



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 05:05 am BST

PDB ID : 3AMZ
Title : Bovine Xanthine Oxidoreductase urate bound form
Authors : Okamoto, K.; Eger, B.T.; Pai, E.F.; Nishino, T.
Deposited on : 2010-08-27
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

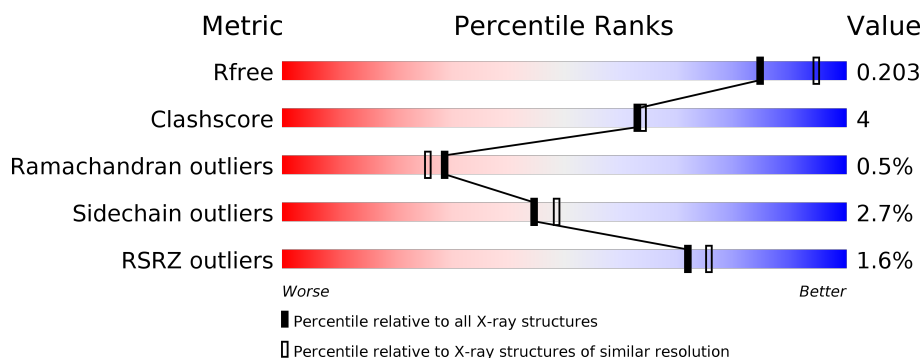
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	1332	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	1332	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	URC	A	1339	-	X	-	-
10	URC	B	1338	-	X	-	-
9	MOS	A	1338	-	-	X	-

2 Entry composition [i](#)

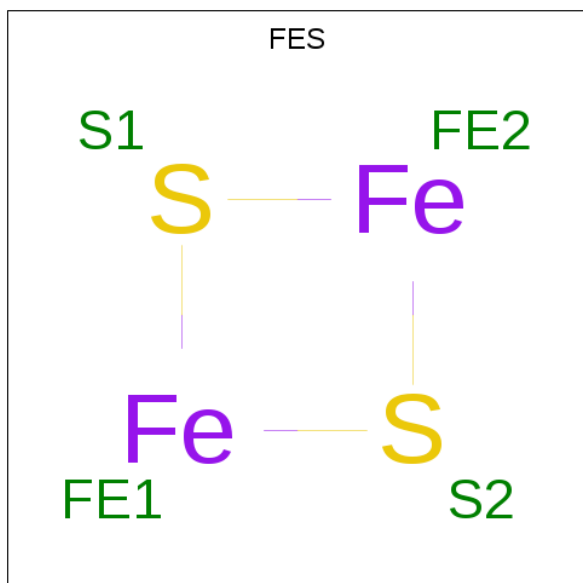
There are 11 unique types of molecules in this entry. The entry contains 22382 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1291	Total	C	N	O	S	0	0	0
			10024	6374	1718	1872	60			
1	B	1289	Total	C	N	O	S	0	0	0
			10013	6368	1716	1869	60			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



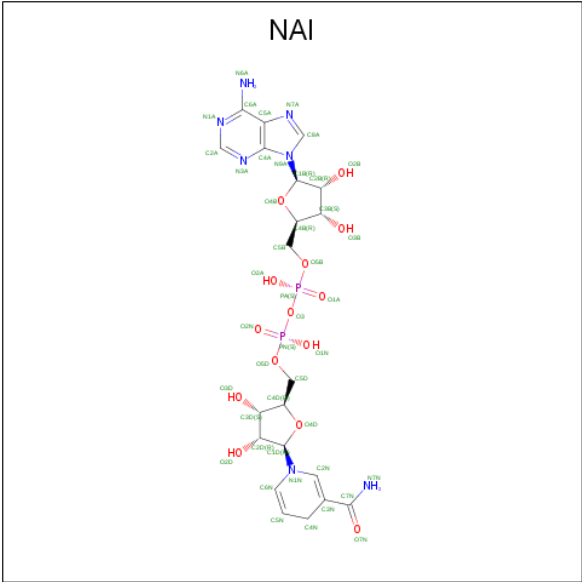
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | B | 1 | Total Ca
1 1 | 0 | 0 |
| 3 | A | 1 | Total Ca
1 1 | 0 | 0 |

- # FAD
-
- The image displays the chemical structure of Flavin Adenine Dinucleotide (FAD), a crucial coenzyme. It is composed of two nucleotides joined by a pyrophosphate bridge. The first nucleotide consists of an adenine base (labeled with N1A, N3A, C2A, C4A, C6A, N6A) attached to a ribose sugar (C1B, C2B, C3B, C4B, C5B). The second nucleotide consists of a flavin base (labeled with C1, C2, C3, C4, C5, C6, C7, C8, N1, N3, N5, C8A, C8B, C8C, C8D, C8E, C8F, C8G, C8H, C8I, C8J, C8K, C8L, C8M, C8N, C8O, C8P, C8Q, C8R, C8S, C8T, C8U, C8V, C8W, C8X, C8Y, C8Z, C8AA, C8AB, C8AC, C8AD, C8AE, C8AF, C8AG, C8AH, C8AI, C8AJ, C8AK, C8AL, C8AM, C8AN, C8AO, C8AP, C8AQ, C8AR, C8AS, C8AT, C8AU, C8AV, C8AW, C8AX, C8AY, C8AZ, C8BA, C8BB, C8BC, C8BD, C8BE, C8BF, C8BG, C8BH, C8BI, C8BJ, C8BK, C8BL, C8BM, C8BN, C8BO, C8BP, C8BQ, C8BR, C8BS, C8BT, C8BU, C8BV, C8BW, C8BX, C8BY, C8BZ, C8CA, C8CB, C8CC, C8CD, C8CE, C8CF, C8CG, C8CH, C8CI, C8CJ, C8CK, C8CL, C8CM, C8CN, C8CO, C8CP, C8CQ, C8CR, C8CS, C8CT, C8CU, C8CV, C8CW, C8CX, C8CY, C8CZ, C8DA, C8DB, C8DC, C8DD, C8DE, C8DF, C8DG, C8DH, C8DI, C8DJ, C8DK, C8DL, C8DM, C8DN, C8DO, C8DP, C8DQ, C8DR, C8DS, C8DT, C8DU, C8DV, C8DW, C8DX, C8DY, C8DZ, C8EA, C8EB, C8EC, C8ED, C8EE, C8EF, C8EG, C8EH, C8EI, C8EJ, C8EK, C8EL, C8EM, C8EN, C8EO, C8EP, C8EQ, C8ER, C8ES, C8ET, C8EU, C8EV, C8EW, C8EX, C8EY, C8EZ, C8FA, C8FB, C8FC, C8FD, C8FE, C8FF, C8FG, C8FH, C8FI, C8FJ, C8FK, C8FL, C8FM, C8FN, C8FO, C8FP, C8FQ, C8FR, C8FS, C8FT, C8FU, C8FV, C8FW, C8FX, C8FY, C8FZ, C8GA, C8GB, C8GC, C8GD, C8GE, C8GF, C8GG, C8GH, C8GI, C8GJ, C8GK, C8GL, C8GM, C8GN, C8GO, C8GP, C8GQ, C8GR, C8GS, C8GT, C8GU, C8GV, C8GW, C8GX, C8GY, C8GZ, C8HA, C8HB, C8HC, C8HD, C8HE, C8HF, C8HG, C8HH, C8HI, C8HJ, C8HK, C8HL, C8HM, C8HN, C8HO, C8HP, C8HQ, C8HR, C8HS, C8HT, C8HU, C8HV, C8HW, C8HX, C8HY, C8HZ, C8IA, C8IB, C8IC, C8ID, C8IE, C8IF, C8IG, C8IH, C8II, C8IJ, C8IK, C8IL, C8IM, C8IN, C8IO, C8IP, C8IQ, C8IR, C8IS, C8IT, C8IU, C8IV, C8IW, C8IX, C8IY, C8IZ, C8JA, C8JB, C8JC, C8JD, C8JE, C8JF, C8JG, C8JH, C8JI, C8JJ, C8JK, C8JL, C8JM, C8JN, C8JO, C8JP, C8JQ, C8JR, C8JS, C8JT, C8JU, C8JV, C8JW, C8JX, C8JY, C8JZ, C8KA, C8KB, C8KC, C8KD, C8KE, C8KF, C8KG, C8KH, C8KI, C8KJ, C8KK, C8KL, C8KM, C8KN, C8KO, C8KP, C8KQ, C8KR, C8KS, C8KT, C8KU, C8KV, C8KW, C8KX, C8KY, C8KZ, C8LA, C8LB, C8LC, C8LD, C8LE, C8LF, C8LG, C8LH, C8LI, C8LJ, C8LK, C8LL, C8LM, C8LN, C8LO, C8LP, C8LQ, C8LR, C8LS, C8LT, C8LU, C8LV, C8LW, C8LX, C8LY, C8LZ, C8MA, C8MB, C8MC, C8MD, C8ME, C8MF, C8MG, C8MH, C8MI, C8MJ, C8MK, C8ML, C8MN, C8MO, C8MP, C8MQ, C8MR, C8MS, C8MT, C8MU, C8MV, C8MW, C8MX, C8MY, C8MZ, C8NA, C8NB, C8NC, C8ND, C8NE, C8NF, C8NG, C8NH, C8NI, C8NJ, C8NK, C8NL, C8NM, C8NO, C8NP, C8NQ, C8NR, C8NS, C8NT, C8NU, C8NV, C8NW, C8NX, C8NY, C8NZ, C8OA, C8OB, C8OC, C8OD, C8OE, C8OF, C8OG, C8OH, C8OI, C8OJ, C8OK, C8OL, C8OM, C8ON, C8OO, C8OP, C8OQ, C8OR, C8OS, C8OT, C8OU, C8OV, C8OW, C8OX, C8OY, C8OZ, C8PA, C8PB, C8PC, C8PD, C8PE, C8PF, C8PG, C8PH, C8PI, C8PJ, C8PK, C8PL, C8PM, C8PN, C8PO, C8PP, C8PQ, C8PR, C8PS, C8PT, C8PU, C8PV, C8PW, C8PX, C8PY, C8PZ, C8QA, C8QB, C8QC, C8QD, C8QE, C8QF, C8QG, C8QH, C8QI, C8QJ, C8QK, C8QL, C8QM, C8QN, C8QO, C8QP, C8QQ, C8QR, C8QS, C8QT, C8QU, C8QV, C8QW, C8QX, C8QY, C8QZ, C8RA, C8RB, C8RC, C8RD, C8RE, C8RF, C8RG, C8RH, C8RI, C8RJ, C8RK, C8RL, C8RM, C8RN, C8RO, C8RP, C8RQ, C8RR, C8RS, C8RT, C8RU, C8RV, C8RW, C8RX, C8RY, C8RZ, C8SA, C8SB, C8SC, C8SD, C8SE, C8SF, C8SG, C8SH, C8SI, C8SJ, C8SK, C8SL, C8SM, C8SN, C8SO, C8SP, C8SQ, C8SR, C8SS, C8ST, C8SU, C8SV, C8SW, C8SX, C8SY, C8SZ, C8TA, C8TB, C8TC, C8TD, C8TE, C8TF, C8TG, C8TH, C8TI, C8TJ, C8TK, C8TL, C8TM, C8TN, C8TO, C8TP, C8TQ, C8TR, C8TS, C8TT, C8TU, C8TV, C8TW, C8TX, C8TY, C8TZ, C8UA, C8UB, C8UC, C8UD, C8UE, C8UF, C8UG, C8UH, C8UI, C8UJ, C8UK, C8UL, C8UM, C8UN, C8UO, C8UP, C8UQ, C8UR, C8US, C8UT, C8UU, C8UV, C8UW, C8UX, C8UY, C8UZ, C8VA, C8VB, C8VC, C8VD, C8VE, C8VF, C8VG, C8VH, C8VI, C8VJ, C8VK, C8VL, C8VM, C8VN, C8VO, C8VP, C8VQ, C8VR, C8VS, C8VT, C8VU, C8VV, C8VW, C8VX, C8VY, C8VZ, C8WA, C8WB, C8WC, C8WD, C8WE, C8WF, C8WG, C8WH, C8WI, C8WJ, C8WK, C8WL, C8WM, C8WN, C8WO, C8WP, C8WQ, C8WR, C8WS, C8WT, C8WU, C8WV, C8WW, C8WX, C8WY, C8WZ, C8XA, C8XB, C8XC, C8XD, C8XE, C8XF, C8XG, C8XH, C8XI, C8XJ, C8XK, C8XL, C8XM, C8XN, C8XO, C8XP, C8XQ, C8XR, C8XS, C8XT, C8XU, C8XV, C8XW, C8XX, C8XY, C8XZ, C8YA, C8YB, C8YC, C8YD, C8YE, C8YF, C8YG, C8YH, C8YI, C8YJ, C8YK, C8YL, C8YM, C8YN, C8YO, C8YP, C8YQ, C8YR, C8YS, C8YT, C8YU, C8YV, C8YW, C8YX, C8YY, C8YZ, C8ZA, C8ZB, C8ZC, C8ZD, C8ZE, C8ZF, C8ZG, C8ZH, C8ZI, C8ZJ, C8ZK, C8ZL, C8ZM, C8ZN, C8ZO, C8ZP, C8ZQ, C8ZR, C8ZS, C8ZT, C8ZU, C8ZV, C8ZW, C8ZX, C8ZY, C8ZZ) attached to a ribose sugar (C1, C2, C3, C4, C5). The pyrophosphate bridge connects the 3' carbon of the first ribose (C3B) to the 5' carbon of the second ribose (C5). The flavin base is a bicyclic system consisting of a benzene ring fused to a pyrimidine ring, with a carbonyl group at C4 and a nitrogen at N1. The adenine base is a purine derivative with a nitrogen at N1 and a carbonyl group at C6. The structure is shown in a 3D representation with stereochemistry indicated by wedges and dashes.

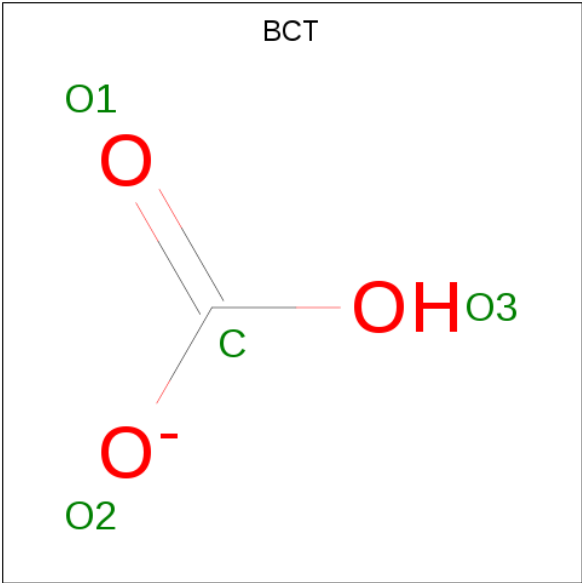
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- 



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



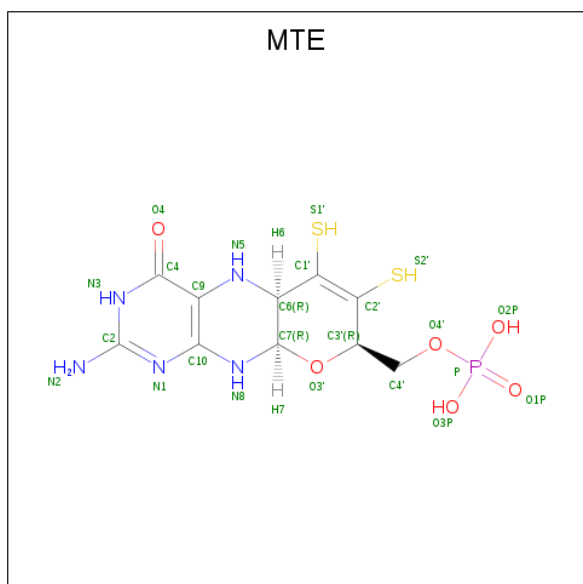
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



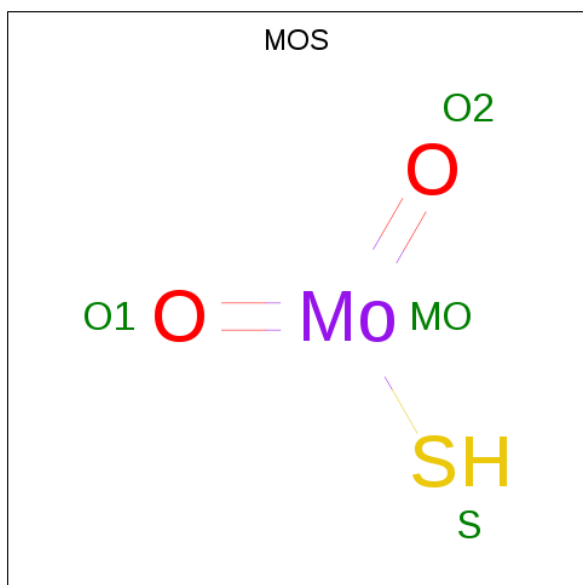
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6P_2S_2$).



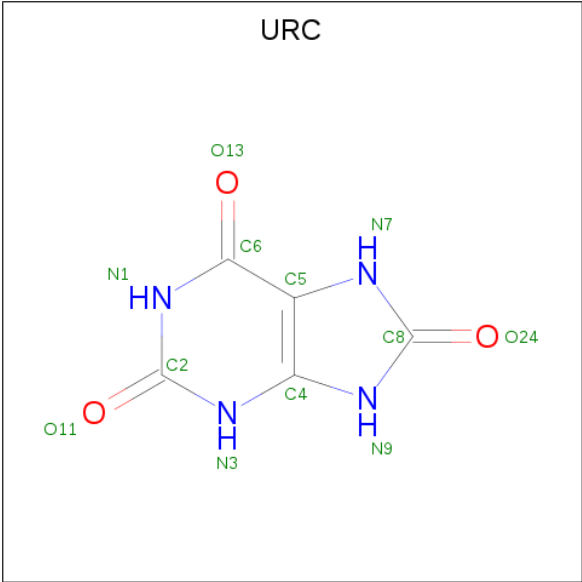
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
8	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	

- Molecule 9 is DIOXOTHIO MOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO_2S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	Mo	O	S		
			3	1	1	1		
9	B	1	Total	Mo	O	S		
			3	1	1	1		

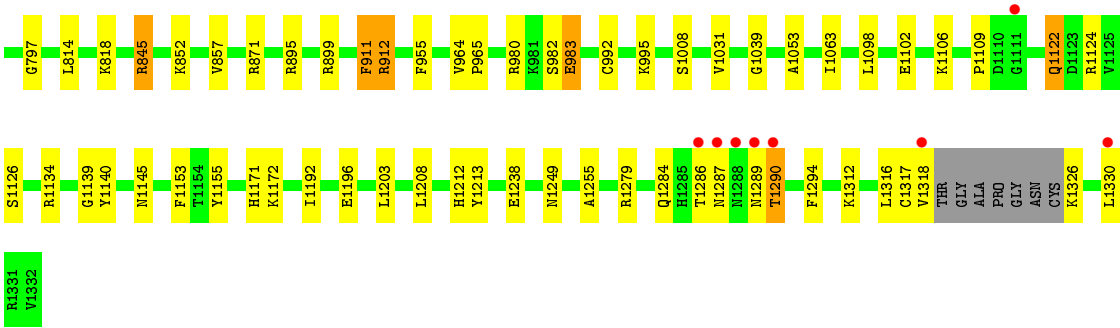
- Molecule 10 is URIC ACID (three-letter code: URC) (formula: $\text{C}_5\text{H}_4\text{N}_4\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			12	5	4	3		
10	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1019	Total	O	0	0
			1019	1019		
11	B	1010	Total	O	0	0
			1010	1010		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.21Å 124.53Å 148.03Å 90.00° 91.07° 90.00°	Depositor
Resolution (Å)	34.83 – 2.10 34.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.83-2.10) 99.4 (34.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.151 , 0.202 0.152 , 0.203	Depositor DCC
R_{free} test set	8881 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22382	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, URC, MOS, CA, NAI, FES, BCT, FAD, MTE

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	1.09	9/10243 (0.1%)	0.96	31/13863 (0.2%)
1	B	1.07	6/10232 (0.1%)	0.94	15/13848 (0.1%)
All	All	1.08	15/20475 (0.1%)	0.95	46/27711 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	1
All	All	1	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	992	CYS	CB-SG	-8.12	1.68	1.82
1	A	983	GLU	CG-CD	7.98	1.64	1.51
1	B	992	CYS	CB-SG	-7.79	1.69	1.82
1	B	699	GLU	CG-CD	7.34	1.62	1.51
1	A	412	SER	CB-OG	-6.95	1.33	1.42

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ARG	NE-CZ-NH2	-16.98	111.81	120.30
1	B	154	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	B	154	ARG	NE-CZ-NH1	15.12	127.86	120.30
1	A	97	ARG	NE-CZ-NH2	-14.60	113.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	ARG	NE-CZ-NH2	-14.59	113.00	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1332	VAL	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1286	THR	Peptide

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	10024	0	10027	92	0
1	B	10013	0	10017	76	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	31	4	0
4	B	53	0	31	6	0
5	A	44	0	25	4	0
5	B	44	0	27	3	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	12	0	16	0	0
7	B	6	0	8	1	0
8	A	24	0	10	1	0
8	B	24	0	10	0	0
9	A	3	0	0	2	0
9	B	3	0	0	1	0
10	A	12	0	4	0	0
10	B	12	0	4	0	0
11	A	1019	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	1010	0	0	19	0
All	All	22382	0	20210	173	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 4.

The worst 5 of 173 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:3:ALA:HB1	1:A:228:ARG:H	1.08	1.09
1:A:60:ARG:O	1:A:61:LEU:HB2	1.47	1.08
1:B:272:ASN:HB3	11:B:1988:HOH:O	1.65	0.95
1:B:217:LEU:O	1:B:220:LYS:HG2	1.70	0.92
1:A:3:ALA:HB1	1:A:228:ARG:N	1.86	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1283/1332 (96%)	1234 (96%)	42 (3%)	7 (0%)	29	26
1	B	1281/1332 (96%)	1239 (97%)	37 (3%)	5 (0%)	34	32
All	All	2564/2664 (96%)	2473 (96%)	79 (3%)	12 (0%)	29	26

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	539	ASP
1	A	61	LEU

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Mol	Chain	Res	Type
1	A	912	ARG
1	A	1008	SER

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	1095/1128 (97%)	1061 (97%)	34 (3%)	40	43
1	B	1094/1128 (97%)	1069 (98%)	25 (2%)	50	55
All	All	2189/2256 (97%)	2130 (97%)	59 (3%)	44	48

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	989	LYS
1	A	1330	LEU
1	B	1208	LEU
1	A	1203	LEU
1	A	1239	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	131	GLN
1	B	333	GLN
1	B	1284	GLN
1	B	146	ASN
1	B	251	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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$
2	FES	B	4001	1	0,4,4	0.00	-	-		
4	FAD	A	3005	-	51,58,58	1.23	5 (9%)	60,89,89	2.27	15 (25%)
2	FES	A	3001	1	0,4,4	0.00	-	-		
4	FAD	B	4005	-	51,58,58	1.53	7 (13%)	60,89,89	2.13	15 (25%)
7	GOL	A	1336	-	5,5,5	0.36	0	5,5,5	0.46	0
8	MTE	B	1336	9	21,26,26	1.80	4 (19%)	21,40,40	2.01	8 (38%)
7	GOL	A	1335	-	5,5,5	1.01	0	5,5,5	1.80	1 (20%)
9	MOS	B	1337	8,10	0,2,3	0.00	-	-		
8	MTE	A	1337	9	21,26,26	1.36	3 (14%)	21,40,40	2.18	11 (52%)
9	MOS	A	1338	8,10	0,2,3	0.00	-	-		
6	BCT	A	1334	-	0,3,3	0.00	-	0,3,3	0.00	-
10	URC	A	1339	9	13,13,13	5.66	10 (76%)	11,19,19	8.97	6 (54%)
6	BCT	B	1334	-	0,3,3	0.00	-	0,3,3	0.00	-
2	FES	A	3002	1	0,4,4	0.00	-	-		
2	FES	B	4002	1	0,4,4	0.00	-	-		
7	GOL	B	1335	-	5,5,5	0.54	0	5,5,5	0.73	0
10	URC	B	1338	9	13,13,13	5.47	8 (61%)	11,19,19	9.85	10 (90%)
5	NAI	A	1333	-	42,48,48	1.49	6 (14%)	47,73,73	1.77	7 (14%)
5	NAI	B	1333	-	42,48,48	1.51	7 (16%)	47,73,73	1.73	7 (14%)

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
2	FES	B	4001	1	-	-	0/1/1/1
4	FAD	A	3005	-	-	0/30/50/50	0/6/6/6
2	FES	A	3001	1	-	-	0/1/1/1
4	FAD	B	4005	-	-	1/30/50/50	0/6/6/6
7	GOL	A	1336	-	-	2/4/4/4	-
8	MTE	B	1336	9	-	1/6/34/34	0/3/3/3
7	GOL	A	1335	-	-	2/4/4/4	-
8	MTE	A	1337	9	-	1/6/34/34	0/3/3/3
10	URC	A	1339	9	-	-	0/2/2/2
2	FES	A	3002	1	-	-	0/1/1/1
2	FES	B	4002	1	-	-	0/1/1/1
7	GOL	B	1335	-	-	4/4/4/4	-
10	URC	B	1338	9	-	-	0/2/2/2
5	NAI	A	1333	-	-	3/25/72/72	0/4/5/5
5	NAI	B	1333	-	-	3/25/72/72	0/4/5/5

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1339	URC	C8-N7	11.59	1.54	1.35
10	B	1338	URC	C8-N7	11.26	1.54	1.35
10	A	1339	URC	C8-N9	8.86	1.50	1.35
10	B	1338	URC	O24-C8	8.36	1.40	1.23
10	A	1339	URC	O24-C8	8.30	1.40	1.23

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1338	URC	C5-C4-N9	23.24	113.40	102.64
10	A	1339	URC	O24-C8-N9	-20.55	96.44	125.94
10	B	1338	URC	O24-C8-N9	-19.18	98.41	125.94
10	A	1339	URC	C5-C4-N9	18.58	111.24	102.64
10	B	1338	URC	N7-C8-N9	-9.04	100.28	108.76

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

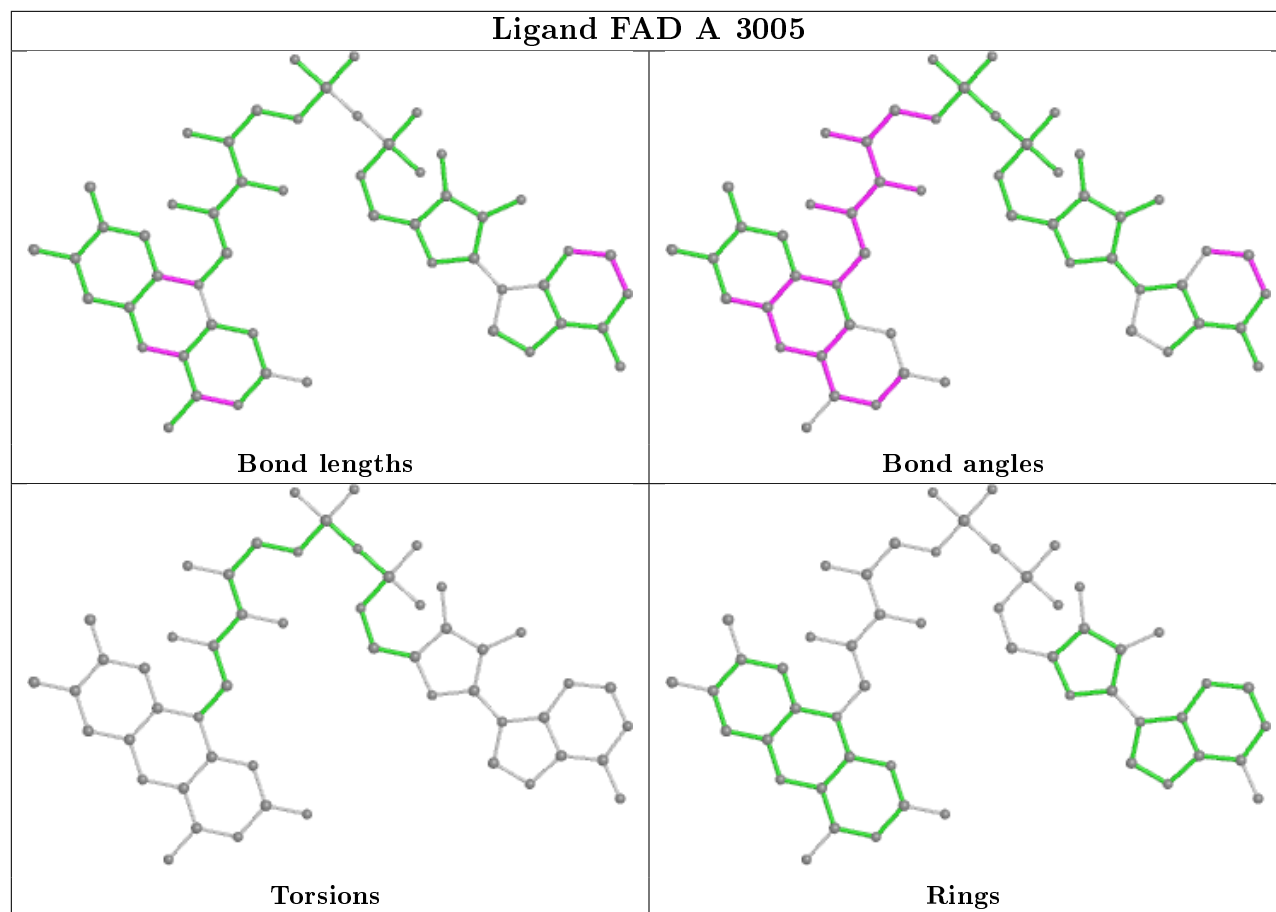
Mol	Chain	Res	Type	Atoms
7	A	1336	GOL	O1-C1-C2-C3
7	B	1335	GOL	C1-C2-C3-O3
5	A	1333	NAI	C2D-C1D-N1N-C6N
5	B	1333	NAI	C2D-C1D-N1N-C6N
8	B	1336	MTE	C3'-C4'-O4'-P

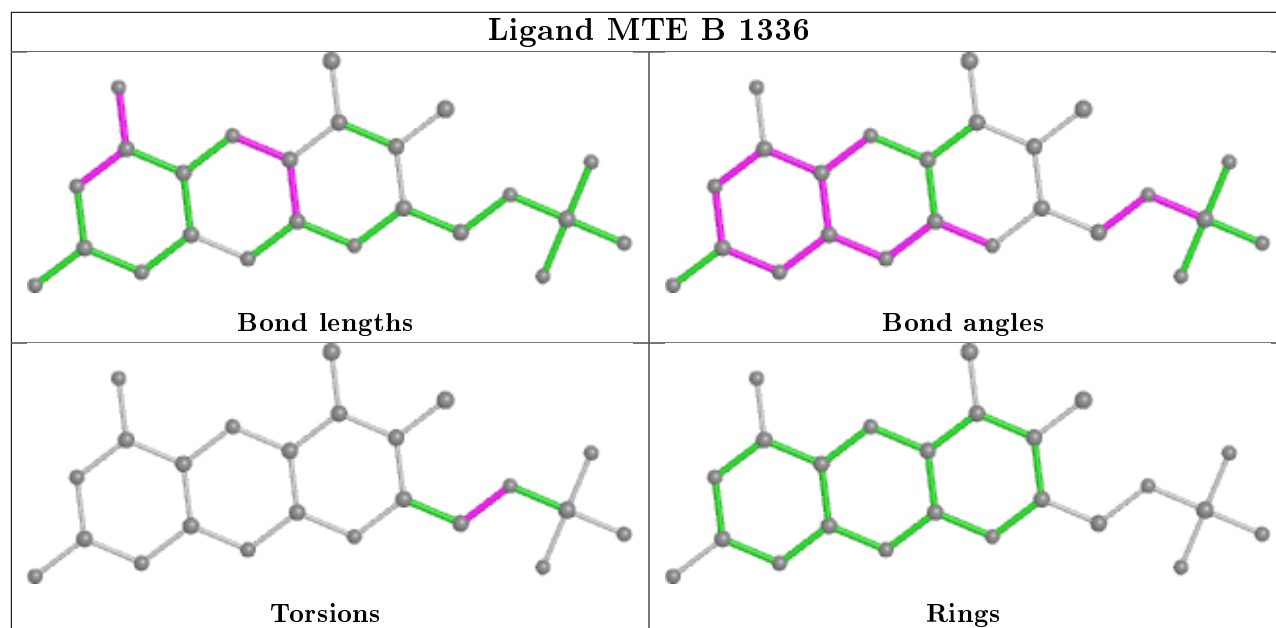
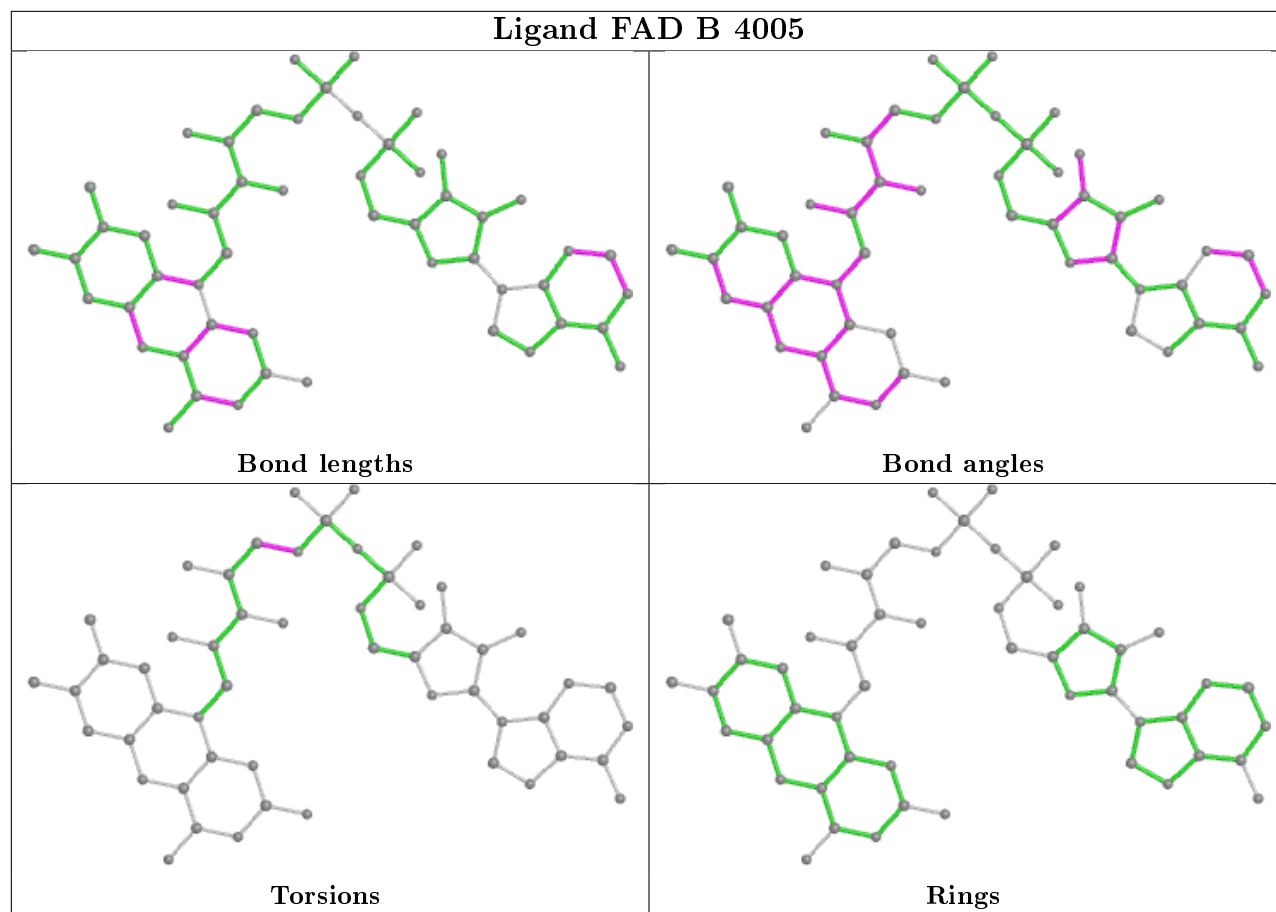
There are no ring outliers.

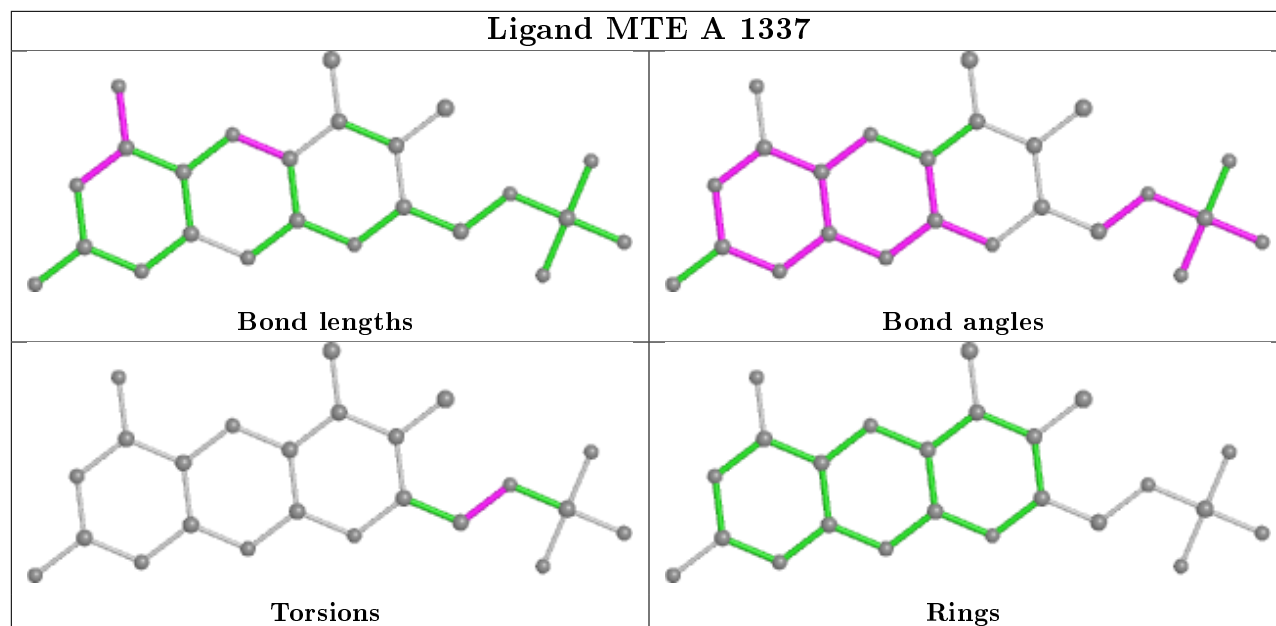
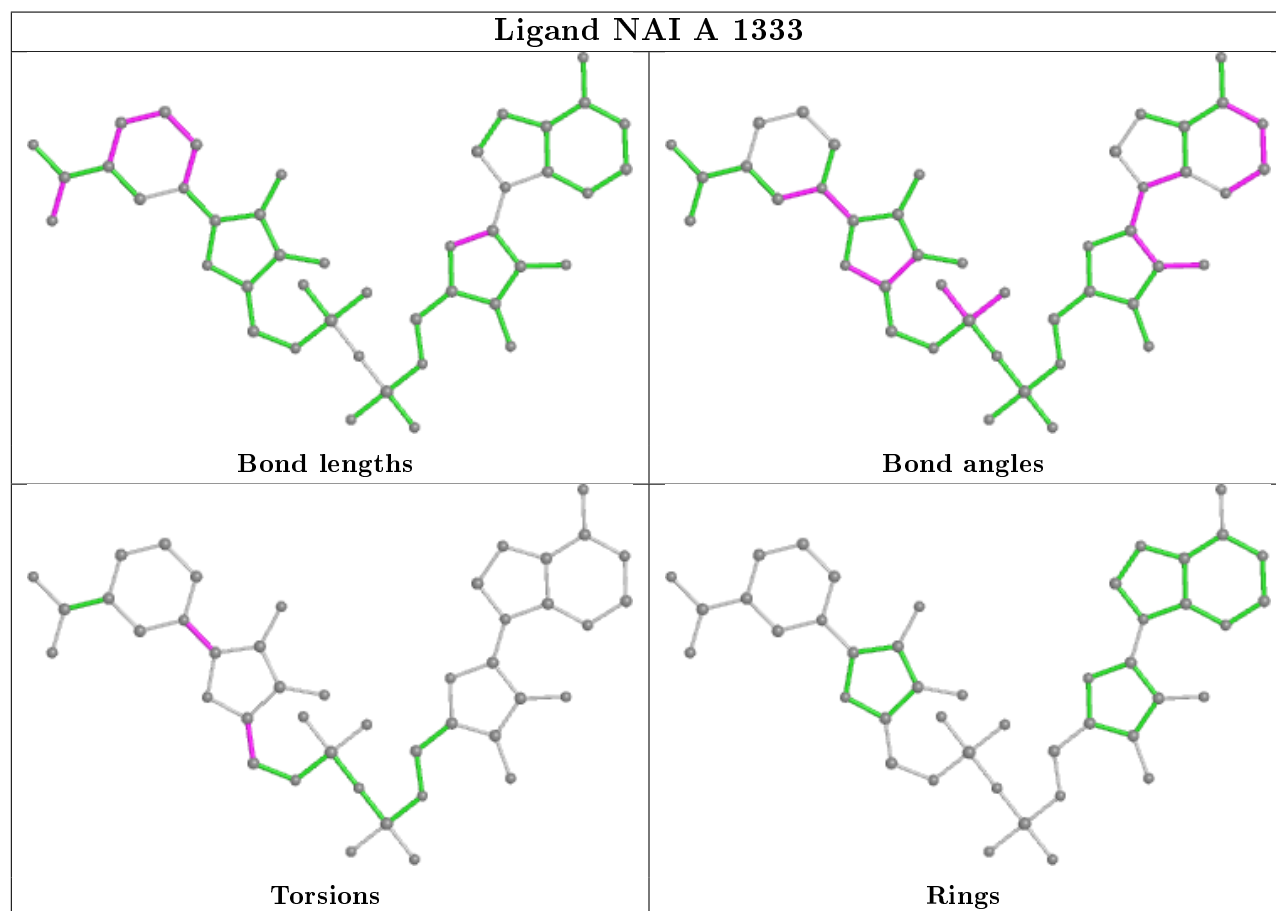
8 monomers are involved in 15 short contacts:

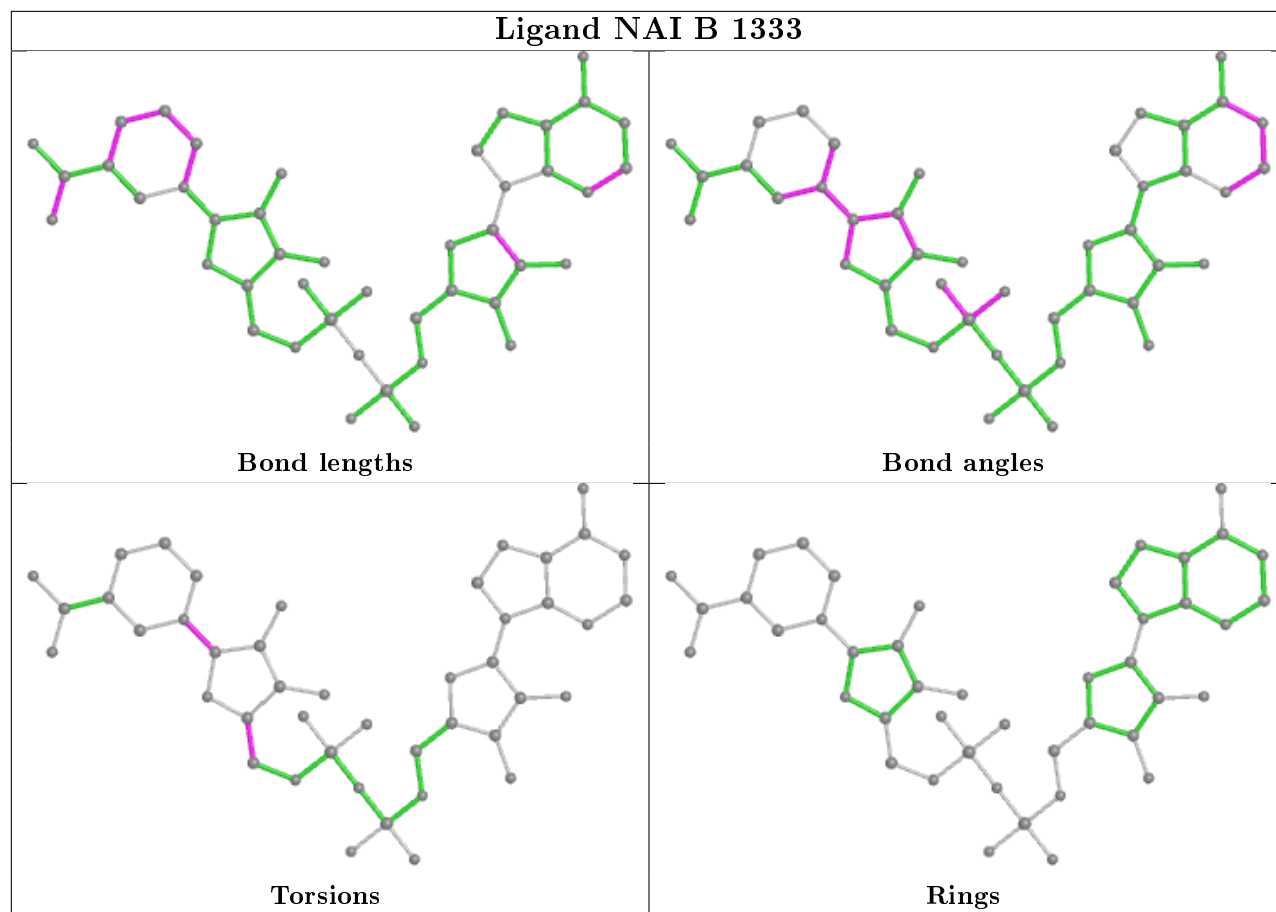
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3005	FAD	4	0
4	B	4005	FAD	6	0
9	B	1337	MOS	1	0
8	A	1337	MTE	1	0
9	A	1338	MOS	2	0
7	B	1335	GOL	1	0
5	A	1333	NAI	4	0
5	B	1333	NAI	3	0

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 MTE A 1337**Ligand NAI A 1333**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1291/1332 (96%)	-0.45	23 (1%) 68 72	12, 22, 39, 66	0
1	B	1289/1332 (96%)	-0.49	19 (1%) 73 77	12, 22, 39, 65	0
All	All	2580/2664 (96%)	-0.47	42 (1%) 72 75	12, 22, 39, 66	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1288	ASN	7.4
1	B	1288	ASN	5.7
1	B	1287	ASN	5.6
1	B	565	ASN	4.6
1	A	565	ASN	4.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

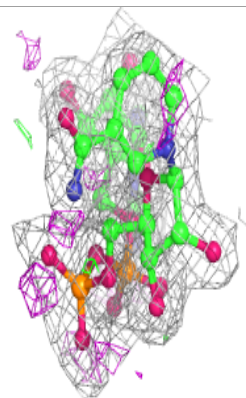
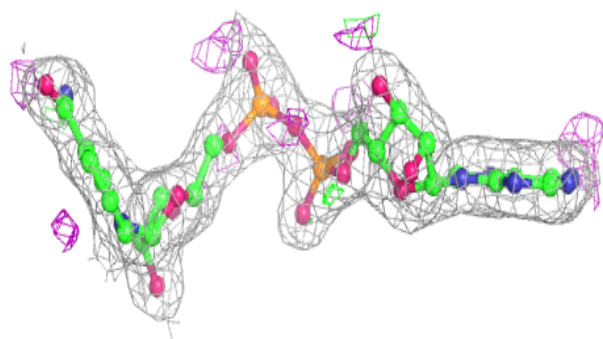
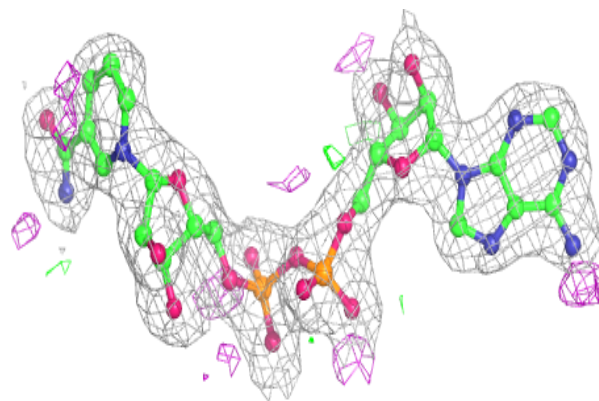
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	URC	A	1339	12/12	0.88	0.13	30,34,37,39	0
7	GOL	A	1335	6/6	0.91	0.14	28,39,39,41	0
10	URC	B	1338	12/12	0.91	0.16	31,38,41,43	0
7	GOL	B	1335	6/6	0.93	0.12	29,35,39,40	0
7	GOL	A	1336	6/6	0.96	0.11	23,27,31,32	0
5	NAI	A	1333	44/44	0.96	0.08	18,25,29,33	0
6	BCT	A	1334	4/4	0.98	0.11	17,20,20,22	0
4	FAD	B	4005	53/53	0.98	0.10	15,18,21,28	0
8	MTE	A	1337	24/24	0.98	0.09	14,19,24,25	0
4	FAD	A	3005	53/53	0.98	0.11	14,19,24,28	0
5	NAI	B	1333	44/44	0.98	0.07	18,25,28,31	0
6	BCT	B	1334	4/4	0.99	0.09	16,17,18,19	0
8	MTE	B	1336	24/24	0.99	0.07	15,20,23,25	0
2	FES	A	3001	4/4	1.00	0.05	15,15,16,17	0
2	FES	A	3002	4/4	1.00	0.07	15,15,17,18	0
3	CA	B	4008	1/1	1.00	0.05	19,19,19,19	0
2	FES	B	4002	4/4	1.00	0.06	14,15,16,16	0
9	MOS	A	1338	3/4	1.00	0.06	25,25,27,40	0
2	FES	B	4001	4/4	1.00	0.05	14,15,16,16	0
3	CA	A	3008	1/1	1.00	0.05	20,20,20,20	0
9	MOS	B	1337	3/4	1.00	0.06	27,27,27,39	0

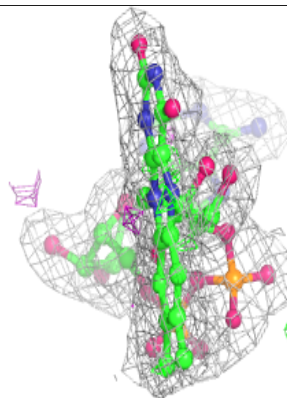
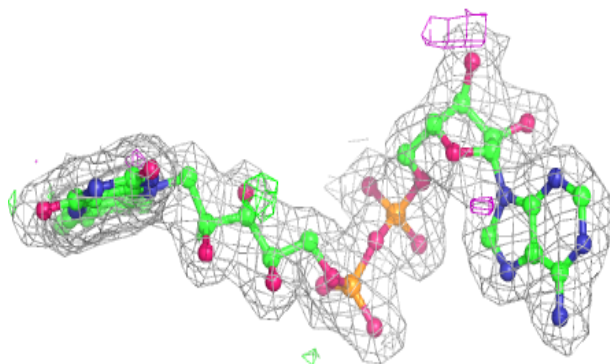
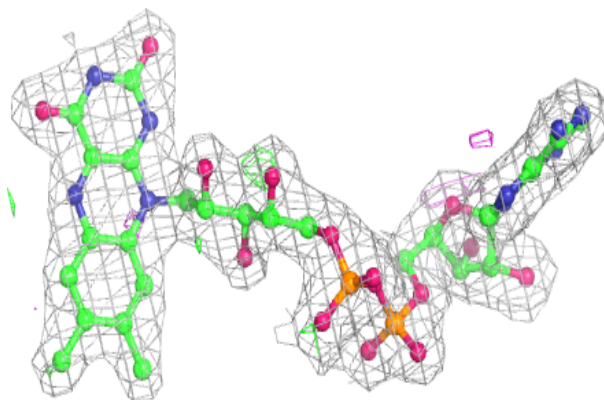
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI A 1333:

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

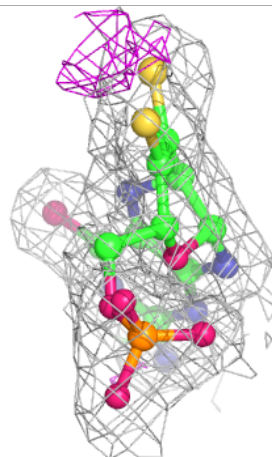
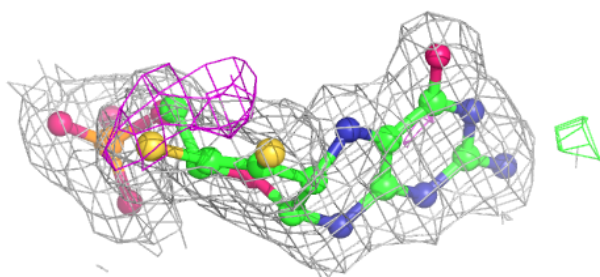
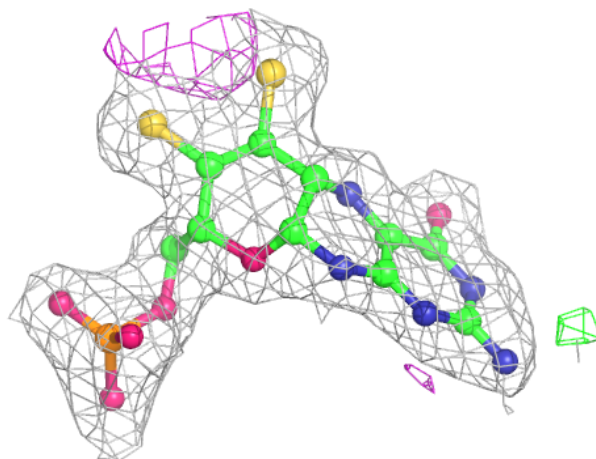
**Electron density around FAD B 4005:**

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



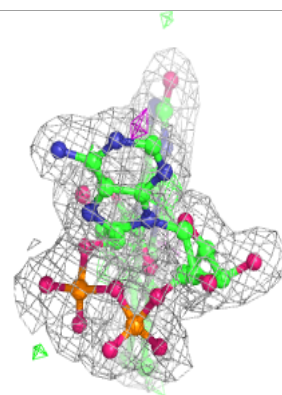
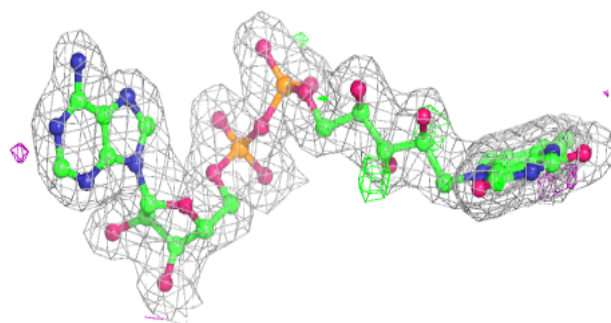
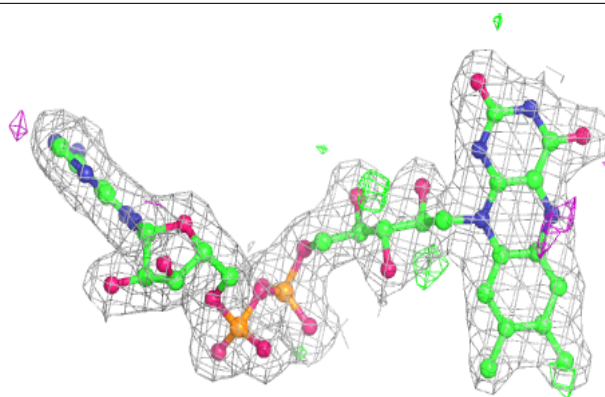
Electron density around MTE A 1337:

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

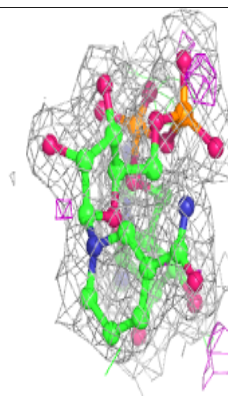
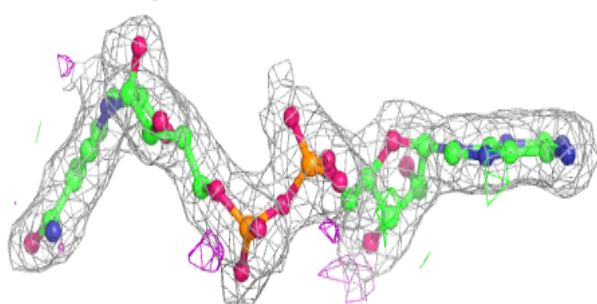
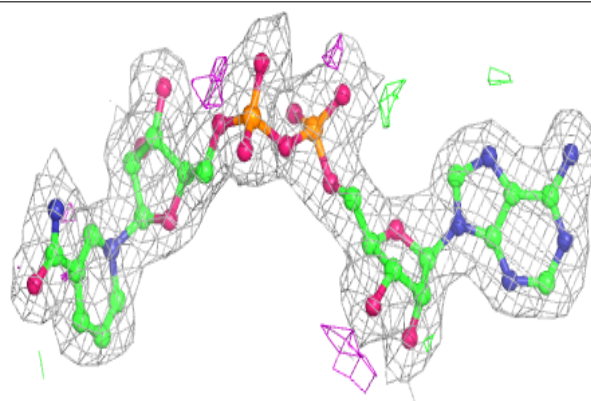


Electron density around FAD A 3005:

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

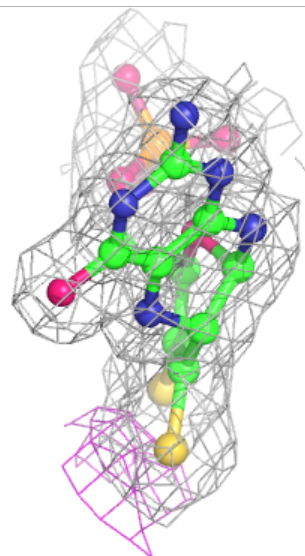
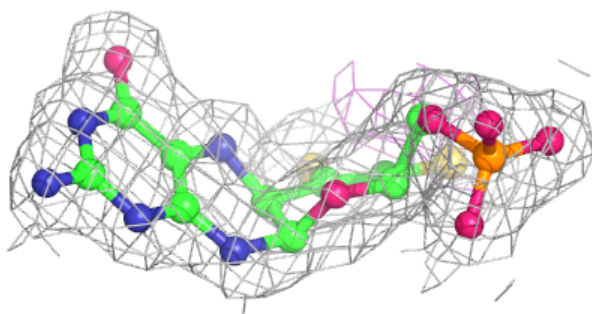
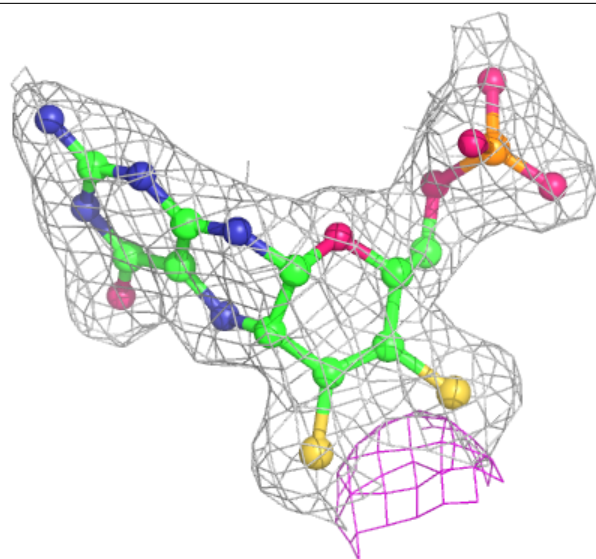
**Electron density around NAI B 1333:**

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



Electron density around MTE B 1336:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.