Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 10:32 AM EDT

PDB ID	:	4KAR
Title	:	Crystal structure of FDTS (TM0449) mutant (H53D) with FAD
Authors	:	Mathews, I.I.
Deposited on	:	2013-04-22
Resolution	:	2.03 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:

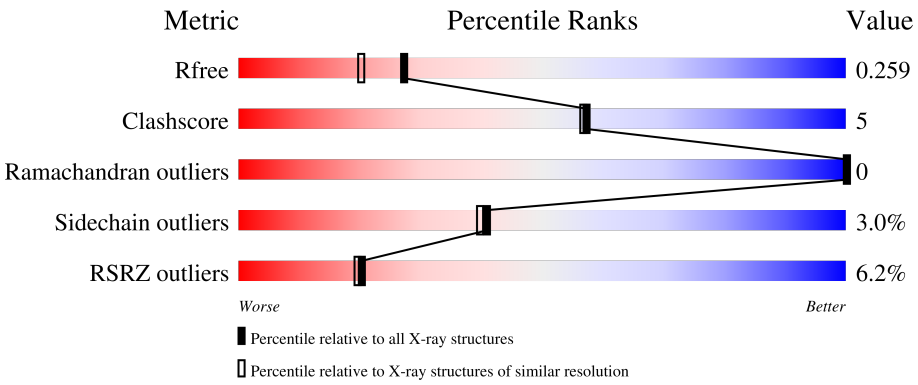
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 <=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	232	7% 75% 16% 8%
1	B	232	5% 78% 13% 9%
1	C	232	6% 82% 12% 6%
1	D	232	5% 83% 9% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7522 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1817	1179	314	318	6	0	2	0
1	B	212	1780	1159	304	312	5	0	0	0
1	C	218	1829	1188	312	324	5	0	0	0
1	D	214	1793	1166	304	318	5	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9WYT0
A	-10	GLY	-	expression tag	UNP Q9WYT0
A	-9	SER	-	expression tag	UNP Q9WYT0
A	-8	ASP	-	expression tag	UNP Q9WYT0
A	-7	LYS	-	expression tag	UNP Q9WYT0
A	-6	ILE	-	expression tag	UNP Q9WYT0
A	-5	HIS	-	expression tag	UNP Q9WYT0
A	-4	HIS	-	expression tag	UNP Q9WYT0
A	-3	HIS	-	expression tag	UNP Q9WYT0
A	-2	HIS	-	expression tag	UNP Q9WYT0
A	-1	HIS	-	expression tag	UNP Q9WYT0
A	0	HIS	-	expression tag	UNP Q9WYT0
A	53	ASP	HIS	engineered mutation	UNP Q9WYT0
B	-11	MET	-	initiating methionine	UNP Q9WYT0
B	-10	GLY	-	expression tag	UNP Q9WYT0
B	-9	SER	-	expression tag	UNP Q9WYT0
B	-8	ASP	-	expression tag	UNP Q9WYT0
B	-7	LYS	-	expression tag	UNP Q9WYT0
B	-6	ILE	-	expression tag	UNP Q9WYT0
B	-5	HIS	-	expression tag	UNP Q9WYT0
B	-4	HIS	-	expression tag	UNP Q9WYT0

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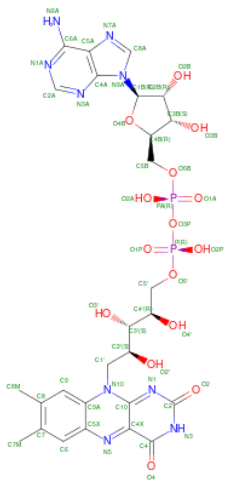
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q9WYT0
B	-2	HIS	-	expression tag	UNP Q9WYT0
B	-1	HIS	-	expression tag	UNP Q9WYT0
B	0	HIS	-	expression tag	UNP Q9WYT0
B	53	ASP	HIS	engineered mutation	UNP Q9WYT0
C	-11	MET	-	initiating methionine	UNP Q9WYT0
C	-10	GLY	-	expression tag	UNP Q9WYT0
C	-9	SER	-	expression tag	UNP Q9WYT0
C	-8	ASP	-	expression tag	UNP Q9WYT0
C	-7	LYS	-	expression tag	UNP Q9WYT0
C	-6	ILE	-	expression tag	UNP Q9WYT0
C	-5	HIS	-	expression tag	UNP Q9WYT0
C	-4	HIS	-	expression tag	UNP Q9WYT0
C	-3	HIS	-	expression tag	UNP Q9WYT0
C	-2	HIS	-	expression tag	UNP Q9WYT0
C	-1	HIS	-	expression tag	UNP Q9WYT0
C	0	HIS	-	expression tag	UNP Q9WYT0
C	53	ASP	HIS	engineered mutation	UNP Q9WYT0
D	-11	MET	-	initiating methionine	UNP Q9WYT0
D	-10	GLY	-	expression tag	UNP Q9WYT0
D	-9	SER	-	expression tag	UNP Q9WYT0
D	-8	ASP	-	expression tag	UNP Q9WYT0
D	-7	LYS	-	expression tag	UNP Q9WYT0
D	-6	ILE	-	expression tag	UNP Q9WYT0
D	-5	HIS	-	expression tag	UNP Q9WYT0
D	-4	HIS	-	expression tag	UNP Q9WYT0
D	-3	HIS	-	expression tag	UNP Q9WYT0
D	-2	HIS	-	expression tag	UNP Q9WYT0
D	-1	HIS	-	expression tag	UNP Q9WYT0
D	0	HIS	-	expression tag	UNP Q9WYT0
D	53	ASP	HIS	engineered mutation	UNP Q9WYT0

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

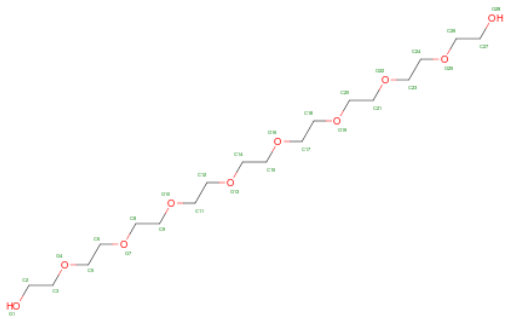
FAD



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	35	15	5	13	2	0	0
			Total	C	N	O	P		
2	B	1	35	15	5	13	2	0	0
			Total	C	N	O	P		
2	C	1	35	15	5	13	2	0	0
			Total	C	N	O	P		
2	D	1	35	15	5	13	2	0	0

- Molecule 3 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).

2PE



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	D	1	13	8	5	0	0

- Molecule 4 is water.

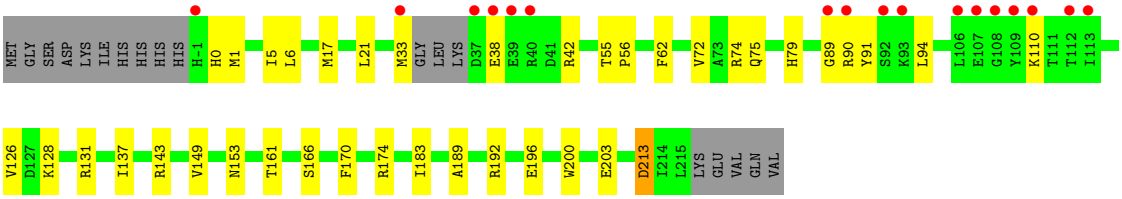
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	44	44	44	0	0
			Total	O		
4	B	32	32	32	0	0
			Total	O		
4	C	36	36	36	0	0
			Total	O		
4	D	38	38	38	0	0

3 Residue-property plots (i)

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

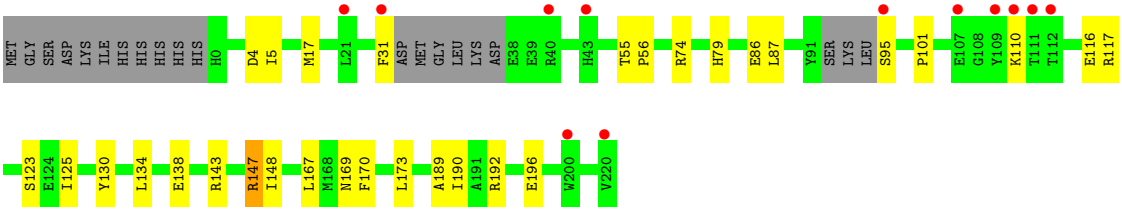
• Molecule 1: Thymidylate synthase

Chain A:



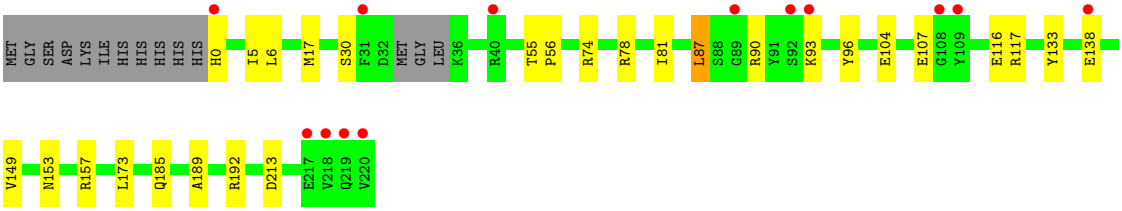
• Molecule 1: Thymidylate synthase

Chain B:



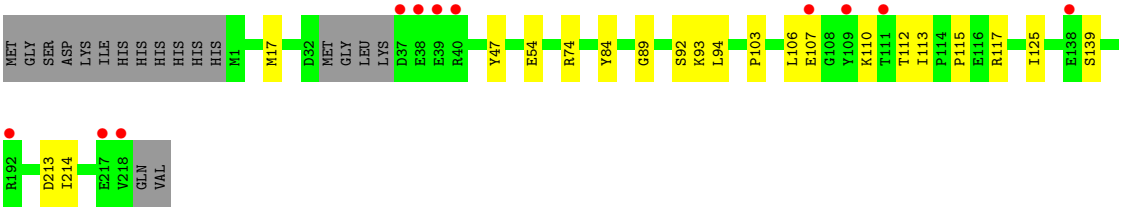
• Molecule 1: Thymidylate synthase

Chain C:



• Molecule 1: Thymidylate synthase

Chain D:


MET GLY SER ASP LYS ILE HIS HIS HIS HIS HIS HIS
M1
M17
D32
MET GLY LEU LYS
D37 E38 E39 R40
Y47
E54
R74
Y84
G89
S92 K93 L94
P103
L106 E107
G108 Y109
K110
T111 T112 I113
P114 P115
E116 R117
I125
E138 S139

R192
D213 I214
E217 V218
GLN VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.99Å 116.64Å 141.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.15 – 2.03 38.15 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.15-2.03) 99.8 (38.15-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.03Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.249 0.204 , 0.259	Depositor DCC
R_{free} test set	2923 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7522	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: 2PE, 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	0.67	0/1867	0.78	3/2524 (0.1%)
1	B	0.70	0/1827	0.76	0/2470
1	C	0.78	0/1877	0.81	0/2536
1	D	0.76	1/1840 (0.1%)	0.79	1/2488 (0.0%)
All	All	0.73	1/7411 (0.0%)	0.79	4/10018 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	84	TYR	CZ-OH	5.45	1.47	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	D	117	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	131	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	192	ARG	NE-CZ-NH2	-5.02	117.79	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	1817	0	1795	29	0
1	B	1780	0	1768	22	0
1	C	1829	0	1819	21	0
1	D	1793	0	1782	13	0
2	A	35	0	20	1	0
2	B	35	0	20	2	0
2	C	35	0	20	2	0
2	D	35	0	20	0	0
3	D	13	0	17	0	0
4	A	44	0	0	2	0
4	B	32	0	0	2	0
4	C	36	0	0	1	0
4	D	38	0	0	0	0
All	All	7522	0	7261	71	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 5.

All (71) 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:17:MET:HB2	1:B:17:MET:HB2	1.66	0.78
1:C:17:MET:HB2	1:D:17:MET:HB2	1.72	0.71
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.72	0.69
1:C:90:ARG:NH2	1:D:47:TYR:OH	2.26	0.68
1:B:167:LEU:HD11	1:B:190:ILE:CG2	2.25	0.66
1:A:0:HIS:CE1	1:B:31:PHE:CE2	2.86	0.63
1:A:89:GLY:N	1:A:94:LEU:HD21	2.15	0.61
1:B:167:LEU:HD11	1:B:190:ILE:HG21	1.83	0.60
1:B:143:ARG:O	1:B:147:ARG:HG3	2.03	0.59
1:A:75:GLN:OE1	1:A:183:ILE:HG13	2.02	0.58
1:A:55:THR:OG1	1:A:56:PRO:HD3	2.02	0.58
1:A:72:VAL:HG13	1:A:183:ILE:HD13	1.85	0.58
1:B:86:GLU:OE2	1:C:74:ARG:NH2	2.37	0.57
1:A:213:ASP:OD1	1:A:213:ASP:N	2.39	0.56
1:A:74:ARG:HG2	1:D:74:ARG:HD3	1.89	0.55
1:A:79[A]:HIS:CE1	1:A:170:PHE:HA	2.42	0.55
1:C:81:ILE:HD11	2:C:301:FAD:H8A	1.89	0.54
1:A:42:ARG:NH2	1:A:203:GLU:OE1	2.41	0.53
1:A:74:ARG:HG2	1:D:74:ARG:CD	2.40	0.51
1:C:116:GLU:CD	1:C:116:GLU:H	2.14	0.51
1:A:74:ARG:CG	1:D:74:ARG:HD3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:FAD:N7A	4:B:424:HOH:O	2.33	0.50
1:D:89:GLY:N	1:D:94:LEU:HD21	2.27	0.49
1:A:79[B]:HIS:HE1	1:A:166:SER:OG	1.95	0.49
1:B:55:THR:N	1:B:56:PRO:CD	2.76	0.49
1:A:128:LYS:HG3	1:D:125:ILE:HD11	1.95	0.49
1:C:30:SER:O	1:C:30:SER:OG	2.28	0.48
1:A:79[B]:HIS:CE1	1:A:166:SER:OG	2.67	0.48
1:B:143:ARG:O	1:B:147:ARG:CG	2.61	0.48
1:D:106:LEU:O	1:D:107:GLU:C	2.53	0.47
1:C:87:LEU:CD1	1:C:157:ARG:NH2	2.77	0.47
1:B:74:ARG:HD3	1:C:74:ARG:CG	2.45	0.46
1:B:116:GLU:H	1:B:116:GLU:CD	2.19	0.46
1:C:104:GLU:HA	1:C:107:GLU:CG	2.46	0.46
1:B:86:GLU:HG2	1:B:87:LEU:O	2.16	0.46
1:A:149:VAL:HB	1:D:125:ILE:HG21	1.97	0.46
1:A:110:LYS:NZ	4:A:431:HOH:O	2.43	0.45
1:B:130:TYR:CE2	1:B:134:LEU:HD11	2.51	0.45
1:A:1:MET:SD	1:A:196:GLU:HG2	2.57	0.45
1:B:79:HIS:HE1	1:B:173:LEU:HD12	1.82	0.45
1:A:38:GLU:HG2	1:A:200:TRP:CH2	2.52	0.45
1:C:55:THR:N	1:C:56:PRO:CD	2.81	0.44
1:C:104:GLU:HA	1:C:107:GLU:HG2	2.00	0.44
1:B:74:ARG:CD	1:C:74:ARG:CG	2.96	0.43
1:A:21:LEU:HD13	1:A:33:MET:HA	2.01	0.43
1:B:4:ASP:C	1:B:5:ILE:HG13	2.38	0.43
1:A:90:ARG:HG3	1:A:91:TYR:CE1	2.53	0.43
1:C:185:GLN:NE2	4:C:430:HOH:O	2.41	0.42
1:D:112:THR:HG22	1:D:112:THR:O	2.19	0.42
1:A:62:PHE:O	1:A:161:THR:HA	2.19	0.42
1:B:79:HIS:CE1	1:B:170:PHE:HA	2.55	0.42
1:C:96:TYR:HH	1:C:133:TYR:HH	1.65	0.42
1:A:55:THR:N	1:A:56:PRO:CD	2.82	0.42
1:B:169:ASN:ND2	2:B:301:FAD:H52A	2.35	0.41
4:B:425:HOH:O	1:C:78:ARG:HD3	2.19	0.41
1:B:125:ILE:HG21	1:C:149:VAL:HB	2.02	0.41
1:C:5:ILE:HD11	1:C:189:ALA:HB2	2.02	0.41
1:D:103:PRO:HB3	1:D:115:PRO:HB2	2.01	0.41
1:A:170:PHE:CE1	1:A:174[B]:ARG:CD	3.04	0.41
2:A:301:FAD:N6A	4:A:420:HOH:O	2.37	0.41
1:A:126:VAL:HG21	1:A:153:ASN:HD21	1.85	0.41
1:B:74:ARG:HD3	1:C:74:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HG3	1:D:125:ILE:CD1	2.51	0.41
1:B:148:ILE:HB	1:C:153:ASN:HB3	2.02	0.41
1:A:5:ILE:HG22	1:A:6:LEU:HG	2.03	0.40
1:D:213:ASP:OD1	1:D:214:ILE:HG23	2.21	0.40
1:A:137:ILE:HD11	1:A:143:ARG:HA	2.04	0.40
1:B:125:ILE:HD12	1:B:125:ILE:HA	1.93	0.40
1:C:5:ILE:HG22	1:C:6:LEU:HG	2.04	0.40
1:B:5:ILE:HD11	1:B:189:ALA:CB	2.52	0.40
1:C:173:LEU:HD13	2:C:301:FAD:O4'	2.22	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	212/232 (91%)	207 (98%)	5 (2%)	0	100	100
1	B	206/232 (89%)	201 (98%)	5 (2%)	0	100	100
1	C	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
1	D	210/232 (90%)	205 (98%)	5 (2%)	0	100	100
All	All	842/928 (91%)	822 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	193/207 (93%)	192 (100%)	1 (0%)	88	91
1	B	189/207 (91%)	180 (95%)	9 (5%)	25	21
1	C	195/207 (94%)	188 (96%)	7 (4%)	35	32
1	D	191/207 (92%)	185 (97%)	6 (3%)	40	38
All	All	768/828 (93%)	745 (97%)	23 (3%)	41	40

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	ASP
1	B	95	SER
1	B	101	PRO
1	B	110	LYS
1	B	117	ARG
1	B	123	SER
1	B	138	GLU
1	B	147	ARG
1	B	192	ARG
1	B	196	GLU
1	C	0	HIS
1	C	87	LEU
1	C	93	LYS
1	C	117	ARG
1	C	138	GLU
1	C	192	ARG
1	C	213	ASP
1	D	54	GLU
1	D	92	SER
1	D	93	LYS
1	D	110	LYS
1	D	113	ILE
1	D	139	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	85	ASN
1	A	169	ASN
1	B	51	HIS

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Mol	Chain	Res	Type
1	B	79	HIS
1	B	169	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)

5 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	$\#\|Z\| > 2$
3	2PE	D	302	-	12,12,27	0.46	0	11,11,26	0.59	0
2	FAD	D	301	-	31,37,58	1.01	1 (3%)	34,56,89	1.48	5 (14%)
2	FAD	C	301	-	31,37,58	1.17	4 (12%)	34,56,89	1.53	7 (20%)
2	FAD	A	301	-	31,37,58	1.06	3 (9%)	34,56,89	1.41	5 (14%)
2	FAD	B	301	-	31,37,58	1.02	3 (9%)	34,56,89	1.43	3 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2PE	D	302	-	-	3/10/10/25	-
2	FAD	D	301	-	-	3/26/46/50	0/3/3/6
2	FAD	C	301	-	-	7/26/46/50	0/3/3/6
2	FAD	A	301	-	-	6/26/46/50	0/3/3/6
2	FAD	B	301	-	-	5/26/46/50	0/3/3/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	FAD	C5A-C4A	3.47	1.50	1.40
2	D	301	FAD	C5A-C4A	3.05	1.49	1.40
2	B	301	FAD	C5A-C4A	3.03	1.49	1.40
2	A	301	FAD	C5A-C4A	3.02	1.48	1.40
2	B	301	FAD	C2A-N3A	2.71	1.36	1.32
2	A	301	FAD	C2A-N3A	2.62	1.36	1.32
2	C	301	FAD	O4B-C1B	2.48	1.44	1.41
2	C	301	FAD	C2A-N3A	2.45	1.36	1.32
2	A	301	FAD	O4B-C1B	2.22	1.44	1.41
2	B	301	FAD	O4B-C1B	2.12	1.44	1.41
2	C	301	FAD	C2A-N1A	2.12	1.37	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	FAD	N3A-C2A-N1A	-4.41	121.78	128.68
2	A	301	FAD	P-O3P-PA	-4.08	118.84	132.83
2	C	301	FAD	N3A-C2A-N1A	-3.93	122.54	128.68
2	C	301	FAD	P-O3P-PA	-3.91	119.41	132.83
2	D	301	FAD	N3A-C2A-N1A	-3.89	122.60	128.68
2	D	301	FAD	C3B-C2B-C1B	3.76	106.64	100.98
2	B	301	FAD	C3B-C2B-C1B	3.50	106.25	100.98
2	A	301	FAD	C4A-C5A-N7A	-3.32	105.94	109.40
2	A	301	FAD	N3A-C2A-N1A	-3.27	123.57	128.68
2	D	301	FAD	P-O3P-PA	-2.90	122.89	132.83
2	B	301	FAD	P-O3P-PA	-2.68	123.62	132.83
2	D	301	FAD	C4A-C5A-N7A	-2.67	106.61	109.40
2	C	301	FAD	O2A-PA-O1A	2.58	124.99	112.24
2	C	301	FAD	C3B-C2B-C1B	2.50	104.74	100.98
2	A	301	FAD	C3B-C2B-C1B	2.48	104.71	100.98
2	C	301	FAD	C2A-N1A-C6A	2.45	122.95	118.75
2	C	301	FAD	C1B-N9A-C4A	-2.23	122.72	126.64
2	D	301	FAD	O2A-PA-O1A	2.19	123.06	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	FAD	C4A-C5A-N7A	-2.13	107.18	109.40
2	A	301	FAD	O2A-PA-O1A	2.05	122.37	112.24

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FAD	P-O3P-PA-O5B
2	A	301	FAD	C3'-C4'-C5'-O5'
2	A	301	FAD	O4'-C4'-C5'-O5'
2	A	301	FAD	C5'-O5'-P-O1P
2	A	301	FAD	C5'-O5'-P-O2P
2	A	301	FAD	C5'-O5'-P-O3P
2	B	301	FAD	P-O3P-PA-O5B
2	B	301	FAD	C5'-O5'-P-O1P
2	B	301	FAD	C5'-O5'-P-O3P
2	C	301	FAD	C3'-C4'-C5'-O5'
2	C	301	FAD	O4'-C4'-C5'-O5'
2	D	301	FAD	C3'-C4'-C5'-O5'
2	D	301	FAD	O4'-C4'-C5'-O5'
2	C	301	FAD	C2'-C3'-C4'-O4'
3	D	302	2PE	O1-C2-C3-O4
3	D	302	2PE	O10-C11-C12-O13
2	B	301	FAD	O4B-C4B-C5B-O5B
2	C	301	FAD	O3'-C3'-C4'-O4'
3	D	302	2PE	O7-C8-C9-O10
2	C	301	FAD	C2'-C3'-C4'-C5'
2	B	301	FAD	C3B-C4B-C5B-O5B
2	C	301	FAD	O3'-C3'-C4'-C5'
2	C	301	FAD	P-O3P-PA-O5B
2	D	301	FAD	PA-O3P-P-O2P

There are no ring outliers.

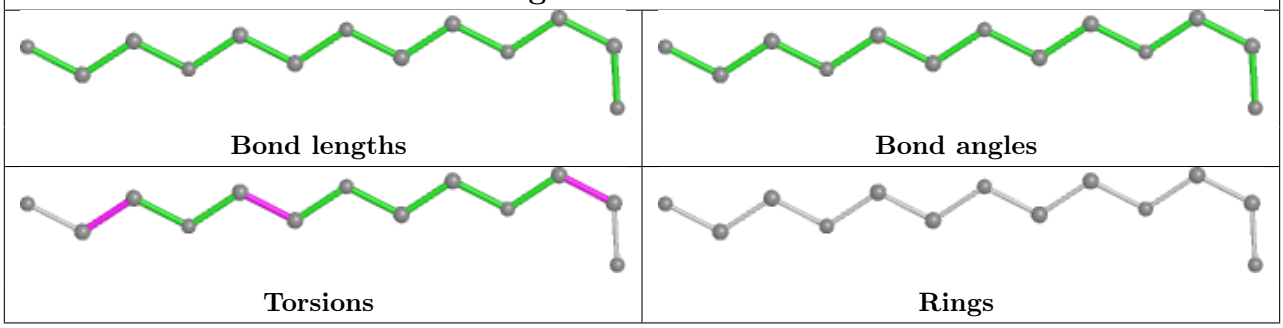
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	FAD	2	0
2	A	301	FAD	1	0
2	B	301	FAD	2	0

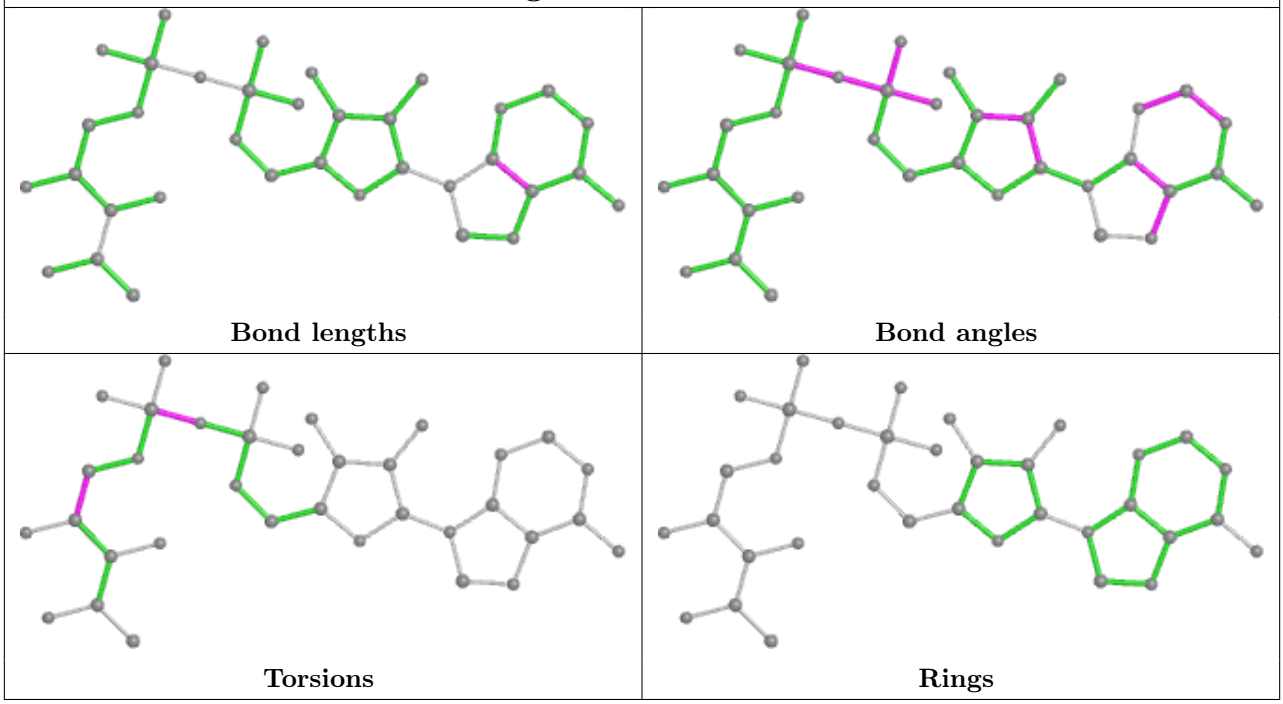
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

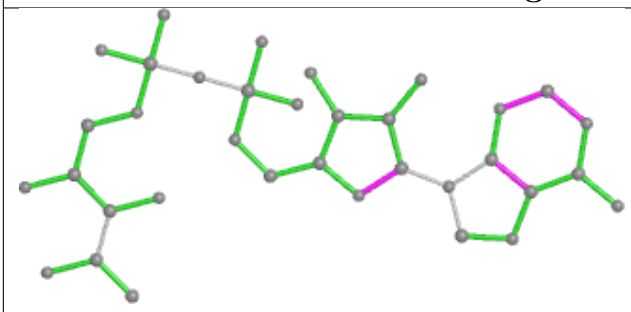
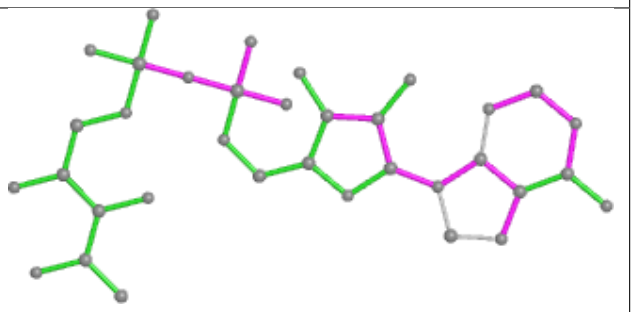
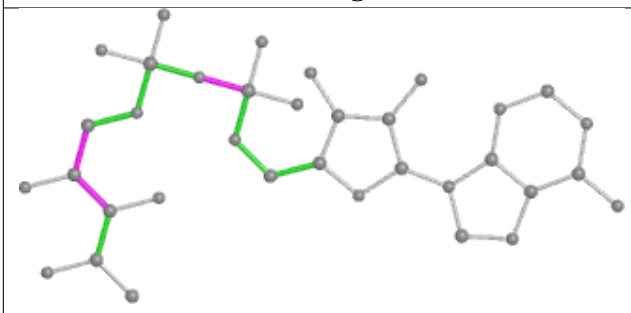
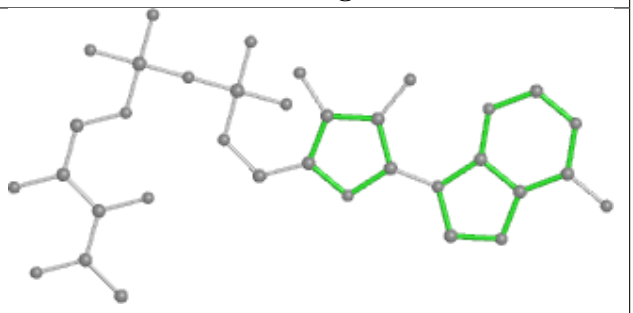
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 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.

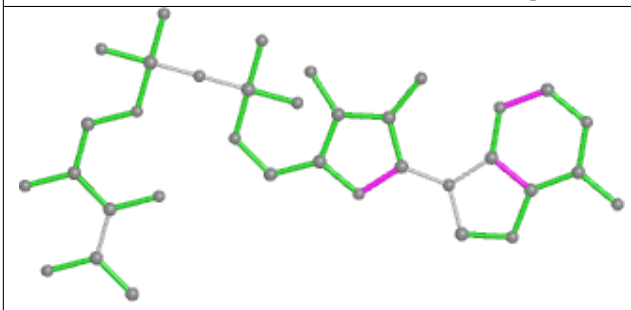
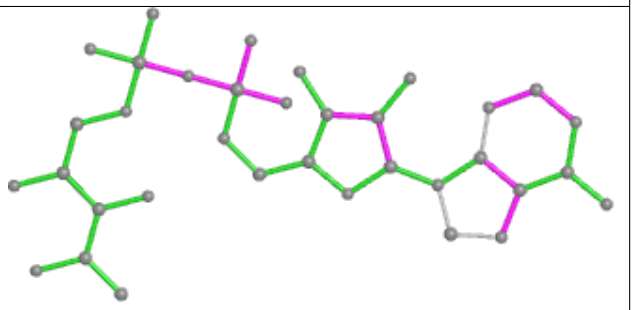
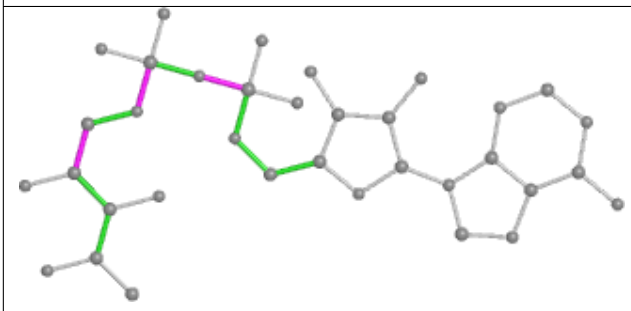
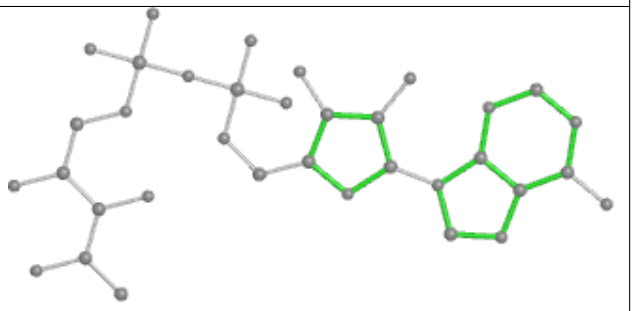
Ligand 2PE D 302

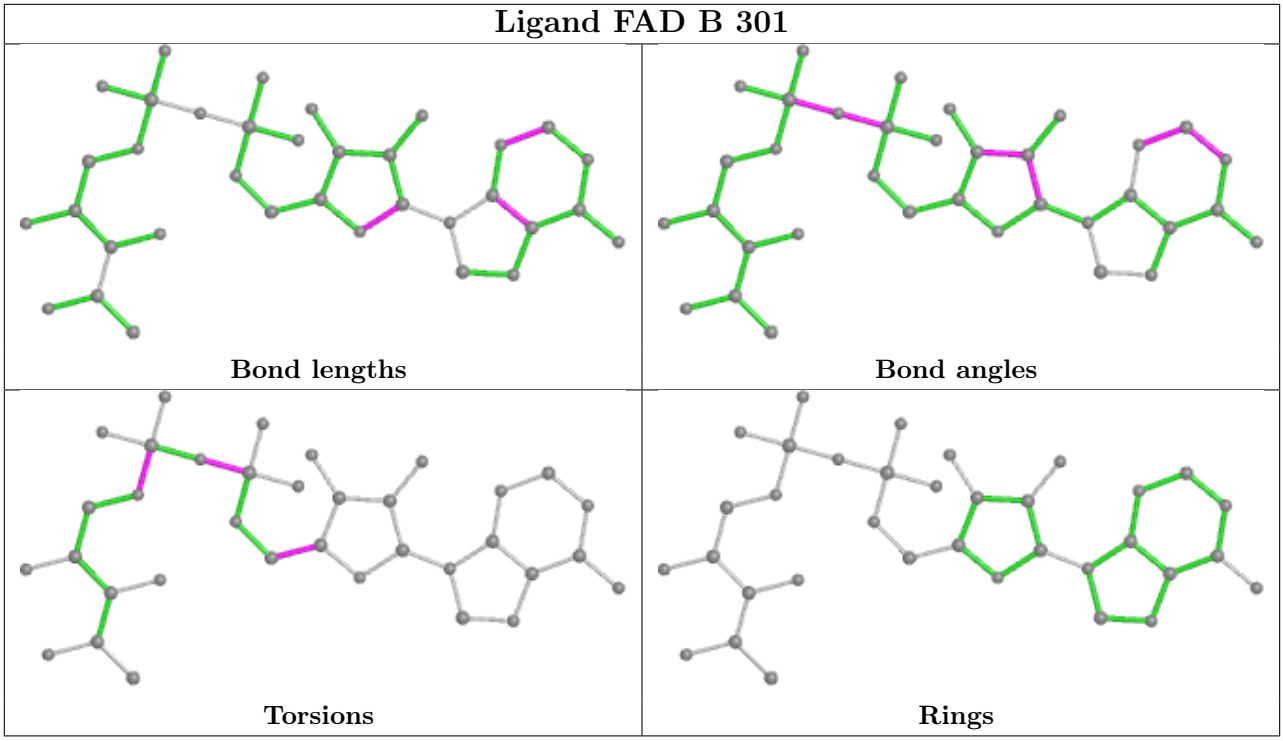


Ligand FAD D 301



Ligand FAD C 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	214/232 (92%)	0.40	17 (7%)	12	12	27, 40, 70, 99	0
1	B	212/232 (91%)	0.27	12 (5%)	23	23	28, 42, 68, 92	0
1	C	218/232 (93%)	0.10	13 (5%)	21	21	25, 39, 69, 86	0
1	D	214/232 (92%)	0.18	11 (5%)	28	27	25, 40, 68, 87	0
All	All	858/928 (92%)	0.24	53 (6%)	20	19	25, 40, 70, 99	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	MET	5.1
1	B	40	ARG	4.7
1	A	90	ARG	4.7
1	D	40	ARG	4.6
1	A	40	ARG	4.0
1	D	109	TYR	3.9
1	A	38	GLU	3.6
1	A	112	THR	3.5
1	A	106	LEU	3.5
1	C	109	TYR	3.5
1	C	220	VAL	3.4
1	C	0	HIS	3.3
1	B	112	THR	3.3
1	A	37	ASP	3.2
1	C	219	GLN	3.1
1	C	218	VAL	3.1
1	D	39	GLU	3.0
1	B	220	VAL	3.0
1	A	107	GLU	3.0
1	C	89	GLY	2.9
1	D	192	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	93	LYS	2.8
1	A	93	LYS	2.6
1	A	113	ILE	2.6
1	B	95	SER	2.6
1	C	217	GLU	2.5
1	D	138	GLU	2.5
1	B	21	LEU	2.5
1	A	89	GLY	2.5
1	C	108	GLY	2.5
1	A	109	TYR	2.5
1	B	109	TYR	2.5
1	B	107	GLU	2.5
1	A	39	GLU	2.4
1	D	107	GLU	2.4
1	C	138	GLU	2.4
1	C	31	PHE	2.3
1	B	110	LYS	2.3
1	A	92	SER	2.3
1	B	31	PHE	2.2
1	A	-1	HIS	2.2
1	B	43	HIS	2.2
1	D	37	ASP	2.2
1	C	92	SER	2.2
1	D	38	GLU	2.1
1	C	40	ARG	2.1
1	A	110	LYS	2.1
1	B	111	THR	2.1
1	B	200	TRP	2.1
1	D	218	VAL	2.0
1	D	217	GLU	2.0
1	D	111	THR	2.0
1	A	108	GLY	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)

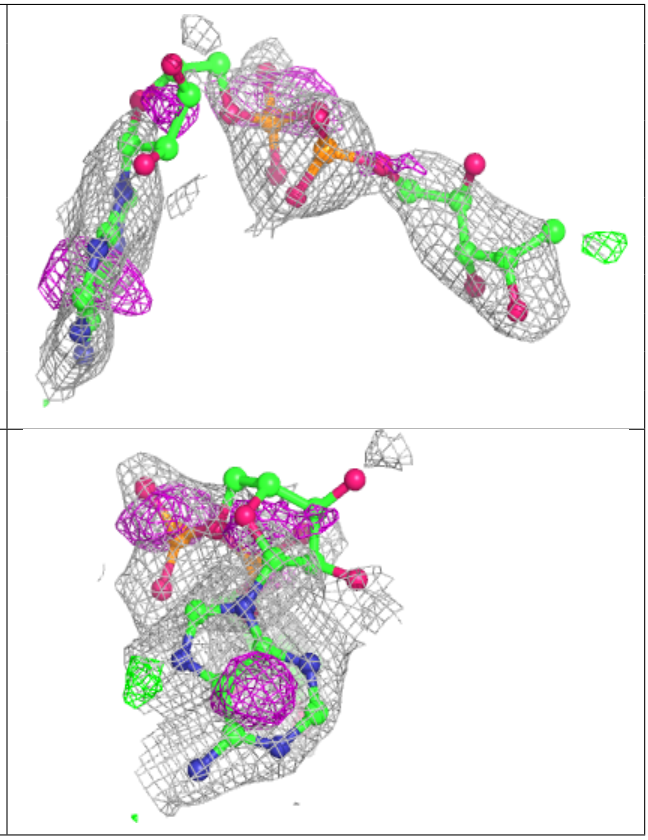
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FAD	C	301	35/53	0.77	0.26	47,77,92,96	0
2	FAD	B	301	35/53	0.82	0.26	50,83,100,104	0
2	FAD	A	301	35/53	0.85	0.23	51,84,108,113	0
2	FAD	D	301	35/53	0.87	0.19	43,67,80,88	0
3	2PE	D	302	13/28	0.89	0.26	65,67,72,75	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

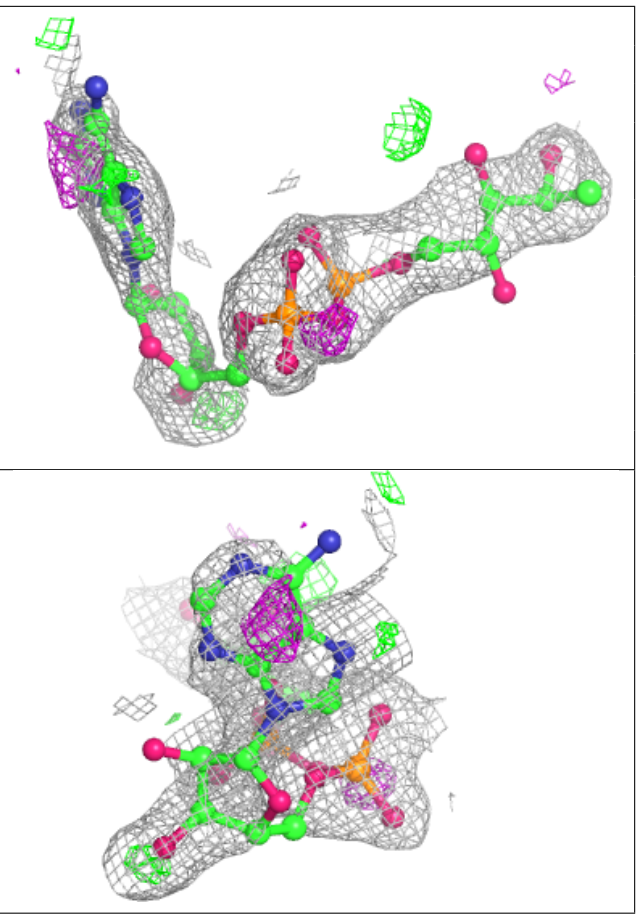
Electron density around FAD C 301:

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



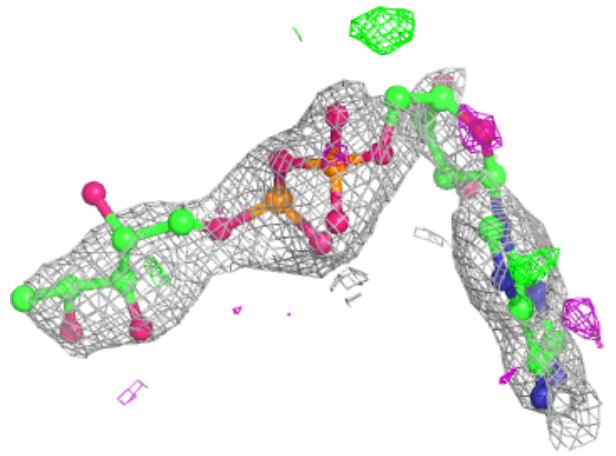
Electron density around FAD B 301:

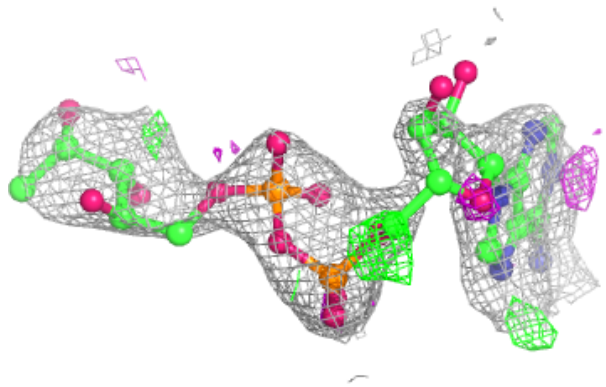
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

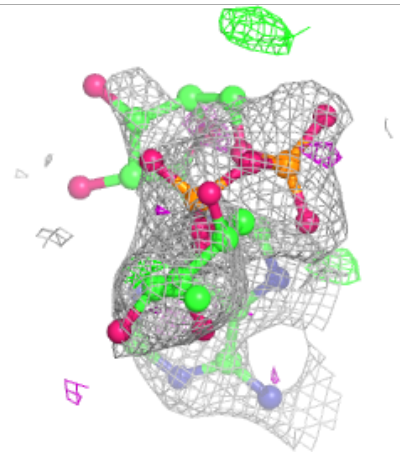


Electron density around FAD A 301:

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

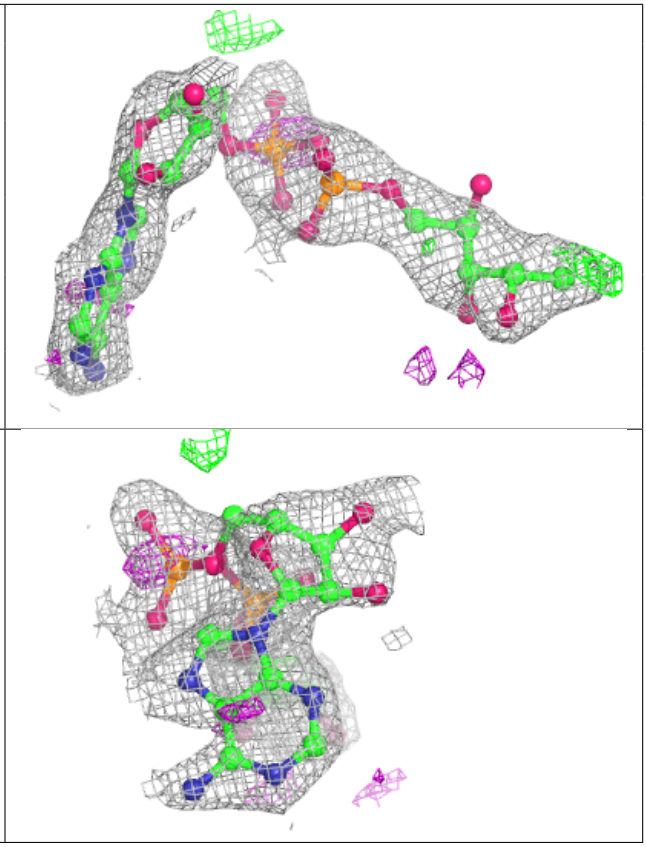






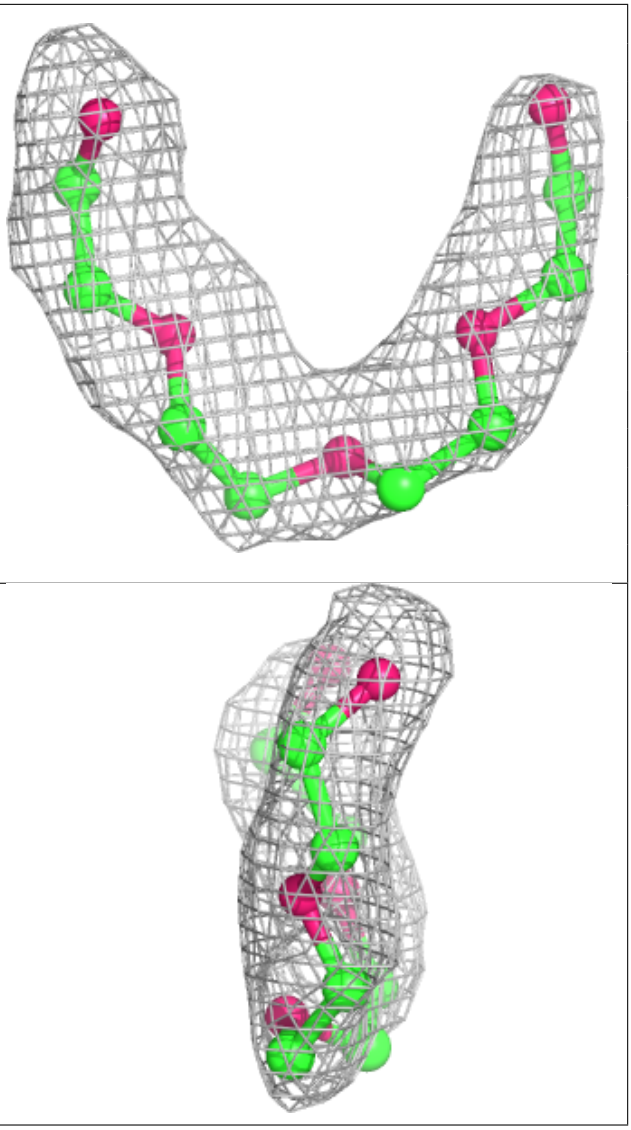
Electron density around FAD D 301:

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



Electron density around 2PE D 302:

$2mF_o$-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.