Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 02:06 AM EDT

PDB ID	:	5L1N
Title	:	Pyrococcus horikoshii CoA Disulfide Reductase Quadruple Mutant
Authors	:	Sea, K.; Chen, B.; Crane III, E.J.; Sazinsky, M.H.
Deposited on	:	2016-07-29
Resolution	:	3.60 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:

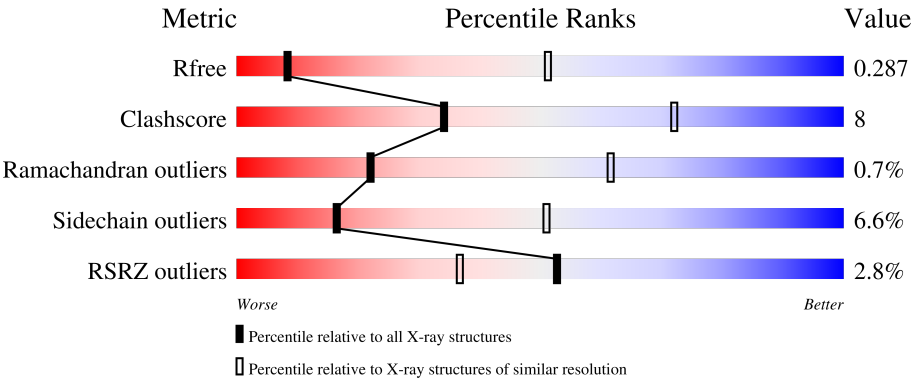
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	453	3% 80% 15%
1	B	453	2% 79% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7023 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.

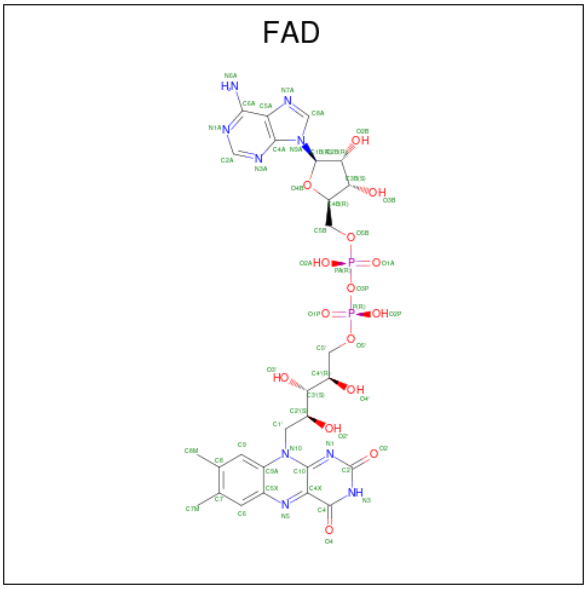
- Molecule 1 is a protein called Coenzyme A disulfide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3407	2187	579	627	14			
1	B	443	Total	C	N	O	S	0	0	0
			3414	2190	579	631	14			

There are 24 discrepancies between the modelled and reference sequences:

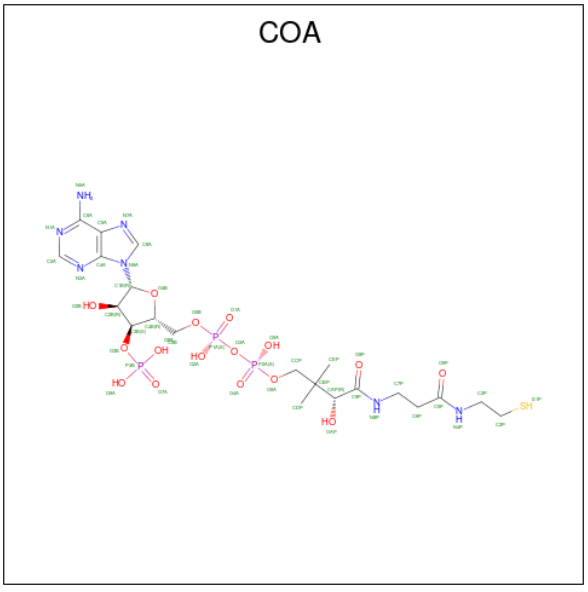
Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ALA	TYR	engineered mutation	UNP O58308
A	66	ALA	TYR	engineered mutation	UNP O58308
A	67	GLY	PRO	engineered mutation	UNP O58308
A	367	ALA	HIS	engineered mutation	UNP O58308
A	446	LEU	-	expression tag	UNP O58308
A	447	GLU	-	expression tag	UNP O58308
A	448	HIS	-	expression tag	UNP O58308
A	449	HIS	-	expression tag	UNP O58308
A	450	HIS	-	expression tag	UNP O58308
A	451	HIS	-	expression tag	UNP O58308
A	452	HIS	-	expression tag	UNP O58308
A	453	HIS	-	expression tag	UNP O58308
B	65	ALA	TYR	engineered mutation	UNP O58308
B	66	ALA	TYR	engineered mutation	UNP O58308
B	67	GLY	PRO	engineered mutation	UNP O58308
B	367	ALA	HIS	engineered mutation	UNP O58308
B	446	LEU	-	expression tag	UNP O58308
B	447	GLU	-	expression tag	UNP O58308
B	448	HIS	-	expression tag	UNP O58308
B	449	HIS	-	expression tag	UNP O58308
B	450	HIS	-	expression tag	UNP O58308
B	451	HIS	-	expression tag	UNP O58308
B	452	HIS	-	expression tag	UNP O58308
B	453	HIS	-	expression tag	UNP O58308

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).

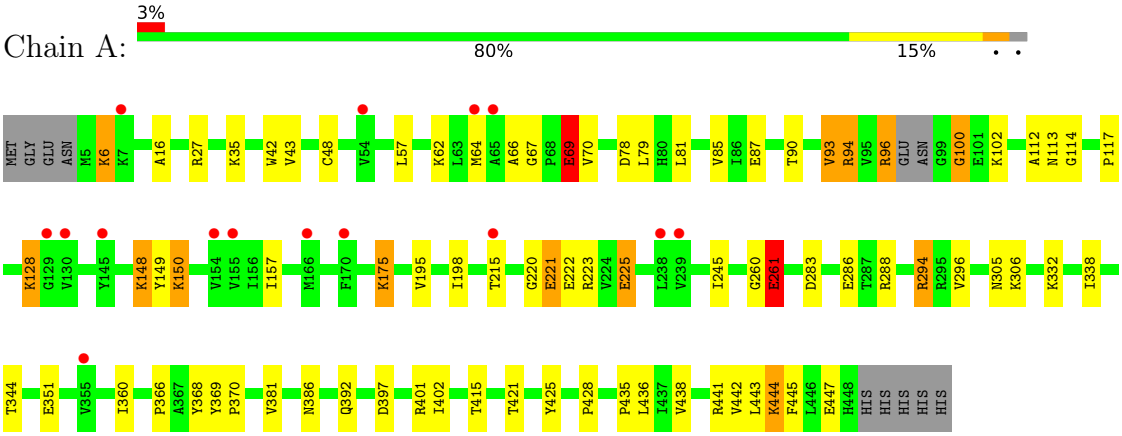


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

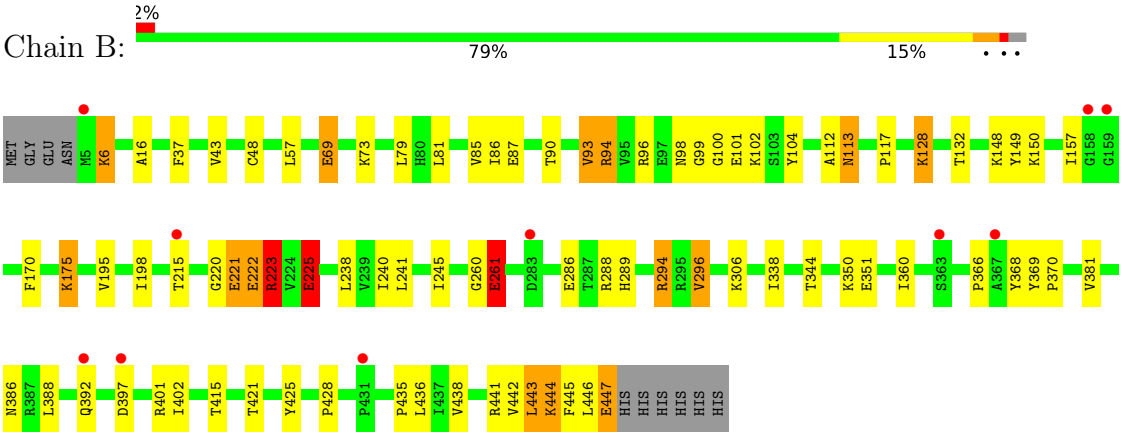
3 Residue-property plots (i)

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: Coenzyme A disulfide reductase



• Molecule 1: Coenzyme A disulfide reductase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	191.97Å 191.97Å 74.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.98 – 3.60 39.26 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (95.98-3.60) 99.7 (39.26-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	3.84 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.245 , 0.290 0.256 , 0.287	Depositor DCC
R_{free} test set	575 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	134.2	Xtriage
Anisotropy	1.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 114.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7023	wwPDB-VP
Average B, all atoms (Å^2)	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: FAD, COA

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	0.51	2/3473 (0.1%)	0.81	7/4702 (0.1%)
1	B	0.52	3/3480 (0.1%)	0.83	11/4713 (0.2%)
All	All	0.52	5/6953 (0.1%)	0.82	18/9415 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	GLU	CD-OE1	7.05	1.33	1.25
1	B	261	GLU	CD-OE1	6.89	1.33	1.25
1	A	261	GLU	CD-OE1	6.75	1.33	1.25
1	B	99	GLY	C-O	-5.46	1.15	1.23
1	A	150	LYS	CD-CE	5.05	1.63	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	223	ARG	CB-CA-C	-13.53	83.33	110.40
1	A	175	LYS	CD-CE-NZ	11.57	138.32	111.70
1	B	175	LYS	CD-CE-NZ	9.45	133.44	111.70
1	B	6	LYS	CA-CB-CG	9.22	133.69	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	LYS	CA-CB-CG	8.16	131.34	113.40
1	B	148	LYS	CA-CB-CG	7.46	129.81	113.40
1	B	6	LYS	CB-CA-C	-7.42	95.57	110.40
1	B	69	GLU	CA-CB-CG	7.40	129.69	113.40
1	A	69	GLU	CA-CB-CG	7.12	129.06	113.40
1	B	148	LYS	CB-CA-C	-7.03	96.35	110.40
1	A	6	LYS	N-CA-CB	6.22	121.79	110.60
1	B	6	LYS	CB-CG-CD	5.90	126.93	111.60
1	A	148	LYS	CG-CD-CE	5.60	128.70	111.90
1	B	148	LYS	CB-CG-CD	5.35	125.52	111.60
1	B	113	ASN	CB-CA-C	5.35	121.10	110.40
1	A	6	LYS	CB-CA-C	-5.34	99.72	110.40
1	A	148	LYS	CD-CE-NZ	5.18	123.61	111.70
1	B	350	LYS	CD-CE-NZ	-5.00	100.20	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ALA	Peptide
1	B	112	ALA	Peptide
1	B	223	ARG	Peptide
1	B	98	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3407	0	3482	56	0
1	B	3414	0	3487	67	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	48	0	32	5	0
3	B	48	0	32	5	0
All	All	7023	0	7095	119	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 8.

All (119) 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:B:221:GLU:HG3	1:B:222:GLU:H	1.27	0.97
1:B:220:GLY:HA2	1:B:225:GLU:HG3	1.46	0.94
1:B:415:THR:OG1	1:B:445:PHE:HB2	1.69	0.93
1:A:48:CYS:SG	3:A:902:COA:S1P	2.59	0.90
1:A:386:ASN:ND2	1:A:445:PHE:CE1	2.40	0.89
1:B:220:GLY:HA2	1:B:225:GLU:CG	2.06	0.85
1:B:128:LYS:HB3	1:B:223:ARG:HB3	1.58	0.84
1:B:48:CYS:HG	3:B:902:COA:HS1	0.92	0.84
1:B:447:GLU:N	1:B:447:GLU:OE2	2.11	0.84
1:A:369:TYR:CE2	1:A:428:PRO:HA	2.17	0.80
1:A:220:GLY:HA2	1:A:225:GLU:HG3	1.66	0.78
1:B:442:VAL:O	1:B:444:LYS:HG3	1.85	0.77
1:B:369:TYR:CE2	1:B:428:PRO:HA	2.20	0.77
1:B:386:ASN:CB	1:B:445:PHE:CD1	2.46	0.76
1:A:368:TYR:OH	1:A:425:TYR:OH	2.04	0.74
1:B:446:LEU:HD23	1:B:446:LEU:N	2.03	0.74
1:B:48:CYS:SG	3:B:902:COA:S1P	2.69	0.73
1:A:438:VAL:O	1:A:442:VAL:HG23	1.90	0.72
1:B:221:GLU:HG3	1:B:222:GLU:N	2.05	0.71
1:B:16:ALA:HB2	3:B:902:COA:H32	1.73	0.69
1:A:415:THR:HG22	1:A:443:LEU:HD13	1.73	0.69
1:B:368:TYR:OH	1:B:425:TYR:OH	2.11	0.68
1:B:438:VAL:O	1:B:442:VAL:HG23	1.94	0.68
1:B:415:THR:HG1	1:B:445:PHE:HB2	1.57	0.66
1:B:261:GLU:OE2	1:B:261:GLU:HA	1.98	0.63
1:A:386:ASN:ND2	1:A:445:PHE:HE1	1.98	0.62
1:A:261:GLU:OE2	1:A:261:GLU:HA	2.01	0.61
1:B:360:ILE:HG21	1:B:442:VAL:HG21	1.83	0.60
1:A:294:ARG:NE	1:A:351:GLU:OE1	2.34	0.60
1:B:221:GLU:O	1:B:223:ARG:N	2.35	0.60
1:A:43:VAL:HG23	1:A:81:LEU:HD21	1.84	0.60
1:A:369:TYR:CD2	1:A:428:PRO:HA	2.36	0.60
1:A:220:GLY:HA2	1:A:225:GLU:CG	2.30	0.60
1:A:128:LYS:HE3	1:A:222:GLU:OE2	2.02	0.59
1:B:294:ARG:NE	1:B:351:GLU:OE1	2.36	0.59
1:B:132:THR:HG22	1:B:241:LEU:HB2	1.84	0.59
1:B:446:LEU:O	1:B:447:GLU:HB3	2.01	0.59
1:A:441:ARG:NH2	3:B:902:COA:O8A	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLU:C	1:B:223:ARG:H	2.06	0.58
1:A:415:THR:HG22	1:A:443:LEU:CD1	2.34	0.58
1:B:170:PHE:HE2	1:B:240:ILE:HG13	1.67	0.58
1:A:381:VAL:HG21	1:A:443:LEU:HD13	1.85	0.57
1:A:445:PHE:CE2	1:A:447:GLU:OE2	2.58	0.57
1:A:360:ILE:HG21	1:A:442:VAL:HG21	1.87	0.56
1:A:386:ASN:CG	1:A:445:PHE:CD1	2.79	0.56
1:B:87:GLU:HB3	1:B:94:ARG:HB2	1.89	0.55
1:A:149:TYR:HB3	1:A:223:ARG:NH1	2.22	0.55
3:A:902:COA:O8A	1:B:441:ARG:NH2	2.40	0.55
1:B:43:VAL:HG23	1:B:81:LEU:HD21	1.89	0.54
1:A:421:THR:O	1:B:306:LYS:NZ	2.42	0.53
1:B:128:LYS:CB	1:B:223:ARG:HB3	2.35	0.53
1:A:306:LYS:NZ	1:B:421:THR:O	2.42	0.53
1:B:149:TYR:HB3	1:B:223:ARG:HH12	1.73	0.53
1:B:221:GLU:C	1:B:223:ARG:N	2.61	0.52
1:B:369:TYR:CD2	1:B:428:PRO:HA	2.43	0.52
1:B:446:LEU:N	1:B:446:LEU:CD2	2.73	0.52
1:A:57:LEU:HD13	1:B:369:TYR:HE1	1.75	0.52
1:A:87:GLU:HB3	1:A:94:ARG:HB2	1.92	0.51
1:B:441:ARG:O	1:B:444:LYS:HG2	2.11	0.50
1:B:447:GLU:HG2	1:B:447:GLU:O	2.10	0.50
1:A:66:ALA:HB1	1:A:70:VAL:HG21	1.94	0.50
1:B:221:GLU:CG	1:B:222:GLU:H	2.06	0.50
1:A:415:THR:CG2	1:A:443:LEU:HD13	2.40	0.49
1:A:67:GLY:HA3	1:A:69:GLU:OE1	2.12	0.49
1:A:443:LEU:O	1:A:444:LYS:HB2	2.11	0.49
1:A:195:VAL:HG12	1:A:338:ILE:HD11	1.94	0.49
1:A:43:VAL:HG21	1:A:79:LEU:HD21	1.95	0.49
1:B:444:LYS:O	1:B:446:LEU:HD22	2.12	0.49
1:A:42:TRP:CE3	1:A:64:MET:HG3	2.47	0.49
1:A:386:ASN:CG	1:A:445:PHE:CE1	2.85	0.49
1:B:223:ARG:O	1:B:223:ARG:HG3	2.12	0.48
1:A:369:TYR:HE1	1:B:57:LEU:HD13	1.78	0.48
1:B:443:LEU:C	1:B:444:LYS:HG3	2.35	0.47
1:A:222:GLU:OE1	1:A:223:ARG:HG3	2.14	0.47
1:B:170:PHE:CE2	1:B:240:ILE:HG13	2.48	0.47
1:A:16:ALA:HB2	3:A:902:COA:H31	1.96	0.47
1:A:369:TYR:CD1	1:A:370:PRO:HD2	2.50	0.47
1:A:386:ASN:HD22	1:A:445:PHE:HE1	1.61	0.47
1:B:195:VAL:HG12	1:B:338:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASN:OD1	1:B:445:PHE:CD1	2.32	0.47
1:A:386:ASN:ND2	1:A:445:PHE:CD1	2.81	0.46
1:A:96:ARG:HA	1:A:100:GLY:O	2.16	0.46
1:A:117:PRO:HA	1:A:245:ILE:HG22	1.98	0.46
1:B:344:THR:HG22	1:B:392:GLN:HE21	1.81	0.46
1:B:43:VAL:HG21	1:B:79:LEU:HD21	1.98	0.46
1:A:441:ARG:CZ	3:B:902:COA:H3B	2.46	0.46
1:A:445:PHE:HE2	1:A:447:GLU:OE2	1.98	0.46
1:B:369:TYR:CD1	1:B:370:PRO:HD2	2.52	0.45
1:B:86:ILE:HD11	1:B:101:GLU:OE2	2.17	0.45
1:B:401:ARG:HG2	1:B:436:LEU:HB2	1.98	0.45
1:B:381:VAL:HG21	1:B:443:LEU:HD13	1.99	0.45
1:A:260:GLY:HA3	1:A:286:GLU:OE1	2.16	0.45
1:A:221:GLU:HG2	1:A:222:GLU:H	1.82	0.45
1:B:117:PRO:HA	1:B:245:ILE:HG22	1.99	0.45
1:B:238:LEU:HD21	1:B:240:ILE:HD11	1.98	0.45
1:A:344:THR:HG22	1:A:392:GLN:HE21	1.83	0.44
1:A:113:ASN:O	1:A:113:ASN:OD1	2.36	0.44
1:A:397:ASP:O	1:A:401:ARG:NH1	2.51	0.44
1:A:366:PRO:HB2	1:A:368:TYR:CE1	2.53	0.44
1:B:366:PRO:HB2	1:B:368:TYR:CE1	2.54	0.43
1:A:35:LYS:NZ	1:A:78:ASP:OD2	2.47	0.43
1:B:401:ARG:HD3	1:B:435:PRO:HB2	2.00	0.43
1:B:85:VAL:HG13	1:B:93:VAL:HG22	2.01	0.43
1:A:27:ARG:CZ	3:A:902:COA:O9A	2.67	0.42
1:A:401:ARG:HG2	1:A:436:LEU:HB2	2.02	0.42
1:B:132:THR:HG22	1:B:241:LEU:CB	2.48	0.42
1:B:397:ASP:O	1:B:401:ARG:NH1	2.52	0.42
1:B:86:ILE:CD1	1:B:101:GLU:OE2	2.68	0.42
1:B:381:VAL:HG22	1:B:388:LEU:HD23	2.02	0.42
1:B:260:GLY:HA3	1:B:286:GLU:OE1	2.20	0.42
1:A:85:VAL:HG13	1:A:93:VAL:HG22	2.02	0.42
1:A:114:GLY:HA2	1:A:283:ASP:HB2	2.01	0.42
1:A:305:ASN:ND2	3:A:902:COA:OAP	2.52	0.42
1:B:447:GLU:N	1:B:447:GLU:CD	2.72	0.41
1:B:37:PHE:CZ	1:B:104:TYR:HD2	2.38	0.41
1:B:289:HIS:HB2	1:B:296:VAL:CG1	2.52	0.40
1:A:401:ARG:HD3	1:A:435:PRO:HB2	2.03	0.40
1:B:48:CYS:SG	2:B:901:FAD:C10	3.10	0.40
1:B:441:ARG:O	1:B:444:LYS:CG	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/453 (97%)	423 (97%)	13 (3%)	2 (0%)	29	68
1	B	441/453 (97%)	421 (96%)	16 (4%)	4 (1%)	17	57
All	All	879/906 (97%)	844 (96%)	29 (3%)	6 (1%)	22	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	221	GLU
1	B	222	GLU
1	A	221	GLU
1	B	444	LYS
1	A	100	GLY
1	B	100	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	354/364 (97%)	331 (94%)	23 (6%)	17	51
1	B	355/364 (98%)	331 (93%)	24 (7%)	16	50
All	All	709/728 (97%)	662 (93%)	47 (7%)	16	51

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	62	LYS
1	A	69	GLU
1	A	90	THR
1	A	93	VAL
1	A	94	ARG
1	A	96	ARG
1	A	102	LYS
1	A	128	LYS
1	A	148	LYS
1	A	150	LYS
1	A	157	ILE
1	A	175	LYS
1	A	198	ILE
1	A	215	THR
1	A	225	GLU
1	A	261	GLU
1	A	288	ARG
1	A	294	ARG
1	A	296	VAL
1	A	332	LYS
1	A	402	ILE
1	A	444	LYS
1	B	6	LYS
1	B	69	GLU
1	B	73	LYS
1	B	90	THR
1	B	93	VAL
1	B	94	ARG
1	B	96	ARG
1	B	102	LYS
1	B	113	ASN
1	B	128	LYS
1	B	150	LYS
1	B	157	ILE
1	B	175	LYS
1	B	198	ILE
1	B	215	THR
1	B	223	ARG
1	B	225	GLU
1	B	261	GLU
1	B	288	ARG
1	B	294	ARG

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Mol	Chain	Res	Type
1	B	296	VAL
1	B	402	ILE
1	B	443	LEU
1	B	447	GLU

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	305	ASN
1	A	321	HIS
1	B	305	ASN
1	B	321	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	FAD	B	901	-	53,58,58	1.49	9 (16%)	68,89,89	1.43	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	COA	A	902	-	41,50,50	1.09	4 (9%)	52,75,75	1.31	8 (15%)
3	COA	B	902	-	41,50,50	1.02	2 (4%)	52,75,75	2.53	14 (26%)
2	FAD	A	901	-	53,58,58	1.48	7 (13%)	68,89,89	1.46	12 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	901	-	-	6/30/50/50	0/6/6/6
3	COA	A	902	-	-	14/44/64/64	0/3/3/3
3	COA	B	902	-	-	20/44/64/64	0/3/3/3
2	FAD	A	901	-	-	3/30/50/50	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	FAD	C9A-C5X	5.99	1.51	1.41
2	B	901	FAD	C9A-C5X	5.92	1.51	1.41
3	A	902	COA	O5P-C5P	3.88	1.31	1.23
2	B	901	FAD	C8-C7	3.80	1.50	1.40
2	A	901	FAD	C8-C7	3.65	1.50	1.40
3	B	902	COA	C5A-C4A	3.10	1.49	1.40
2	A	901	FAD	C10-N10	2.78	1.43	1.37
3	A	902	COA	C5A-C4A	2.70	1.48	1.40
2	B	901	FAD	C5A-C4A	2.66	1.48	1.40
2	B	901	FAD	C10-N10	2.62	1.43	1.37
3	B	902	COA	C2A-N3A	2.50	1.36	1.32
2	A	901	FAD	C5A-C4A	2.45	1.47	1.40
2	A	901	FAD	C5X-N5	-2.34	1.35	1.39
2	B	901	FAD	C5X-N5	-2.26	1.35	1.39
3	A	902	COA	C2A-N3A	2.25	1.35	1.32
2	B	901	FAD	C4-N3	-2.23	1.34	1.38
2	A	901	FAD	C2A-N3A	2.18	1.35	1.32
2	A	901	FAD	C4-N3	-2.15	1.34	1.38
2	B	901	FAD	O4B-C1B	2.14	1.44	1.41
2	B	901	FAD	C2A-N3A	2.10	1.35	1.32
3	A	902	COA	O4B-C1B	2.09	1.44	1.41
2	B	901	FAD	C4X-N5	2.09	1.34	1.30

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	902	COA	CEP-CBP-CCP	9.14	123.14	108.23
3	B	902	COA	CEP-CBP-CAP	-7.23	96.29	108.82
3	B	902	COA	CDP-CBP-CAP	-6.21	98.05	108.82
3	B	902	COA	CEP-CBP-CDP	4.76	118.87	109.17
3	B	902	COA	CDP-CBP-CCP	4.37	115.37	108.23
3	B	902	COA	C3P-N4P-C5P	-4.32	114.81	122.84
3	B	902	COA	O6A-CCP-CBP	-3.71	104.58	110.55
2	A	901	FAD	N3A-C2A-N1A	-3.57	123.10	128.68
3	A	902	COA	N3A-C2A-N1A	-3.52	123.18	128.68
2	B	901	FAD	N3A-C2A-N1A	-3.48	123.24	128.68
2	A	901	FAD	C4X-C10-N1	-3.46	116.71	124.73
3	B	902	COA	N3A-C2A-N1A	-3.36	123.43	128.68
2	B	901	FAD	C4X-C10-N1	-3.33	117.00	124.73
2	A	901	FAD	C4'-C3'-C2'	2.95	119.50	113.36
3	B	902	COA	C1B-N9A-C4A	2.74	131.46	126.64
3	A	902	COA	P2A-O3A-P1A	-2.66	123.69	132.83
2	B	901	FAD	C3B-C2B-C1B	2.65	104.96	100.98
2	B	901	FAD	C4A-C5A-N7A	-2.63	106.65	109.40
2	B	901	FAD	C10-N1-C2	2.58	122.07	116.90
2	A	901	FAD	C4A-C5A-N7A	-2.58	106.71	109.40
2	A	901	FAD	C10-N1-C2	2.57	122.05	116.90
2	A	901	FAD	C4X-C10-N10	2.54	120.20	116.48
3	B	902	COA	C6P-C7P-N8P	2.50	116.94	111.90
3	B	902	COA	C6P-C5P-N4P	-2.48	112.25	116.42
2	A	901	FAD	P-O3P-PA	-2.44	124.45	132.83
2	B	901	FAD	C4X-C10-N10	2.41	120.01	116.48
2	A	901	FAD	C9A-N10-C10	-2.39	117.05	120.77
3	A	902	COA	C4A-C5A-N7A	-2.35	106.95	109.40
3	A	902	COA	C3B-C2B-C1B	2.34	105.08	99.89
2	B	901	FAD	C4'-C3'-C2'	2.31	118.17	113.36
3	A	902	COA	CEP-CBP-CAP	2.28	112.77	108.82
3	B	902	COA	C4A-C5A-N7A	-2.25	107.06	109.40
2	A	901	FAD	O2-C2-N1	-2.25	118.10	121.83
3	A	902	COA	CDP-CBP-CAP	2.22	112.66	108.82
3	A	902	COA	C7P-C6P-C5P	-2.21	108.67	112.36
3	B	902	COA	O4B-C1B-C2B	-2.21	103.69	106.93
2	B	901	FAD	C9A-N10-C10	-2.19	117.35	120.77
2	A	901	FAD	O4-C4-C4X	-2.19	120.80	126.60
2	A	901	FAD	O5'-C5'-C4'	2.13	115.06	109.36
3	B	902	COA	P2A-O3A-P1A	-2.13	125.52	132.83
2	B	901	FAD	O2-C2-N1	-2.12	118.32	121.83
3	A	902	COA	CDP-CBP-CCP	2.10	111.66	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	FAD	C5X-N5-C4X	2.06	121.49	118.07
2	B	901	FAD	C2A-N1A-C6A	2.02	122.21	118.75
2	B	901	FAD	C5X-N5-C4X	2.01	121.42	118.07

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	FAD	O4'-C4'-C5'-O5'
2	B	901	FAD	C5B-O5B-PA-O1A
2	B	901	FAD	C5B-O5B-PA-O3P
2	B	901	FAD	O4'-C4'-C5'-O5'
2	B	901	FAD	PA-O3P-P-O5'
3	A	902	COA	C3B-O3B-P3B-O7A
3	A	902	COA	C5B-O5B-P1A-O1A
3	A	902	COA	C5B-O5B-P1A-O3A
3	A	902	COA	C6P-C5P-N4P-C3P
3	A	902	COA	O5P-C5P-N4P-C3P
3	A	902	COA	S1P-C2P-C3P-N4P
3	B	902	COA	C3B-O3B-P3B-O9A
3	B	902	COA	C5B-O5B-P1A-O1A
3	B	902	COA	C5B-O5B-P1A-O2A
3	B	902	COA	CCP-O6A-P2A-O4A
3	B	902	COA	C6P-C5P-N4P-C3P
3	B	902	COA	O5P-C5P-N4P-C3P
3	A	902	COA	C3B-C4B-C5B-O5B
3	A	902	COA	O4B-C4B-C5B-O5B
3	B	902	COA	C3B-C4B-C5B-O5B
3	B	902	COA	O4B-C4B-C5B-O5B
3	A	902	COA	C4B-C3B-O3B-P3B
3	B	902	COA	C4B-C3B-O3B-P3B
3	A	902	COA	C2B-C3B-O3B-P3B
3	B	902	COA	C2B-C3B-O3B-P3B
2	A	901	FAD	PA-O3P-P-O5'
3	B	902	COA	P2A-O3A-P1A-O5B
3	B	902	COA	C3B-O3B-P3B-O7A
3	B	902	COA	CEP-CBP-CCP-O6A
2	B	901	FAD	C3'-C4'-C5'-O5'
3	A	902	COA	C5B-O5B-P1A-O2A
3	A	902	COA	O9P-C9P-CAP-OAP
3	B	902	COA	CDP-CBP-CCP-O6A
3	A	902	COA	C5P-C6P-C7P-N8P

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Mol	Chain	Res	Type	Atoms
3	A	902	COA	C2P-C3P-N4P-C5P
3	B	902	COA	C2P-C3P-N4P-C5P
2	B	901	FAD	O4B-C4B-C5B-O5B
3	B	902	COA	C5B-O5B-P1A-O3A
3	B	902	COA	CCP-O6A-P2A-O3A
2	A	901	FAD	O4B-C4B-C5B-O5B
3	B	902	COA	P1A-O3A-P2A-O5A
3	B	902	COA	CBP-CCP-O6A-P2A
3	B	902	COA	C6P-C7P-N8P-C9P

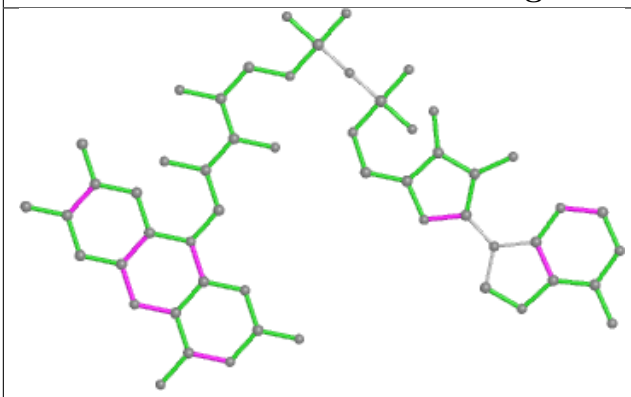
There are no ring outliers.

3 monomers are involved in 11 short contacts:

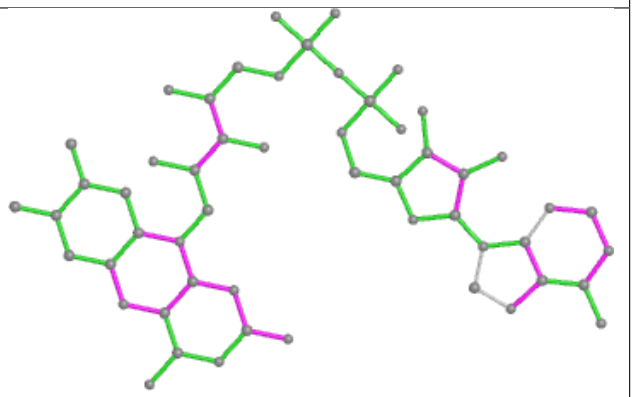
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	FAD	1	0
3	A	902	COA	5	0
3	B	902	COA	5	0

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.

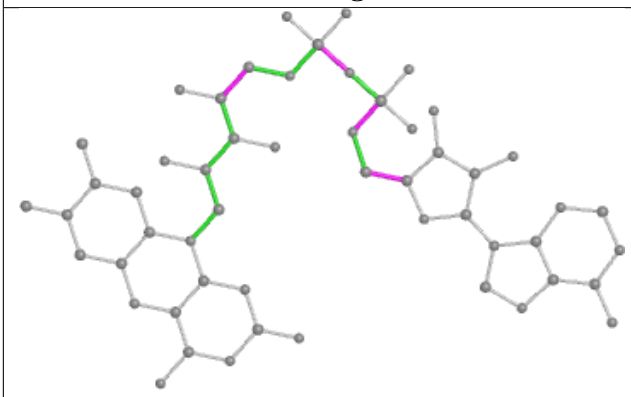
Ligand FAD B 901



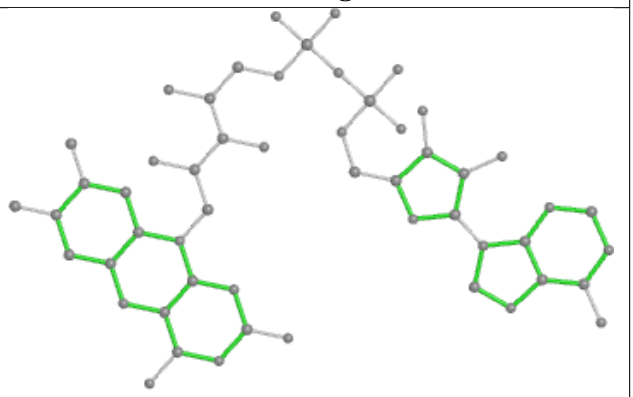
Bond lengths



Bond angles

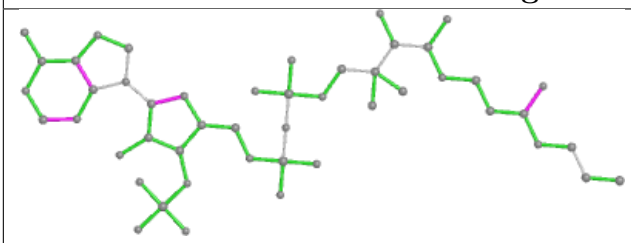


Torsions

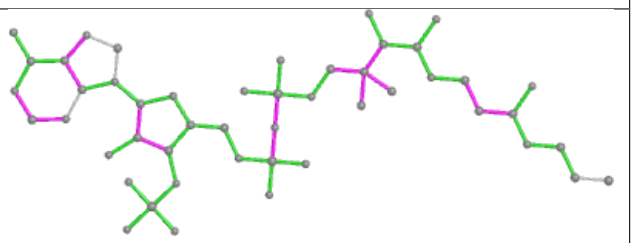


Rings

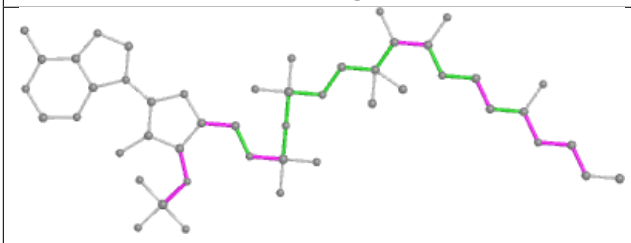
Ligand COA A 902



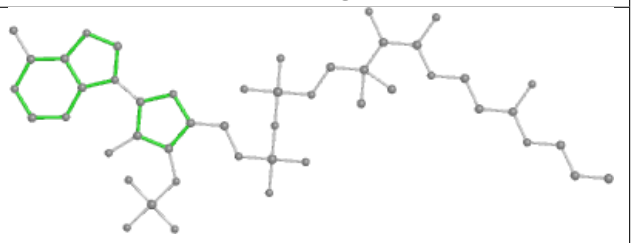
Bond lengths



Bond angles

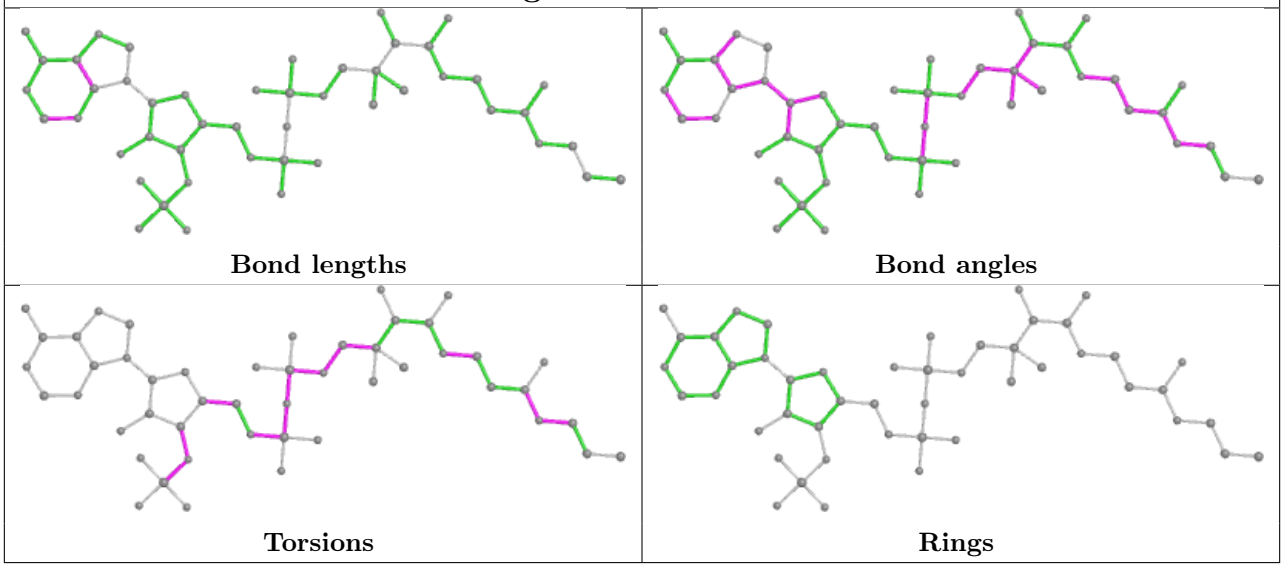


Torsions

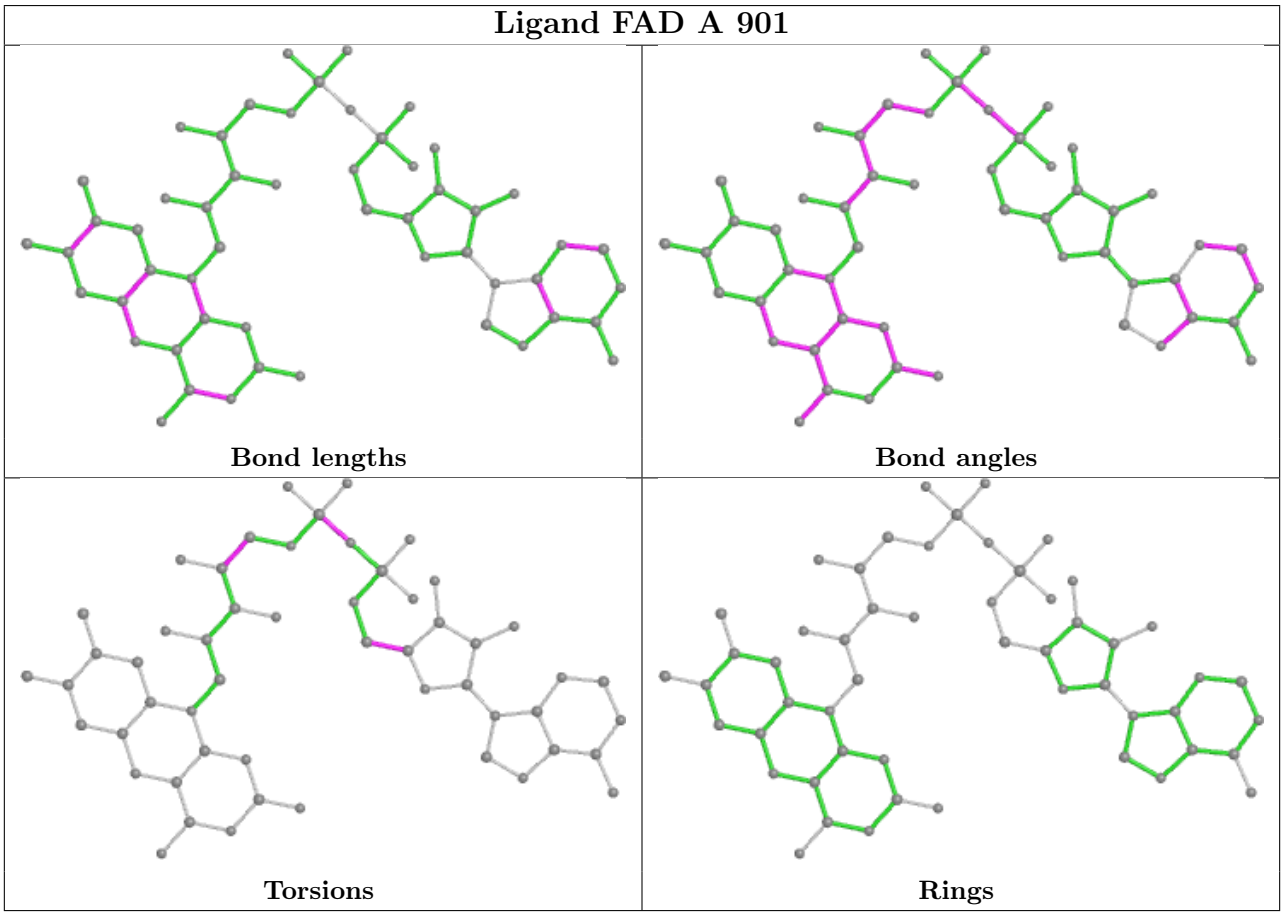


Rings

Ligand COA B 902



Ligand FAD A 901



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	442/453 (97%)	0.04	15 (3%)	45	30	111, 178, 225, 269	0
1	B	443/453 (97%)	0.02	10 (2%)	60	44	110, 177, 226, 266	0
All	All	885/906 (97%)	0.03	25 (2%)	53	37	110, 178, 226, 269	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	GLY	4.3
1	A	238	LEU	4.2
1	A	145	TYR	3.9
1	B	431	PRO	3.5
1	A	215	THR	3.4
1	A	154	VAL	3.3
1	A	54	VAL	3.2
1	A	155	VAL	3.0
1	B	158	GLY	2.9
1	A	65	ALA	2.8
1	A	130	VAL	2.8
1	B	363	SER	2.5
1	B	367	ALA	2.5
1	A	64	MET	2.4
1	B	283	ASP	2.3
1	A	7	LYS	2.2
1	A	166	MET	2.2
1	A	355	VAL	2.2
1	B	215	THR	2.2
1	A	170	PHE	2.2
1	B	159	GLY	2.2
1	B	392	GLN	2.2
1	A	239	VAL	2.1
1	B	5	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	397	ASP	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)

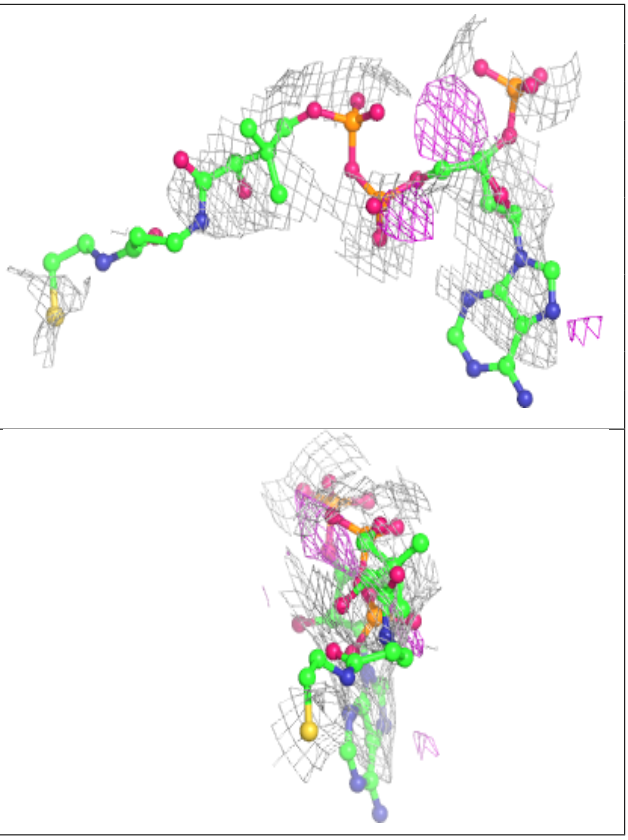
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

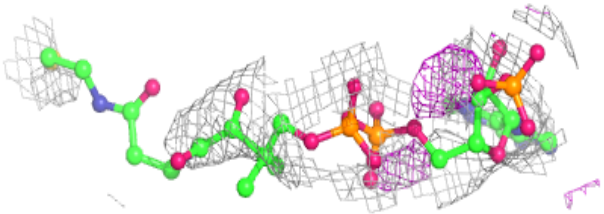
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	COA	B	902	48/48	0.76	0.32	189,219,243,247	0
3	COA	A	902	48/48	0.81	0.39	182,220,241,249	0
2	FAD	A	901	53/53	0.86	0.31	144,205,243,245	0
2	FAD	B	901	53/53	0.90	0.29	146,208,226,237	0

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 COA B 902:

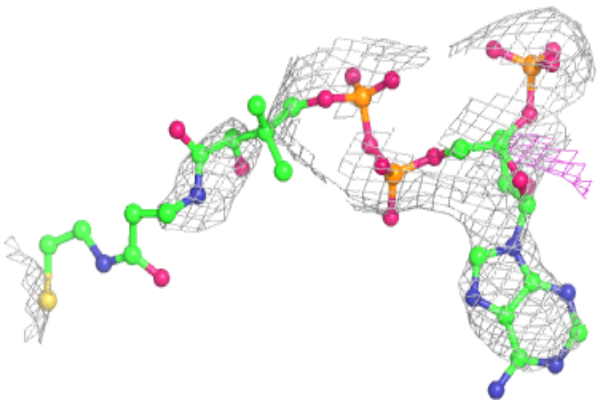
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

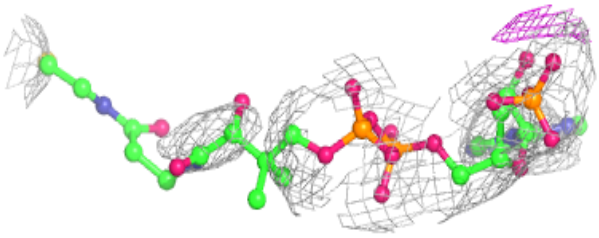


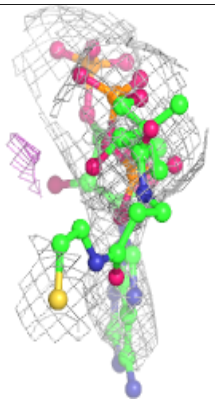


Electron density around COA A 902:

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

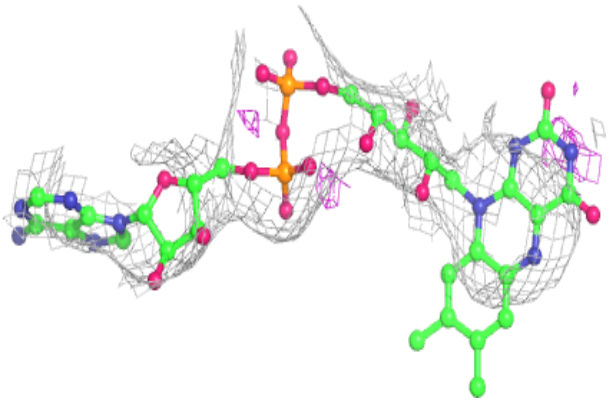


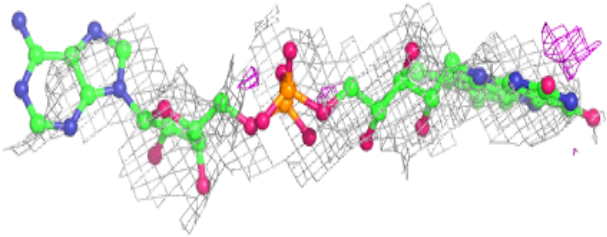


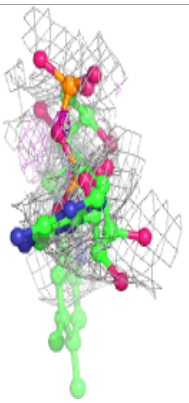


Electron density around FAD A 901:

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

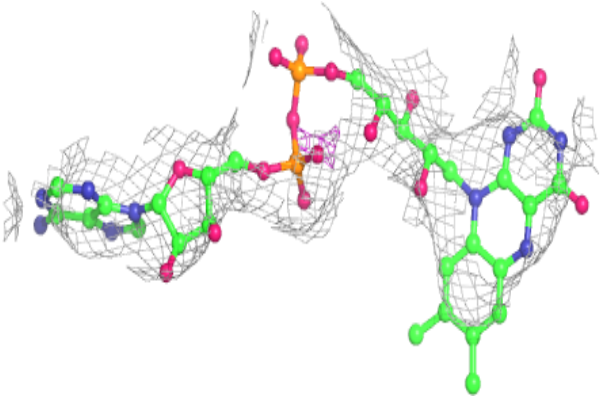


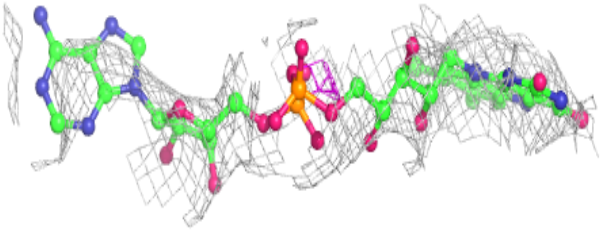


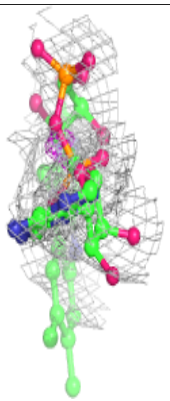


Electron density around FAD B 901:

$2mF_o$-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.