



Full wwPDB X-ray Structure Validation 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 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 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

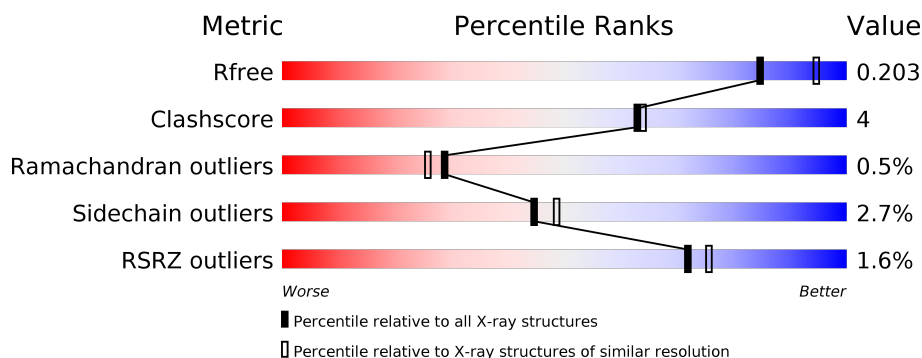
1 Overall quality at a glance ⓘ

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](#)

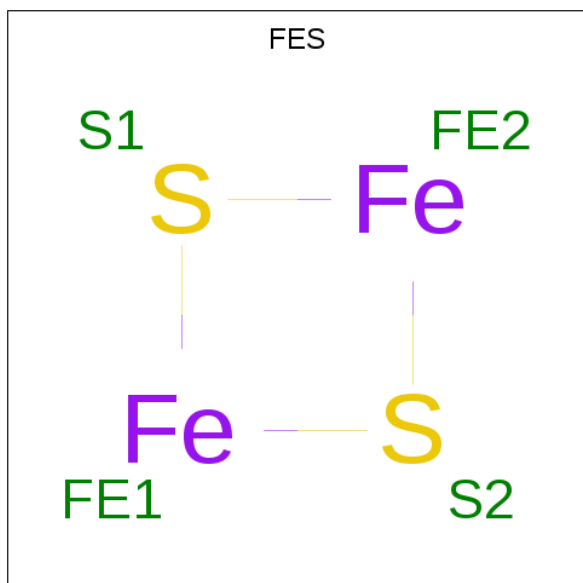
There are 11 unique types of molecules in this entry. The entry contains 22382 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

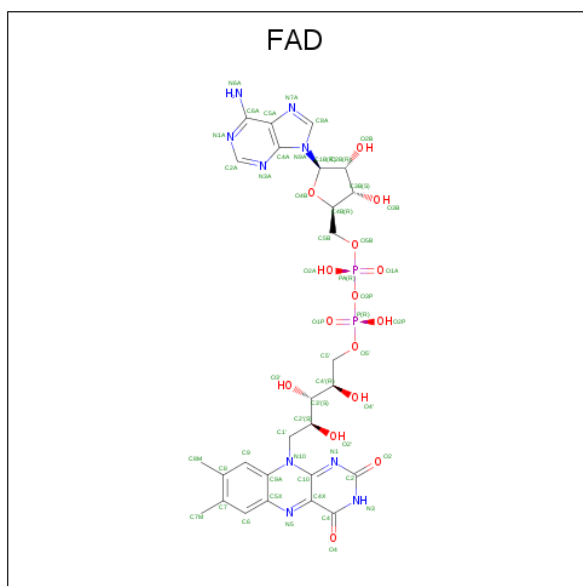


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

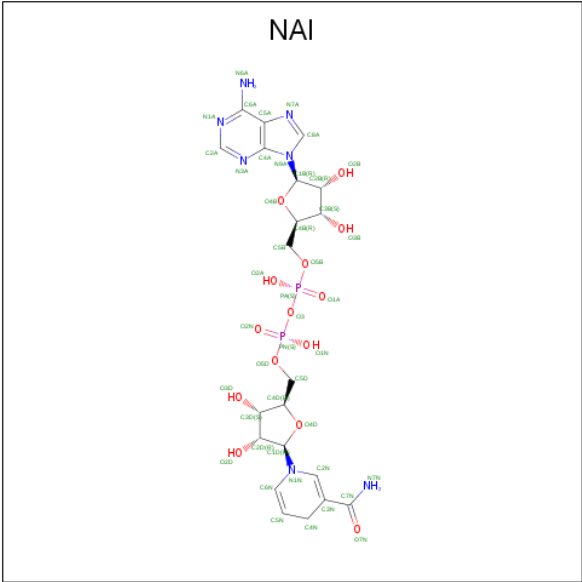
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



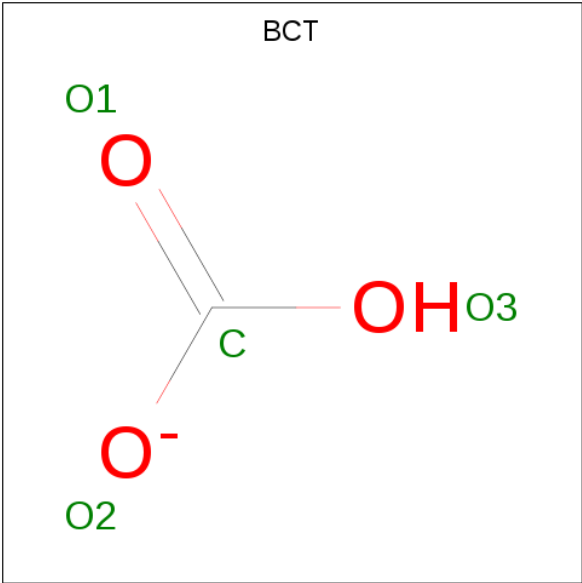
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



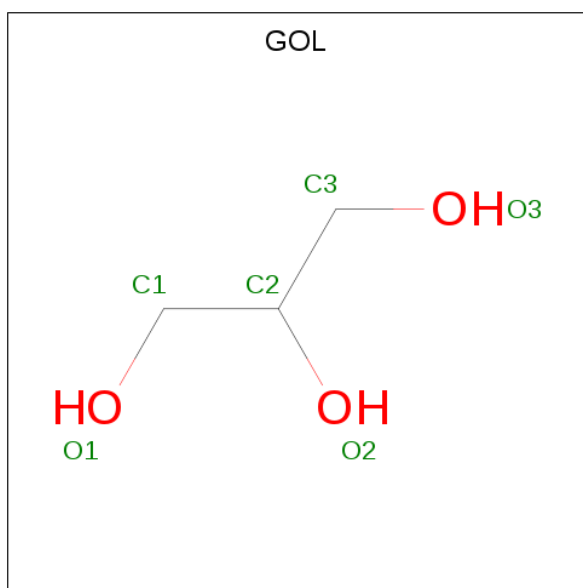
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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



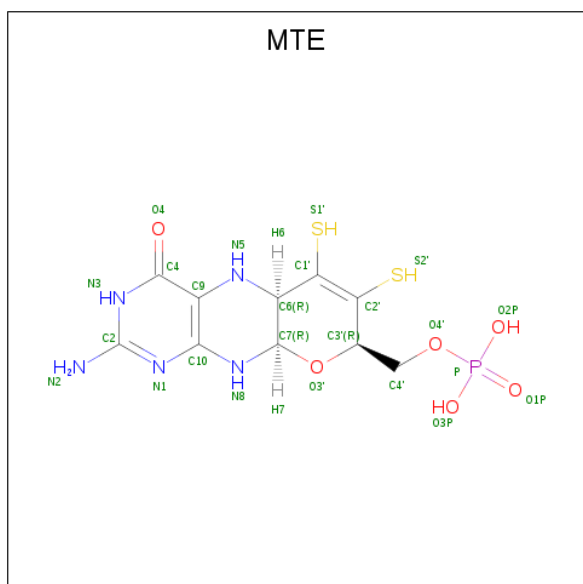
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		

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



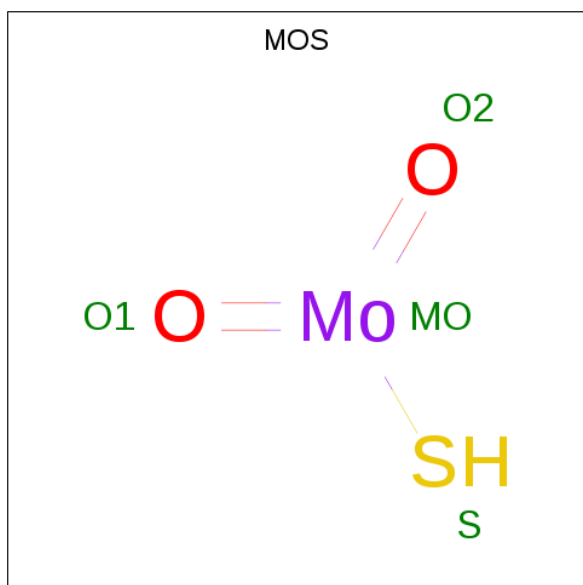
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- 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: $C_{10}H_{14}N_5O_6P_2S_2$).



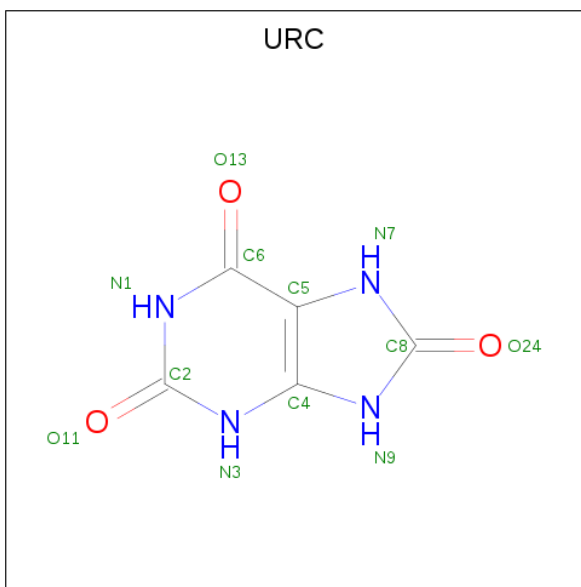
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
8	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	

- 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: $\text{C}_5\text{H}_4\text{N}_4\text{O}_3$).



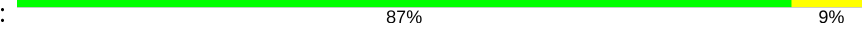
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			12	5	4	3		
10	B	1	Total	C	N	O	0	0
			12	5	4	3		

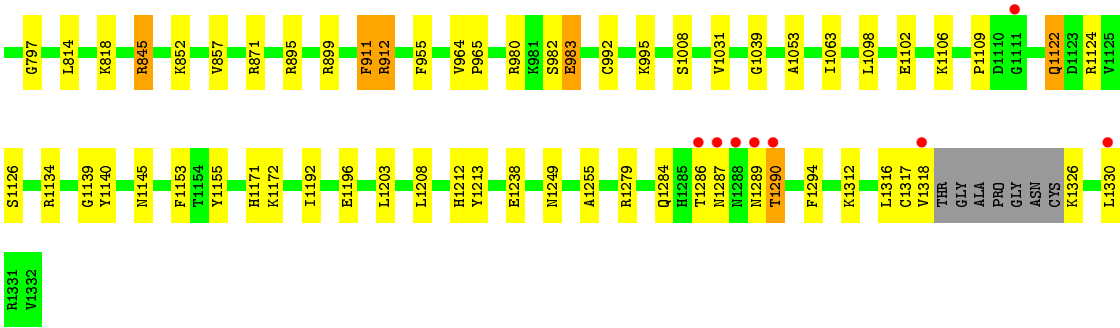
- Molecule 11 is water.

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 96% 9% 5%
- 0 100

- Chain B: 



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

All (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
1	B	645	GLU	CD-OE2	6.73	1.33	1.25
1	A	73	CYS	CB-SG	6.12	1.92	1.82
1	A	645	GLU	CG-CD	5.93	1.60	1.51
1	A	153	TYR	CD2-CE2	5.64	1.47	1.39
1	B	645	GLU	CG-CD	5.61	1.60	1.51
1	B	983	GLU	CG-CD	5.58	1.60	1.51
1	A	645	GLU	CD-OE2	5.44	1.31	1.25
1	A	699	GLU	CG-CD	5.25	1.59	1.51
1	A	983	GLU	CD-OE2	5.10	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	508	ARG	CD-NE	-5.07	1.37	1.46

All (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
1	B	508	ARG	NE-CZ-NH2	-14.59	113.00	120.30
1	B	508	ARG	NE-CZ-NH1	14.14	127.37	120.30
1	B	427	ARG	NE-CZ-NH2	-12.93	113.84	120.30
1	A	980	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	A	154	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	A	980	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	97	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	B	427	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	A	1332	VAL	CB-CA-C	7.77	126.16	111.40
1	B	1124	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	A	61	LEU	CA-CB-CG	7.03	131.46	115.30
1	B	1316	LEU	CA-CB-CG	7.01	131.42	115.30
1	A	398	LEU	CA-CB-CG	6.96	131.30	115.30
1	A	1306	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	386	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	1330	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	684	VAL	CG1-CB-CG2	6.56	121.40	110.90
1	A	719	LEU	CA-CB-CG	-6.54	100.27	115.30
1	A	1203	LEU	CA-CB-CG	6.39	130.00	115.30
1	B	621	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	4	ASP	CB-CA-C	6.24	122.88	110.40
1	B	621	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	1124	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	1332	VAL	CG1-CB-CG2	-5.98	101.33	110.90
1	A	97	ARG	CG-CD-NE	-5.95	99.30	111.80
1	A	598	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	412	SER	N-CA-CB	-5.90	101.65	110.50
1	A	89	GLU	CA-CB-CG	5.82	126.20	113.40
1	B	845	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	598	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	621	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	1306	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	380	ARG	NE-CZ-NH2	-5.54	117.53	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	871	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	312	LEU	CB-CG-CD1	5.19	119.82	111.00
1	A	966	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	1208	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	1208	LEU	CB-CG-CD1	5.11	119.68	111.00
1	A	1186	LEU	CB-CG-CD1	-5.09	102.34	111.00
1	A	748	CYS	CA-CB-SG	-5.05	104.91	114.00
1	A	97	ARG	CD-NE-CZ	5.01	130.62	123.60
1	A	4	ASP	CB-CG-OD1	5.01	122.81	118.30

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 ⓘ

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
4:A:3005:FAD:C4X	5:A:1333:NAI:C6N	2.50	0.90
4:B:4005:FAD:C4X	5:B:1333:NAI:C6N	2.52	0.88
1:B:37:ARG:HD3	11:B:1467:HOH:O	1.74	0.88
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.77	0.85
1:A:377:ARG:NE	11:A:2032:HOH:O	2.09	0.84
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.41	0.83
1:A:60:ARG:O	1:A:61:LEU:CB	2.27	0.83
1:A:237:ILE:HD12	1:A:277:MET:HE2	1.61	0.82
1:B:131:GLN:HE21	1:B:133:GLU:H	1.27	0.80
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.44	0.80
1:A:154:ARG:CD	1:A:1196:GLU:OE2	2.29	0.80
1:A:57:LYS:HD2	11:A:1470:HOH:O	1.81	0.79
1:A:1330:LEU:HG	11:A:2358:HOH:O	1.83	0.78
1:B:165:LYS:HE3	1:B:165:LYS:O	1.84	0.77
1:B:506:GLU:HG3	11:B:1384:HOH:O	1.86	0.76
1:A:552:HIS:HB2	11:A:2208:HOH:O	1.85	0.75
1:A:3:ALA:O	1:A:4:ASP:C	2.23	0.75
1:B:323:LYS:NZ	11:B:1485:HOH:O	2.18	0.75
1:B:552:HIS:CE1	1:B:1172:LYS:HZ2	2.06	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.51	0.74
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.85	0.73
1:A:154:ARG:HD2	11:A:1444:HOH:O	1.89	0.72
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.56	0.70
1:A:3:ALA:O	1:A:5:GLU:N	2.25	0.69
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.57	0.68
1:A:439:ARG:HB3	1:A:439:ARG:HH11	1.58	0.68
1:B:467:LEU:O	1:B:471:GLN:HG2	1.94	0.67
1:A:415:ASP:OD2	1:A:444:PRO:HA	1.95	0.66
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.95	0.66
1:A:1178:ILE:CG2	1:A:1180:MET:HE2	2.26	0.66
1:A:131:GLN:HE21	1:A:133:GLU:H	1.44	0.66
1:A:237:ILE:HD12	1:A:277:MET:CE	2.25	0.66
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.92	0.65
1:B:1212:HIS:HD2	11:B:2345:HOH:O	1.80	0.64
1:B:154:ARG:HD2	11:B:1705:HOH:O	1.98	0.63
1:A:1249:ASN:O	1:A:1255:ALA:HA	1.98	0.63
1:B:433:LYS:HE2	1:B:504:MET:SD	2.38	0.63
1:B:1312:LYS:HE2	11:B:2314:HOH:O	1.99	0.62
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.64	0.62
1:A:1319:THR:HG22	11:A:2095:HOH:O	2.00	0.62
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.48	0.61
1:B:627:LYS:NZ	11:B:2302:HOH:O	2.28	0.61
1:A:154:ARG:HD2	1:A:1196:GLU:OE2	2.00	0.61
1:A:624:GLU:HB3	11:A:2199:HOH:O	2.00	0.60
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.50	0.60
9:A:1338:MOS:MO	9:A:1338:MOS:O1	1.72	0.59
1:B:348:LEU:HD13	1:B:407:ILE:HD13	1.84	0.58
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.85	0.58
4:A:3005:FAD:C4	5:A:1333:NAI:C6N	2.81	0.58
1:A:562:GLU:HB2	11:A:2245:HOH:O	2.04	0.58
1:B:425:SER:OG	1:B:433:LYS:NZ	2.38	0.57
1:B:427:ARG:NH2	1:B:1171:HIS:O	2.37	0.57
1:B:645:GLU:HG2	1:B:650:ASN:ND2	2.16	0.57
1:A:237:ILE:CD1	1:A:277:MET:CE	2.82	0.57
1:A:645:GLU:HG2	1:A:650:ASN:ND2	2.19	0.57
4:B:4005:FAD:C4	5:B:1333:NAI:C6N	2.83	0.57
1:B:552:HIS:CE1	1:B:1172:LYS:NZ	2.73	0.57
1:A:144:GLN:HE21	1:A:429:ASP:H	1.53	0.56
1:B:695:ILE:HG23	1:B:700:ASP:HB3	1.87	0.56
1:A:541:THR:HG23	1:A:992:CYS:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:LYS:N	1:A:1327:PRO:CD	2.70	0.55
1:B:980:ARG:HD2	11:B:2278:HOH:O	2.07	0.55
1:A:197:ASN:O	1:A:200:GLU:HG3	2.06	0.54
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.55	0.54
1:B:1106:LYS:O	1:B:1109:PRO:HD3	2.08	0.54
1:A:322:GLN:O	1:A:412:SER:HB3	2.08	0.54
1:B:264:ILE:HD11	4:B:4005:FAD:H3B	1.89	0.54
1:B:346:ALA:HB1	4:B:4005:FAD:H4'	1.90	0.53
1:A:1140:TYR:OH	1:A:1145:ASN:ND2	2.41	0.53
1:A:508:ARG:O	1:A:512:THR:HG23	2.08	0.52
1:A:256:LYS:HG3	1:A:275:PHE:CD2	2.45	0.52
1:A:655:PHE:HE1	1:A:814:LEU:CD2	2.23	0.52
1:A:220:LYS:HG2	1:A:221:ASP:N	2.25	0.51
1:A:719:LEU:HD22	1:A:860:GLU:HG3	1.93	0.51
1:A:37:ARG:HD3	1:A:595:ASP:O	2.11	0.51
1:A:980:ARG:HD2	11:A:2318:HOH:O	2.12	0.50
1:B:508:ARG:O	1:B:512:THR:HG23	2.11	0.50
1:A:263:GLU:HB2	11:A:2103:HOH:O	2.11	0.50
1:A:59:ASP:OD2	1:A:62:GLN:HB2	2.12	0.50
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.44	0.50
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.47	0.49
1:A:220:LYS:HE3	11:A:2267:HOH:O	2.11	0.49
1:A:1057:PRO:HD2	1:A:1060:LYS:HD2	1.95	0.49
1:A:1212:HIS:HD2	11:A:1528:HOH:O	1.95	0.48
1:A:237:ILE:CD1	1:A:277:MET:HE3	2.43	0.48
1:A:35:GLY:N	11:A:2071:HOH:O	2.47	0.48
1:B:401:GLU:HB2	11:B:1713:HOH:O	2.13	0.48
1:B:428:GLU:HG2	11:B:1891:HOH:O	2.12	0.48
1:B:473:GLN:HE21	1:B:482:LEU:HD12	1.79	0.48
1:A:529:LYS:HG2	11:A:2066:HOH:O	2.13	0.48
1:B:271:LYS:HE2	11:B:2010:HOH:O	2.13	0.48
1:B:414:GLU:O	1:B:415:ASP:HB2	2.13	0.48
1:A:539:ASP:OD1	1:A:541:THR:HB	2.14	0.48
1:B:1203:LEU:C	1:B:1203:LEU:HD23	2.34	0.48
4:A:3005:FAD:C4	5:A:1333:NAI:H6N	2.44	0.48
1:A:1178:ILE:CG2	1:A:1180:MET:CE	2.92	0.47
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.49	0.47
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.96	0.47
1:A:376:SER:HB3	1:A:379:THR:OG1	2.15	0.47
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.15	0.46
1:B:247:ASP:OD1	1:B:377:ARG:HD3	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1289:ASN:O	1:B:1290:THR:HB	2.16	0.46
1:B:912:ARG:N	9:B:1337:MOS:S	2.89	0.46
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.80	0.46
1:A:154:ARG:HD3	1:A:1196:GLU:CD	2.35	0.46
1:B:468:LYS:HG3	11:B:1428:HOH:O	2.15	0.46
1:B:555:ALA:O	1:B:1238:GLU:HA	2.16	0.46
1:B:263:GLU:HB3	4:B:4005:FAD:H52A	1.98	0.45
1:A:723:PHE:CE2	1:A:847:LYS:HG2	2.51	0.45
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.47	0.45
1:A:474:LEU:O	1:A:475:SER:HB2	2.16	0.45
1:A:217:LEU:O	1:A:220:LYS:HD3	2.16	0.45
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.97	0.45
1:A:618:LYS:HA	1:A:618:LYS:HD2	1.67	0.45
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.52	0.45
1:B:1213:TYR:HD1	11:B:2360:HOH:O	2.00	0.45
1:B:1122:GLN:NE2	11:B:1906:HOH:O	2.50	0.44
1:A:1082:SER:HB2	8:A:1337:MTE:O3P	2.17	0.44
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.44
1:A:217:LEU:HA	1:A:217:LEU:HD12	1.77	0.44
1:B:112:GLN:HB3	1:B:1039:GLY:O	2.17	0.44
1:A:723:PHE:CZ	1:A:847:LYS:HG2	2.53	0.44
1:A:35:GLY:HA2	11:A:2071:HOH:O	2.17	0.44
4:A:3005:FAD:C4X	5:A:1333:NAI:C5N	2.96	0.44
1:A:195:LEU:HD22	1:A:1189:ALA:HA	2.00	0.44
1:A:1212:HIS:HE1	11:A:1816:HOH:O	2.00	0.44
1:A:970:GLU:HG2	1:A:1179:VAL:HG21	2.00	0.44
1:A:256:LYS:HE2	1:A:275:PHE:CE2	2.52	0.43
1:A:613:ALA:O	1:A:904:ASN:HB3	2.19	0.43
1:B:325:GLU:HB2	1:B:412:SER:HB3	2.00	0.43
1:A:598:ARG:HG3	1:B:600:GLU:HG2	2.00	0.43
1:B:1212:HIS:HE1	11:B:2011:HOH:O	2.00	0.43
1:B:268:MET:CE	11:B:2245:HOH:O	2.67	0.43
1:B:113:CYS:HA	1:B:1039:GLY:HA2	2.00	0.43
1:A:55:LEU:CD2	1:A:85:VAL:HG22	2.49	0.43
1:B:1140:TYR:OH	1:B:1145:ASN:ND2	2.51	0.43
1:B:1279:ARG:HG2	1:B:1294:PHE:HE2	1.84	0.43
1:B:374:ILE:HD13	1:B:398:LEU:HD22	2.01	0.43
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.18	0.43
1:A:362:ASN:N	1:A:363:PRO:CD	2.82	0.43
1:A:348:LEU:HD13	1:A:407:ILE:HD13	2.01	0.43
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.22	0.43
1:B:308:VAL:HG21	1:B:348:LEU:HG	2.01	0.43
1:A:712:LEU:HG	11:A:1380:HOH:O	2.19	0.42
4:B:4005:FAD:C4	5:B:1333:NAI:H6N	2.49	0.42
1:A:325:GLU:HB2	1:A:412:SER:OG	2.19	0.42
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.63	0.42
1:B:1031:VAL:HB	1:B:1063:ILE:HG12	2.01	0.42
1:B:911:PHE:O	1:B:912:ARG:C	2.57	0.42
1:A:599:TYR:HA	1:B:599:TYR:HA	2.02	0.42
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.20	0.41
1:A:1178:ILE:HG21	1:A:1180:MET:CE	2.50	0.41
1:A:447:MET:O	1:A:477:PHE:HA	2.20	0.41
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	2.02	0.41
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.64	0.41
1:B:1134:ARG:HG2	11:B:1419:HOH:O	2.20	0.41
1:A:541:THR:HG22	1:A:542:TYR:HD1	1.84	0.41
1:A:912:ARG:N	9:A:1338:MOS:S	2.94	0.41
1:A:35:GLY:CA	11:A:2071:HOH:O	2.69	0.41
1:B:272:ASN:CB	11:B:1988:HOH:O	2.42	0.41
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.86	0.41
1:B:645:GLU:CG	1:B:650:ASN:HD22	2.26	0.40
1:B:675:PRO:HB3	7:B:1335:GOL:H12	2.03	0.40
1:B:1102:GLU:OE1	1:B:1106:LYS:HD2	2.22	0.40
1:A:555:ALA:O	1:A:1238:GLU:HA	2.20	0.40
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.02	0.40
1:B:618:LYS:HD2	1:B:618:LYS:HA	1.91	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	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

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	539	ASP
1	A	61	LEU
1	A	912	ARG
1	A	1008	SER
1	B	1008	SER
1	B	912	ARG
1	A	1139	GLY
1	A	797	GLY
1	B	797	GLY
1	B	1139	GLY
1	B	1290	THR

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

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	61	LEU
1	A	62	GLN
1	A	64	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	89	GLU
1	A	154	ARG
1	A	165	LYS
1	A	200	GLU
1	A	211	ILE
1	A	225	LYS
1	A	256	LYS
1	A	312	LEU
1	A	348	LEU
1	A	439	ARG
1	A	462	ARG
1	A	468	LYS
1	A	541	THR
1	A	548	LEU
1	A	551	LYS
1	A	562	GLU
1	A	684	VAL
1	A	719	LEU
1	A	743	TYR
1	A	857	VAL
1	A	911	PHE
1	A	983	GLU
1	A	989	LYS
1	A	1203	LEU
1	A	1208	LEU
1	A	1239	PHE
1	A	1287	ASN
1	A	1316	LEU
1	A	1326	LYS
1	A	1330	LEU
1	B	64	LYS
1	B	132	PRO
1	B	154	ARG
1	B	165	LYS
1	B	321	THR
1	B	348	LEU
1	B	375	VAL
1	B	537	LYS
1	B	551	LYS
1	B	600	GLU
1	B	743	TYR
1	B	818	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	845	ARG
1	B	852	LYS
1	B	857	VAL
1	B	899	ARG
1	B	911	PHE
1	B	982	SER
1	B	983	GLU
1	B	1122	GLN
1	B	1208	LEU
1	B	1287	ASN
1	B	1317	CYS
1	B	1318	VAL
1	B	1326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	GLN
1	A	251	GLN
1	A	473	GLN
1	A	567	GLN
1	A	650	ASN
1	A	728	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1212	HIS
1	A	1284	GLN
1	B	131	GLN
1	B	146	ASN
1	B	251	GLN
1	B	333	GLN
1	B	471	GLN
1	B	473	GLN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	1088	GLN
1	B	1122	GLN
1	B	1145	ASN
1	B	1212	HIS
1	B	1284	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1288	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 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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

All (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
10	B	1338	URC	C8-N9	8.21	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1338	URC	C4-N3	-7.43	1.37	1.46
10	A	1339	URC	C4-N3	-6.86	1.37	1.46
5	B	1333	NAI	C4N-C3N	-5.23	1.39	1.49
8	B	1336	MTE	O4-C4	5.04	1.37	1.24
10	A	1339	URC	C5-C6	-5.00	1.44	1.52
10	B	1338	URC	C4-N9	-4.97	1.38	1.44
10	A	1339	URC	C4-N9	-4.82	1.38	1.44
10	B	1338	URC	C5-C6	-4.79	1.44	1.52
4	B	4005	FAD	C2A-N3A	4.66	1.39	1.32
5	A	1333	NAI	C4N-C3N	-4.63	1.40	1.49
4	A	3005	FAD	C4X-N5	4.60	1.39	1.33
4	B	4005	FAD	C2A-N1A	4.20	1.41	1.33
5	B	1333	NAI	C6N-C5N	3.77	1.40	1.33
8	A	1337	MTE	O4-C4	3.76	1.34	1.24
5	A	1333	NAI	C6N-C5N	3.52	1.39	1.33
5	A	1333	NAI	C7N-N7N	-3.48	1.24	1.33
4	B	4005	FAD	C4-N3	3.33	1.38	1.33
8	B	1336	MTE	C6-N5	3.25	1.49	1.45
4	B	4005	FAD	C4X-C10	3.24	1.42	1.38
5	A	1333	NAI	C4N-C5N	-3.20	1.40	1.48
10	A	1339	URC	O11-C2	3.19	1.30	1.23
4	B	4005	FAD	C9A-N10	3.14	1.42	1.38
4	A	3005	FAD	C2A-N3A	3.14	1.37	1.32
4	B	4005	FAD	C10-N1	2.96	1.37	1.33
5	B	1333	NAI	C4N-C5N	-2.96	1.41	1.48
5	B	1333	NAI	C6N-N1N	2.95	1.44	1.37
8	B	1336	MTE	C4-N3	2.92	1.38	1.33
4	A	3005	FAD	C2A-N1A	2.83	1.39	1.33
5	A	1333	NAI	O4B-C1B	2.80	1.45	1.41
5	B	1333	NAI	C2A-N3A	2.80	1.36	1.32
10	A	1339	URC	C5-N7	-2.78	1.40	1.45
5	B	1333	NAI	C7N-N7N	-2.78	1.25	1.33
10	B	1338	URC	C5-N7	-2.71	1.40	1.45
8	B	1336	MTE	C7-C6	2.68	1.55	1.53
10	A	1339	URC	C6-N1	2.60	1.41	1.37
4	A	3005	FAD	C4-N3	2.56	1.37	1.33
4	A	3005	FAD	C9A-N10	2.40	1.41	1.38
8	A	1337	MTE	C4-N3	2.39	1.37	1.33
8	A	1337	MTE	C6-N5	2.37	1.48	1.45
10	A	1339	URC	C2-N3	2.34	1.39	1.34
5	A	1333	NAI	C6N-N1N	2.19	1.42	1.37
4	B	4005	FAD	C5X-N5	2.09	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1338	URC	O11-C2	2.07	1.27	1.23
5	B	1333	NAI	C2B-C1B	-2.02	1.50	1.53

All (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
10	A	1339	URC	N7-C8-N9	-8.94	100.37	108.76
5	A	1333	NAI	N3A-C2A-N1A	-7.06	117.64	128.68
4	A	3005	FAD	C4X-N5-C5X	6.79	123.55	116.77
5	B	1333	NAI	N3A-C2A-N1A	-6.78	118.08	128.68
4	B	4005	FAD	C4X-N5-C5X	6.45	123.22	116.77
4	B	4005	FAD	N3A-C2A-N1A	-6.31	118.81	128.68
4	B	4005	FAD	C1'-N10-C9A	6.20	123.17	118.29
4	A	3005	FAD	N3A-C2A-N1A	-6.15	119.06	128.68
4	A	3005	FAD	C4-N3-C2	5.96	120.18	115.14
4	A	3005	FAD	O3'-C3'-C2'	-5.23	96.18	108.81
10	B	1338	URC	C4-N9-C8	-5.19	109.36	112.89
4	A	3005	FAD	C10-C4X-N5	-4.93	117.85	121.26
8	B	1336	MTE	C4-C9-C10	4.52	118.58	114.57
5	A	1333	NAI	C1D-N1N-C2N	-4.50	113.61	121.11
5	B	1333	NAI	C1D-N1N-C2N	-4.45	113.70	121.11
4	B	4005	FAD	C4-N3-C2	4.31	118.78	115.14
4	B	4005	FAD	C10-C4X-N5	-4.25	118.32	121.26
4	A	3005	FAD	C4X-C4-N3	-4.19	117.69	123.43
4	B	4005	FAD	O3'-C3'-C2'	-3.83	99.55	108.81
4	A	3005	FAD	C1'-N10-C9A	3.81	121.29	118.29
4	A	3005	FAD	O2'-C2'-C1'	3.78	118.69	109.59
5	A	1333	NAI	O1N-PN-O2N	3.74	130.75	112.24
8	A	1337	MTE	C4-C9-N5	3.74	122.26	119.12
8	B	1336	MTE	C4-C9-N5	3.64	122.17	119.12
7	A	1335	GOL	O2-C2-C3	-3.60	93.27	109.12
10	A	1339	URC	C4-N9-C8	-3.53	110.49	112.89
5	B	1333	NAI	O1N-PN-O2N	3.37	128.91	112.24
4	B	4005	FAD	C4X-C4-N3	-3.35	118.85	123.43
4	B	4005	FAD	C5'-C4'-C3'	-3.32	105.79	112.20
5	B	1333	NAI	C2A-N1A-C6A	3.27	124.36	118.75
4	A	3005	FAD	C9A-C5X-N5	-3.20	117.36	122.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1333	NAI	O2B-C2B-C1B	-3.18	99.10	110.85
10	B	1338	URC	O24-C8-N7	3.12	130.41	125.94
10	B	1338	URC	O13-C6-N1	-3.12	115.46	121.01
10	B	1338	URC	C6-N1-C2	-3.09	122.11	126.25
10	B	1338	URC	O11-C2-N3	-3.07	116.80	122.92
8	A	1337	MTE	C9-C10-N8	3.05	120.92	118.13
8	A	1337	MTE	O2P-P-O4'	-3.04	98.66	106.73
4	A	3005	FAD	C5'-C4'-C3'	-3.03	106.35	112.20
8	B	1336	MTE	N3-C2-N1	-3.01	120.70	125.42
10	A	1339	URC	O24-C8-N7	2.99	130.23	125.94
4	A	3005	FAD	O4'-C4'-C3'	2.91	116.18	109.10
8	A	1337	MTE	O2P-P-O1P	2.83	121.77	110.68
4	A	3005	FAD	C6-C5X-C9A	2.77	122.69	119.05
4	B	4005	FAD	O4B-C1B-C2B	-2.76	102.89	106.93
4	B	4005	FAD	O2'-C2'-C3'	-2.76	102.40	109.10
8	A	1337	MTE	C2-N1-C10	2.75	120.69	114.54
5	B	1333	NAI	O4D-C1D-N1N	2.66	113.26	108.06
4	B	4005	FAD	C1'-N10-C10	-2.65	116.04	118.41
5	A	1333	NAI	C2A-N1A-C6A	2.63	123.25	118.75
8	A	1337	MTE	P-O4'-C4'	2.62	125.51	118.30
5	A	1333	NAI	O4D-C4D-C3D	-2.61	99.94	105.11
4	A	3005	FAD	O5'-C5'-C4'	-2.60	102.43	109.36
4	B	4005	FAD	C6-C5X-C9A	2.51	122.34	119.05
8	B	1336	MTE	C4-N3-C2	2.51	119.92	115.93
10	A	1339	URC	C6-N1-C2	-2.50	122.90	126.25
4	A	3005	FAD	O2'-C2'-C3'	-2.50	103.01	109.10
4	A	3005	FAD	C4-C4X-N5	2.49	121.44	118.60
8	A	1337	MTE	C10-N8-C7	-2.41	118.95	123.67
8	B	1336	MTE	C2-N1-C10	2.41	119.93	114.54
4	B	4005	FAD	C9A-C5X-N5	-2.41	118.60	122.36
10	B	1338	URC	O13-C6-C5	2.37	124.69	119.86
5	B	1333	NAI	C1D-N1N-C6N	-2.36	115.74	120.83
8	B	1336	MTE	O3'-C7-N8	2.35	110.99	108.57
10	B	1338	URC	N1-C2-N3	2.35	118.59	116.12
8	A	1337	MTE	N3-C2-N1	-2.31	121.79	125.42
8	A	1337	MTE	O3'-C7-C6	-2.28	107.44	108.96
8	A	1337	MTE	O3'-C7-N8	2.22	110.85	108.57
8	B	1336	MTE	P-O4'-C4'	2.16	124.24	118.30
4	B	4005	FAD	O3B-C3B-C4B	-2.14	104.86	111.05
5	B	1333	NAI	C3D-C2D-C1D	2.08	105.39	101.43
8	B	1336	MTE	C9-C10-N8	2.07	120.02	118.13
4	B	4005	FAD	C7-C6-C5X	-2.06	118.30	121.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1337	MTE	C4-N3-C2	2.06	119.20	115.93
5	A	1333	NAI	C1B-N9A-C4A	-2.00	123.12	126.64

There are no chirality outliers.

All (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
7	A	1335	GOL	C1-C2-C3-O3
7	B	1335	GOL	O1-C1-C2-C3
7	A	1336	GOL	O1-C1-C2-O2
8	A	1337	MTE	C3'-C4'-O4'-P
7	B	1335	GOL	O2-C2-C3-O3
7	B	1335	GOL	O1-C1-C2-O2
5	A	1333	NAI	O4D-C1D-N1N-C6N
7	A	1335	GOL	O1-C1-C2-C3
4	B	4005	FAD	C4'-C5'-O5'-P
5	B	1333	NAI	O4D-C4D-C5D-O5D
5	B	1333	NAI	O4D-C1D-N1N-C6N
5	A	1333	NAI	O4D-C4D-C5D-O5D

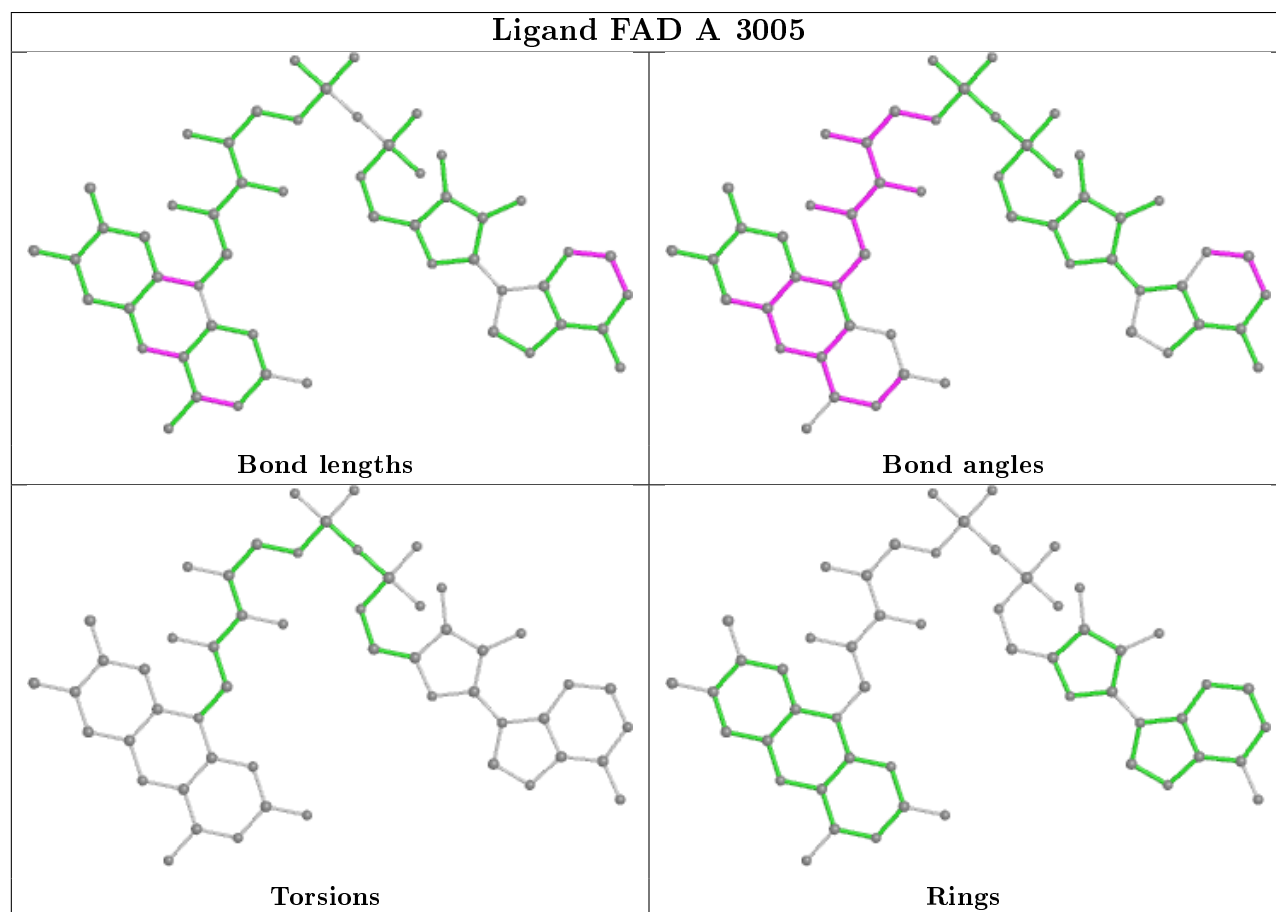
There are no ring outliers.

8 monomers are involved in 15 short contacts:

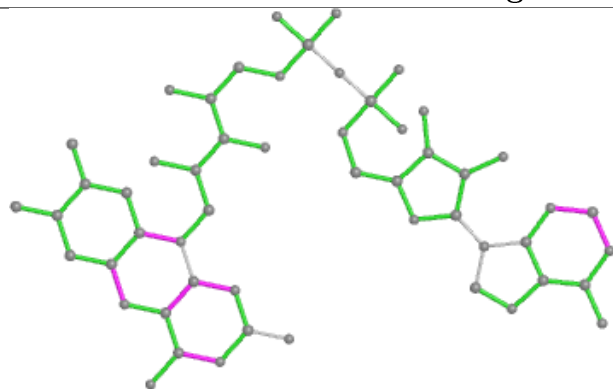
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3005	FAD	4	0
4	B	4005	FAD	6	0
9	B	1337	MOS	1	0
8	A	1337	MTE	1	0
9	A	1338	MOS	2	0
7	B	1335	GOL	1	0
5	A	1333	NAI	4	0
5	B	1333	NAI	3	0

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

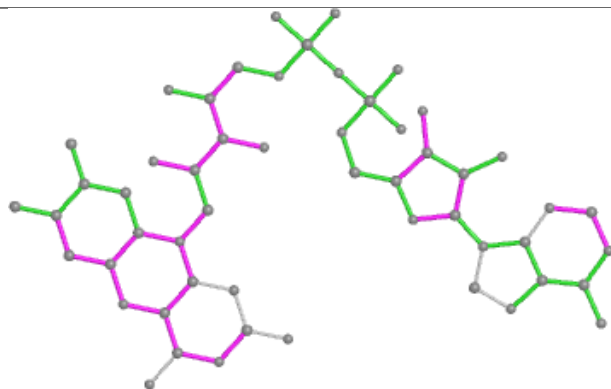
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



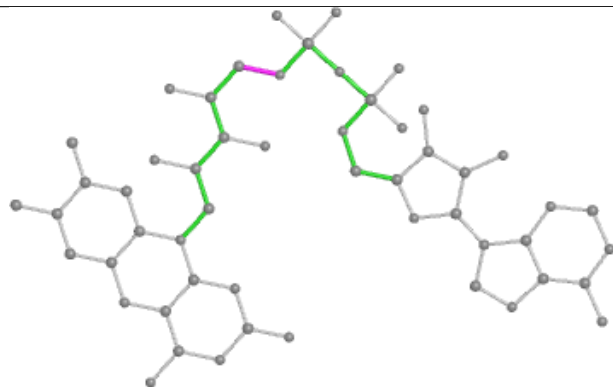
Ligand FAD B 4005



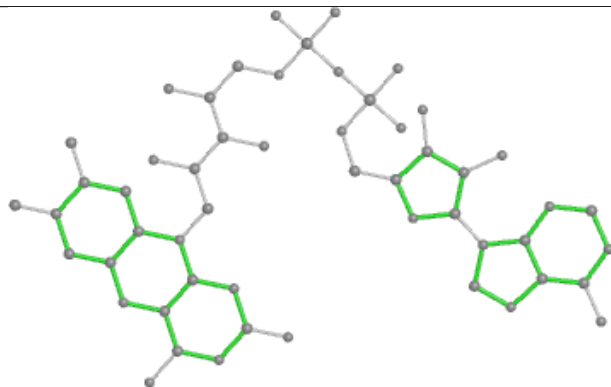
Bond lengths



Bond angles

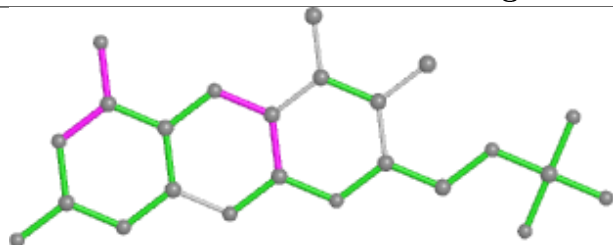


Torsions

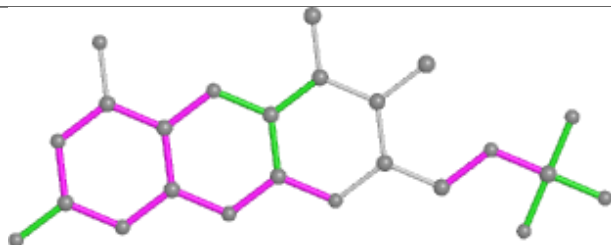


Rings

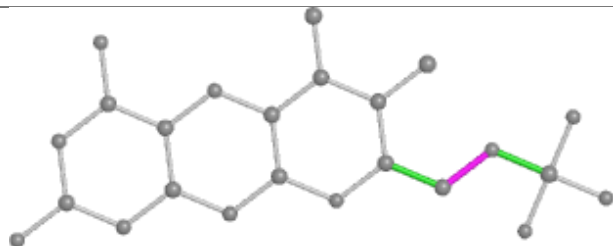
Ligand MTE B 1336



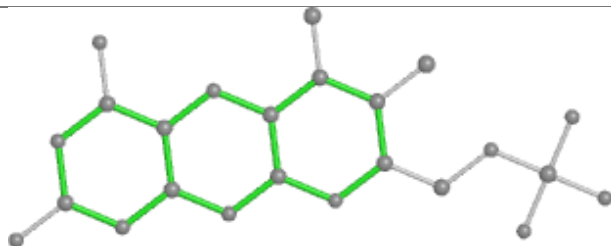
Bond lengths



Bond angles

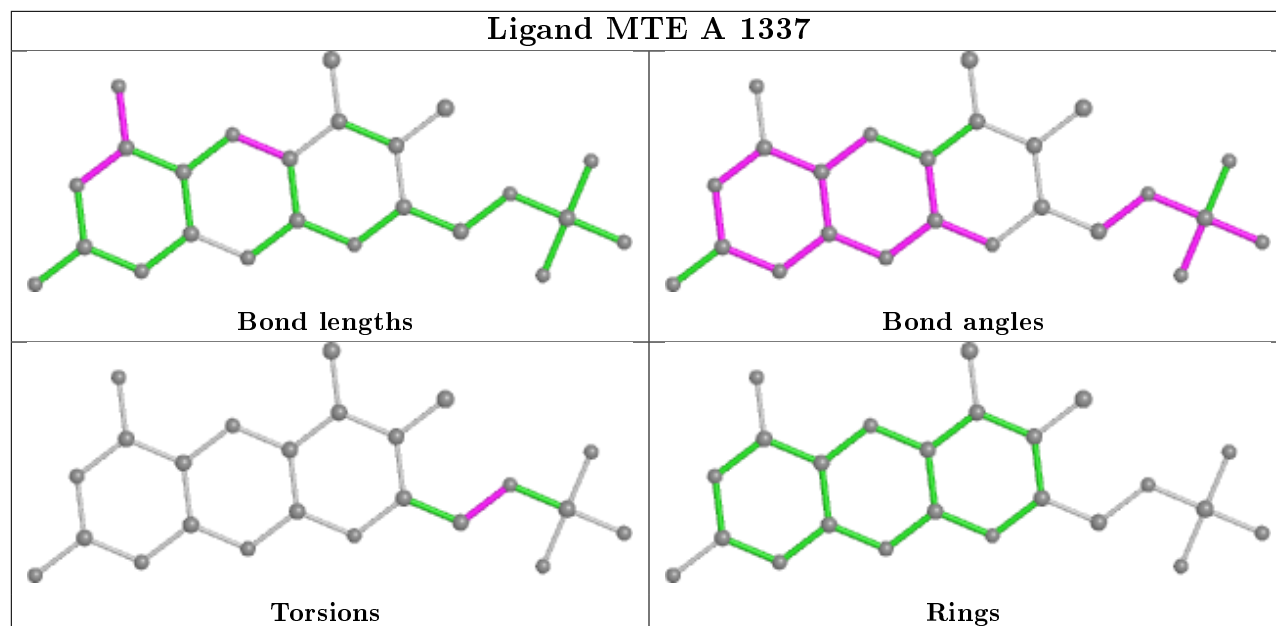


Torsions

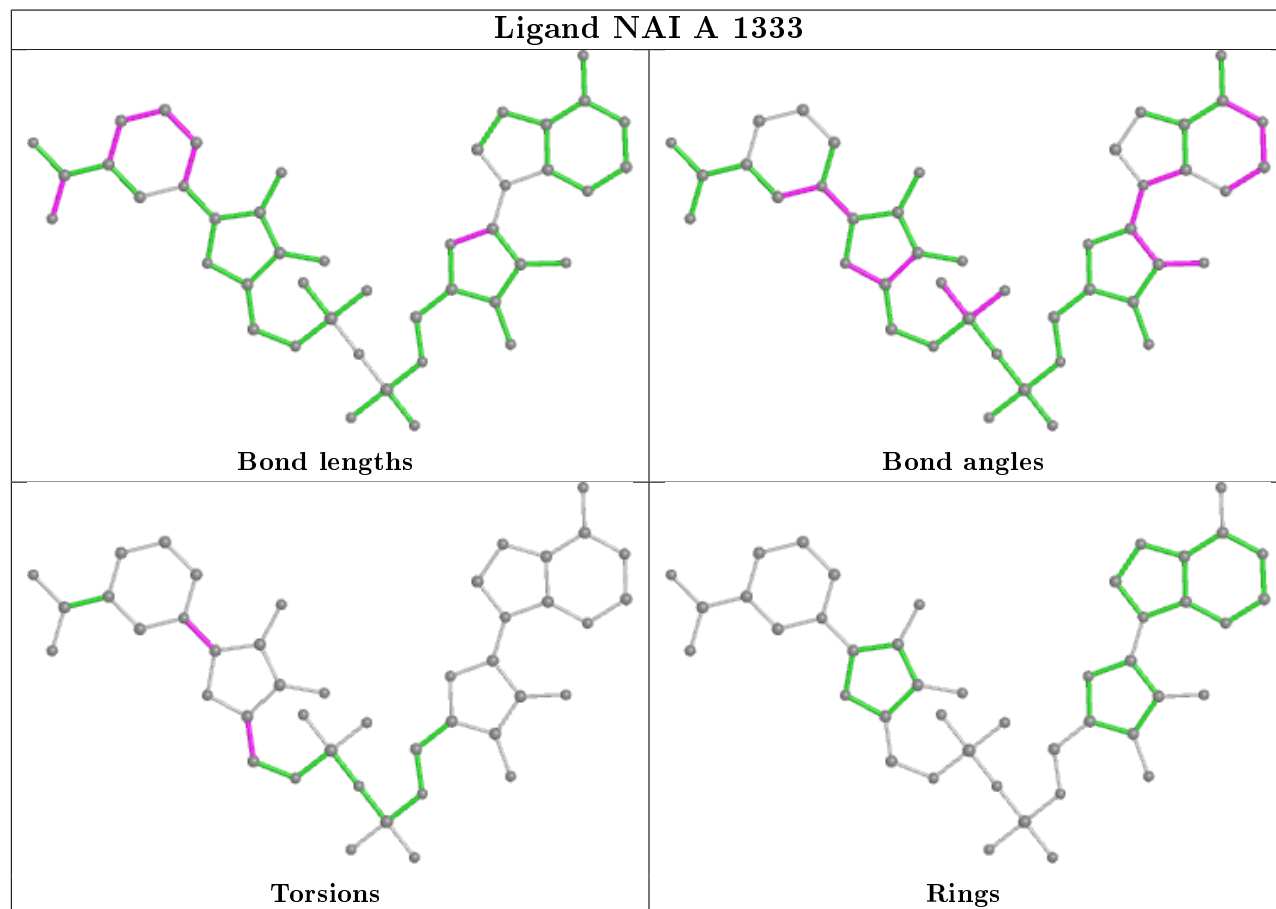


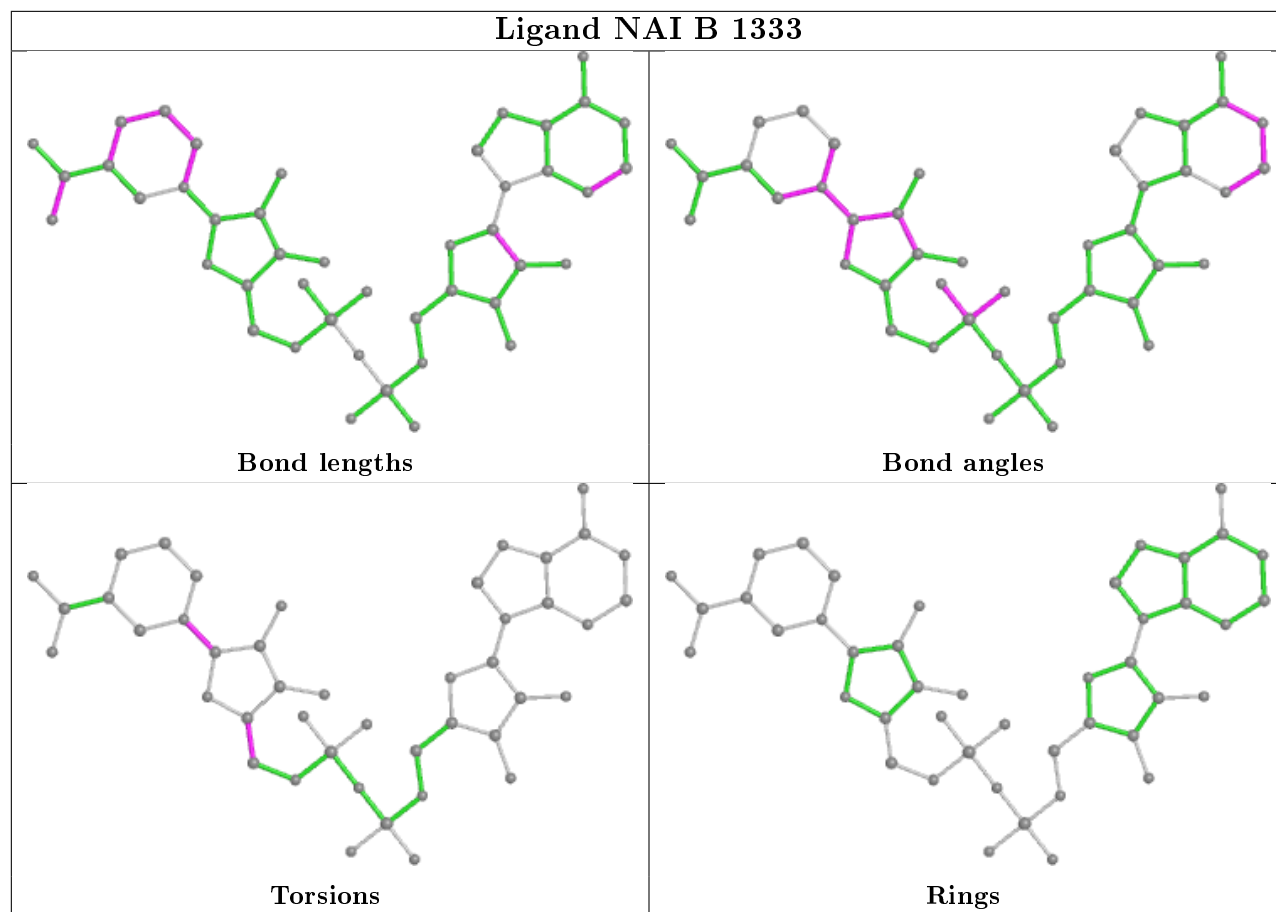
Rings

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 ⓘ

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	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

All (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
1	A	1287	ASN	4.4
1	A	1320	GLY	4.3
1	A	1319	THR	4.2
1	A	552	HIS	4.0
1	A	1318	VAL	4.0
1	A	528	GLY	3.9
1	A	378	GLY	3.8
1	A	60	ARG	3.6
1	B	60	ARG	3.6
1	B	1318	VAL	3.6
1	A	192	SER	3.5
1	A	566	GLY	3.5
1	B	192	SER	3.3
1	B	61	LEU	3.2
1	B	223	PRO	3.2
1	A	529	LYS	3.2
1	B	537	LYS	3.1
1	A	538	LEU	3.1
1	B	552	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1289	ASN	2.8
1	B	1286	THR	2.8
1	A	540	PRO	2.5
1	B	540	PRO	2.4
1	A	61	LEU	2.4
1	A	471	GLN	2.3
1	A	221	ASP	2.3
1	B	553	PRO	2.3
1	A	1290	THR	2.2
1	B	1111	GLY	2.2
1	A	63	ASP	2.2
1	B	221	ASP	2.2
1	A	498	PRO	2.2
1	A	1286	THR	2.1
1	A	705	ASN	2.1
1	B	1290	THR	2.0
1	B	569	LYS	2.0
1	B	1330	LEU	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 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.

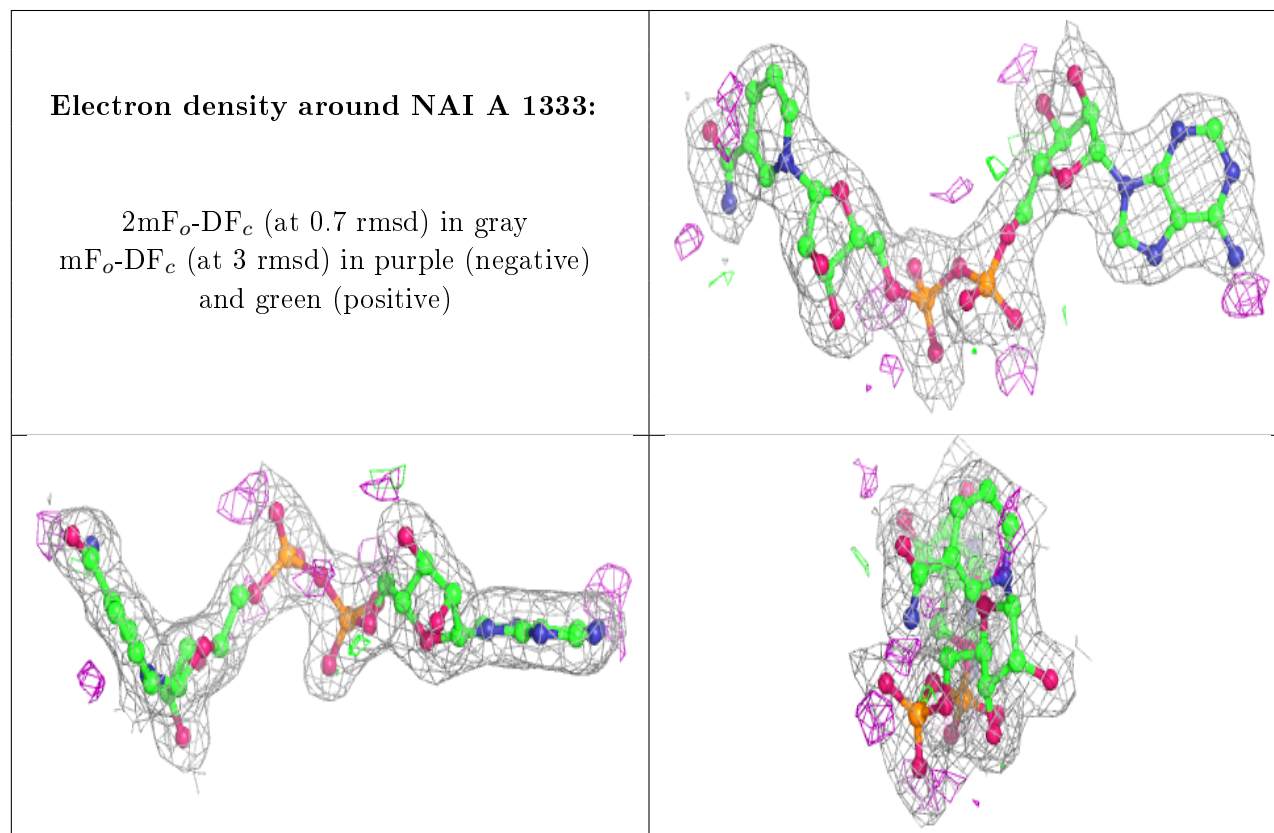
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	URC	A	1339	12/12	0.88	0.13	30,34,37,39	0
7	GOL	A	1335	6/6	0.91	0.14	28,39,39,41	0
10	URC	B	1338	12/12	0.91	0.16	31,38,41,43	0
7	GOL	B	1335	6/6	0.93	0.12	29,35,39,40	0
7	GOL	A	1336	6/6	0.96	0.11	23,27,31,32	0

Continued on next page...

Continued from previous page...

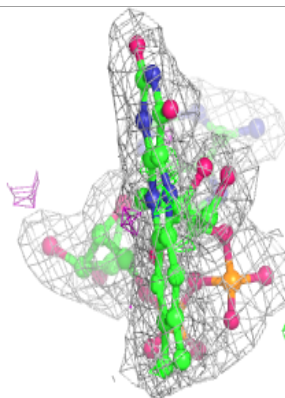
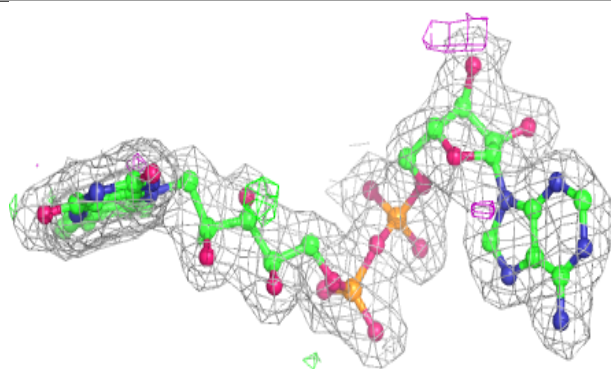
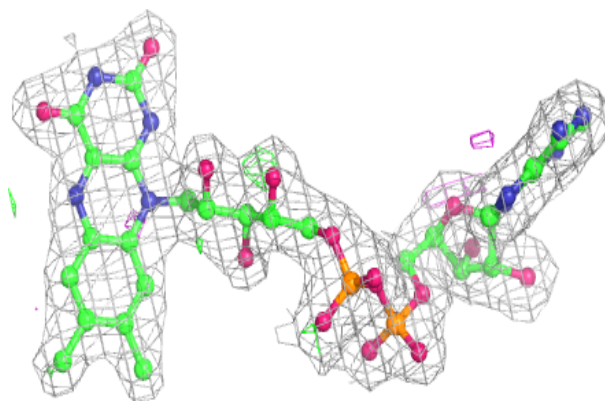
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAI	A	1333	44/44	0.96	0.08	18,25,29,33	0
6	BCT	A	1334	4/4	0.98	0.11	17,20,20,22	0
4	FAD	B	4005	53/53	0.98	0.10	15,18,21,28	0
8	MTE	A	1337	24/24	0.98	0.09	14,19,24,25	0
4	FAD	A	3005	53/53	0.98	0.11	14,19,24,28	0
5	NAI	B	1333	44/44	0.98	0.07	18,25,28,31	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.



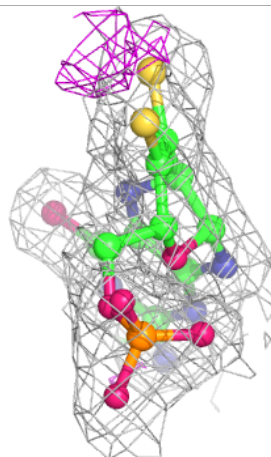
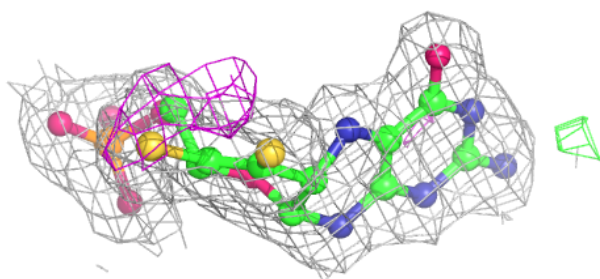
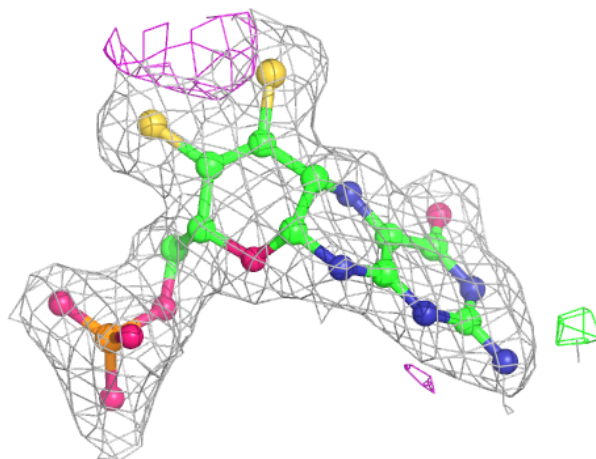
Electron density around FAD B 4005:

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



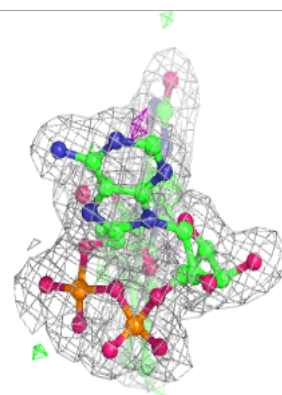
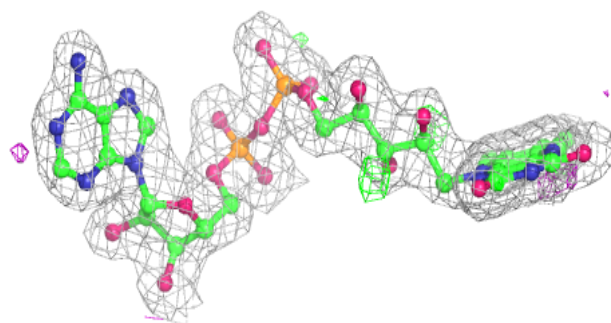
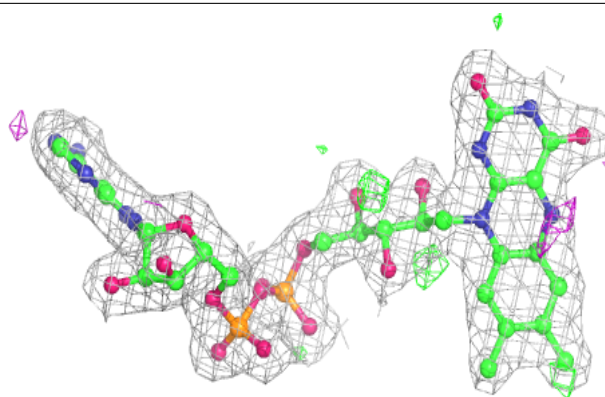
Electron density around MTE A 1337:

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

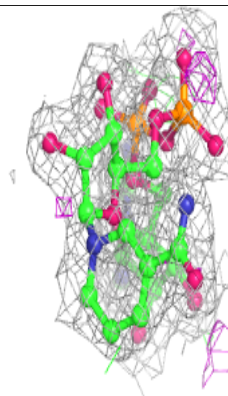
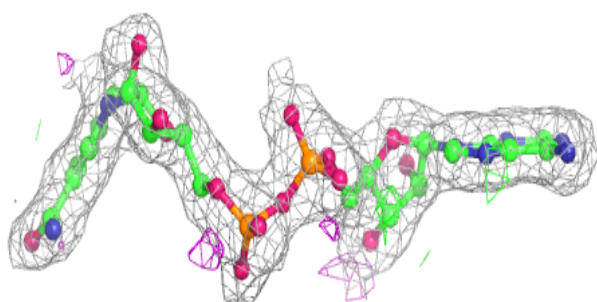
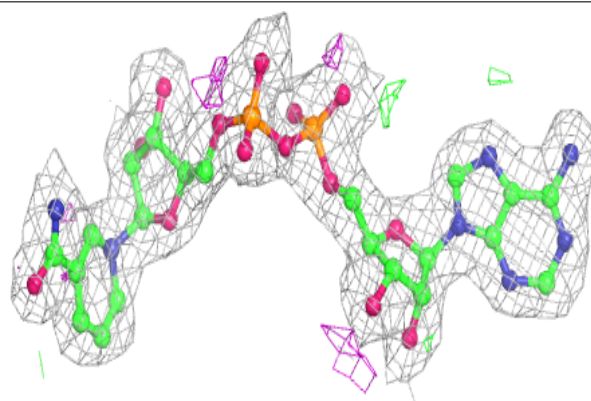


Electron density around FAD A 3005:

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

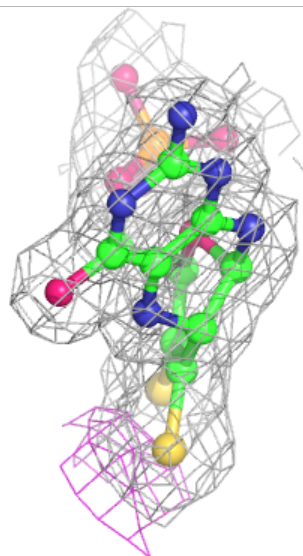
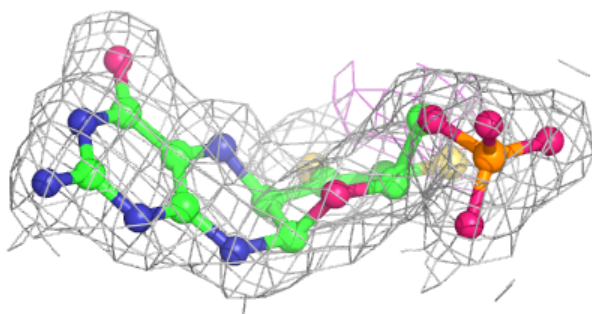
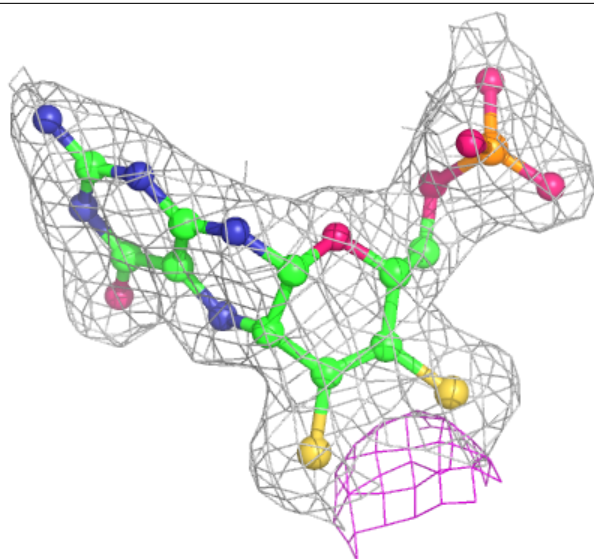
**Electron density around NAI B 1333:**

$2mF_o-DF_c$ (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.