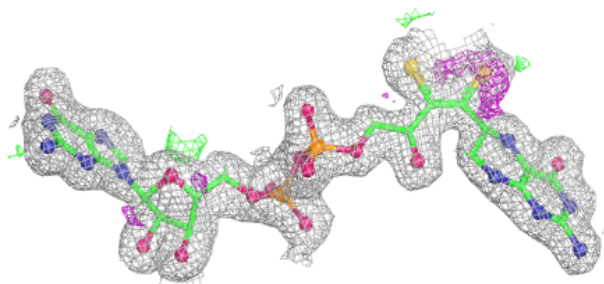


Electron density around MD1 C 1004:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.