Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 06:41 AM EDT

PDB ID	:	1LQT
Title	:	A covalent modification of NADP+ revealed by the atomic resolution structure of FprA, a Mycobacterium tuberculosis oxidoreductase
Authors	:	Bossi, R.T.; Aliverti, A.; Raimondi, D.; Fischer, F.; Zanetti, G.; Ferrari, D.; Tahallah, N.; Maier, C.S.; Heck, A.J.R.; Rizzi, M.; Mattevi, A.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2002-05-13
Resolution	:	1.05 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:

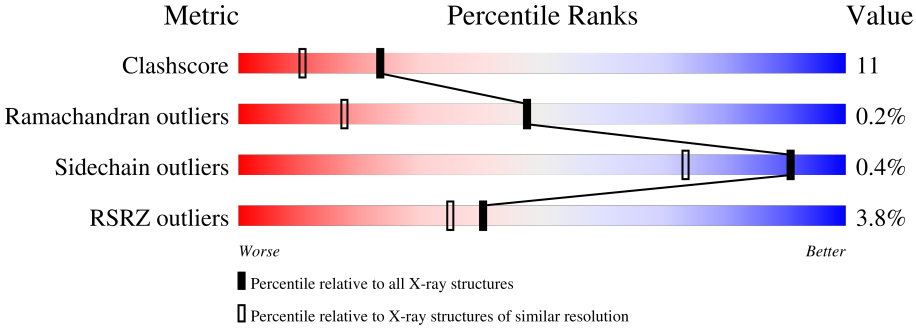
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.05 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))
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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	456	3% 86% 12%
1	B	456	5% 89% 10%

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
2	ACT	A	1866	-	-	X	-
2	ACT	B	1867	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	1868	-	-	X	-
2	ACT	B	1873	-	-	X	-
2	ACT	B	1874	-	-	X	-
2	ACT	B	1875	-	-	X	-
2	ACT	B	1876	-	-	X	-
4	ODP	A	2458	X	-	-	-
4	ODP	B	3458	X	-	-	-

2 Entry composition (i)

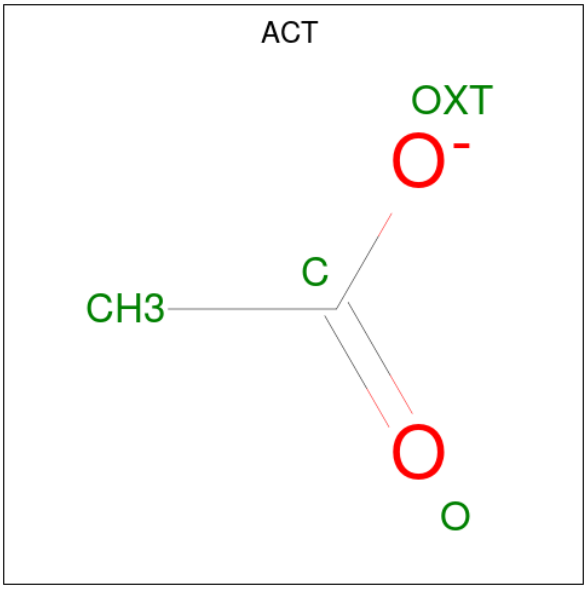
There are 5 unique types of molecules in this entry. The entry contains 20280 atoms, of which 11064 are hydrogens and 0 are deuteriums.

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 FprA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	452	7214	2261	3629	641	673	10	187	23	0
1	B	454	7073	2222	3554	627	662	8	182	12	0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	7	2	3	2	0	0
2	A	1	7	2	3	2	0	0
2	A	1	7	2	3	2	0	0
2	A	1	7	2	3	2	0	0

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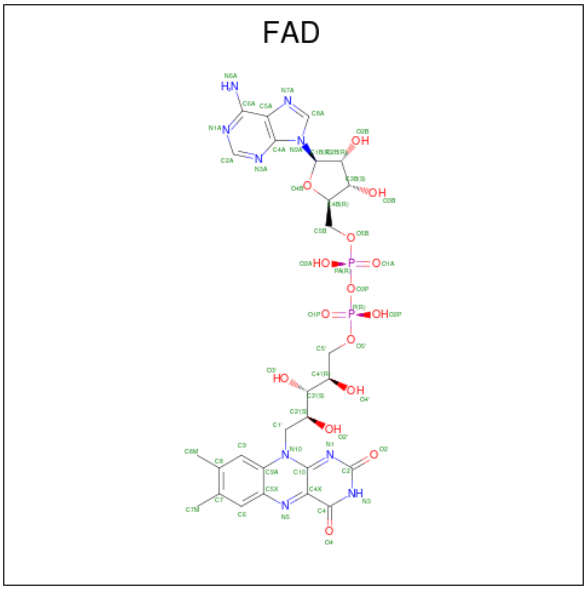
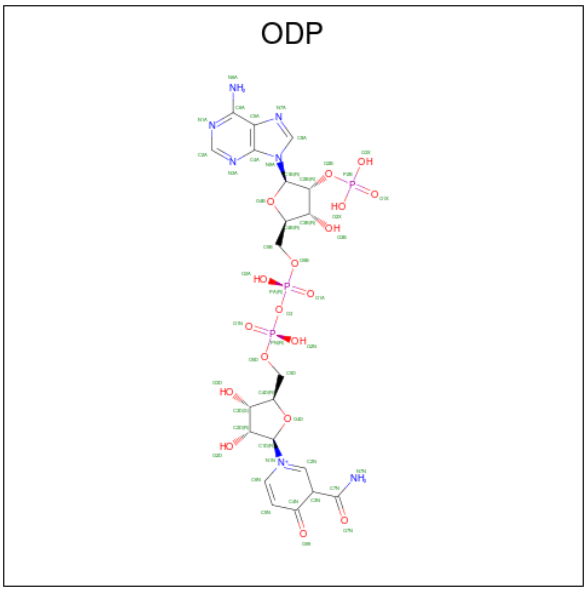
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O			
2	A	1	7	2	3	2		0	0
			Total	C	H	O			
2	B	1	7	2	3	2		0	0
			Total	C	H	O			
2	B	1	7	2	3	2		0	0
			Total	C	H	O			
2	B	1	7	2	3	2		0	0
			Total	C	H	O			
2	B	1	7	2	3	2		0	0
			Total	C	H	O			
2	B	1	7	2	3	2		0	0
			Total	C	H	O			
2	B	1	7	2	3	2		0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
3	A	1	86	27	33	9	15	2	9	0
			Total	C	H	N	O	P		
3	B	1	86	27	33	9	15	2	9	0

- Molecule 4 is 4-OXO-NICOTINAMIDE-ADENINE DINUCLEOTIDE PHOSPHATE (three-letter code: ODP) (formula: $C_{21}H_{29}N_7O_{18}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
4	A	1	76	21	27	7	18	3	10	0
			Total	C	H	N	O	P		
4	B	1	76	21	27	7	18	3	10	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
5	A	971	2913	1942	971	1942	0
			Total	H	O		
5	B	893	2679	1786	893	1786	0

3 Residue-property plots (i)

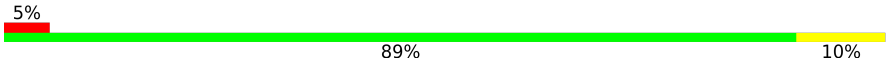
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

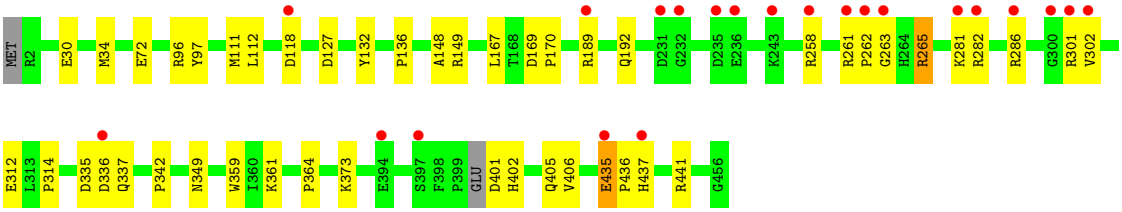
• Molecule 1: FprA

Chain A:

• Molecule 1: FprA

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.33Å 89.22Å 160.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.05 10.00 – 1.05	Depositor EDS
% Data completeness (in resolution range)	95.4 (40.00-1.05) 95.5 (10.00-1.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.134 , 0.153 0.137 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	9.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.49 , 61.5	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	0.98	EDS
Total number of atoms	20280	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, ODP, FAD

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	0.66	0/3704	0.87	11/5024 (0.2%)
1	B	0.64	0/3632	0.85	4/4934 (0.1%)
All	All	0.65	0/7336	0.86	15/9958 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	441	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	A	33	ASP	CB-CG-OD2	6.68	124.32	118.30
1	A	441	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	265	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	401	ASP	CB-CG-OD2	6.28	123.96	118.30
1	A	164	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	320	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	336	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	96	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	441	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	270	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	118	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	217	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	31[A]	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	31[B]	ASP	CB-CG-OD2	5.07	122.86	118.30

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	3585	3629	3620	76	0
1	B	3519	3554	3551	67	0
2	A	20	15	15	9	0
2	B	24	18	17	27	2
3	A	53	33	31	3	0
3	B	53	33	31	0	0
4	A	49	27	24	4	0
4	B	49	27	24	13	0
5	A	971	1942	0	38	8
5	B	893	1786	0	46	6
All	All	9216	11064	7313	165	9

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 11.

All (165) 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:349[A]:ASN:ND2	1:B:342[A]:PRO:HG3	1.44	1.29
1:A:60[B]:ILE:HG13	5:A:2865:HOH:O	1.42	1.20
1:A:344[B]:VAL:HG23	1:A:349[B]:ASN:ND2	1.57	1.17
1:B:361:LYS:HD2	5:B:4329:HOH:O	1.47	1.14
2:B:1876:ACT:H2	4:B:3458:ODP:O1A	1.43	1.12
1:B:361:LYS:CD	5:B:4329:HOH:O	1.95	1.11
1:B:192:GLN:HG3	5:B:4269:HOH:O	1.54	1.08
1:B:127[B]:ASP:OD1	5:B:3885:HOH:O	1.69	1.07
1:A:344[B]:VAL:CG2	5:A:3234:HOH:O	2.03	1.07
2:B:1876:ACT:H3	4:B:3458:ODP:O1A	1.45	1.07
1:A:344[B]:VAL:CG2	1:A:349[B]:ASN:HD21	1.69	1.05
1:A:2:ARG:N	5:A:3386:HOH:O	1.87	1.05
2:B:1876:ACT:CH3	4:B:3458:ODP:H3D	1.87	1.05
1:A:127[B]:ASP:OD1	5:A:2848:HOH:O	1.77	1.02
1:A:286[B]:ARG:NH1	1:A:312:GLU:OE1	1.93	1.00
1:A:344[B]:VAL:CG2	1:A:349[B]:ASN:ND2	2.24	1.00
1:A:264:HIS:CD2	5:A:3408:HOH:O	2.16	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:HIS:NE2	5:A:3408:HOH:O	1.99	0.95
1:B:265:ARG:NE	5:B:4299:HOH:O	2.03	0.91
1:B:118:ASP:OD1	5:B:4330:HOH:O	1.89	0.91
1:A:349[A]:ASN:HD21	1:B:342[A]:PRO:HG3	1.13	0.91
2:B:1876:ACT:H3	4:B:3458:ODP:H3D	1.51	0.90
1:B:336:ASP:CB	5:B:4297:HOH:O	2.20	0.90
2:B:1874:ACT:H1	5:B:3536:HOH:O	1.71	0.90
1:A:349[A]:ASN:ND2	1:B:342[A]:PRO:CG	2.32	0.88
1:B:336:ASP:HB3	5:B:4297:HOH:O	1.72	0.88
1:A:286[B]:ARG:NH2	5:A:3139:HOH:O	1.94	0.87
1:B:437:HIS:CD2	5:B:4138:HOH:O	2.26	0.86
1:A:60[B]:ILE:CG1	5:A:2865:HOH:O	2.11	0.86
1:B:435:GLU:HG2	5:B:3664:HOH:O	1.75	0.86
1:B:192:GLN:HG3	5:B:4142:HOH:O	1.77	0.83
2:B:1876:ACT:H1	4:B:3458:ODP:H3D	1.59	0.83
2:B:1876:ACT:H1	4:B:3458:ODP:C3D	2.11	0.81
1:A:60[A]:ILE:HG21	5:A:2691:HOH:O	1.81	0.80
1:A:60[B]:ILE:HD12	5:A:2691:HOH:O	1.81	0.80
1:B:405:GLN:HG3	5:B:4026:HOH:O	1.81	0.79
1:B:265:ARG:CZ	5:B:4299:HOH:O	2.30	0.78
1:B:189:ARG:HH21	1:B:265:ARG:CZ	1.97	0.78
1:A:342:PRO:HB3	5:B:3912:HOH:O	1.84	0.77
1:B:435:GLU:CG	5:B:3664:HOH:O	2.32	0.77
1:B:263:GLY:HA3	5:B:3716:HOH:O	1.85	0.76
1:B:263:GLY:CA	5:B:3716:HOH:O	2.34	0.76
1:A:295[B]:VAL:HG23	5:A:3092:HOH:O	1.85	0.76
1:B:336:ASP:CG	5:B:4297:HOH:O	2.23	0.75
1:B:258:ARG:CZ	5:B:3899:HOH:O	2.35	0.75
1:A:59:LYS:HB2	2:A:1870:ACT:H2	1.67	0.74
2:B:1874:ACT:H2	5:B:3849:HOH:O	1.86	0.74
2:B:1876:ACT:H3	4:B:3458:ODP:PA	2.27	0.74
1:A:214:GLU:OE2	5:A:3427:HOH:O	2.07	0.72
1:B:437:HIS:HD2	5:B:4138:HOH:O	1.68	0.72
1:A:31[B]:ASP:OD2	5:A:3067:HOH:O	2.07	0.72
1:A:449:GLU:OE1	5:A:2657:HOH:O	2.08	0.70
2:A:1866:ACT:H3	4:A:2458:ODP:N6A	2.05	0.70
1:A:295[C]:VAL:HG13	5:A:3092:HOH:O	1.91	0.70
1:A:405:GLN:HG2	5:A:3325:HOH:O	1.90	0.70
2:B:1874:ACT:CH3	5:B:3849:HOH:O	2.38	0.70
1:A:189:ARG:HH21	1:A:265:ARG:CZ	2.06	0.69
2:B:1876:ACT:CH3	4:B:3458:ODP:C3D	2.66	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:NH2	5:A:2933:HOH:O	2.25	0.68
1:B:337:GLN:NE2	5:B:4346:HOH:O	2.24	0.68
1:B:118:ASP:OD1	5:B:4240:HOH:O	2.10	0.68
1:A:395:CYS:SG	5:A:3416:HOH:O	2.52	0.67
1:B:435:GLU:HG2	5:B:4333:HOH:O	1.94	0.67
2:B:1875:ACT:CH3	4:B:3458:ODP:H62A	2.07	0.67
1:B:361:LYS:CE	5:B:4329:HOH:O	2.33	0.67
2:A:1866:ACT:H3	4:A:2458:ODP:H62A	1.60	0.66
1:A:60[A]:ILE:HG23	5:A:2895:HOH:O	1.96	0.66
2:B:1876:ACT:CH3	5:B:3470:HOH:O	2.44	0.65
1:A:189:ARG:HD2	5:A:3060:HOH:O	1.96	0.65
1:B:72:GLU:OE1	5:B:4133:HOH:O	2.14	0.65
1:B:111:MET:O	2:B:1875:ACT:H3	1.97	0.65
1:B:96:ARG:O	1:B:402:HIS:HE1	1.80	0.64
1:A:349[A]:ASN:ND2	1:B:335[A]:ASP:HB2	2.12	0.64
1:A:135:HIS:HE1	1:A:137:HIS:CD2	2.16	0.63
2:B:1876:ACT:H1	5:B:3470:HOH:O	1.99	0.61
2:A:1866:ACT:C	4:A:2458:ODP:H62A	2.15	0.60
1:B:435:GLU:CG	5:B:4333:HOH:O	2.49	0.60
1:A:345[A]:GLY:HA3	5:A:3379:HOH:O	2.01	0.60
1:B:361:LYS:HE3	5:B:4329:HOH:O	1.96	0.60
2:B:1875:ACT:CH3	4:B:3458:ODP:N6A	2.66	0.59
2:B:1875:ACT:C	4:B:3458:ODP:H62A	2.16	0.58
1:A:2:ARG:N	5:A:3314:HOH:O	2.36	0.58
1:A:335:ASP:HB2	1:B:349:ASN:ND2	2.19	0.57
1:A:60[A]:ILE:HD13	3:A:2457:FAD:N3	2.18	0.57
1:B:148:ALA:HB1	2:B:1867:ACT:H1	1.87	0.56
1:B:30:GLU:HG3	5:B:4021:HOH:O	2.05	0.56
2:A:1866:ACT:CH3	4:A:2458:ODP:H62A	2.19	0.56
1:B:281:LYS:HA	5:B:4313:HOH:O	2.06	0.56
1:A:167:LEU:O	1:A:265:ARG:CZ	2.55	0.55
1:A:41[B]:MET:HB2	1:A:83:VAL:HG22	1.88	0.55
1:B:136:PRO:O	5:B:3924:HOH:O	2.18	0.54
1:A:381:THR:OG1	5:A:3379:HOH:O	2.11	0.54
1:A:97:TYR:OH	1:A:406[B]:VAL:HG11	2.07	0.54
1:B:258:ARG:NE	5:B:3899:HOH:O	2.41	0.54
1:A:295[B]:VAL:CG2	5:A:3092:HOH:O	2.52	0.53
1:A:189:ARG:HH21	1:A:265:ARG:NH2	2.06	0.53
1:A:449:GLU:HG2	5:A:3403:HOH:O	2.07	0.53
1:A:60[A]:ILE:HG23	5:A:2636:HOH:O	2.09	0.53
1:B:282:ARG:N	5:B:4313:HOH:O	2.03	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:GLU:HB2	5:B:4114:HOH:O	2.08	0.53
1:B:167:LEU:O	1:B:265:ARG:CZ	2.57	0.53
1:A:347[A]:ARG:HD2	1:A:351:SER:O	2.09	0.52
1:B:189:ARG:HH21	1:B:265:ARG:NH2	2.07	0.52
1:B:192:GLN:HB2	2:B:1867:ACT:H2	1.91	0.52
1:B:373:LYS:HD3	5:B:3958:HOH:O	2.09	0.52
1:A:60[B]:ILE:HD13	3:A:2457:FAD:N3	2.24	0.52
1:A:96:ARG:O	1:A:402:HIS:HE1	1.92	0.51
2:B:1876:ACT:H2	5:B:3470:HOH:O	2.09	0.51
1:A:96:ARG:O	1:A:402:HIS:CE1	2.64	0.50
1:A:349[A]:ASN:HD21	1:B:342[A]:PRO:CG	2.02	0.49
1:B:286:ARG:HD2	1:B:312:GLU:OE2	2.12	0.49
1:A:374:ASP:OD2	5:A:3389:HOH:O	2.18	0.49
1:B:127[A]:ASP:OD2	5:B:4098:HOH:O	2.20	0.49
1:B:111:MET:O	2:B:1875:ACT:CH3	2.60	0.49
1:B:373:LYS:CD	5:B:3958:HOH:O	2.61	0.49
1:B:402:HIS:CE1	1:B:406[C]:VAL:CG2	2.96	0.49
1:B:112:LEU:HA	2:B:1875:ACT:H2	1.95	0.49
1:A:189:ARG:NH1	5:A:2864:HOH:O	2.45	0.49
1:A:135:HIS:CE1	1:A:137:HIS:CD2	2.99	0.48
2:B:1876:ACT:H1	4:B:3458:ODP:C2D	2.43	0.48
1:A:422:HIS:HB3	1:A:454:GLY:O	2.14	0.48
2:B:1875:ACT:H1	4:B:3458:ODP:H62A	1.77	0.48
1:A:292:ASN:OD1	2:A:1872:ACT:H3	2.15	0.47
1:B:258:ARG:NH1	5:B:4215:HOH:O	2.48	0.47
1:A:210:LEU:O	1:A:214:GLU:HG3	2.15	0.47
1:A:388:ASN:ND2	5:A:3020:HOH:O	2.44	0.46
1:A:422:HIS:CD2	5:A:2803:HOH:O	2.67	0.46
1:B:261:ARG:NH1	5:B:4298:HOH:O	2.13	0.46
1:B:281:LYS:O	1:B:282:ARG:HB2	2.15	0.46
1:A:359:TRP:CD2	1:A:364:PRO:HA	2.51	0.46
1:A:110:ARG:NH1	2:A:1866:ACT:H2	2.30	0.46
1:A:344[B]:VAL:HG23	1:A:349[B]:ASN:HD21	1.29	0.46
1:B:435:GLU:N	1:B:436:PRO:CD	2.79	0.46
1:B:263:GLY:N	5:B:3716:HOH:O	2.45	0.46
1:B:402:HIS:CE1	1:B:406[C]:VAL:HG21	2.52	0.45
1:A:349[B]:ASN:ND2	5:A:3234:HOH:O	0.61	0.45
1:A:345[A]:GLY:CA	5:A:3379:HOH:O	2.61	0.45
1:A:455:LEU:HA	5:A:2935:HOH:O	2.15	0.45
1:A:60[A]:ILE:HD13	3:A:2457:FAD:HN3	1.81	0.45
2:B:1874:ACT:H3	5:B:3849:HOH:O	2.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60[A]:ILE:HG12	5:A:2636:HOH:O	2.18	0.43
1:B:189:ARG:HH21	1:B:265:ARG:NH1	2.15	0.43
1:A:34[B]:MET:HE2	1:A:34[B]:MET:HB3	1.08	0.43
1:A:344[B]:VAL:HG22	1:A:349[B]:ASN:HD21	1.70	0.43
1:B:97:TYR:CZ	1:B:406[C]:VAL:HG11	2.54	0.43
1:A:31[B]:ASP:OD1	5:A:3150:HOH:O	2.21	0.42
1:A:131:TRP:CH2	1:A:182:ALA:HA	2.54	0.42
1:B:359:TRP:CD2	1:B:364:PRO:HA	2.53	0.42
1:A:167:LEU:O	1:A:265:ARG:NH1	2.53	0.42
1:B:301:ARG:HG3	1:B:302:VAL:N	2.35	0.42
1:A:382:LEU:C	1:A:382:LEU:HD23	2.40	0.41
1:A:449:GLU:CG	5:A:3403:HOH:O	2.67	0.41
1:B:169:ASP:HA	1:B:170[A]:PRO:HD2	1.98	0.41
1:B:34[B]:MET:HB3	1:B:34[B]:MET:HE2	1.15	0.41
1:B:149:ARG:HD2	1:B:314:PRO:O	2.20	0.41
1:A:2:ARG:CA	5:A:3386:HOH:O	2.57	0.40
1:A:344[B]:VAL:HB	1:A:347[B]:ARG:NH2	2.36	0.40
1:A:6:ILE:HG13	1:A:34[B]:MET:HE1	2.02	0.40
1:A:365:THR:OG1	5:A:3346:HOH:O	2.22	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1868:ACT:OXT	5:A:3320:HOH:O[1_565]	0.65	1.55
2:B:1868:ACT:C	5:A:3320:HOH:O[1_565]	1.82	0.38
5:A:3325:HOH:O	5:B:3803:HOH:O[3_545]	1.84	0.36
5:A:2970:HOH:O	5:A:3396:HOH:O[4_445]	1.99	0.21
5:A:2684:HOH:O	5:B:4333:HOH:O[1_545]	2.01	0.19
5:A:3425:HOH:O	5:B:3695:HOH:O[4_455]	2.02	0.18
5:A:3383:HOH:O	5:B:4315:HOH:O[1_545]	2.07	0.13
5:A:3363:HOH:O	5:B:4202:HOH:O[3_545]	2.10	0.10
5:B:4173:HOH:O	5:B:4183:HOH:O[1_455]	2.12	0.08

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	471/456 (103%)	461 (98%)	9 (2%)	1 (0%)	47	17
1	B	464/456 (102%)	452 (97%)	11 (2%)	1 (0%)	47	17
All	All	935/912 (102%)	913 (98%)	20 (2%)	2 (0%)	47	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	TRP
1	B	262	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/365 (105%)	383 (100%)	1 (0%)	92	75
1	B	377/365 (103%)	375 (100%)	2 (0%)	88	66
All	All	761/730 (104%)	758 (100%)	3 (0%)	91	73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	TYR
1	B	132	TYR
1	B	435	GLU

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

Mol	Chain	Res	Type
1	A	137	HIS
1	A	385	ASN

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Mol	Chain	Res	Type
1	A	388	ASN
1	A	402	HIS
1	A	405	GLN
1	B	264	HIS
1	B	349	ASN
1	B	385	ASN
1	B	388	ASN
1	B	402	HIS
1	B	437	HIS

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)

15 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	$\#\|Z\| > 2$
2	ACT	A	1869	-	3,3,3	0.95	0	3,3,3	0.65	0
3	FAD	A	2457	-	53,58,58	0.91	1 (1%)	68,89,89	1.06	5 (7%)
3	FAD	B	3457	-	53,58,58	0.91	2 (3%)	68,89,89	1.05	3 (4%)
2	ACT	B	1867	-	3,3,3	0.76	0	3,3,3	2.25	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	A	1871	-	3,3,3	0.85	0	3,3,3	1.49	1 (33%)
2	ACT	B	1875	-	3,3,3	0.87	0	3,3,3	0.66	0
4	ODP	B	3458	2	42,53,53	1.26	2 (4%)	51,82,82	1.13	2 (3%)
2	ACT	A	1870	-	3,3,3	0.73	0	3,3,3	0.94	0
2	ACT	A	1866	-	3,3,3	1.00	0	3,3,3	0.62	0
2	ACT	A	1872	-	3,3,3	0.91	0	3,3,3	1.22	0
2	ACT	B	1876	4	3,3,3	0.60	0	3,3,3	1.54	1 (33%)
2	ACT	B	1874	-	3,3,3	0.61	0	3,3,3	1.89	1 (33%)
4	ODP	A	2458	-	42,53,53	1.22	3 (7%)	51,82,82	1.17	6 (11%)
2	ACT	B	1868	-	3,3,3	0.75	0	3,3,3	1.20	0
2	ACT	B	1873	1	3,3,3	0.77	0	3,3,3	0.69	0

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
3	FAD	A	2457	-	-	5/30/50/50	0/6/6/6
4	ODP	A	2458	-	1/1/18/18	4/26/80/80	0/4/5/5
3	FAD	B	3457	-	-	6/30/50/50	0/6/6/6
4	ODP	B	3458	2	1/1/18/18	3/26/80/80	0/4/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3458	ODP	C2D-C1D	-6.36	1.44	1.53
4	A	2458	ODP	C2D-C1D	-4.13	1.47	1.53
3	A	2457	FAD	C4X-N5	3.83	1.38	1.30
3	B	3457	FAD	C4X-N5	3.26	1.37	1.30
4	A	2458	ODP	O99-C4N	3.13	1.27	1.22
4	B	3458	ODP	C2A-N3A	2.57	1.36	1.32
3	B	3457	FAD	C2A-N3A	2.56	1.36	1.32
4	A	2458	ODP	C6N-C5N	2.25	1.41	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1867	ACT	OXT-C-CH3	2.93	127.29	115.18
3	A	2457	FAD	O4B-C1B-C2B	-2.85	102.77	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2458	ODP	C3D-C2D-C1D	2.77	105.15	100.98
4	A	2458	ODP	O99-C4N-C3N	2.75	124.16	120.22
2	B	1874	ACT	O-C-CH3	-2.64	112.07	122.33
3	B	3457	FAD	C5A-C6A-N6A	2.51	124.16	120.35
3	B	3457	FAD	C4X-C10-N10	2.46	120.08	116.48
3	A	2457	FAD	C5A-C6A-N6A	2.44	124.06	120.35
4	A	2458	ODP	O2D-C2D-C3D	2.41	119.63	111.82
4	A	2458	ODP	N3A-C2A-N1A	-2.38	124.96	128.68
2	B	1867	ACT	OXT-C-O	-2.34	113.44	122.05
4	A	2458	ODP	C5A-C6A-N6A	2.30	123.85	120.35
3	A	2457	FAD	O3'-C3'-C4'	-2.29	103.29	108.81
3	B	3457	FAD	C5X-C9A-N10	2.18	120.21	117.95
4	B	3458	ODP	C3D-C2D-C1D	2.17	104.25	100.98
3	A	2457	FAD	C4X-C10-N10	2.13	119.60	116.48
2	B	1876	ACT	O-C-CH3	-2.13	114.05	122.33
4	B	3458	ODP	O99-C4N-C3N	2.12	123.26	120.22
3	A	2457	FAD	C9A-C5X-N5	-2.07	120.18	122.43
4	A	2458	ODP	O7N-C7N-N7N	2.07	126.60	123.00
2	A	1871	ACT	OXT-C-O	-2.03	114.57	122.05

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2458	ODP	C3N
4	B	3458	ODP	C3N

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2458	ODP	C2B-O2B-P2B-O2X
4	B	3458	ODP	C2B-O2B-P2B-O2X
3	B	3457	FAD	C2'-C3'-C4'-O4'
3	A	2457	FAD	C2'-C3'-C4'-O4'
3	A	2457	FAD	PA-O3P-P-O5'
3	B	3457	FAD	PA-O3P-P-O5'
4	A	2458	ODP	C2B-O2B-P2B-O1X
3	A	2457	FAD	O3'-C3'-C4'-O4'
3	B	3457	FAD	O3'-C3'-C4'-O4'
3	A	2457	FAD	O4B-C4B-C5B-O5B
3	B	3457	FAD	O4B-C4B-C5B-O5B
3	B	3457	FAD	C2'-C3'-C4'-C5'
4	A	2458	ODP	C4N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
4	B	3458	ODP	C4N-C3N-C7N-O7N
4	A	2458	ODP	O4B-C4B-C5B-O5B
4	B	3458	ODP	O4B-C4B-C5B-O5B
3	A	2457	FAD	O3'-C3'-C4'-C5'
3	B	3457	FAD	O3'-C3'-C4'-C5'

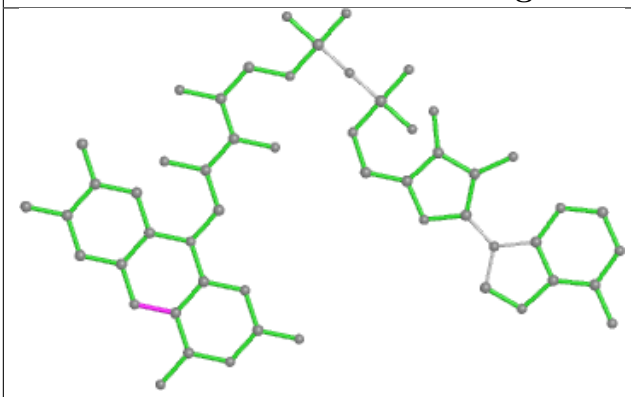
There are no ring outliers.

12 monomers are involved in 41 short contacts:

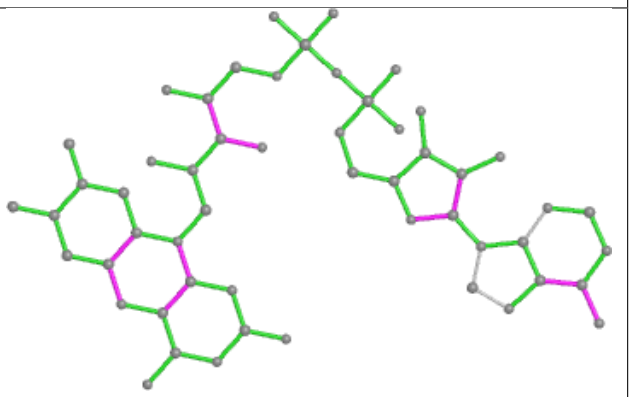
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2457	FAD	3	0
2	B	1867	ACT	2	0
2	B	1875	ACT	7	0
4	B	3458	ODP	13	0
2	A	1870	ACT	1	0
2	A	1866	ACT	7	0
2	A	1872	ACT	1	0
2	B	1876	ACT	12	0
2	B	1874	ACT	4	0
4	A	2458	ODP	4	0
2	B	1868	ACT	0	2
2	B	1873	ACT	2	0

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.

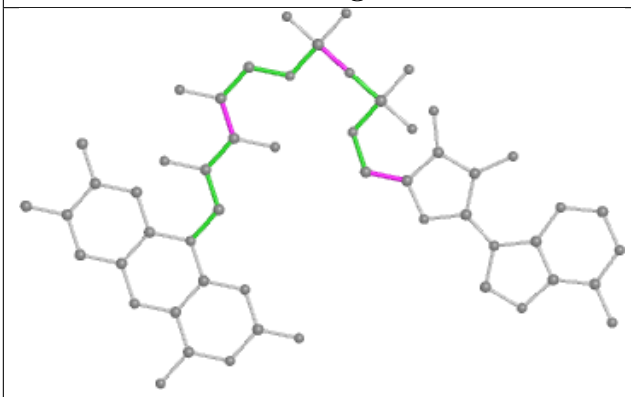
Ligand FAD A 2457



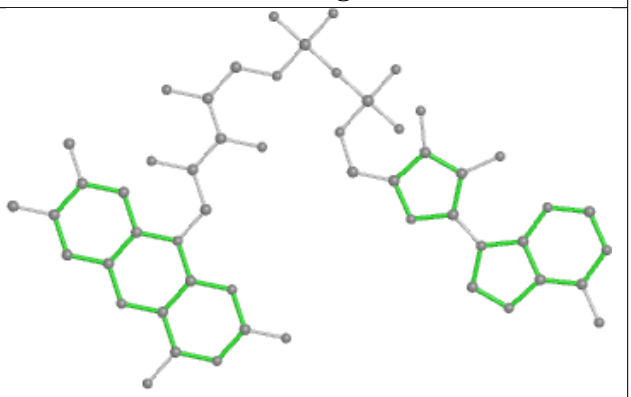
Bond lengths



Bond angles

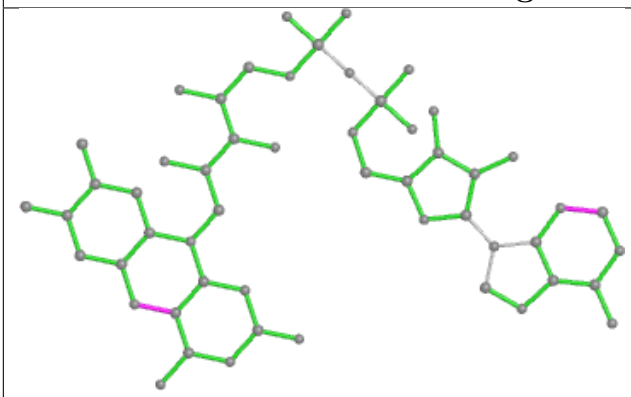


Torsions



Rings

Ligand FAD B 3457



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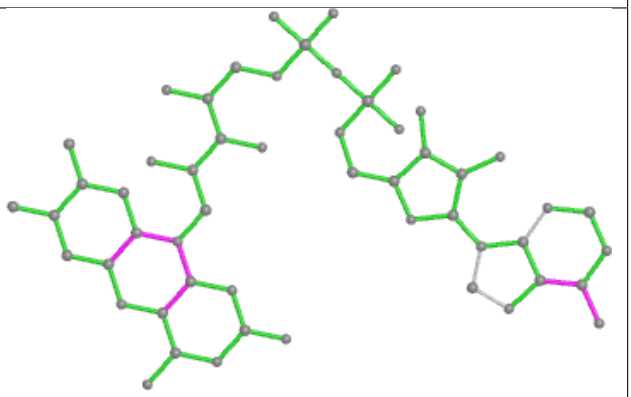
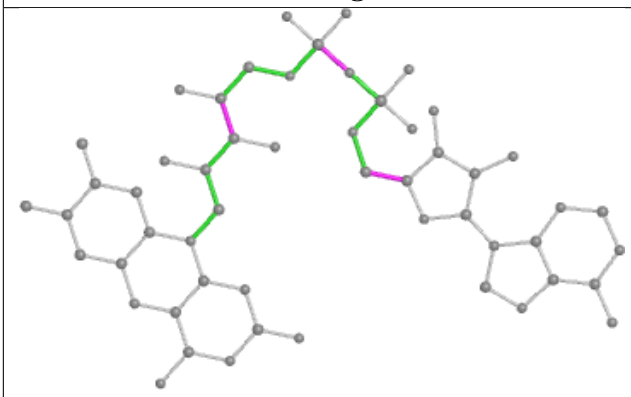
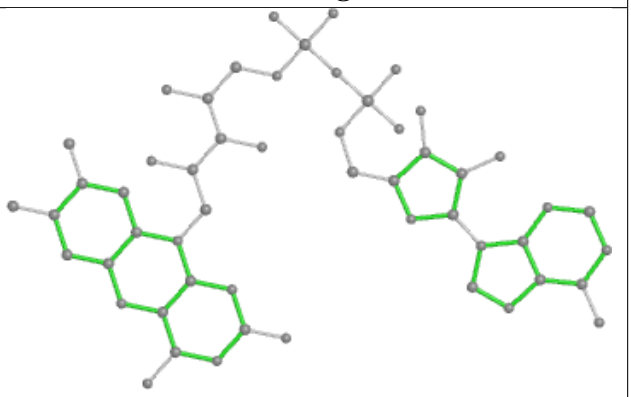


Bond angles

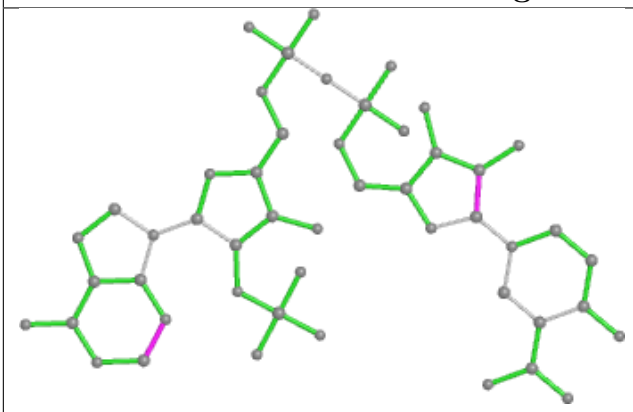


Torsions

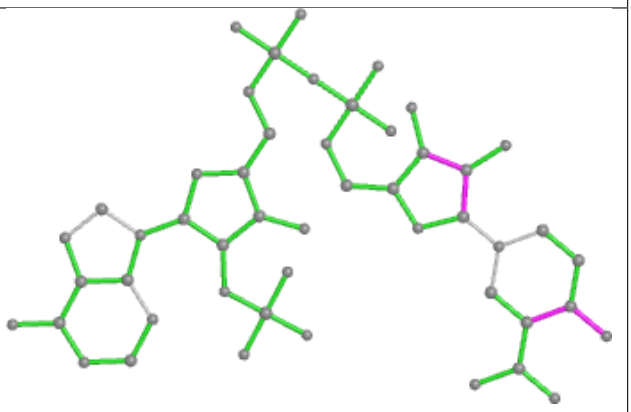


Rings

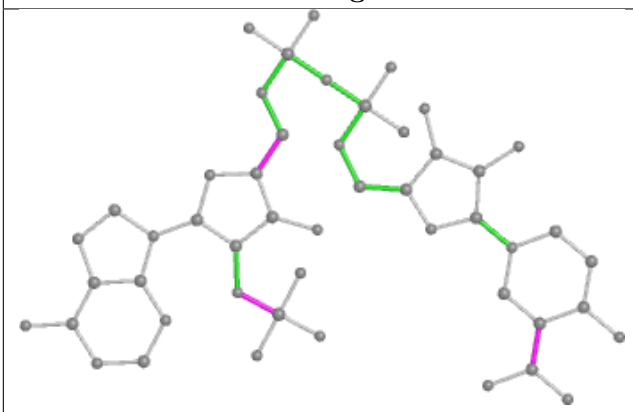
Ligand ODP B 3458



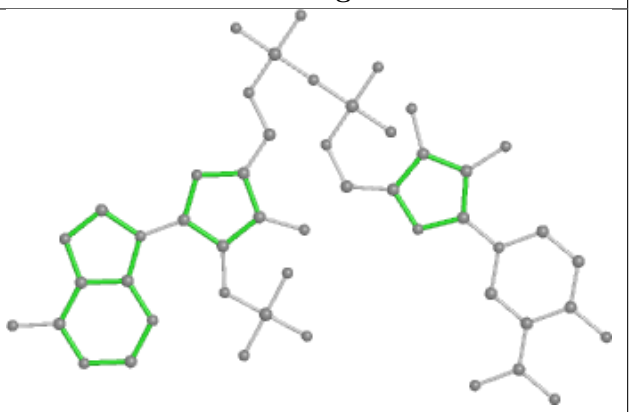
Bond lengths



Bond angles

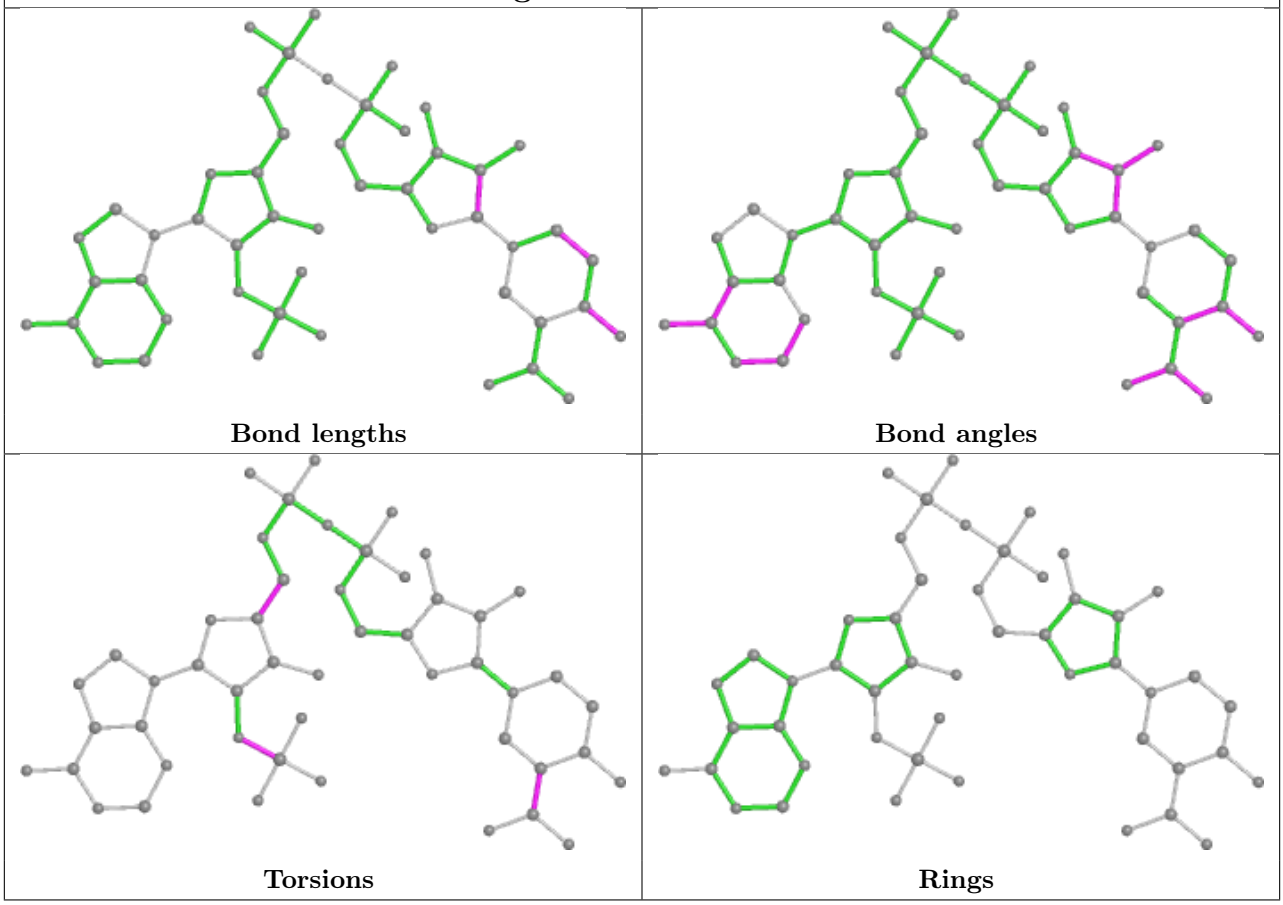


Torsions



Rings

Ligand ODP A 2458



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	452/456 (99%)	-0.08	12 (2%)	54	49	8, 12, 22, 36	0
1	B	454/456 (99%)	0.01	22 (4%)	30	27	7, 13, 24, 36	0
All	All	906/912 (99%)	-0.04	34 (3%)	40	35	7, 13, 23, 36	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	ALA	8.2
1	B	263	GLY	7.7
1	B	282	ARG	6.4
1	B	231	ASP	5.8
1	B	281	LYS	5.6
1	B	262	PRO	5.1
1	B	232	GLY	5.0
1	B	236	GLU	5.0
1	B	261	ARG	4.9
1	A	394	GLU	4.7
1	A	392	GLY	3.9
1	A	261	ARG	3.9
1	B	437	HIS	3.6
1	A	281	LYS	3.5
1	A	60[A]	ILE	3.4
1	B	302	VAL	3.4
1	B	435	GLU	3.1
1	B	235	ASP	3.1
1	B	189	ARG	2.9
1	A	258	ARG	2.8
1	B	286	ARG	2.7
1	B	243	LYS	2.7
1	A	189	ARG	2.7
1	A	395	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	336	ASP	2.6
1	B	118	ASP	2.5
1	B	397	SER	2.5
1	A	282	ARG	2.4
1	B	258	ARG	2.2
1	B	300	GLY	2.2
1	A	456	GLY	2.2
1	A	301	ARG	2.1
1	B	301	ARG	2.1
1	B	394	GLU	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(Å^2)	Q<0.9
2	ACT	B	1873	4/4	0.21	0.28	47,47,47,48	0
2	ACT	A	1869	4/4	0.72	0.23	27,29,29,29	0
2	ACT	A	1872	4/4	0.74	0.19	24,27,27,27	0
2	ACT	B	1875	4/4	0.76	0.31	27,30,30,31	0
2	ACT	A	1866	4/4	0.79	0.36	25,27,28,28	0
2	ACT	B	1876	4/4	0.79	0.38	25,30,30,31	0
2	ACT	A	1870	4/4	0.80	0.19	29,31,31,33	0
2	ACT	B	1868	4/4	0.90	0.12	19,20,20,21	0
2	ACT	B	1867	4/4	0.91	0.20	14,16,24,24	0
2	ACT	B	1874	4/4	0.92	0.08	15,16,18,18	0
2	ACT	A	1871	4/4	0.94	0.09	15,16,16,18	0
3	FAD	A	2457	53/53	0.98	0.09	5,8,10,12	13
3	FAD	B	3457	53/53	0.98	0.08	4,7,9,10	13

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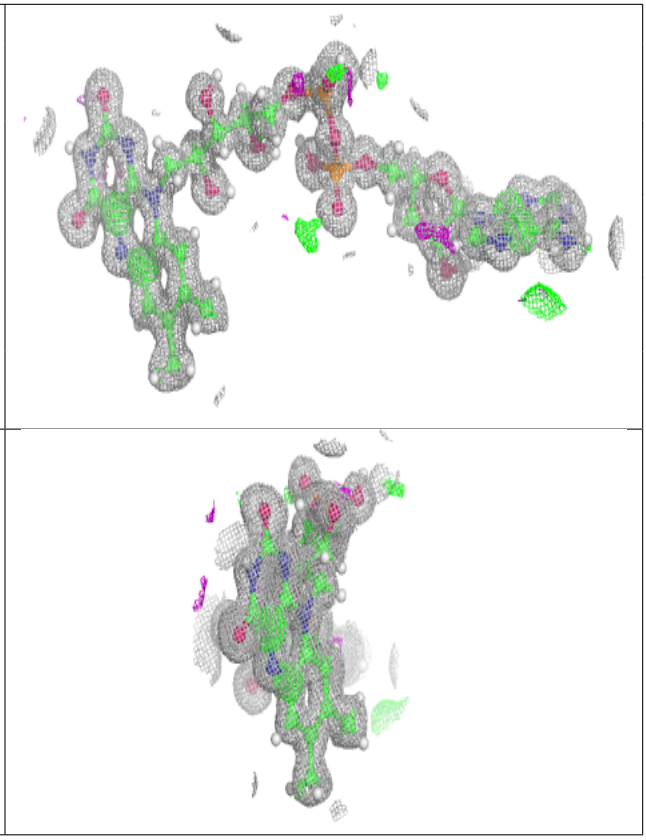
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ODP	A	2458	49/49	0.99	0.06	6,10,13,16	10
4	ODP	B	3458	49/49	0.99	0.07	7,10,13,14	10

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.

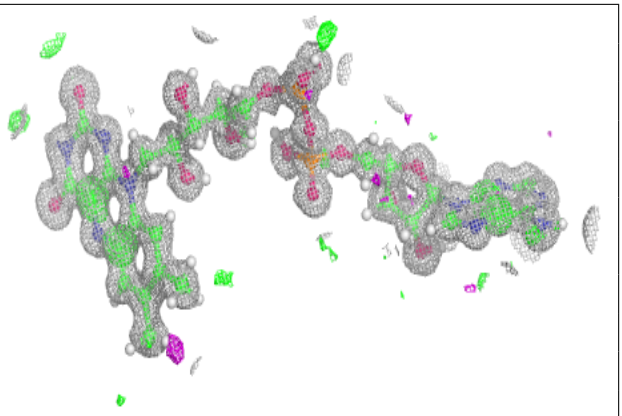
Electron density around FAD A 2457:

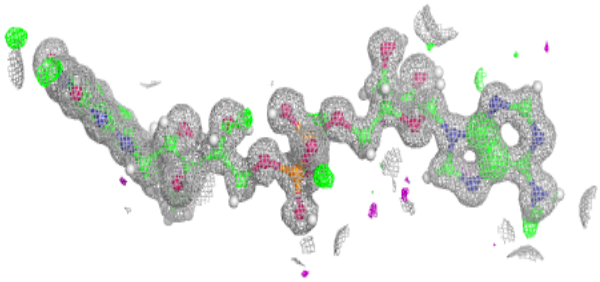
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

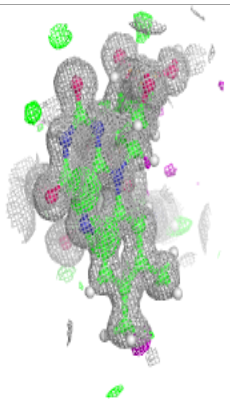


Electron density around FAD B 3457:

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

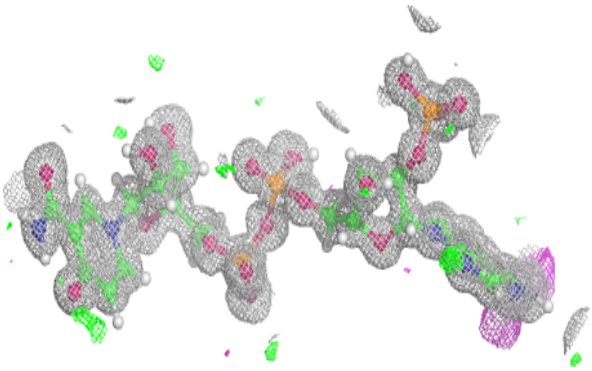


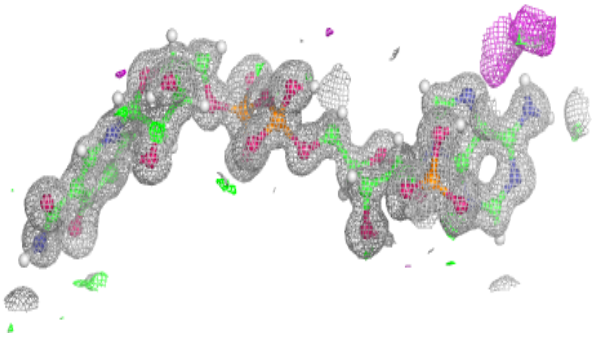


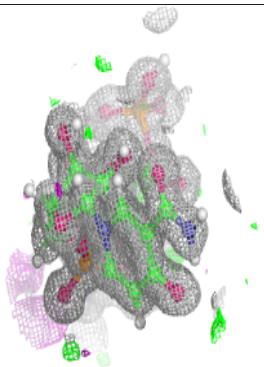


Electron density around ODP A 2458:

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

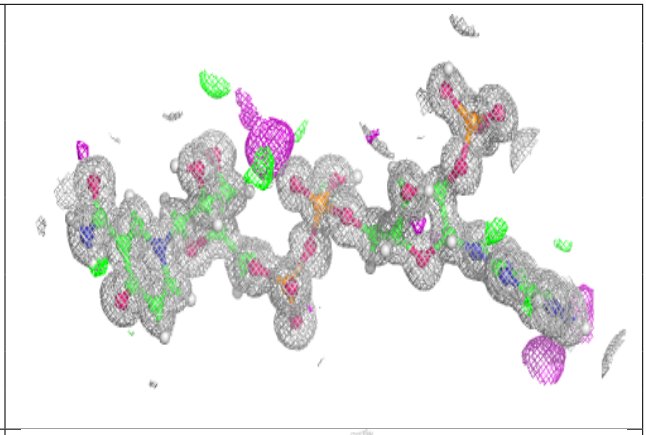


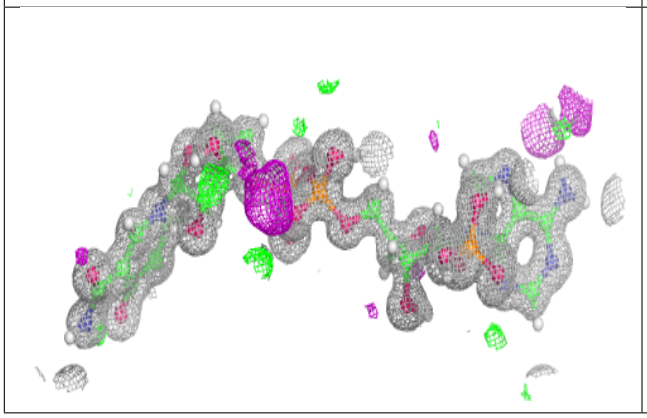


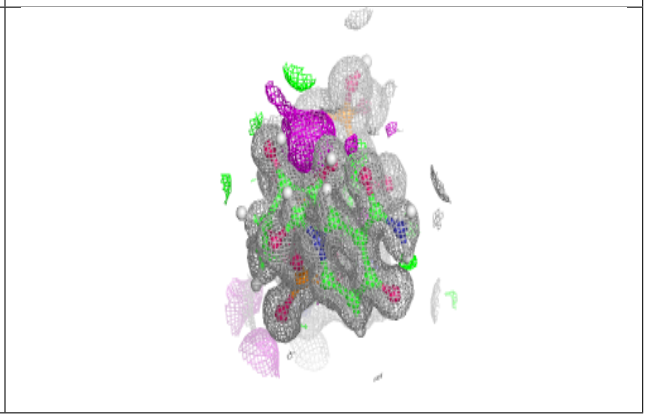


Electron density around ODP B 3458:

$2mF_o$-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.