Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 01:33 pm GMT

PDB ID	:	4UHX
Title	:	Human aldehyde oxidase in complex with phthalazine and thioridazine
Authors	:	Coelho, C.; Romao, M.J.; Santos-Silva, T.
Deposited on	:	2015-03-26
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

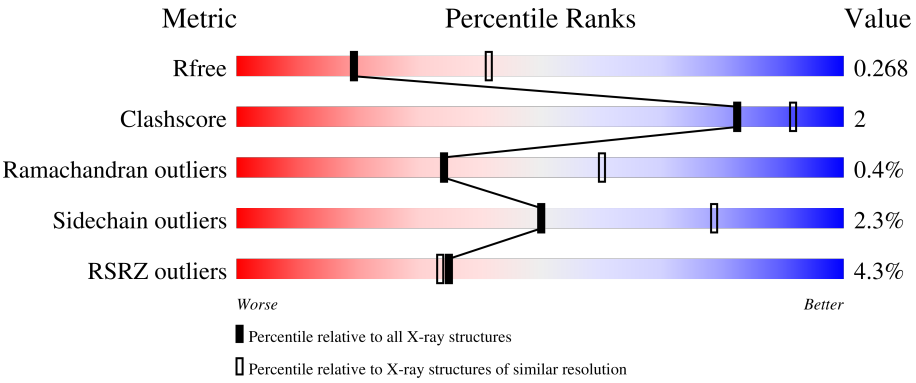
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	1338	4% 89% 7% .

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
6	4FT	A	3007	-	-	-	X

2 Entry composition

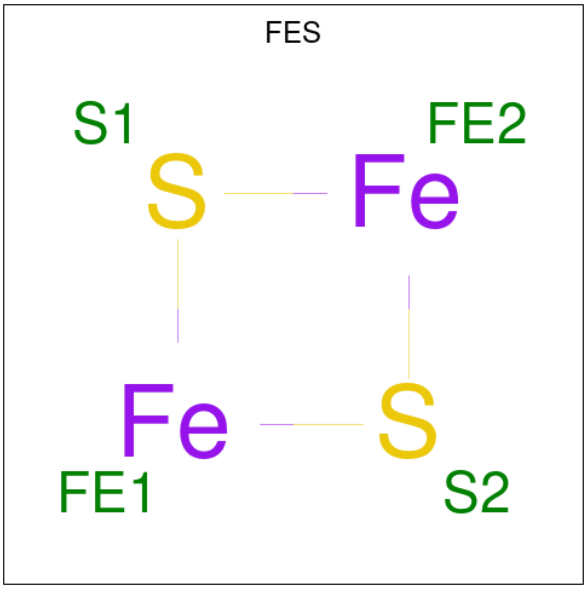
There are 10 unique types of molecules in this entry. The entry contains 10223 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALDEHYDE OXIDASE.

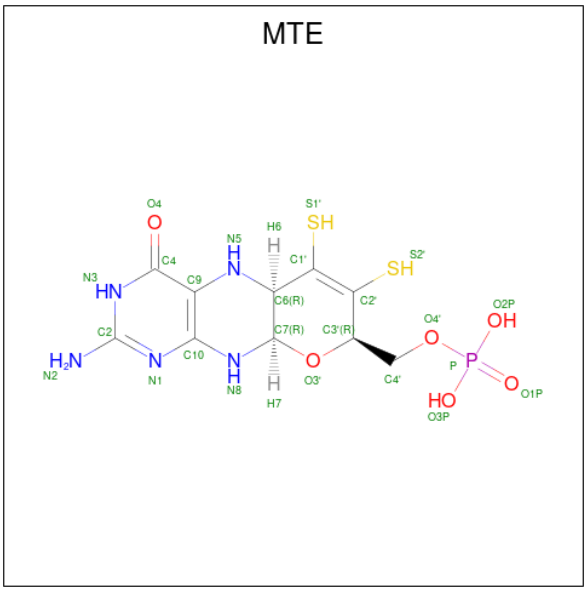
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1290	Total	C	N	O	S	0	0	0
			10000	6356	1724	1840	80			

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



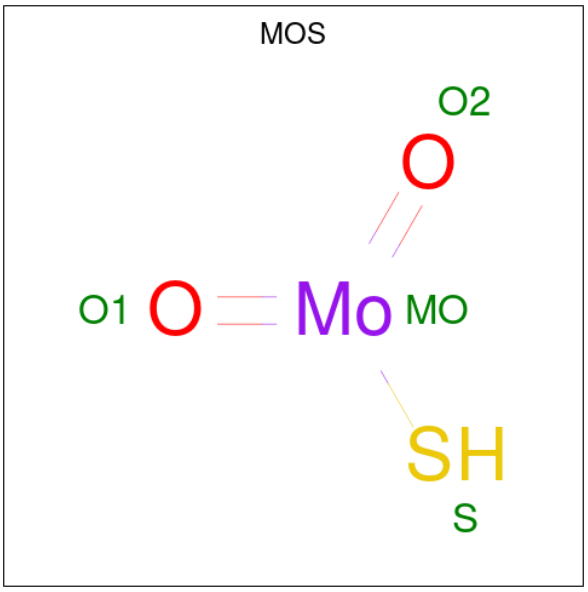
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 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: $C_{10}H_{14}N_5O_6PS_2$).



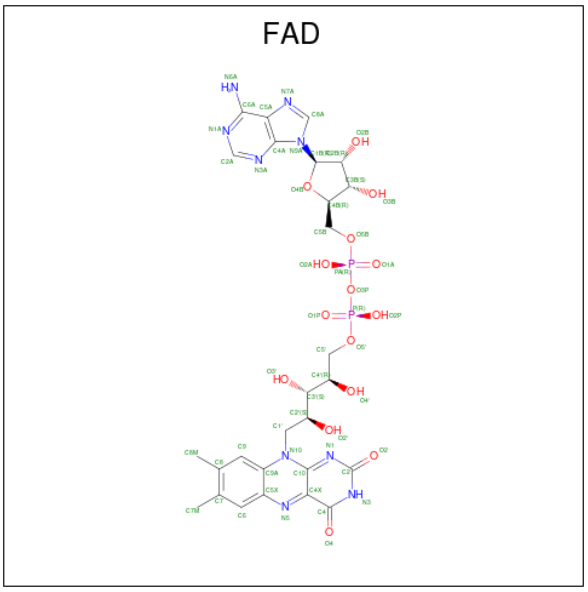
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



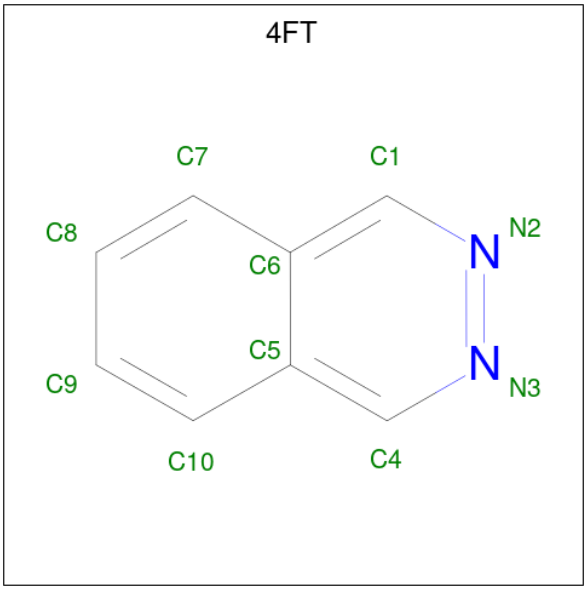
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



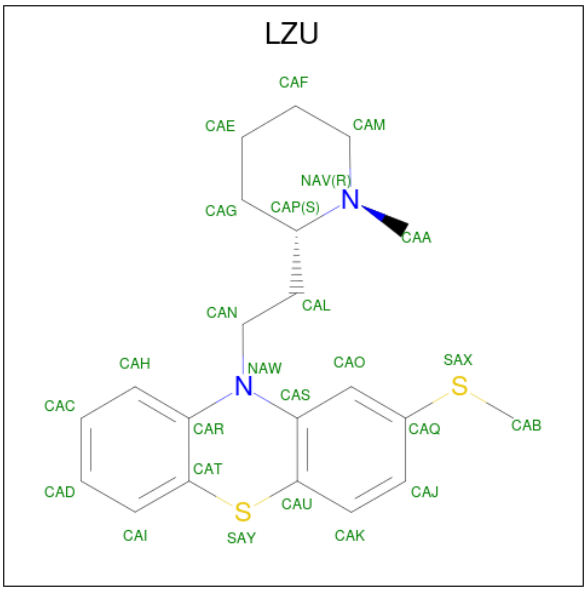
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is phthalazine (three-letter code: 4FT) (formula: $C_8H_6N_2$).



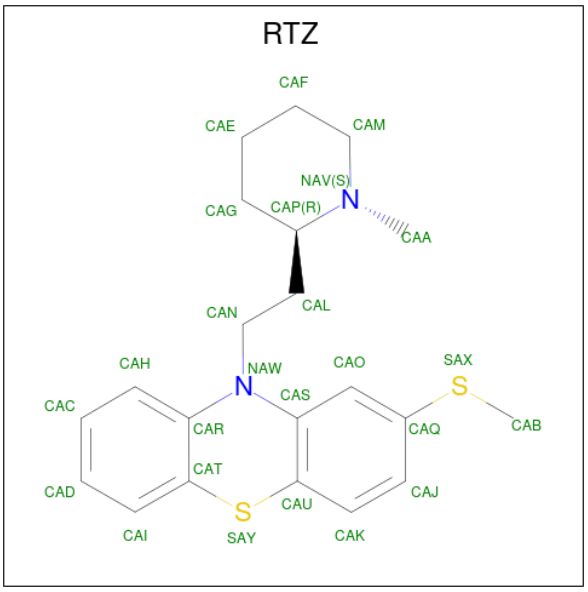
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N		0	0
			10	8	2			

- Molecule 7 is 10-{2-[(2S)-1-methylpiperidin-2-yl]ethyl}-2-(methylsulfanyl)-10H-phenothiazine (three-letter code: LZU) (formula: $C_{21}H_{26}N_2S_2$).



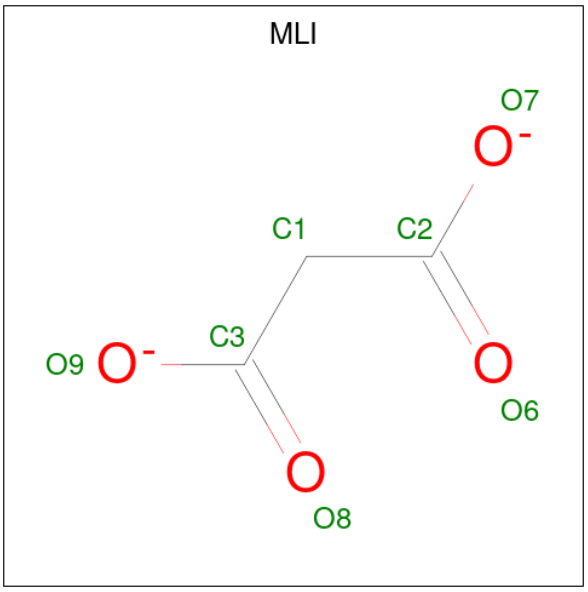
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
7	A	1	25	21	2	2	0	1

- Molecule 8 is 10-{2-[(2R)-1-methylpiperidin-2-yl]ethyl}-2-(methylsulfanyl)-10H-phenothiazine (three-letter code: RTZ) (formula: $C_{21}H_{26}N_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
8	A	1	25	21	2	2	0	1

- Molecule 9 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 7 3 4	0	0
9	A	1	Total C O 7 3 4	0	0

- Molecule 10 is water.

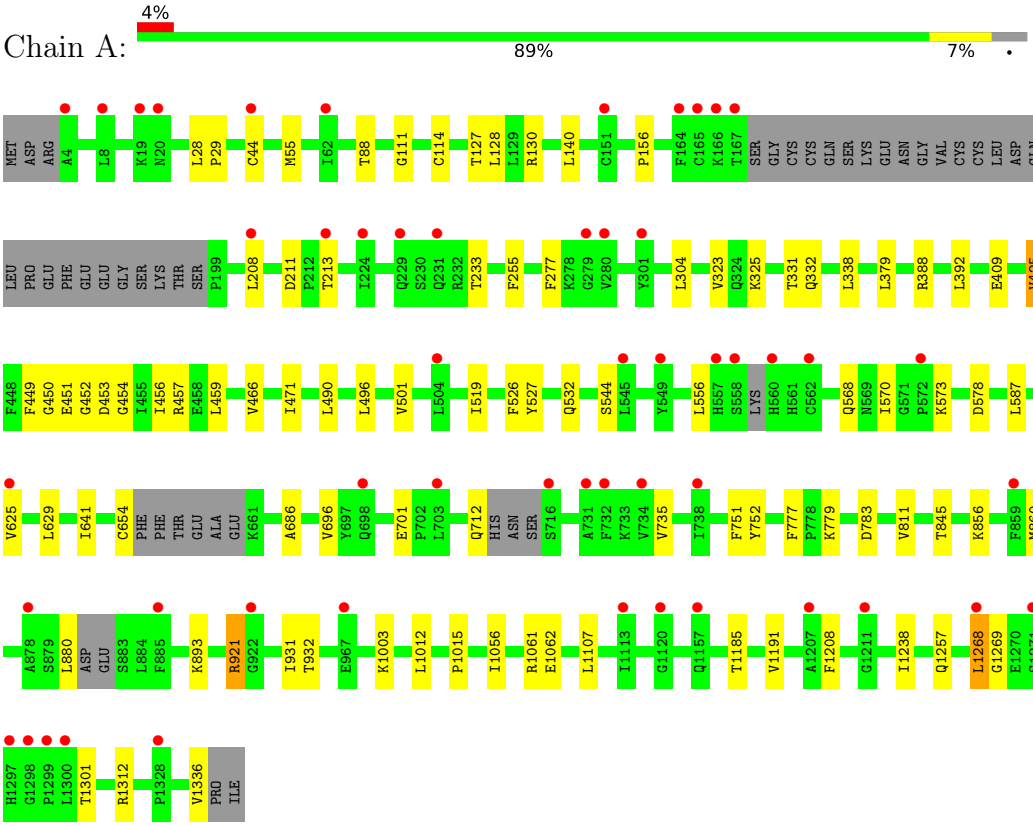
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	60	Total O 60 60	0	0

3 Residue-property plots (i)

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: ALDEHYDE OXIDASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	148.73Å 148.73Å 132.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.17 – 2.70 40.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (105.17-2.70) 99.8 (40.80-2.70)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.195 , 0.244 0.232 , 0.268	Depositor DCC
R_{free} test set	2085 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10223	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: RTZ, FES, 4FT, FAD, LZU, MOS, MLI, 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	0.36	0/10210	0.58	0/13805

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

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	10000	0	10065	44	0
2	A	8	0	0	0	0
3	A	24	0	10	0	0
4	A	4	0	0	1	0
5	A	53	0	31	0	0
6	A	10	0	6	0	0
7	A	25	0	26	2	0
8	A	25	0	26	3	0
9	A	14	0	4	0	0
10	A	60	0	0	0	0
All	All	10223	0	10168	50	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 2.

All (50) 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)
8:A:3009[B]:RTZ:HALA	8:A:3009[B]:RTZ:CAH	1.92	0.95
1:A:449:PHE:CE1	1:A:456:ILE:HG22	2.02	0.95
1:A:453:ASP:OD1	1:A:454:GLY:N	1.98	0.95
1:A:450:GLY:O	1:A:452:GLY:N	2.01	0.92
8:A:3009[B]:RTZ:HALA	8:A:3009[B]:RTZ:HAH	1.55	0.88
1:A:449:PHE:HE1	1:A:456:ILE:HG22	1.39	0.84
7:A:3008[A]:LZU:H20	7:A:3008[A]:LZU:CAH	2.19	0.71
8:A:3009[B]:RTZ:CAH	8:A:3009[B]:RTZ:CAL	2.69	0.68
4:A:3004:MOS:MO	4:A:3004:MOS:O2	1.72	0.60
1:A:379:LEU:HD21	1:A:392:LEU:HD12	1.86	0.58
1:A:466:VAL:HG11	1:A:519:ILE:HD11	1.85	0.58
1:A:453:ASP:CG	1:A:454:GLY:N	2.57	0.58
7:A:3008[A]:LZU:CAH	7:A:3008[A]:LZU:CAL	2.78	0.58
1:A:1185:THR:HG21	1:A:1208:PHE:CZ	2.40	0.56
1:A:870:MET:SD	1:A:931:ILE:HD13	2.46	0.55
1:A:433:ARG:NH1	1:A:1238:ILE:O	2.41	0.54
1:A:323:VAL:HG12	1:A:331:THR:HB	1.90	0.52
1:A:1191:VAL:HG23	1:A:1268:LEU:CD2	2.40	0.52
1:A:55:MET:CE	1:A:127:THR:HA	2.40	0.51
1:A:111:GLY:HA2	1:A:156:PRO:HB2	1.93	0.51
1:A:332:GLN:HG3	1:A:425:VAL:HG23	1.93	0.51
1:A:471:ILE:HD12	1:A:501:VAL:HG12	1.93	0.50
1:A:613:THR:HG22	1:A:686:ALA:HB1	1.93	0.50
1:A:501:VAL:HG23	1:A:501:VAL:O	2.13	0.48
1:A:447:VAL:HG12	1:A:459:LEU:CD1	2.44	0.47
1:A:578:ASP:OD2	1:A:1061:ARG:NH1	2.47	0.47
1:A:447:VAL:HG13	1:A:526:PHE:CZ	2.50	0.46
1:A:921:ARG:NE	1:A:1269:GLY:O	2.46	0.46
1:A:211:ASP:OD1	1:A:213:THR:HG22	2.15	0.46
1:A:1191:VAL:O	1:A:1191:VAL:HG22	2.14	0.46
1:A:233:THR:HG21	1:A:255:PHE:CE2	2.51	0.45
1:A:893:LYS:HG2	1:A:1015:PRO:HG2	1.99	0.45
1:A:570:ILE:HD11	1:A:573:LYS:HE3	1.98	0.45
1:A:625:VAL:HG23	1:A:696:VAL:HG23	1.98	0.45
1:A:55:MET:HE1	1:A:130:ARG:HG3	1.99	0.45
1:A:1012:LEU:HB2	1:A:1275:LEU:HD21	1.98	0.44
1:A:128:LEU:HD22	1:A:140:LEU:HA	1.99	0.44
1:A:629:LEU:HD22	1:A:641:ILE:HG21	1.99	0.44
1:A:587:LEU:HD11	1:A:1056:ILE:HG13	2.00	0.43
1:A:931:ILE:HD12	1:A:932:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LEU:HD11	1:A:527:TYR:CG	2.55	0.42
1:A:28:LEU:HB3	1:A:29:PRO:HD3	2.02	0.42
1:A:450:GLY:C	1:A:452:GLY:N	2.73	0.42
1:A:388:ARG:NH1	1:A:409:GLU:OE2	2.53	0.41
1:A:449:PHE:O	1:A:457:ARG:HD2	2.20	0.41
1:A:625:VAL:CG2	1:A:696:VAL:HG23	2.50	0.41
1:A:556:LEU:HD11	1:A:1003:LYS:HE3	2.03	0.41
1:A:735:VAL:HA	1:A:860:MET:CE	2.51	0.41
1:A:779:LYS:NZ	1:A:783:ASP:OD2	2.53	0.41
1:A:1062:GLU:O	1:A:1107:LEU:HD11	2.21	0.40

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	1278/1338 (96%)	1237 (97%)	36 (3%)	5 (0%)	34 60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	GLU
1	A	1257	GLN
1	A	532	GLN
1	A	921	ARG
1	A	811	VAL

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	1094/1136 (96%)	1069 (98%)	25 (2%)	50 78

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	CYS
1	A	88	THR
1	A	114	CYS
1	A	208	LEU
1	A	277	PHE
1	A	304	LEU
1	A	325	LYS
1	A	338	LEU
1	A	425	VAL
1	A	496	LEU
1	A	544	SER
1	A	568	GLN
1	A	654	CYS
1	A	701	GLU
1	A	712	GLN
1	A	751	PHE
1	A	752	TYR
1	A	777	PHE
1	A	845	THR
1	A	856	LYS
1	A	880	LEU
1	A	1268	LEU
1	A	1301	THR
1	A	1312	ARG
1	A	1336	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	147	ASN
1	A	231	GLN
1	A	568	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
8	RTZ	A	3009[B]	-	27,28,28	1.67	5 (18%)	35,39,39	1.34	6 (17%)
9	MLI	A	3010	-	6,6,6	1.15	0	7,7,7	1.21	1 (14%)
3	MTE	A	3003	4	21,26,26	1.59	2 (9%)	21,40,40	2.02	6 (28%)
2	FES	A	3002	1	0,4,4	-	-	-		
9	MLI	A	3011	-	6,6,6	1.12	0	7,7,7	0.91	0
6	4FT	A	3007	-	11,11,11	1.35	1 (9%)	14,14,14	1.55	2 (14%)
2	FES	A	3001	1	0,4,4	-	-	-		
4	MOS	A	3004	3	0,3,3	-	-	-		
5	FAD	A	3006	-	53,58,58	1.43	8 (15%)	68,89,89	1.34	10 (14%)
7	LZU	A	3008[A]	-	27,28,28	1.65	4 (14%)	35,39,39	1.26	3 (8%)

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
8	RTZ	A	3009[B]	-	-	6/7/30/30	0/4/4/4
3	MTE	A	3003	4	-	1/6/34/34	0/3/3/3
7	LZU	A	3008[A]	-	-	5/7/30/30	0/4/4/4
2	FES	A	3002	1	-	-	0/1/1/1
9	MLI	A	3011	-	-	0/4/4/4	-
6	4FT	A	3007	-	-	-	0/2/2/2
2	FES	A	3001	1	-	-	0/1/1/1
5	FAD	A	3006	-	-	0/30/50/50	0/6/6/6
9	MLI	A	3010	-	-	0/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3008[A]	LZU	CAT-SAY	-5.89	1.66	1.76
5	A	3006	FAD	C9A-C5X	5.82	1.50	1.41
8	A	3009[B]	RTZ	CAT-SAY	-5.70	1.66	1.76
3	A	3003	MTE	C9-C4	5.24	1.48	1.41
3	A	3003	MTE	C9-C10	3.85	1.48	1.41
5	A	3006	FAD	C8-C7	3.74	1.50	1.40
8	A	3009[B]	RTZ	CAS-NAW	-3.36	1.35	1.40
7	A	3008[A]	LZU	CAR-NAW	-3.15	1.35	1.40
7	A	3008[A]	LZU	CAS-NAW	-3.13	1.35	1.40
7	A	3008[A]	LZU	CAU-SAY	-3.10	1.70	1.76
8	A	3009[B]	RTZ	CAR-NAW	-3.06	1.35	1.40
8	A	3009[B]	RTZ	CAU-SAY	-3.03	1.71	1.76
5	A	3006	FAD	C5A-C4A	2.64	1.47	1.40
5	A	3006	FAD	C10-N10	2.29	1.42	1.37
5	A	3006	FAD	C4X-N5	2.29	1.35	1.30
5	A	3006	FAD	C4-N3	-2.29	1.34	1.38
6	A	3007	4FT	C1-N2	2.18	1.35	1.31
5	A	3006	FAD	C2A-N3A	2.06	1.35	1.32
8	A	3009[B]	RTZ	CAG-CAP	2.06	1.57	1.52
5	A	3006	FAD	C5X-N5	-2.02	1.35	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	3008[A]	LZU	CAM-NAV-CAP	-5.42	102.34	112.75
3	A	3003	MTE	C4-C9-N5	4.75	123.11	119.12
8	A	3009[B]	RTZ	CAE-CAF-CAM	-4.28	102.90	111.19
3	A	3003	MTE	C2-N3-C4	3.88	122.09	115.93
5	A	3006	FAD	N3A-C2A-N1A	-3.80	122.73	128.68
6	A	3007	4FT	C5-C4-N3	-3.78	120.60	124.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	3007	4FT	C6-C1-N2	-3.74	120.64	124.56
5	A	3006	FAD	P-O3P-PA	-3.08	122.26	132.83
5	A	3006	FAD	C4X-C10-N1	-3.04	117.67	124.73
8	A	3009[B]	RTZ	CAF-CAM-NAV	-2.96	106.49	111.35
3	A	3003	MTE	C2-N1-C10	2.95	121.16	114.54
8	A	3009[B]	RTZ	CAM-NAV-CAP	-2.76	107.45	112.75
3	A	3003	MTE	O3'-C7-N8	2.62	111.26	108.57
5	A	3006	FAD	C4A-C5A-N7A	-2.55	106.74	109.40
5	A	3006	FAD	C10-N1-C2	2.55	122.00	116.90
5	A	3006	FAD	C4-C4X-N5	2.48	121.76	118.23
3	A	3003	MTE	C10-C9-C4	2.42	116.72	114.57
7	A	3008[A]	LZU	CAN-NAW-CAS	2.35	122.08	119.03
8	A	3009[B]	RTZ	CAB-SAX-CAQ	2.32	108.96	103.38
8	A	3009[B]	RTZ	CAL-CAP-CAG	-2.29	109.09	112.58
7	A	3008[A]	LZU	CAB-SAX-CAQ	2.22	108.72	103.38
5	A	3006	FAD	C4X-C10-N10	2.18	119.67	116.48
3	A	3003	MTE	O3'-C7-C6	-2.17	107.51	108.96
8	A	3009[B]	RTZ	CAF-CAE-CAG	-2.17	106.99	111.42
5	A	3006	FAD	C2A-N1A-C6A	2.11	122.36	118.75
5	A	3006	FAD	O4-C4-C4X	-2.10	121.02	126.60
9	A	3010	MLI	O7-C2-C1	2.05	121.09	114.54
5	A	3006	FAD	O2-C2-N1	-2.04	118.45	121.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	3008[A]	LZU	CAP-CAL-CAN-NAW
7	A	3008[A]	LZU	CAL-CAN-NAW-CAR
8	A	3009[B]	RTZ	CAN-CAL-CAP-CAG
8	A	3009[B]	RTZ	CAN-CAL-CAP-NAV
8	A	3009[B]	RTZ	CAL-CAN-NAW-CAR
8	A	3009[B]	RTZ	CAL-CAN-NAW-CAS
3	A	3003	MTE	C3'-C4'-O4'-P
7	A	3008[A]	LZU	CAL-CAN-NAW-CAS
7	A	3008[A]	LZU	CAJ-CAQ-SAX-CAB
8	A	3009[B]	RTZ	CAJ-CAQ-SAX-CAB
8	A	3009[B]	RTZ	CAO-CAQ-SAX-CAB
7	A	3008[A]	LZU	CAO-CAQ-SAX-CAB

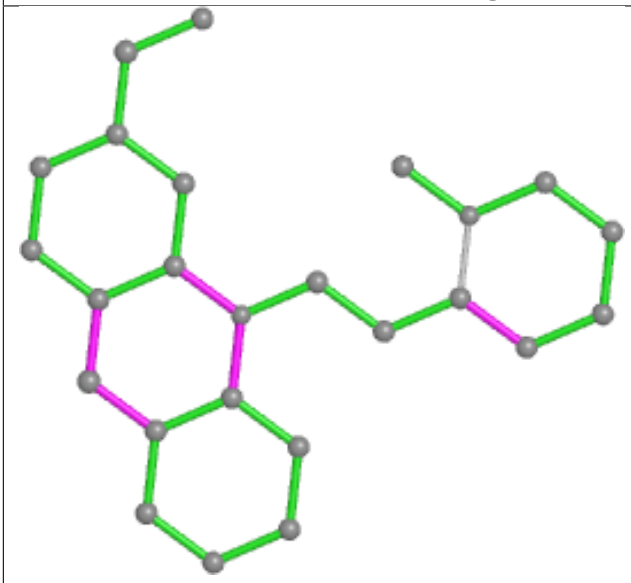
There are no ring outliers.

3 monomers are involved in 6 short contacts:

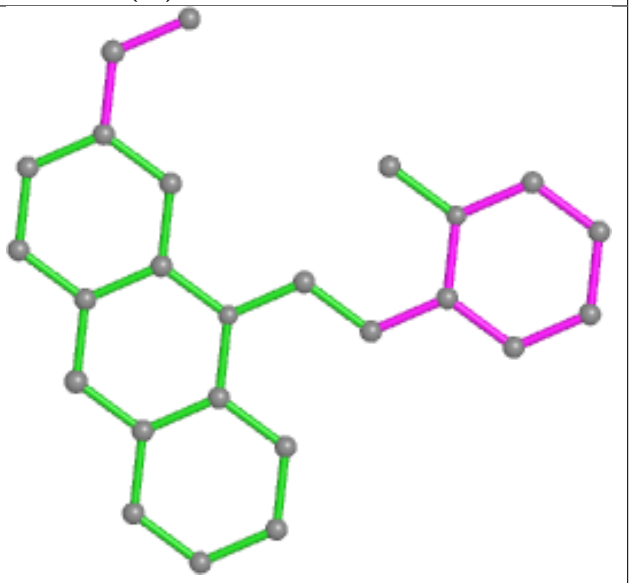
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	3009[B]	RTZ	3	0
4	A	3004	MOS	1	0
7	A	3008[A]	LZU	2	0

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 then 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.

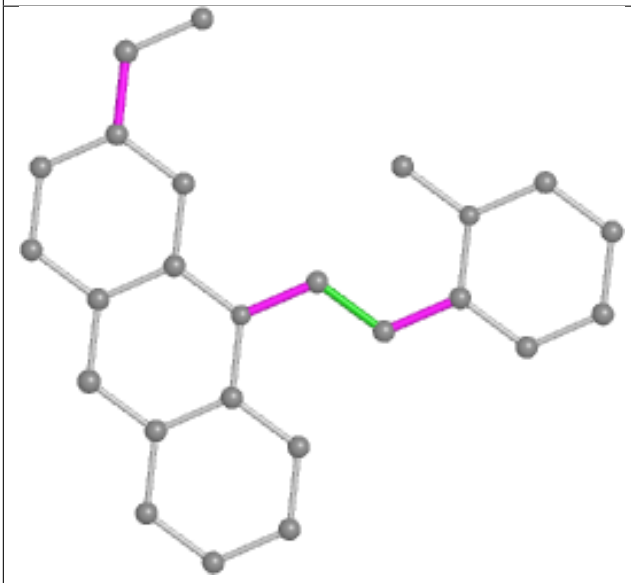
Ligand RTZ A 3009 (B)



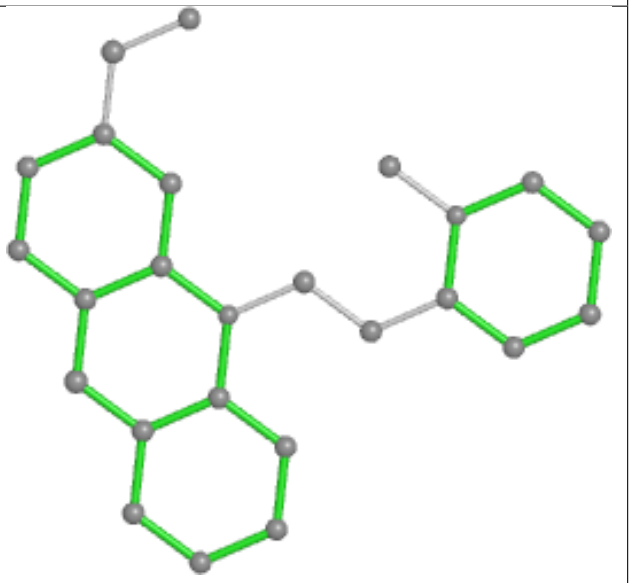
Bond lengths



Bond angles

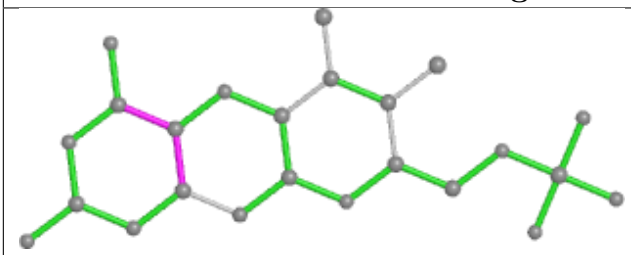


Torsions

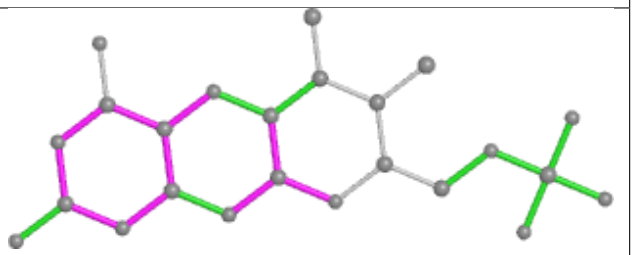


Rings

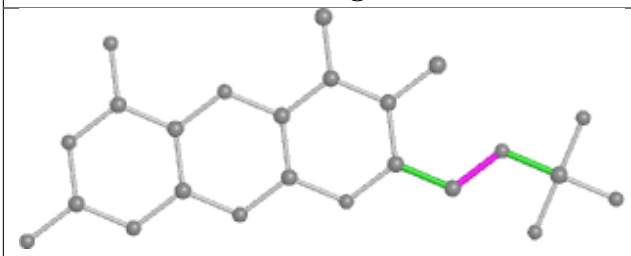
Ligand MTE A 3003



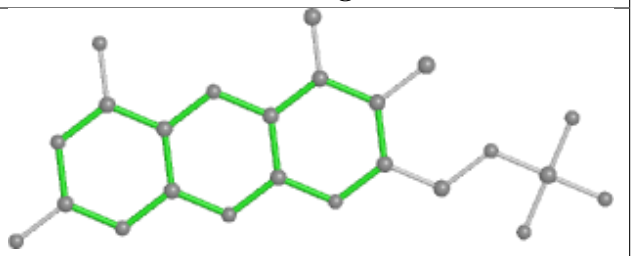
Bond lengths



Bond angles

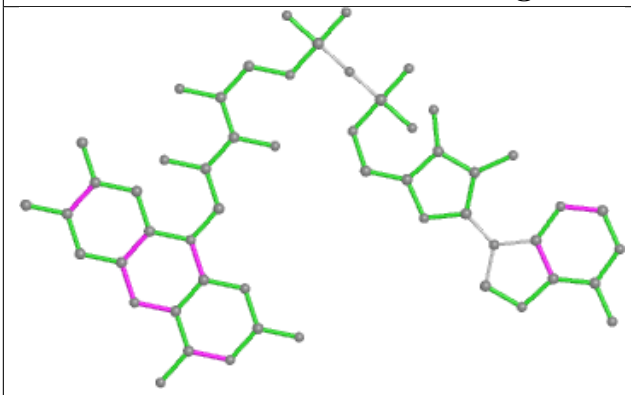


Torsions

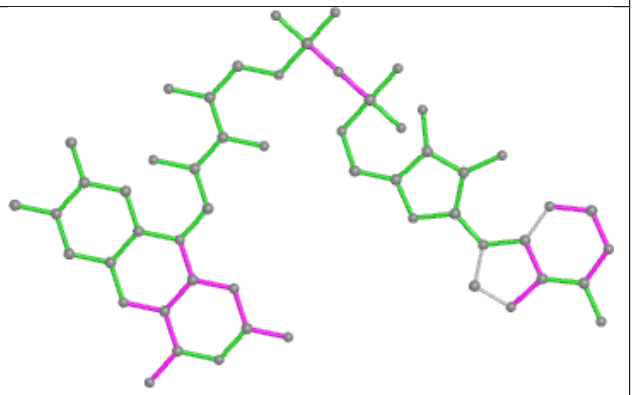


Rings

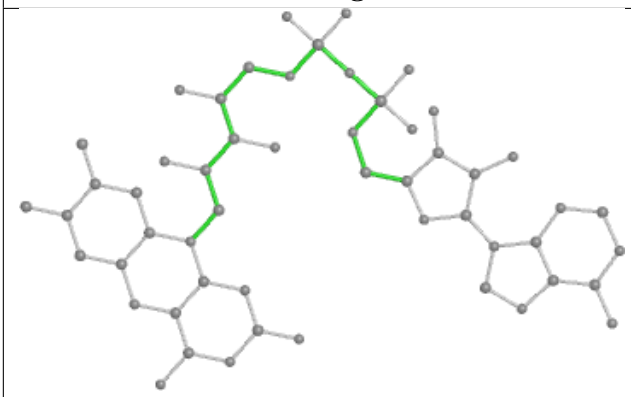
Ligand FAD A 3006



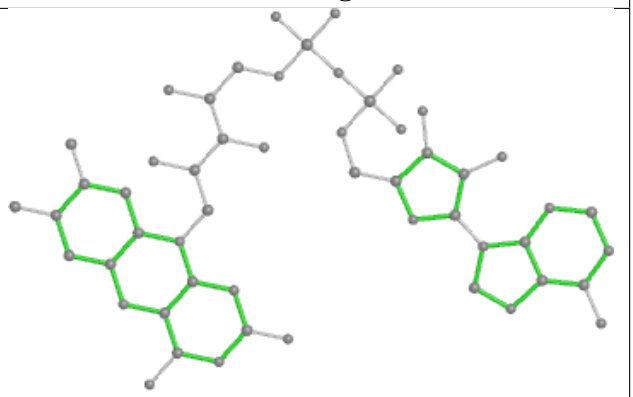
Bond lengths



Bond angles

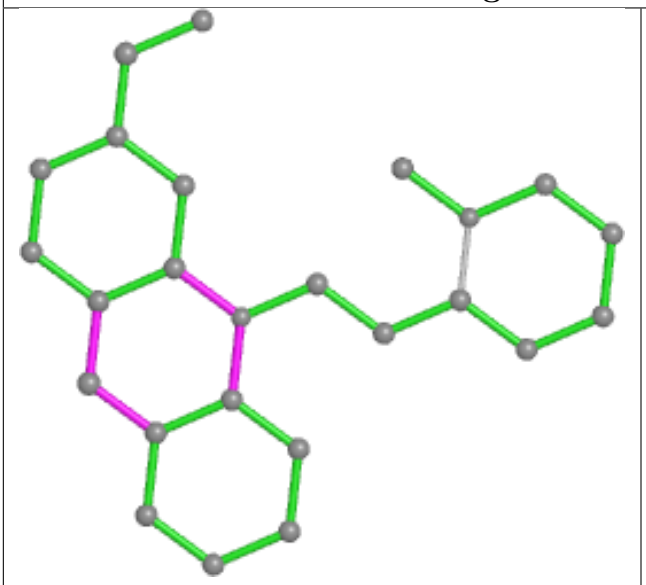


Torsions

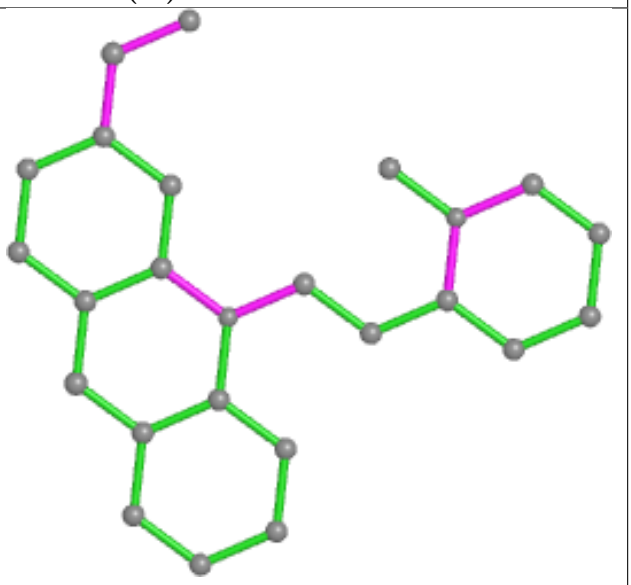


Rings

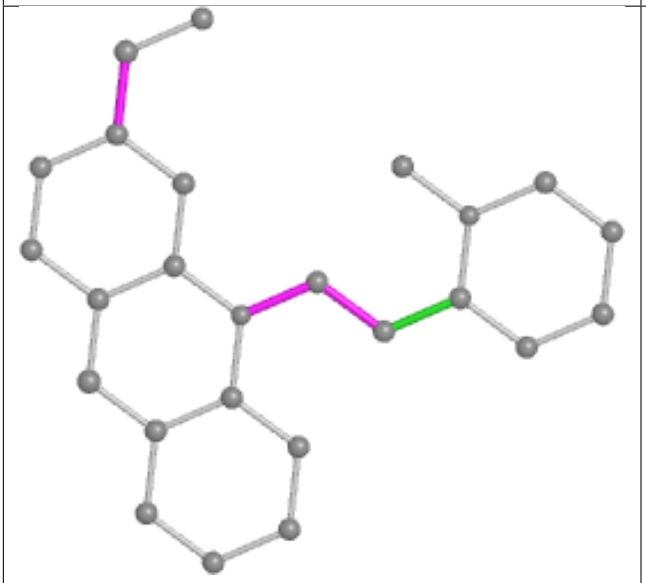
Ligand LZU A 3008 (A)



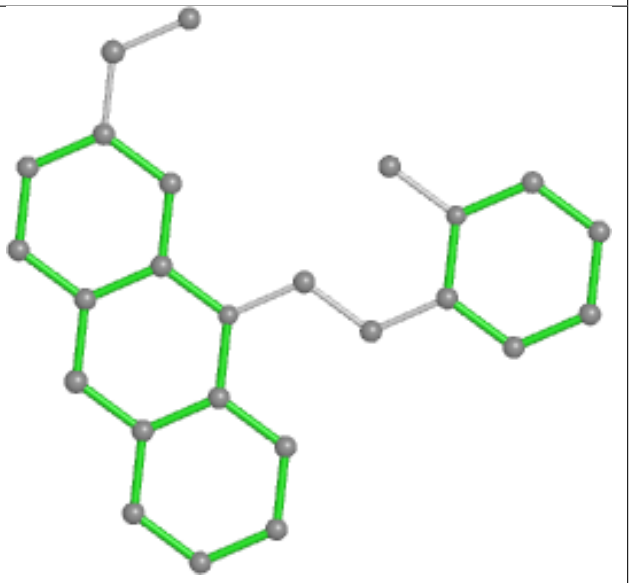
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1290/1338 (96%)	0.31	56 (4%) 35 33	48, 76, 106, 134	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	557	HIS	5.5
1	A	167	THR	4.0
1	A	731	ALA	3.7
1	A	967	GLU	3.7
1	A	734	VAL	3.6
1	A	1299	PRO	3.6
1	A	1328	PRO	3.5
1	A	572	PRO	3.4
1	A	8	LEU	3.4
1	A	738	ILE	3.4
1	A	4	ALA	3.4
1	A	1296	LEU	3.3
1	A	301	TYR	3.2
1	A	549	TYR	3.2
1	A	208	LEU	3.2
1	A	732	PHE	3.2
1	A	229	GLN	3.2
1	A	1271	SER	3.1
1	A	213	THR	3.1
1	A	560	HIS	3.1
1	A	868	LEU	3.0
1	A	280	VAL	2.9
1	A	166	LYS	2.8
1	A	623	LYS	2.8
1	A	279	GLY	2.8
1	A	558	SER	2.8
1	A	62	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1300	LEU	2.8
1	A	625	VAL	2.6
1	A	1297	HIS	2.6
1	A	1207	ALA	2.6
1	A	44	CYS	2.5
1	A	1157	GLN	2.5
1	A	19	LYS	2.5
1	A	164	PHE	2.5
1	A	545	LEU	2.4
1	A	716	SER	2.4
1	A	624	ILE	2.4
1	A	562	CYS	2.4
1	A	878	ALA	2.3
1	A	885	PHE	2.3
1	A	922	GLY	2.3
1	A	698	GLN	2.2
1	A	703	LEU	2.2
1	A	224	ILE	2.2
1	A	1268	LEU	2.2
1	A	1211	GLY	2.2
1	A	165	CYS	2.2
1	A	231	GLN	2.1
1	A	504	LEU	2.1
1	A	1113	ILE	2.1
1	A	20	ASN	2.1
1	A	1298	GLY	2.1
1	A	1120	GLY	2.1
1	A	859	PHE	2.0
1	A	151	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

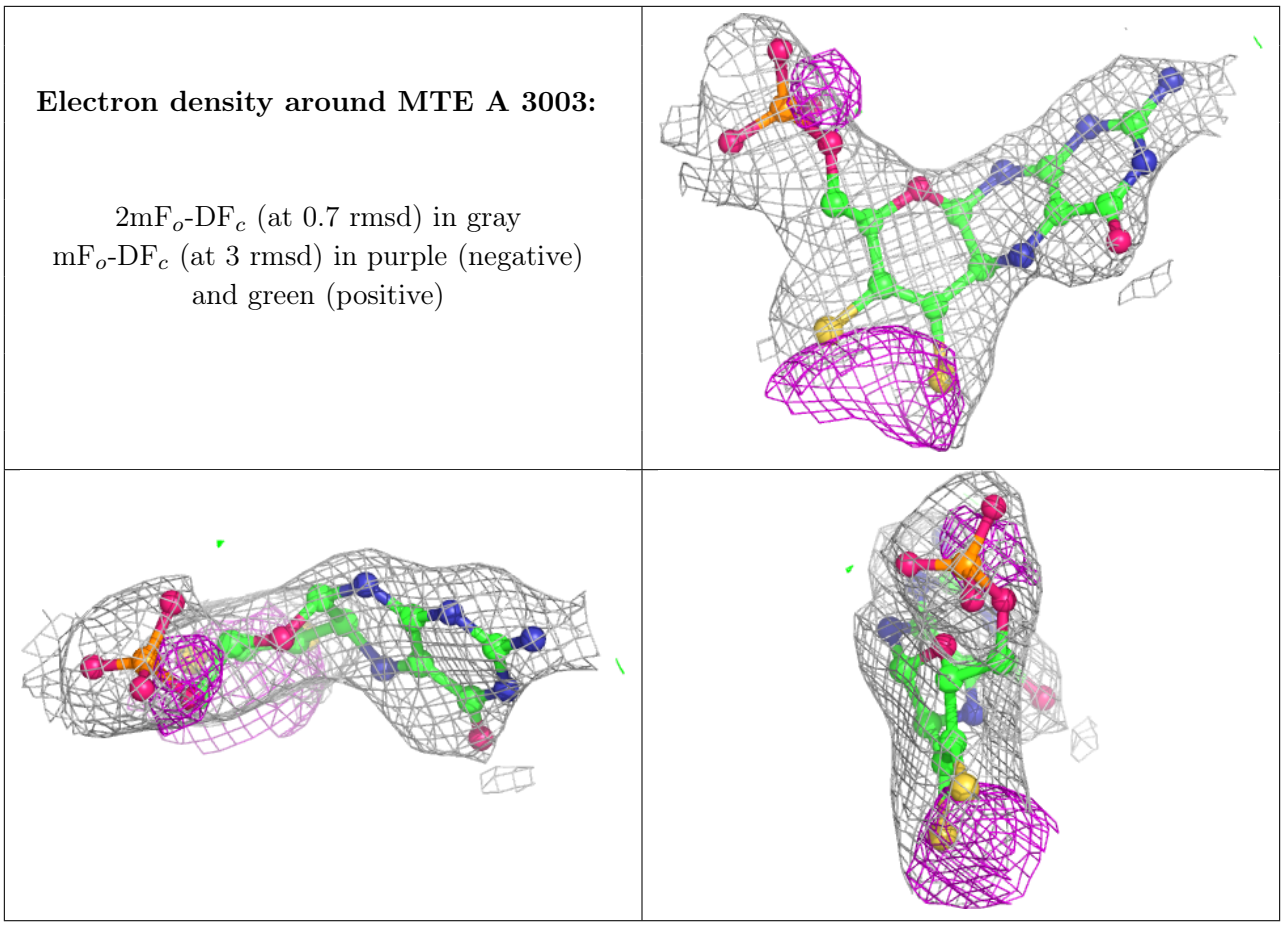
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	4FT	A	3007	10/10	0.74	0.41	102,102,103,103	0
9	MLI	A	3010	7/7	0.80	0.38	62,64,64,64	7
9	MLI	A	3011	7/7	0.84	0.53	67,68,69,71	7
3	MTE	A	3003	24/24	0.90	0.19	79,85,87,89	0
8	RTZ	A	3009[B]	25/25	0.93	0.19	74,84,88,89	25
4	MOS	A	3004	4/4	0.93	0.19	110,113,113,115	1
7	LZU	A	3008[A]	25/25	0.93	0.18	80,92,98,100	25
5	FAD	A	3006	53/53	0.94	0.20	55,60,67,68	0
2	FES	A	3001	4/4	0.95	0.18	47,49,49,52	0
2	FES	A	3002	4/4	0.98	0.12	89,90,90,92	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.

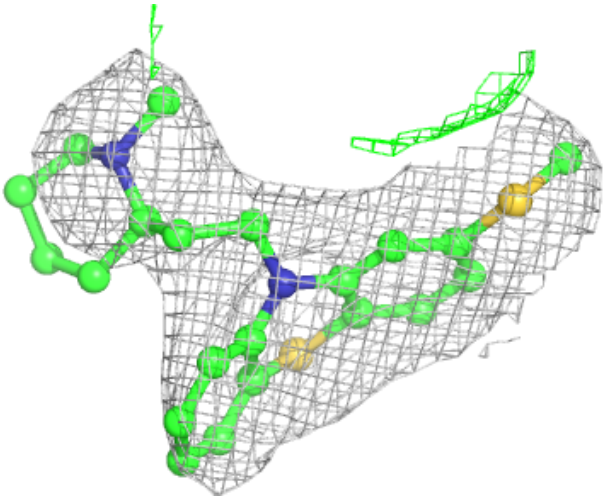
Electron density around MTE A 3003:

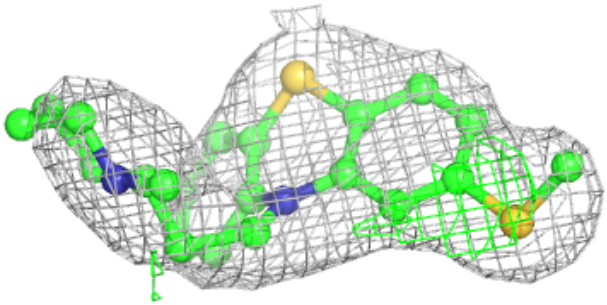
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

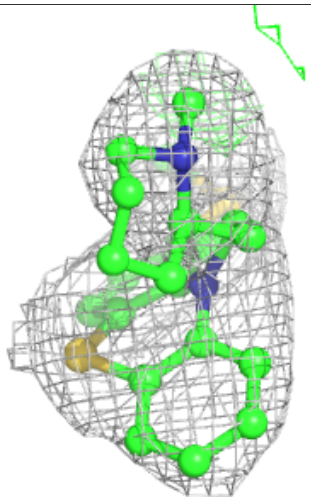


Electron density around RTZ A 3009 (B):

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

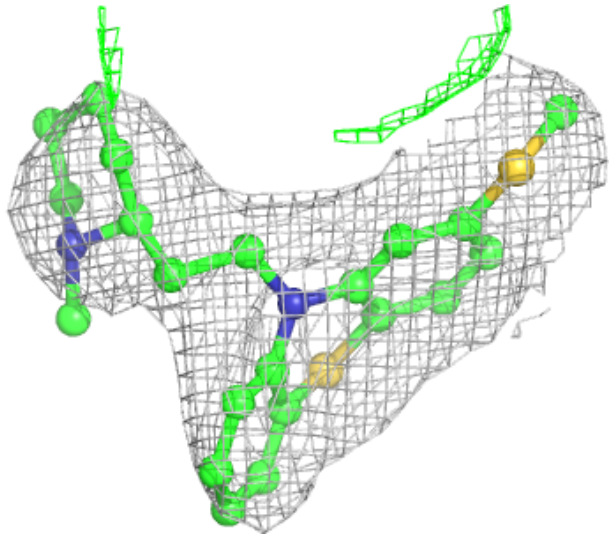


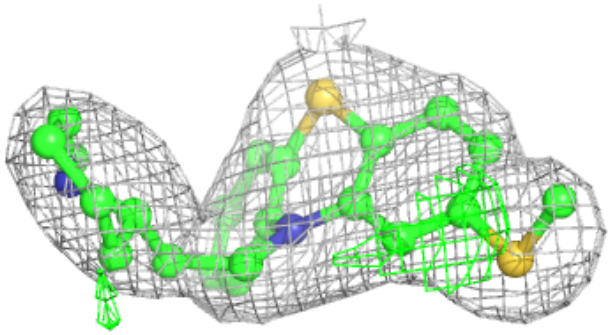


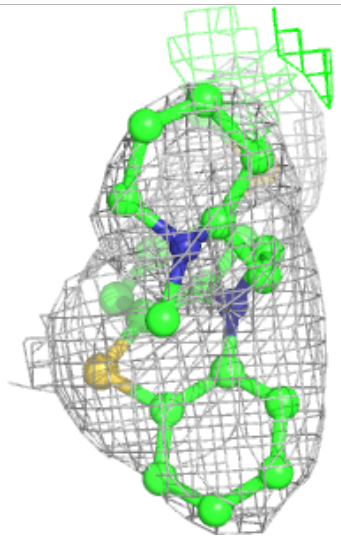


Electron density around LZU A 3008 (A):

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

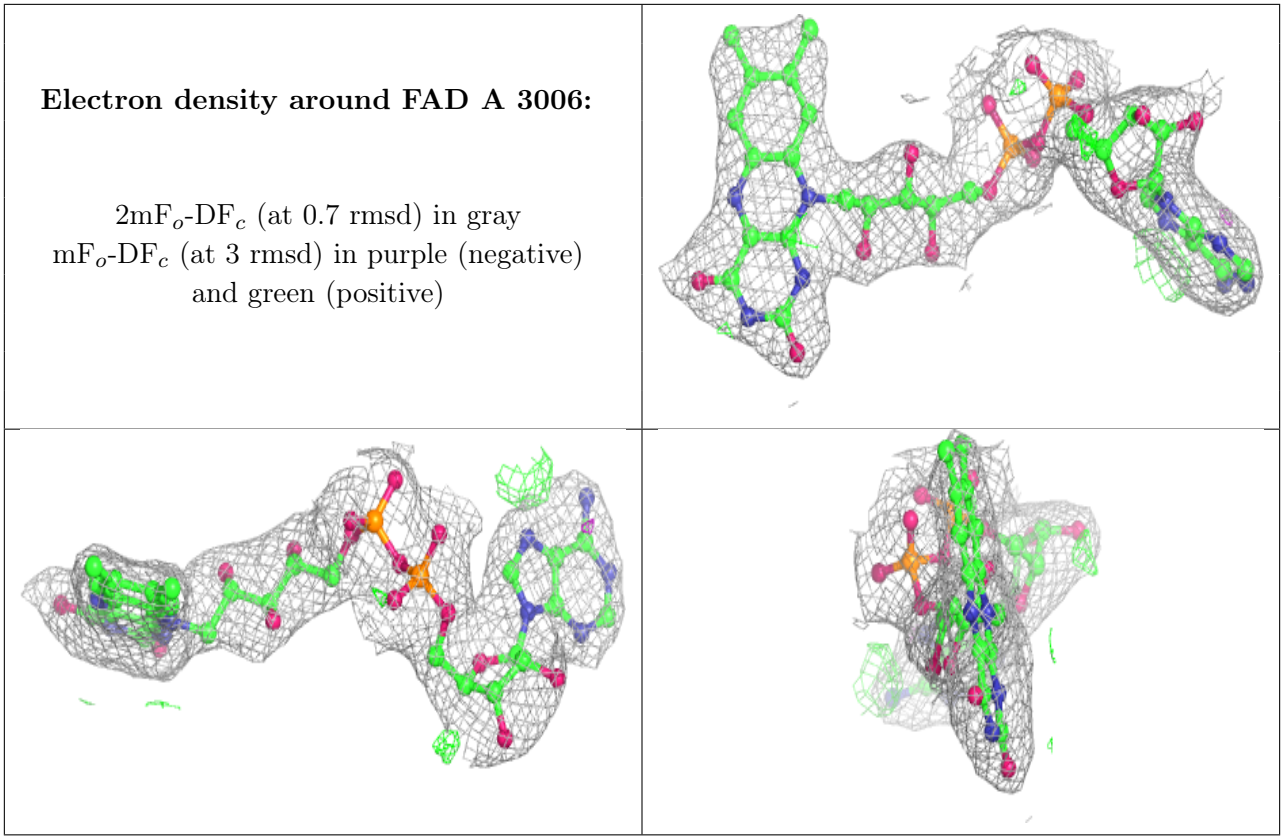






Electron density around FAD A 3006:

$2mF_o$-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.