



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2022 – 08:59 PM JST

PDB ID : 7D6O
Title : Oxidized structure of bovine xanthine oxidoreductase bound with oxypurinol.
Authors : Okamoto, K.
Deposited on : 2020-10-01
Resolution : 1.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

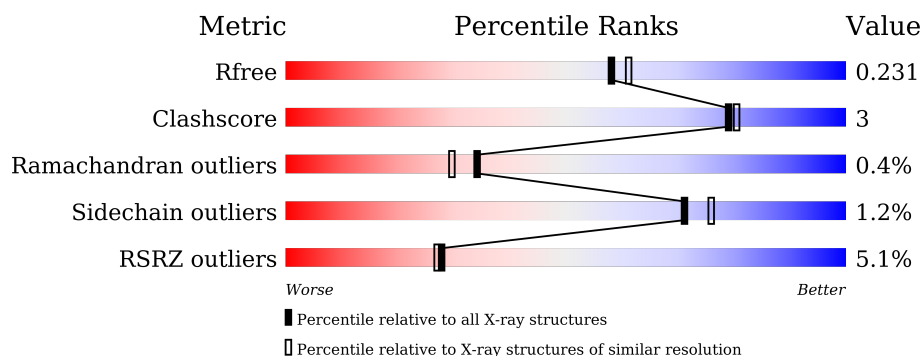
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	1332	<div> <div>4%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	B	1332	<div> <div>5%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>

2 Entry composition [i](#)

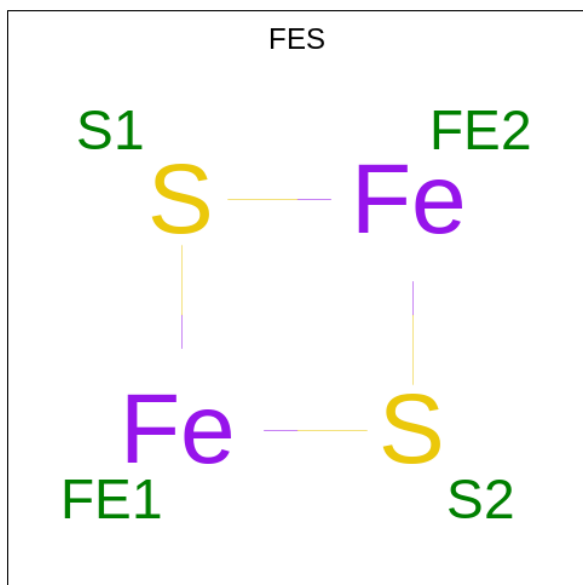
There are 9 unique types of molecules in this entry. The entry contains 20740 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

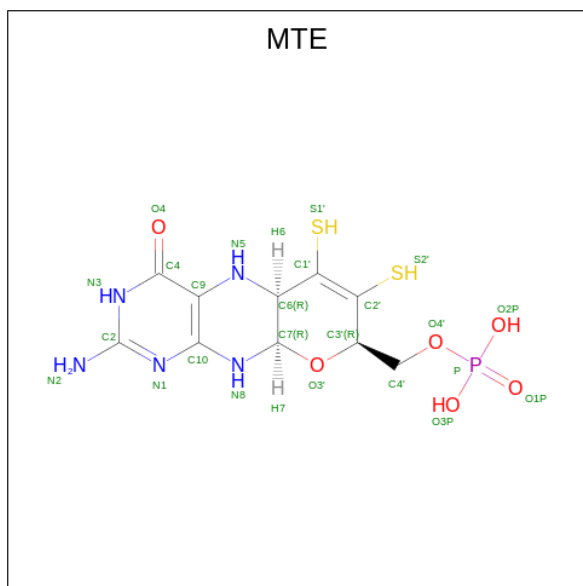
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1285	Total	C	N	O	S	0	0	0
			9980	6346	1708	1866	60			
1	B	1288	Total	C	N	O	S	0	0	0
			10000	6358	1711	1870	61			

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



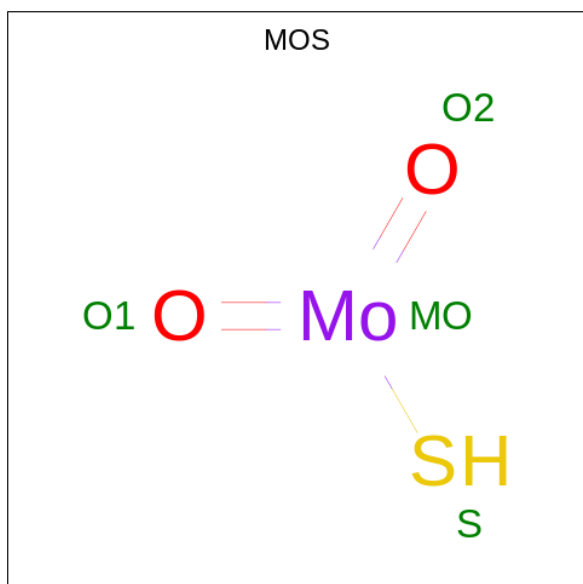
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8 A,9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMET HYL)ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$) (labeled as "Ligand of Interest" by depositor).



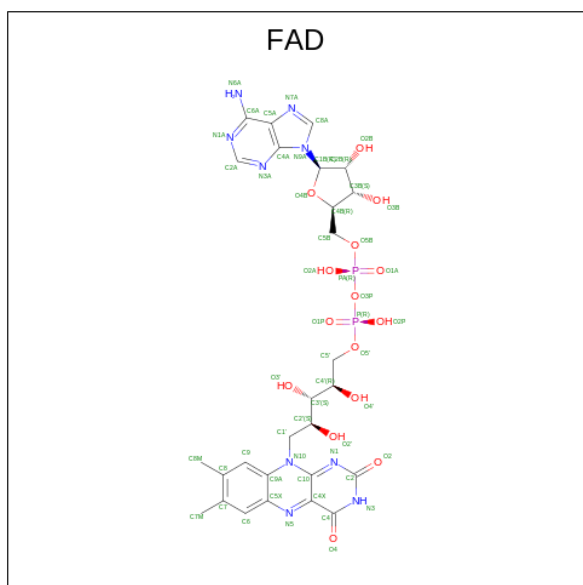
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

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



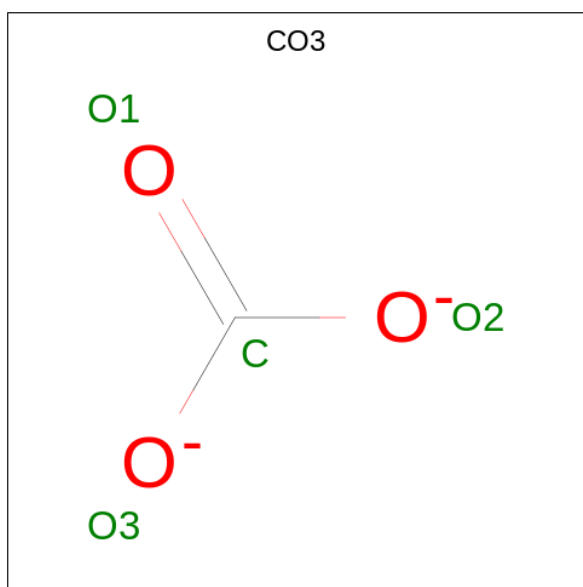
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	Mo 1	O 2	S 1	0	0
4	B	1	Total 4	Mo 1	O 2	S 1	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).

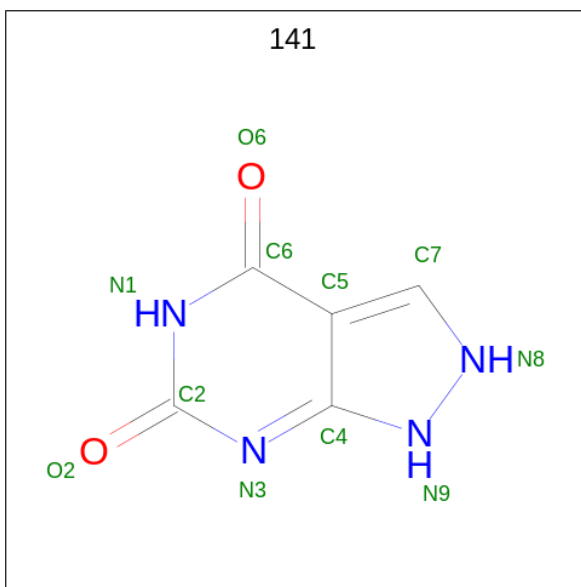


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is Oxypurinol (three-letter code: 141) (formula: C₅H₄N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			11	5	4	2		

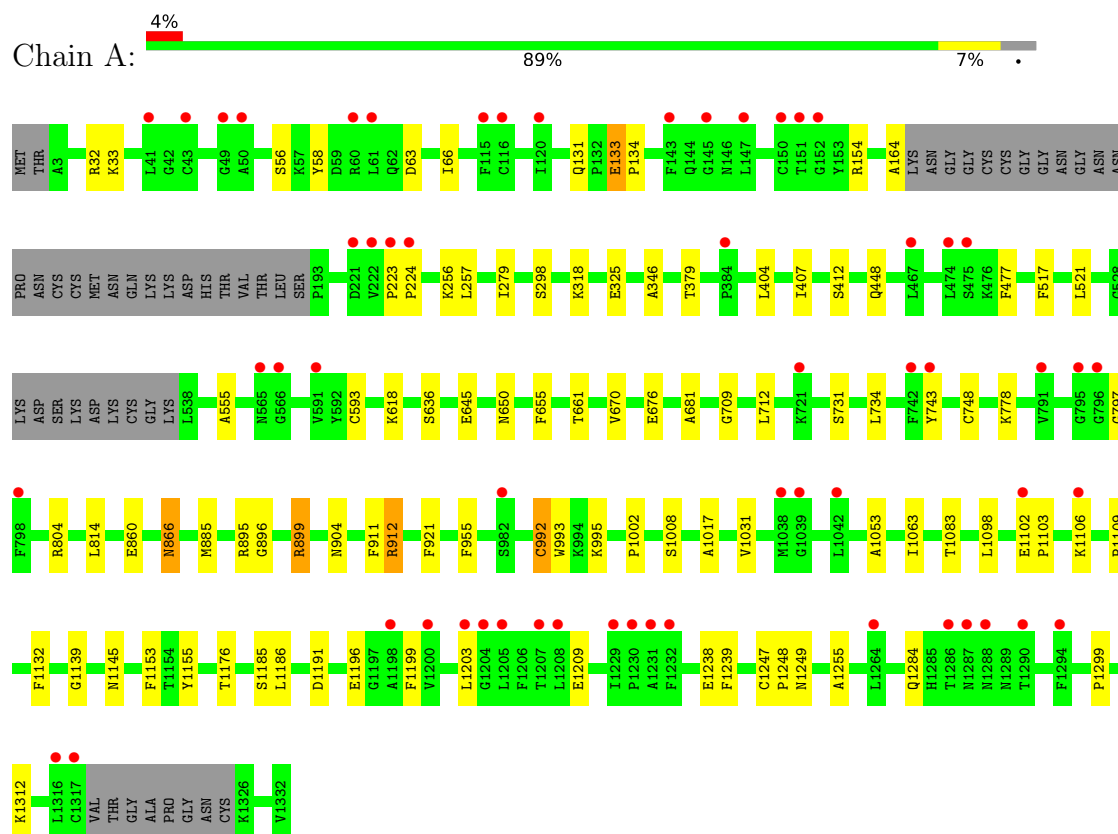
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	273	Total	O	0	0
			273	273		
9	B	288	Total	O	0	0
			288	288		

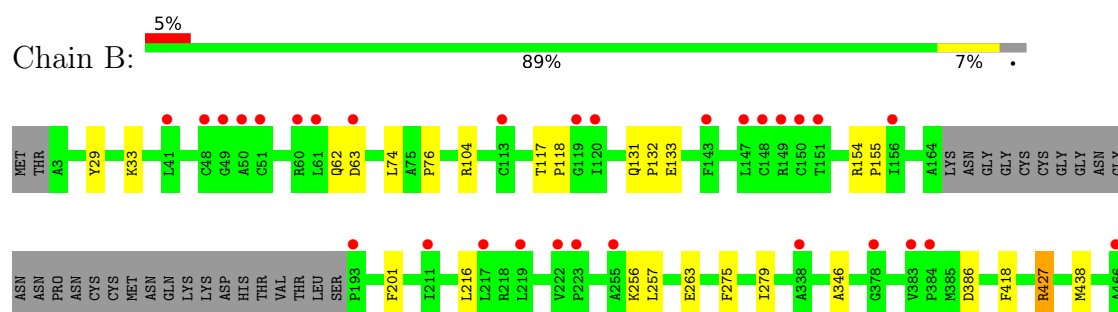
3 Residue-property plots

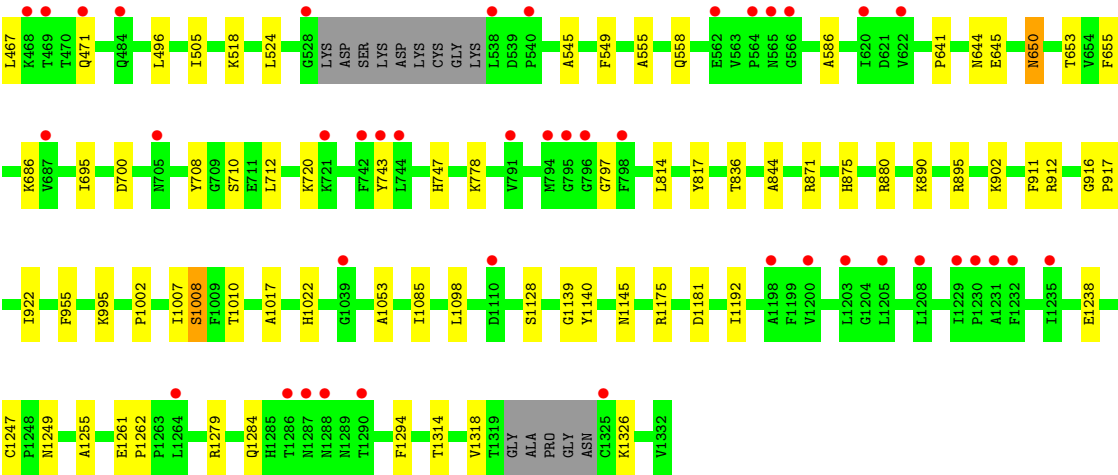
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.70Å 123.49Å 150.09Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	48.48 – 1.99 48.43 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.48-1.99) 99.6 (48.43-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.190 , 0.228 0.198 , 0.231	Depositor DCC
R_{free} test set	10299 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20740	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CO3, 141, MTE, CA, FAD, MOS

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	0.74	0/10198	0.85	0/13803
1	B	0.74	0/10218	0.86	1/13831 (0.0%)
All	All	0.74	0/20416	0.86	1/27634 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	871	ARG	NE-CZ-NH1	5.19	122.90	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9980	0	9975	56	0
1	B	10000	0	9996	56	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	24	0	10	0	0
3	B	24	0	10	0	0
4	A	4	0	0	1	0
4	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	53	0	31	1	0
5	B	53	0	31	3	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	11	0	4	3	0
9	A	273	0	0	4	0
9	B	288	0	0	0	0
All	All	20740	0	20057	112	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 3.

All (112) 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:1247:CYS:HB3	9:A:1745:HOH:O	0.96	1.14
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.32	0.91
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.39	0.84
1:B:880:ARG:HH21	8:B:1408:141:H2	1.29	0.80
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.46	0.80
1:A:131:GLN:HE21	1:A:133:GLU:H	1.34	0.75
1:B:467:LEU:O	1:B:471:GLN:HG2	1.86	0.75
1:B:131:GLN:HE21	1:B:133:GLU:H	1.38	0.71
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.71	0.71
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.89	0.69
1:B:1181:ASP:OD1	1:B:1247:CYS:SG	2.53	0.67
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.94	0.66
1:A:709:GLY:O	1:A:899:ARG:NH2	2.30	0.65
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.62	0.64
1:A:645:GLU:HG2	1:A:650:ASN:ND2	2.17	0.59
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.67	0.59
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.52	0.57
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.04	0.57
1:B:257:LEU:O	5:B:1405:FAD:H2B	2.04	0.57
1:B:496:LEU:HB2	1:B:505:ILE:HG23	1.87	0.56
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.05	0.56
1:A:655:PHE:HE2	1:A:814:LEU:HD23	1.70	0.55
1:B:1140:TYR:OH	1:B:1145:ASN:ND2	2.39	0.55
1:A:1247:CYS:SG	9:A:1581:HOH:O	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1247:CYS:CB	9:A:1745:HOH:O	1.83	0.54
1:B:880:ARG:NH2	8:B:1408:141:H2	2.04	0.54
1:A:655:PHE:CE2	1:A:814:LEU:HD23	2.43	0.53
1:B:645:GLU:HG2	1:B:650:ASN:ND2	2.17	0.52
1:B:1010:THR:H	8:B:1408:141:H5	1.57	0.52
1:A:1209:GLU:O	1:A:1299:PRO:HG3	2.10	0.52
1:B:74:LEU:O	1:B:76:PRO:HD3	2.11	0.51
1:A:1185:SER:OG	1:A:1191:ASP:OD2	2.28	0.51
1:A:1247:CYS:N	1:A:1248:PRO:CD	2.74	0.51
1:A:346:ALA:HB1	5:A:1405:FAD:H4'	1.92	0.51
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.58	0.49
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	1.94	0.49
1:B:708:TYR:CE1	1:B:902:LYS:HD3	2.47	0.49
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.47	0.49
1:B:995:LYS:HZ1	1:B:1284:GLN:HE21	1.60	0.48
1:A:1106:LYS:O	1:A:1109:PRO:HD3	2.13	0.48
1:A:404:LEU:CD2	1:A:407:ILE:HD11	2.41	0.48
1:A:1203:LEU:C	1:A:1203:LEU:HD23	2.33	0.48
1:A:866:ASN:C	1:A:866:ASN:HD22	2.17	0.47
1:B:257:LEU:HA	1:B:279:ILE:O	2.14	0.47
1:B:641:PRO:HG3	1:B:817:TYR:CE2	2.50	0.47
1:A:1153:PHE:HB2	1:A:1155:TYR:CZ	2.48	0.47
1:B:655:PHE:HE2	1:B:814:LEU:HD23	1.78	0.47
1:A:134:PRO:O	1:A:164:ALA:HA	2.15	0.47
1:B:154:ARG:N	1:B:155:PRO:HD2	2.30	0.46
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.80	0.46
1:A:555:ALA:O	1:A:1238:GLU:HA	2.16	0.46
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.16	0.46
1:B:644:ASN:O	1:B:653:THR:HA	2.16	0.46
1:A:58:TYR:OH	1:A:63:ASP:OD1	2.25	0.45
1:A:636:SER:HB2	9:A:1517:HOH:O	2.16	0.45
1:B:518:LYS:HE2	1:B:545:ALA:O	2.16	0.45
1:B:1022:HIS:CE1	1:B:1128:SER:HG	2.32	0.45
1:A:257:LEU:HA	1:A:279:ILE:O	2.16	0.45
1:A:448:GLN:HB2	1:A:477:PHE:CE2	2.52	0.45
1:B:104:ARG:HD3	1:B:201:PHE:CD2	2.52	0.45
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	1.99	0.45
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.17	0.45
1:A:734:LEU:HD21	1:A:921:PHE:CE2	2.52	0.44
1:B:1314:THR:O	1:B:1318:VAL:HG13	2.17	0.44
1:A:1083:THR:HG21	1:A:1186:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.80	0.44
1:B:117:THR:HB	1:B:118:PRO:HD3	1.98	0.44
1:B:346:ALA:HB1	5:B:1405:FAD:H4'	1.99	0.44
1:B:555:ALA:O	1:B:1238:GLU:HA	2.18	0.44
1:A:1247:CYS:SG	1:A:1247:CYS:O	2.76	0.44
1:B:1279:ARG:HG2	1:B:1294:PHE:HE1	1.83	0.44
1:A:804:ARG:HA	1:A:804:ARG:HD2	1.83	0.43
1:B:386:ASP:OD1	1:B:386:ASP:C	2.57	0.43
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.00	0.43
1:B:916:GLY:N	1:B:917:PRO:CD	2.82	0.43
1:B:1175:ARG:HA	1:B:1238:GLU:O	2.19	0.43
1:A:885:MET:SD	1:A:896:GLY:HA3	2.59	0.43
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.22	0.43
1:A:1176:THR:HG21	1:A:1199:PHE:CZ	2.54	0.42
1:A:593:CYS:HB3	1:A:748:CYS:SG	2.58	0.42
1:B:844:ALA:HB2	1:B:922:ILE:HD13	2.00	0.42
1:A:860:GLU:HA	1:A:895:ARG:O	2.20	0.42
1:A:56:SER:HA	1:A:66:ILE:O	2.20	0.42
1:A:618:LYS:HA	1:A:618:LYS:HE2	2.01	0.42
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.88	0.42
1:B:29:TYR:CZ	1:B:33:LYS:HG2	2.55	0.42
1:B:131:GLN:NE2	1:B:133:GLU:H	2.13	0.42
1:A:712:LEU:N	1:A:712:LEU:HD12	2.34	0.42
1:B:1007:ILE:O	1:B:1008:SER:OG	2.21	0.42
1:B:117:THR:HG22	1:B:586:ALA:HA	2.02	0.42
1:B:1017:ALA:HB2	1:B:1085:ILE:HD12	2.02	0.41
1:B:256:LYS:HE3	1:B:275:PHE:CE1	2.56	0.41
1:B:1247:CYS:SG	1:B:1247:CYS:O	2.78	0.41
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.23	0.41
1:A:1017:ALA:O	1:A:1132:PHE:HA	2.20	0.41
1:A:1031:VAL:HB	1:A:1063:ILE:HG12	2.01	0.41
1:B:427:ARG:HD3	1:B:549:PHE:CE2	2.56	0.41
1:A:325:GLU:HB2	1:A:412:SER:HB3	2.03	0.41
1:A:661:THR:O	1:A:904:ASN:HA	2.20	0.41
1:A:992:CYS:HB3	1:A:993:TRP:CD1	2.55	0.41
1:B:524:LEU:HD23	1:B:524:LEU:HA	1.97	0.41
1:B:695:ILE:HG23	1:B:700:ASP:HB3	2.03	0.41
1:A:154:ARG:HE	1:A:1196:GLU:CD	2.24	0.41
1:A:912:ARG:N	4:A:1404:MOS:S	2.94	0.41
1:B:418:PHE:HA	1:B:438:MET:O	2.20	0.40
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:PHE:CZ	1:A:521:LEU:HD11	2.56	0.40
1:B:712:LEU:HD21	1:B:875:HIS:NE2	2.36	0.40
1:A:298:SER:HA	1:A:407:ILE:O	2.20	0.40
1:A:645:GLU:CG	1:A:650:ASN:HD22	2.32	0.40
1:B:131:GLN:NE2	1:B:132:PRO:HD2	2.36	0.40
1:B:263:GLU:HB2	5:B:1405:FAD:H52A	2.04	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	1277/1332 (96%)	1231 (96%)	42 (3%)	4 (0%)	41	37
1	B	1280/1332 (96%)	1242 (97%)	33 (3%)	5 (0%)	34	30
All	All	2557/2664 (96%)	2473 (97%)	75 (3%)	9 (0%)	34	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1008	SER
1	A	912	ARG
1	A	1008	SER
1	B	63	ASP
1	B	912	ARG
1	B	1139	GLY
1	A	797	GLY
1	A	1139	GLY
1	B	797	GLY

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	1090/1128 (97%)	1076 (99%)	14 (1%)	69	74
1	B	1093/1128 (97%)	1081 (99%)	12 (1%)	73	78
All	All	2183/2256 (97%)	2157 (99%)	26 (1%)	71	76

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	133	GLU
1	A	256	LYS
1	A	318	LYS
1	A	379	THR
1	A	731	SER
1	A	743	TYR
1	A	866	ASN
1	A	899	ARG
1	A	911	PHE
1	A	992	CYS
1	A	1002	PRO
1	A	1239	PHE
1	A	1312	LYS
1	B	62	GLN
1	B	427	ARG
1	B	650	ASN
1	B	686	LYS
1	B	710	SER
1	B	720	LYS
1	B	743	TYR
1	B	890	LYS
1	B	895	ARG
1	B	911	PHE
1	B	1002	PRO
1	B	1326	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	272	ASN
1	A	292	HIS
1	A	471	GLN
1	A	473	GLN
1	A	650	ASN
1	A	866	ASN
1	A	1145	ASN
1	A	1284	GLN
1	B	131	GLN
1	B	292	HIS
1	B	473	GLN
1	B	626	GLN
1	B	650	ASN
1	B	1088	GLN
1	B	1145	ASN
1	B	1284	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\# Z > 2$
5	FAD	A	1405	-	53,58,58	0.72	1 (1%)	68,89,89	0.79	1 (1%)
2	FES	A	1401	1	0,4,4	-	-	-		
5	FAD	B	1405	-	53,58,58	0.67	0	68,89,89	0.90	4 (5%)
6	CO3	B	1406	-	2,3,3	0.56	0	2,3,3	0.16	0
3	MTE	B	1403	4	21,26,26	1.39	2 (9%)	21,40,40	2.07	10 (47%)
2	FES	B	1401	1	0,4,4	-	-	-		
3	MTE	A	1403	4	21,26,26	1.26	1 (4%)	21,40,40	2.38	7 (33%)
4	MOS	B	1404	3	0,3,3	-	-	-		
2	FES	A	1402	1	0,4,4	-	-	-		
6	CO3	A	1406	-	2,3,3	0.75	0	2,3,3	0.10	0
4	MOS	A	1404	3	0,3,3	-	-	-		
8	141	B	1408	-	10,12,12	1.26	0	10,17,17	1.22	1 (10%)
2	FES	B	1402	1	0,4,4	-	-	-		

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
5	FAD	A	1405	-	-	2/30/50/50	0/6/6/6
2	FES	A	1401	1	-	-	0/1/1/1
5	FAD	B	1405	-	-	3/30/50/50	0/6/6/6
3	MTE	B	1403	4	-	2/6/34/34	0/3/3/3
2	FES	B	1401	1	-	-	0/1/1/1
3	MTE	A	1403	4	-	3/6/34/34	0/3/3/3
2	FES	A	1402	1	-	-	0/1/1/1
8	141	B	1408	-	-	-	0/2/2/2
2	FES	B	1402	1	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1403	MTE	C4-N3	4.05	1.40	1.33
3	B	1403	MTE	C4-N3	4.02	1.40	1.33
5	A	1405	FAD	C9-C8	-2.29	1.36	1.39
3	B	1403	MTE	P-O2P	-2.26	1.46	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1403	MTE	C10-C9-C4	5.72	119.65	114.57
3	A	1403	MTE	C2-N3-C4	4.71	123.41	115.93
3	B	1403	MTE	C2-N3-C4	4.13	122.50	115.93
3	A	1403	MTE	O3'-C7-N8	3.58	112.24	108.57
3	B	1403	MTE	C10-C9-C4	3.33	117.53	114.57
3	A	1403	MTE	C9-C4-N3	-3.06	115.31	124.01
3	A	1403	MTE	N1-C2-N3	-2.83	120.98	125.42
3	B	1403	MTE	N1-C2-N3	-2.76	121.08	125.42
3	B	1403	MTE	O2P-P-O4'	-2.49	100.11	106.73
3	B	1403	MTE	C4-C9-N5	2.39	121.13	119.12
3	B	1403	MTE	O3P-P-O2P	2.38	116.72	107.64
3	A	1403	MTE	C9-C10-N8	2.37	120.30	118.13
5	B	1405	FAD	C5A-C6A-N6A	2.36	123.94	120.35
3	B	1403	MTE	C9-C4-N3	-2.35	117.33	124.01
5	A	1405	FAD	C5A-C6A-N6A	2.26	123.78	120.35
5	B	1405	FAD	O2'-C2'-C1'	2.20	115.11	109.80
5	B	1405	FAD	C4-N3-C2	-2.15	121.67	125.64
3	A	1403	MTE	C4-C9-N5	2.14	120.92	119.12
3	B	1403	MTE	O3P-P-O4'	-2.14	101.05	106.73
3	B	1403	MTE	N2-C2-N1	2.13	120.57	117.25
3	B	1403	MTE	O3'-C7-N8	2.10	110.72	108.57
5	B	1405	FAD	O2P-P-O1P	2.03	122.25	112.24
8	B	1408	141	O2-C2-N3	-2.02	118.47	121.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

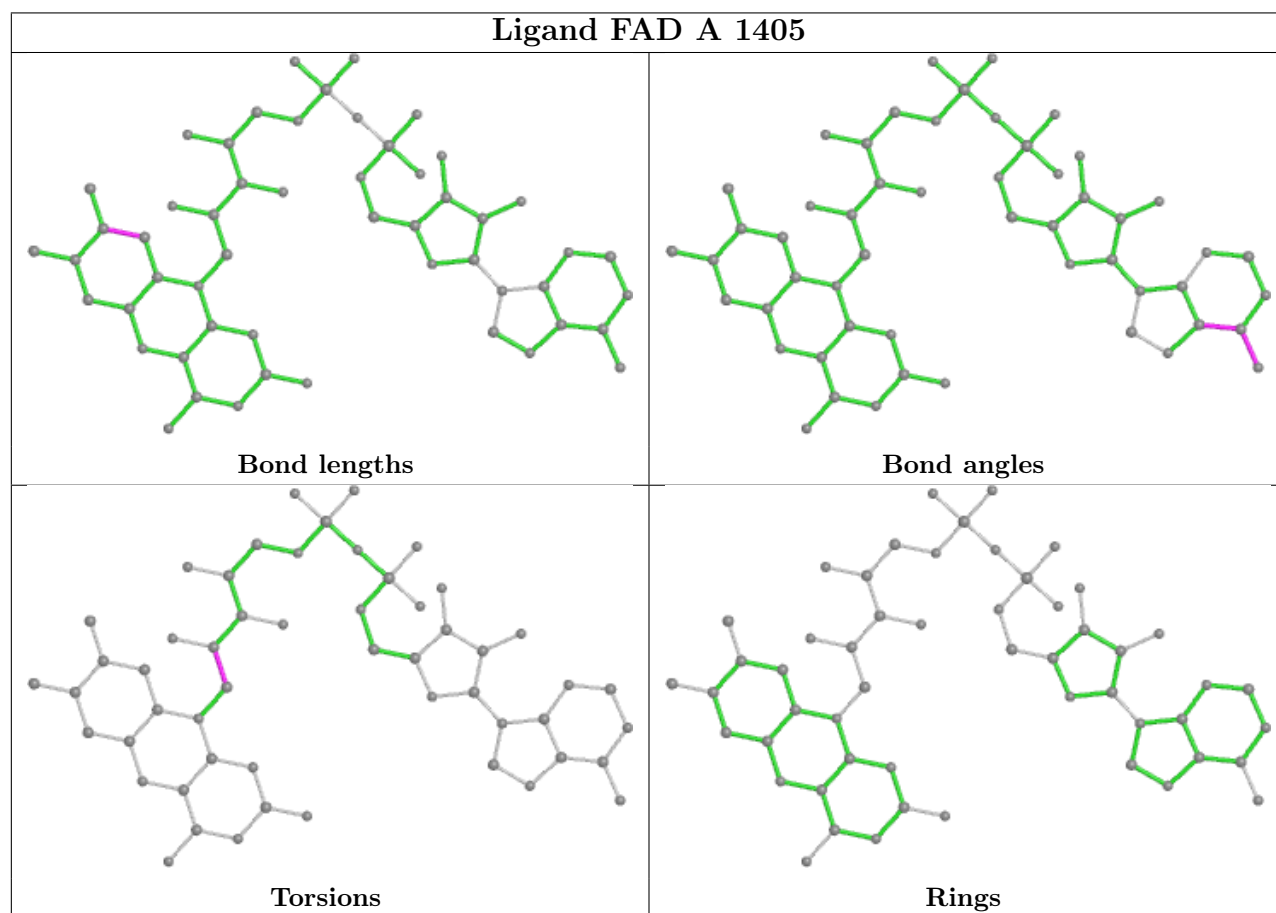
Mol	Chain	Res	Type	Atoms
3	A	1403	MTE	C4'-O4'-P-O1P
5	A	1405	FAD	N10-C1'-C2'-O2'
5	A	1405	FAD	N10-C1'-C2'-C3'
5	B	1405	FAD	N10-C1'-C2'-O2'
5	B	1405	FAD	N10-C1'-C2'-C3'
3	B	1403	MTE	C3'-C4'-O4'-P
3	A	1403	MTE	C3'-C4'-O4'-P
3	A	1403	MTE	C4'-O4'-P-O3P
3	B	1403	MTE	C4'-O4'-P-O3P
5	B	1405	FAD	C2'-C3'-C4'-O4'

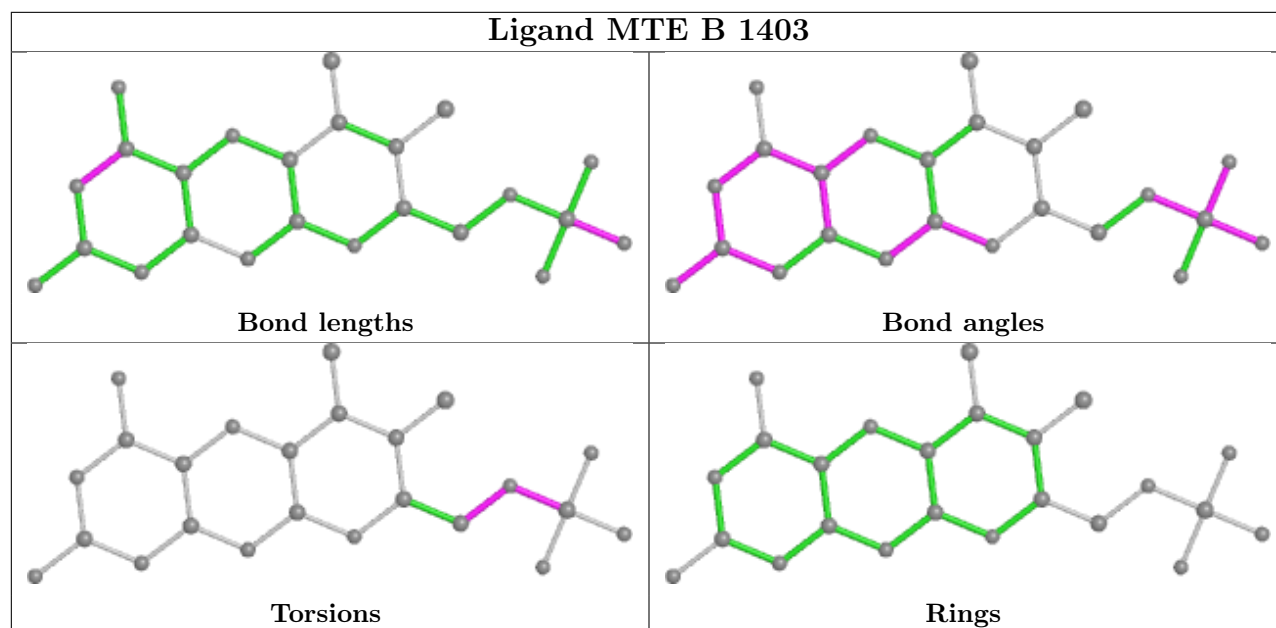
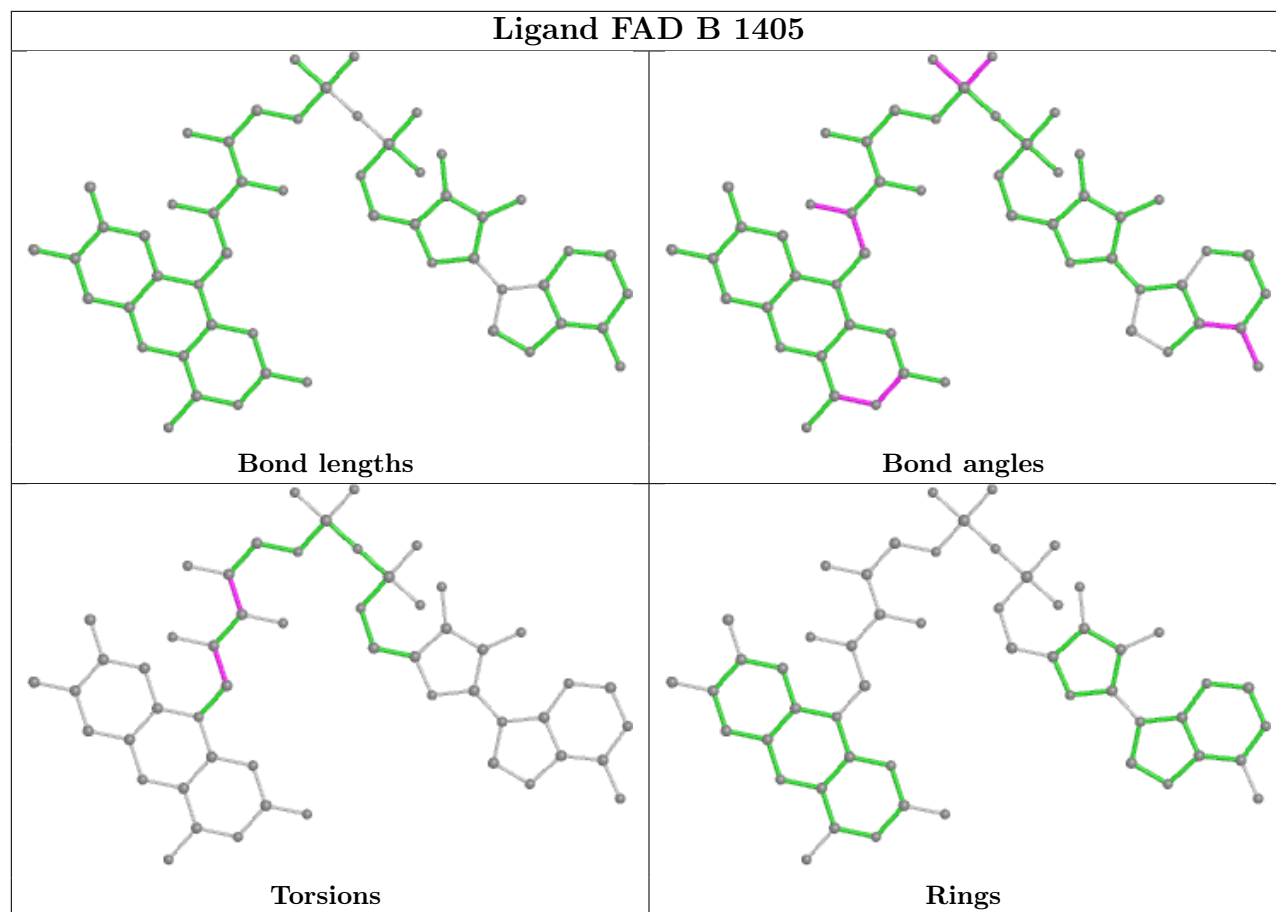
There are no ring outliers.

4 monomers are involved in 8 short contacts:

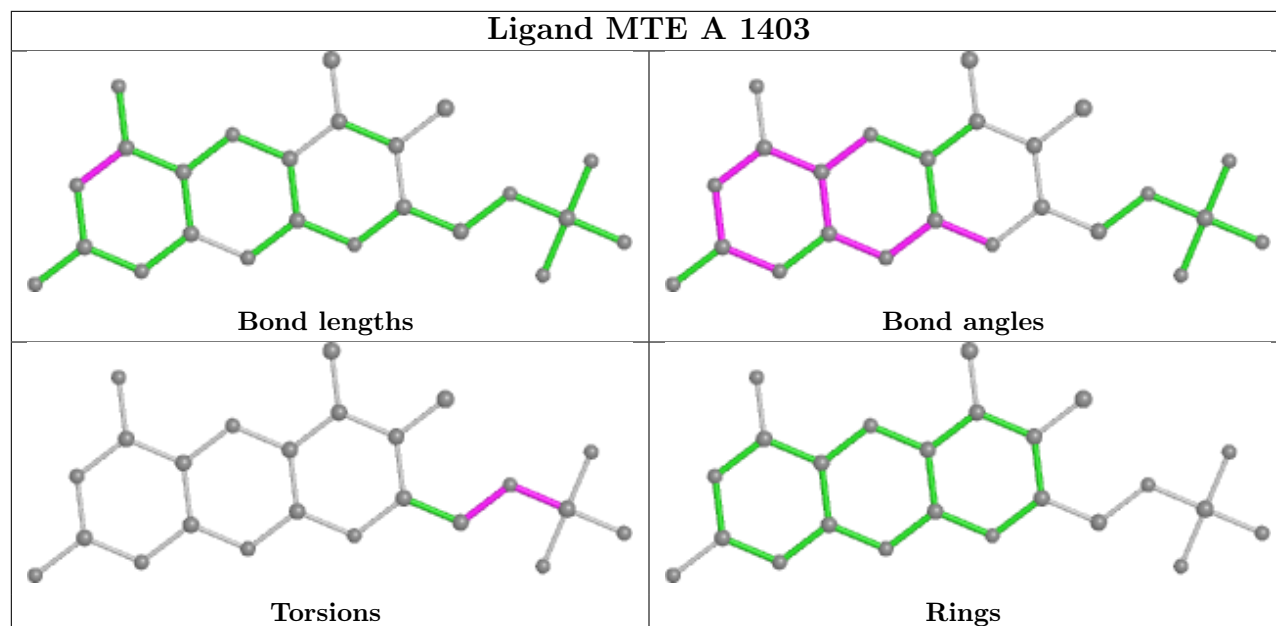
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1405	FAD	1	0
5	B	1405	FAD	3	0
4	A	1404	MOS	1	0
8	B	1408	141	3	0

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.

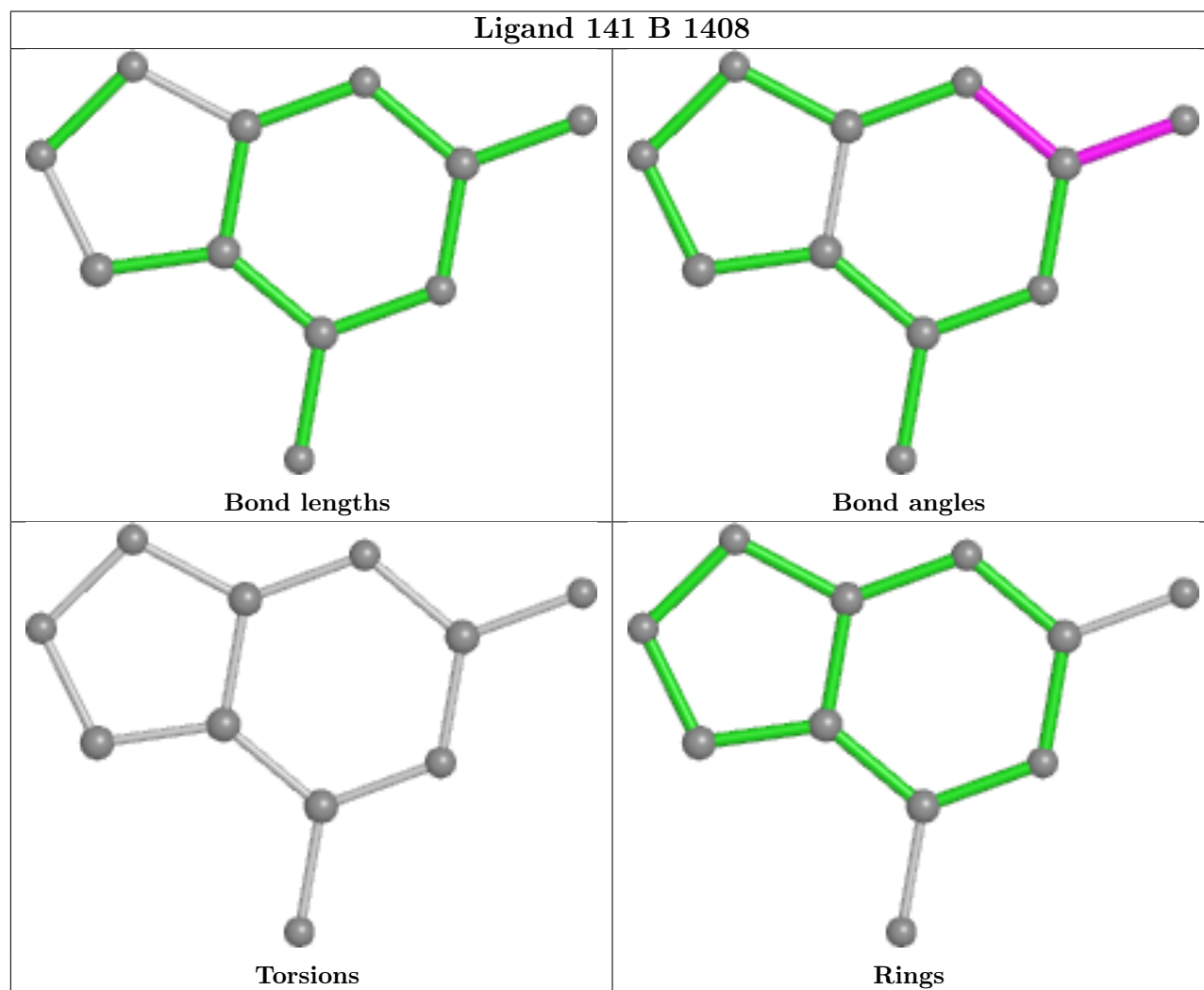




Ligand MTE A 1403



Ligand 141 B 1408



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	1285/1332 (96%)	0.48	58 (4%) 33 32	20, 30, 47, 80	0
1	B	1288/1332 (96%)	0.52	72 (5%) 24 23	19, 30, 47, 83	0
All	All	2573/2664 (96%)	0.50	130 (5%) 28 27	19, 30, 47, 83	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	566	GLY	8.3
1	B	565	ASN	7.5
1	B	1288	ASN	5.9
1	A	565	ASN	5.1
1	A	223	PRO	4.5
1	B	1229	ILE	4.3
1	A	61	LEU	4.2
1	A	1288	ASN	4.1
1	B	1205	LEU	4.0
1	A	1290	THR	4.0
1	A	221	ASP	4.0
1	B	223	PRO	3.9
1	B	1200	VAL	3.9
1	B	378	GLY	3.7
1	A	1316	LEU	3.7
1	B	1287	ASN	3.7
1	B	211	ILE	3.7
1	A	1205	LEU	3.6
1	B	147	LEU	3.5
1	B	222	VAL	3.5
1	A	798	PHE	3.5
1	A	1200	VAL	3.4
1	B	150	CYS	3.4
1	B	1325	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	60	ARG	3.3
1	A	1229	ILE	3.3
1	B	564	PRO	3.3
1	A	1203	LEU	3.2
1	B	1231	ALA	3.2
1	B	61	LEU	3.2
1	B	1264	LEU	3.1
1	A	147	LEU	3.1
1	B	744	LEU	3.0
1	A	152	GLY	3.0
1	B	255	ALA	3.0
1	A	150	CYS	3.0
1	B	1208	LEU	3.0
1	B	798	PHE	2.9
1	B	471	GLN	2.9
1	B	538	LEU	2.9
1	B	540	PRO	2.9
1	B	721	LYS	2.9
1	A	1039	GLY	2.8
1	B	1203	LEU	2.8
1	A	1231	ALA	2.8
1	B	1232	PHE	2.8
1	A	1208	LEU	2.8
1	B	1290	THR	2.7
1	A	721	LYS	2.7
1	A	1286	THR	2.7
1	B	468	LYS	2.7
1	A	224	PRO	2.7
1	B	151	THR	2.7
1	B	50	ALA	2.6
1	B	1235	ILE	2.6
1	B	469	THR	2.6
1	A	43	CYS	2.6
1	A	467	LEU	2.6
1	A	120	ILE	2.6
1	A	1294	PHE	2.5
1	A	743	TYR	2.5
1	A	796	GLY	2.5
1	B	383	VAL	2.5
1	B	1198	ALA	2.5
1	A	1230	PRO	2.5
1	A	474	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	794	MET	2.5
1	A	1204	GLY	2.5
1	A	1287	ASN	2.4
1	A	742	PHE	2.4
1	B	219	LEU	2.4
1	B	742	PHE	2.4
1	B	119	GLY	2.4
1	B	620	ILE	2.4
1	B	1230	PRO	2.4
1	B	41	LEU	2.4
1	A	791	VAL	2.4
1	A	143	PHE	2.4
1	B	143	PHE	2.4
1	B	743	TYR	2.4
1	B	49	GLY	2.4
1	A	1317	CYS	2.4
1	B	484	GLN	2.4
1	A	145	GLY	2.3
1	B	1039	GLY	2.3
1	B	193	PRO	2.3
1	B	705	ASN	2.3
1	B	384	PRO	2.3
1	A	115	PHE	2.3
1	B	622	VAL	2.3
1	B	791	VAL	2.3
1	A	50	ALA	2.3
1	A	475	SER	2.3
1	A	1038	MET	2.2
1	A	591	VAL	2.2
1	A	49	GLY	2.2
1	B	149	ARG	2.2
1	B	156	ILE	2.2
1	A	982	SER	2.2
1	A	1106	LYS	2.2
1	B	1286	THR	2.2
1	A	1232	PHE	2.2
1	B	338	ALA	2.2
1	B	120	ILE	2.2
1	A	151	THR	2.1
1	B	562	GLU	2.1
1	A	1198	ALA	2.1
1	A	116	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	795	GLY	2.1
1	B	63	ASP	2.1
1	B	795	GLY	2.1
1	A	1102	GLU	2.1
1	B	1110	ASP	2.1
1	A	566	GLY	2.1
1	B	528	GLY	2.1
1	B	217	LEU	2.1
1	B	687	VAL	2.1
1	B	51	CYS	2.1
1	B	113	CYS	2.1
1	A	384	PRO	2.1
1	B	466	ALA	2.1
1	A	41	LEU	2.1
1	A	1042	LEU	2.1
1	B	48	CYS	2.1
1	B	796	GLY	2.1
1	B	60	ARG	2.0
1	A	222	VAL	2.0
1	B	148	CYS	2.0
1	A	1207	THR	2.0
1	A	1264	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 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, 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
8	141	B	1408	11/11	0.67	0.29	47,50,53,56	0

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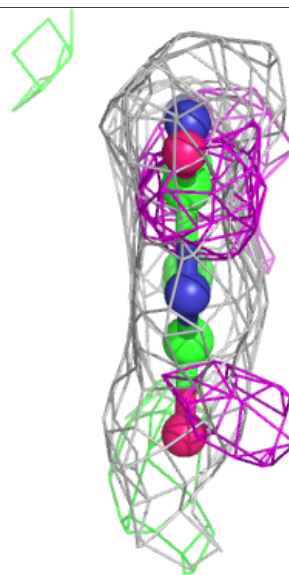
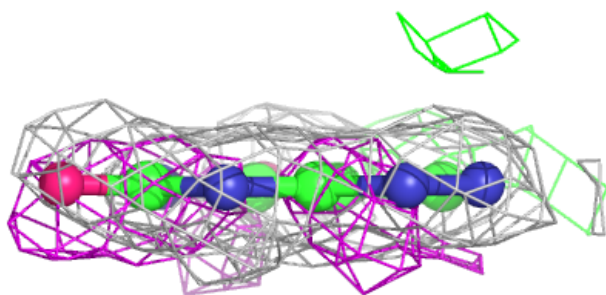
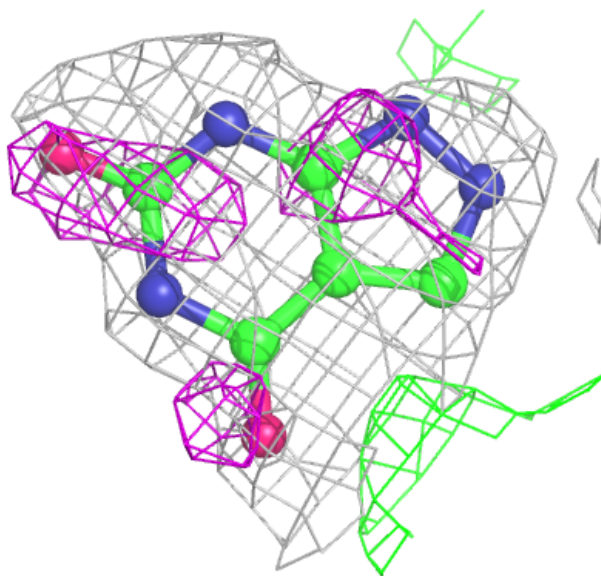
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	FAD	B	1405	53/53	0.96	0.11	22,26,31,33	0
6	CO3	B	1406	4/4	0.96	0.14	26,28,29,30	0
5	FAD	A	1405	53/53	0.96	0.11	22,27,30,33	0
6	CO3	A	1406	4/4	0.97	0.15	21,24,24,27	0
3	MTE	A	1403	24/24	0.97	0.15	18,24,30,32	0
3	MTE	B	1403	24/24	0.97	0.14	17,22,27,29	0
4	MOS	B	1404	4/4	0.99	0.09	27,28,35,41	0
2	FES	B	1401	4/4	0.99	0.14	20,22,22,24	0
2	FES	B	1402	4/4	0.99	0.12	22,22,23,23	0
2	FES	A	1401	4/4	0.99	0.14	20,21,22,22	0
2	FES	A	1402	4/4	0.99	0.11	23,23,25,27	0
7	CA	A	1407	1/1	0.99	0.11	25,25,25,25	0
4	MOS	A	1404	4/4	0.99	0.09	28,30,31,43	0
7	CA	B	1407	1/1	1.00	0.09	25,25,25,25	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.

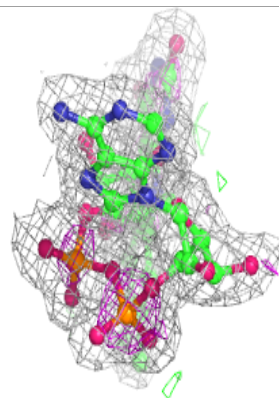
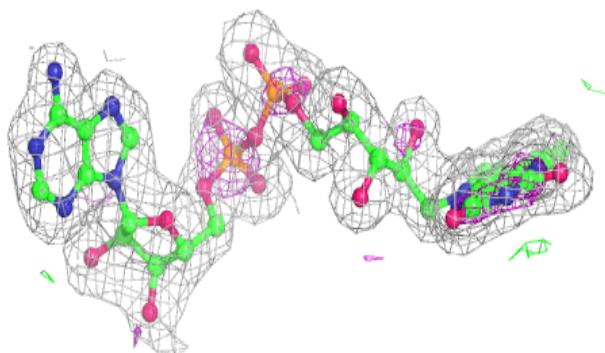
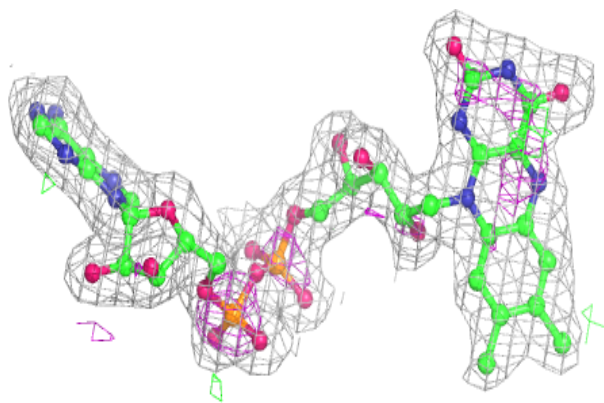
Electron density around 141 B 1408:

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

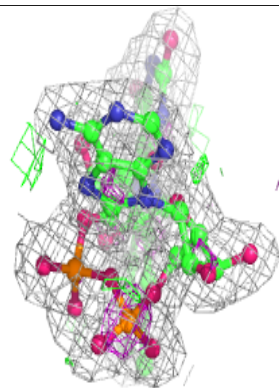
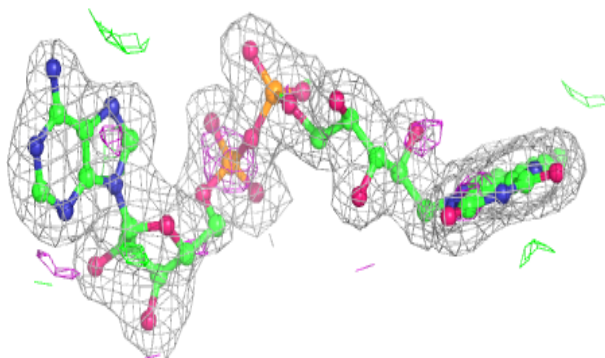
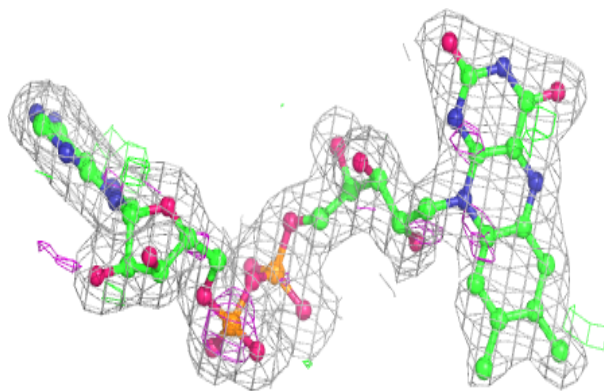


Electron density around FAD B 1405:

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

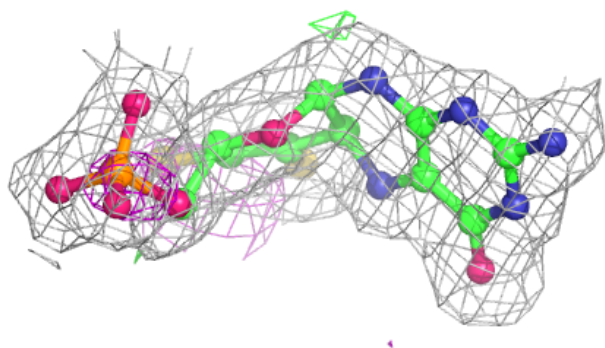
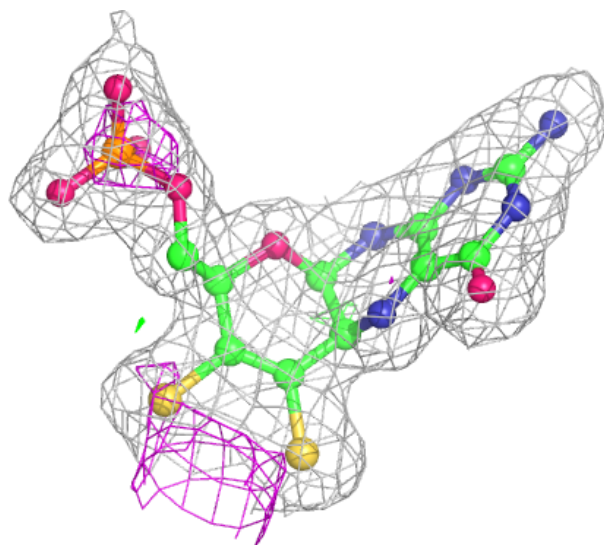
**Electron density around FAD A 1405:**

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



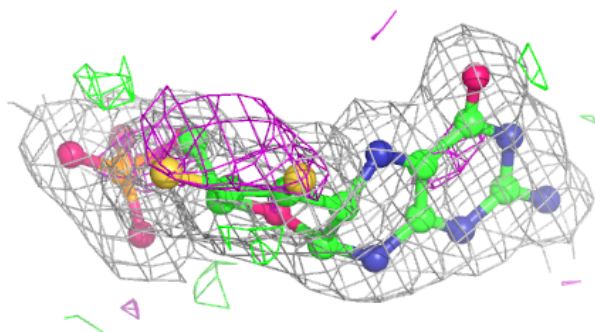
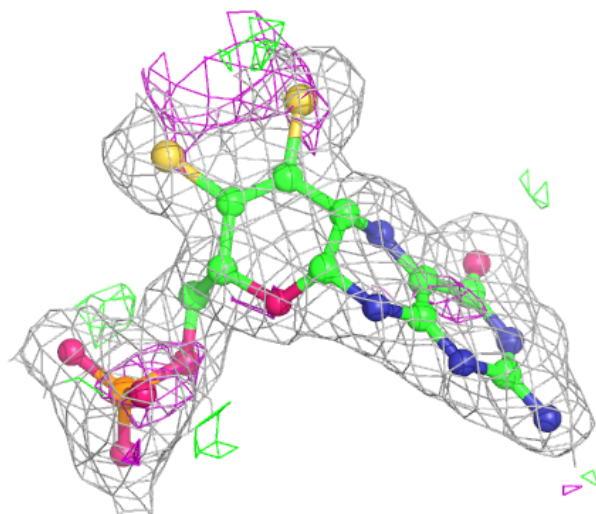
Electron density around MTE A 1403:

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



Electron density around MTE B 1403:

$2mF_o-DF_c$ (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.