Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 08:46 PM JST

PDB ID	:	5H75
Title	:	Crystal structure of the MrsD-Protein A fusion protein
Authors	:	Youn, S.J.; Kwon, N.Y.; Lee, J.H.; Kim, J.H.; Lee, H.; Lee, J.O.
Deposited on	:	2016-11-17
Resolution	:	2.74 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:

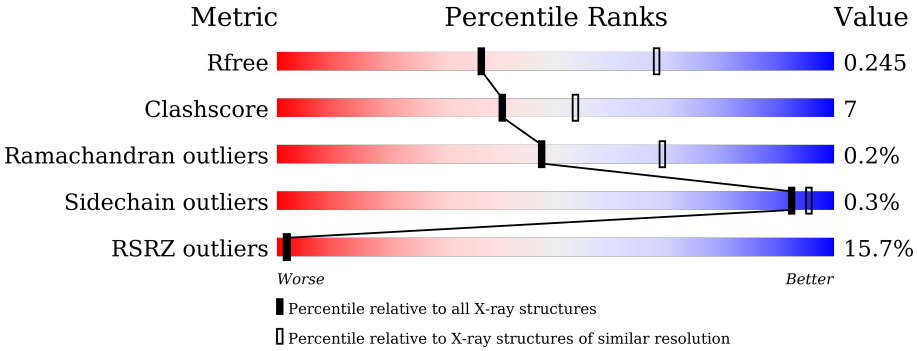
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	238	20% 76% 13% 11%
1	B	238	14% 68% 16% 16%
1	C	238	16% 72% 13% 15%
1	D	238	6% 83% 12% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6812 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 Mersacidin decarboxylase,Immunoglobulin G-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	1666	1067	282	309	8	0	0	0
1	B	200	1576	1011	266	292	7	0	0	0
1	C	202	1592	1023	268	294	7	0	0	0
1	D	225	1754	1122	298	325	9	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q9RC23
A	-5	SER	-	expression tag	UNP Q9RC23
A	-4	GLY	-	expression tag	UNP Q9RC23
A	-3	GLY	-	expression tag	UNP Q9RC23
A	-2	GLY	-	expression tag	UNP Q9RC23
A	-1	GLY	-	expression tag	UNP Q9RC23
A	0	SER	-	expression tag	UNP Q9RC23
A	182	GLN	LYS	engineered mutation	UNP Q9RC23
A	202	ALA	GLY	engineered mutation	UNP P38507
B	-6	GLY	-	expression tag	UNP Q9RC23
B	-5	SER	-	expression tag	UNP Q9RC23
B	-4	GLY	-	expression tag	UNP Q9RC23
B	-3	GLY	-	expression tag	UNP Q9RC23
B	-2	GLY	-	expression tag	UNP Q9RC23
B	-1	GLY	-	expression tag	UNP Q9RC23
B	0	SER	-	expression tag	UNP Q9RC23
B	182	GLN	LYS	engineered mutation	UNP Q9RC23
B	202	ALA	GLY	engineered mutation	UNP P38507
C	-6	GLY	-	expression tag	UNP Q9RC23
C	-5	SER	-	expression tag	UNP Q9RC23

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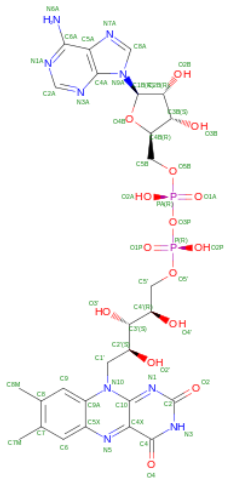
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q9RC23
C	-3	GLY	-	expression tag	UNP Q9RC23
C	-2	GLY	-	expression tag	UNP Q9RC23
C	-1	GLY	-	expression tag	UNP Q9RC23
C	0	SER	-	expression tag	UNP Q9RC23
C	182	GLN	LYS	engineered mutation	UNP Q9RC23
C	202	ALA	GLY	engineered mutation	UNP P38507
D	-6	GLY	-	expression tag	UNP Q9RC23
D	-5	SER	-	expression tag	UNP Q9RC23
D	-4	GLY	-	expression tag	UNP Q9RC23
D	-3	GLY	-	expression tag	UNP Q9RC23
D	-2	GLY	-	expression tag	UNP Q9RC23
D	-1	GLY	-	expression tag	UNP Q9RC23
D	0	SER	-	expression tag	UNP Q9RC23
D	182	GLN	LYS	engineered mutation	UNP Q9RC23
D	202	ALA	GLY	engineered mutation	UNP P38507

- 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	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0
2	C	1	53	27	9	15	2	0	0

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

- Molecule 3 is water.

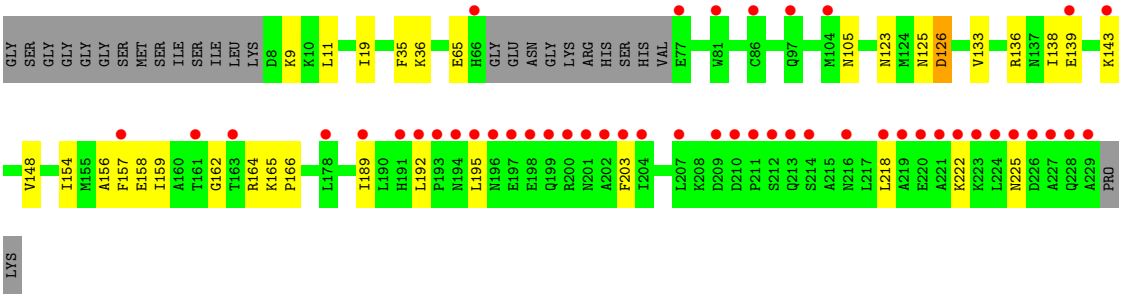
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	1	1	1	0	0
			Total	O		
3	C	5	5	5	0	0
			Total	O		
3	D	6	6	6	0	0

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.

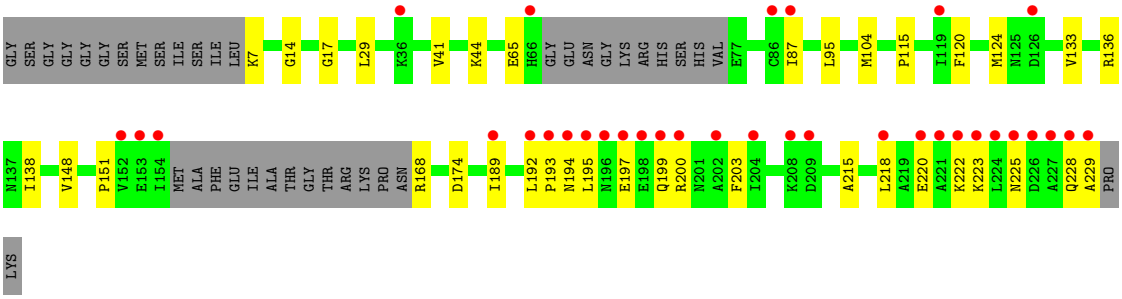
• Molecule 1: Mersacidin decarboxylase,Immunoglobulin G-binding protein A

Chain A:



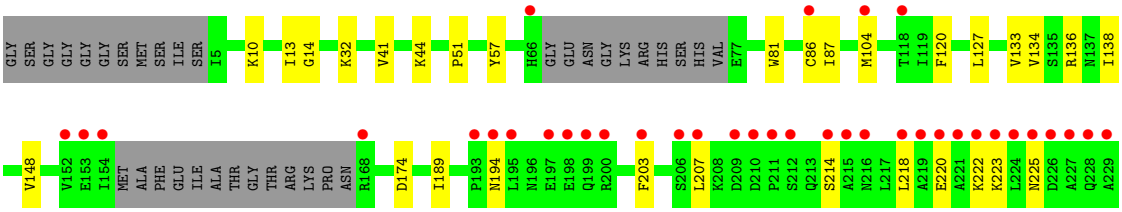
• Molecule 1: Mersacidin decarboxylase,Immunoglobulin G-binding protein A

Chain B:



• Molecule 1: Mersacidin decarboxylase,Immunoglobulin G-binding protein A

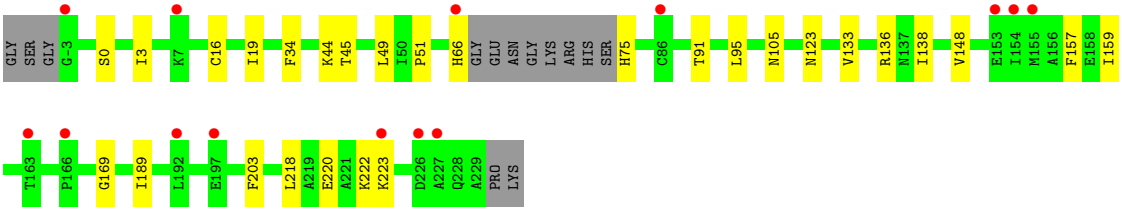
Chain C:



PRO
LYS

• Molecule 1: Mersacidin decarboxylase,Immunoglobulin G-binding protein A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	167.73Å 167.73Å 167.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.62 – 2.74 30.62 – 2.74	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.62-2.74) 95.2 (30.62-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.72Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.204 , 0.243 0.206 , 0.245	Depositor DCC
R_{free} test set	1998 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	76.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 76.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6812	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: 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	0.30	0/1700	0.47	0/2306
1	B	0.31	0/1607	0.48	0/2178
1	C	0.34	0/1623	0.46	0/2200
1	D	0.37	0/1789	0.53	0/2424
All	All	0.33	0/6719	0.49	0/9108

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	1666	0	1672	22	0
1	B	1576	0	1583	25	0
1	C	1592	0	1605	20	0
1	D	1754	0	1770	22	0
2	A	53	0	31	10	0
2	B	53	0	31	4	0
2	C	53	0	31	5	0
2	D	53	0	31	4	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
3	D	6	0	0	1	0
All	All	6812	0	6754	98	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 7.

All (98) 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)
2:A:301:FAD:C2A	2:C:301:FAD:H62A	1.82	0.92
2:A:301:FAD:N3A	2:C:301:FAD:N6A	2.21	0.89
2:A:301:FAD:O2'	2:A:301:FAD:O4'	1.99	0.80
1:A:156:ALA:HB3	1:A:164:ARG:HA	1.66	0.76
2:A:301:FAD:N3A	2:A:301:FAD:H2B	2.01	0.76
2:A:301:FAD:C2A	2:C:301:FAD:N6A	2.46	0.76
1:C:189:ILE:HD13	1:C:203:PHE:HB3	1.68	0.75
1:D:45:THR:OG1	2:D:301:FAD:O2A	2.04	0.73
1:D:218:LEU:HG	1:D:222:LYS:NZ	2.06	0.70
1:D:218:LEU:HG	1:D:222:LYS:HZ2	1.57	0.70
1:B:189:ILE:HD13	1:B:203:PHE:HB3	1.74	0.69
1:A:19:ILE:HG12	1:A:159:ILE:HD11	1.76	0.67
1:B:115:PRO:HA	1:C:127:LEU:HD11	1.77	0.67
1:D:220:GLU:OE2	1:D:223:LYS:HD3	1.96	0.66
1:A:189:ILE:HD13	1:A:203:PHE:HB3	1.79	0.65
2:A:301:FAD:H9	2:A:301:FAD:H2'	1.77	0.65
2:B:301:FAD:H5'2	2:B:301:FAD:H1'1	1.77	0.65
1:B:199:GLN:HE22	1:B:228:GLN:HE22	1.42	0.64
1:D:123:ASN:ND2	1:D:169:GLY:HA2	2.13	0.62
1:C:138:ILE:HD12	1:C:148:VAL:HG11	1.82	0.61
1:B:194:ASN:ND2	1:B:229:ALA:HA	2.15	0.61
1:D:138:ILE:HD12	1:D:148:VAL:HG11	1.83	0.60
2:A:301:FAD:H2A	2:C:301:FAD:N6A	2.16	0.60
1:A:218:LEU:HG	1:A:222:LYS:NZ	2.18	0.59
1:B:194:ASN:HD22	1:B:229:ALA:HA	1.68	0.58
1:B:138:ILE:HD12	1:B:148:VAL:HG11	1.87	0.57
1:B:192:LEU:HD13	1:B:195:LEU:HD13	1.87	0.56
1:B:220:GLU:OE2	1:B:223:LYS:HD3	2.05	0.56
2:A:301:FAD:HO4'	2:A:301:FAD:HO2'	1.45	0.55
1:A:125:ASN:OD1	1:A:126:ASP:N	2.40	0.55
2:A:301:FAD:H2'	2:A:301:FAD:C9	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLY:N	2:B:301:FAD:O1P	2.39	0.55
1:C:218:LEU:HG	1:C:222:LYS:NZ	2.23	0.54
1:B:192:LEU:O	1:B:200:ARG:NH2	2.40	0.54
1:B:151:PRO:HG2	1:B:168:ARG:HD2	1.89	0.53
1:D:19:ILE:HG12	1:D:159:ILE:HD11	1.90	0.53
1:A:138:ILE:HD12	1:A:148:VAL:HG11	1.90	0.53
1:C:10:LYS:HD2	1:C:81:TRP:O	2.08	0.53
1:A:154:ILE:O	1:A:166:PRO:HA	2.09	0.52
1:A:156:ALA:CB	1:A:165:LYS:H	2.22	0.51
1:D:133:VAL:HG12	1:D:136:ARG:NH2	2.25	0.51
2:A:301:FAD:H2A	2:C:301:FAD:H62A	1.68	0.51
1:A:192:LEU:HB3	1:A:195:LEU:HD13	1.92	0.51
1:D:189:ILE:HD13	1:D:203:PHE:HB3	1.92	0.50
1:C:218:LEU:HG	1:C:222:LYS:HZ2	1.75	0.50
1:A:156:ALA:HB1	1:A:158:GLU:N	2.27	0.50
1:D:75:HIS:N	3:D:401:HOH:O	2.44	0.50
1:A:139:GLU:HG3	1:A:143:LYS:NZ	2.27	0.49
1:A:9:LYS:HA	1:A:36:LYS:HE2	1.94	0.49
1:C:194:ASN:ND2	1:C:225:ASN:O	2.45	0.49
1:B:124:MET:O	1:B:168:ARG:HB3	2.12	0.49
2:B:301:FAD:H1'1	2:B:301:FAD:C5'	2.43	0.49
1:D:49:LEU:HD21	2:D:301:FAD:HM72	1.94	0.49
2:D:301:FAD:O2A	2:D:301:FAD:H4B	2.13	0.49
1:C:14:GLY:HA2	1:C:41:VAL:O	2.13	0.49
1:B:44:LYS:HE3	1:B:65:GLU:HG2	1.95	0.48
1:D:16:CYS:HB3	1:D:91:THR:HG23	1.96	0.48
1:B:133:VAL:HG12	1:B:136:ARG:NH2	2.29	0.47
1:C:87:ILE:HD12	1:C:120:PHE:CE2	2.49	0.47
1:B:14:GLY:HA2	1:B:41:VAL:O	2.15	0.46
1:D:19:ILE:CG1	1:D:159:ILE:HD11	2.45	0.46
1:D:95:LEU:HD13	1:D:138:ILE:HD11	1.97	0.46
1:A:156:ALA:HB1	1:A:157:PHE:CA	2.46	0.46
1:B:218:LEU:HG	1:B:222:LYS:NZ	2.31	0.46
1:A:156:ALA:HB2	1:A:165:LYS:H	1.80	0.45
1:A:218:LEU:HG	1:A:222:LYS:HZ2	1.81	0.45
1:D:3:ILE:HG23	1:D:34:PHE:HD1	1.81	0.45
1:C:174:ASP:N	1:C:174:ASP:OD1	2.50	0.45
1:A:222:LYS:O	1:A:225:ASN:HB3	2.17	0.45
1:A:133:VAL:HG12	1:A:136:ARG:NH2	2.32	0.45
1:B:87:ILE:HD12	1:B:120:PHE:CE2	2.52	0.45
1:D:44:LYS:HA	1:D:44:LYS:HD2	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:HIS:O	1:D:66:HIS:ND1	2.48	0.44
1:B:174:ASP:N	1:B:174:ASP:OD1	2.51	0.44
1:A:156:ALA:HB1	1:A:157:PHE:HA	1.98	0.44
1:C:220:GLU:OE2	1:C:223:LYS:HD3	2.18	0.44
1:C:133:VAL:HG12	1:C:136:ARG:NH2	2.33	0.44
1:A:156:ALA:HB1	1:A:157:PHE:C	2.38	0.43
1:C:51:PRO:HD3	1:D:51:PRO:HD3	2.00	0.43
1:D:0:SER:O	1:D:0:SER:OG	2.36	0.43
1:A:65:GLU:OE2	1:A:105:ASN:HB2	2.19	0.43
1:B:95:LEU:HD13	1:B:138:ILE:HD11	2.01	0.43
2:B:301:FAD:H5'2	2:B:301:FAD:C1'	2.47	0.43
1:C:57:TYR:CD1	1:D:159:ILE:HG23	2.54	0.42
1:B:222:LYS:O	1:B:225:ASN:HB3	2.20	0.42
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.85	0.42
1:C:32:LYS:HZ3	1:D:157:PHE:HZ	1.62	0.42
1:A:157:PHE:CE2	1:A:159:ILE:HD13	2.55	0.41
1:B:197:GLU:H	1:B:197:GLU:HG2	1.70	0.41
1:B:218:LEU:HG	1:B:222:LYS:HZ2	1.84	0.41
1:C:207:LEU:HD21	1:C:214:SER:HA	2.01	0.41
1:C:134:VAL:O	1:C:138:ILE:HG12	2.21	0.41
1:A:11:LEU:HB2	1:A:35:PHE:CD2	2.56	0.41
1:B:104:MET:HE3	1:C:104:MET:HE3	2.02	0.41
1:C:44:LYS:HD2	1:C:44:LYS:HA	1.87	0.41
1:B:7:LYS:HG3	1:B:215:ALA:HB2	2.02	0.40
1:C:13:ILE:HA	1:C:86:CYS:O	2.21	0.40
1:D:105:ASN:HB3	2:D:301:FAD:H2A	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/238 (87%)	199 (96%)	8 (4%)	1 (0%)	29	48
1	B	194/238 (82%)	187 (96%)	6 (3%)	1 (0%)	29	48
1	C	196/238 (82%)	191 (97%)	5 (3%)	0	100	100
1	D	221/238 (93%)	214 (97%)	7 (3%)	0	100	100
All	All	819/952 (86%)	791 (97%)	26 (3%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	PRO
1	A	162	GLY

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	182/201 (90%)	180 (99%)	2 (1%)	73	84
1	B	173/201 (86%)	173 (100%)	0	100	100
1	C	175/201 (87%)	175 (100%)	0	100	100
1	D	192/201 (96%)	192 (100%)	0	100	100
All	All	722/804 (90%)	720 (100%)	2 (0%)	92	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	126	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	196	ASN

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Mol	Chain	Res	Type
1	B	228	GLN
1	C	123	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)

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	A	301	-	53,58,58	1.28	5 (9%)	68,89,89	1.35	10 (14%)
2	FAD	C	301	-	53,58,58	1.28	5 (9%)	68,89,89	1.35	10 (14%)
2	FAD	D	301	-	53,58,58	1.28	5 (9%)	68,89,89	1.35	10 (14%)
2	FAD	B	301	-	53,58,58	1.28	5 (9%)	68,89,89	1.35	10 (14%)

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	A	301	-	-	14/30/50/50	0/6/6/6
2	FAD	C	301	-	-	7/30/50/50	0/6/6/6
2	FAD	D	301	-	-	10/30/50/50	0/6/6/6
2	FAD	B	301	-	-	16/30/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	FAD	C9A-C5X	5.05	1.49	1.41
2	A	301	FAD	C9A-C5X	5.02	1.49	1.41
2	B	301	FAD	C9A-C5X	5.02	1.49	1.41
2	C	301	FAD	C9A-C5X	5.01	1.49	1.41
2	B	301	FAD	C8-C7	3.34	1.49	1.40
2	D	301	FAD	C8-C7	3.30	1.49	1.40
2	C	301	FAD	C8-C7	3.30	1.49	1.40
2	A	301	FAD	C8-C7	3.29	1.49	1.40
2	A	301	FAD	C4X-N5	2.54	1.35	1.30
2	A	301	FAD	C5A-C4A	2.53	1.47	1.40
2	B	301	FAD	C5A-C4A	2.50	1.47	1.40
2	D	301	FAD	C4X-N5	2.50	1.35	1.30
2	C	301	FAD	C4X-N5	2.48	1.35	1.30
2	C	301	FAD	C5A-C4A	2.48	1.47	1.40
2	B	301	FAD	C4X-N5	2.47	1.35	1.30
2	D	301	FAD	C5A-C4A	2.46	1.47	1.40
2	B	301	FAD	C4-N3	-2.45	1.34	1.38
2	A	301	FAD	C4-N3	-2.45	1.34	1.38
2	C	301	FAD	C4-N3	-2.45	1.34	1.38
2	D	301	FAD	C4-N3	-2.43	1.34	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	FAD	P-O3P-PA	-3.60	120.47	132.83
2	C	301	FAD	P-O3P-PA	-3.60	120.49	132.83
2	D	301	FAD	P-O3P-PA	-3.59	120.51	132.83
2	B	301	FAD	P-O3P-PA	-3.59	120.52	132.83
2	C	301	FAD	C3B-C2B-C1B	3.44	106.16	100.98
2	B	301	FAD	C3B-C2B-C1B	3.44	106.16	100.98
2	D	301	FAD	C3B-C2B-C1B	3.43	106.15	100.98
2	A	301	FAD	C3B-C2B-C1B	3.42	106.13	100.98
2	B	301	FAD	N3A-C2A-N1A	-3.20	123.68	128.68
2	D	301	FAD	N3A-C2A-N1A	-3.20	123.68	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	FAD	N3A-C2A-N1A	-3.19	123.69	128.68
2	A	301	FAD	N3A-C2A-N1A	-3.17	123.72	128.68
2	B	301	FAD	C4-C4X-N5	2.76	122.16	118.23
2	C	301	FAD	C4-C4X-N5	2.74	122.13	118.23
2	D	301	FAD	C4-C4X-N5	2.72	122.10	118.23
2	A	301	FAD	C4-C4X-N5	2.72	122.10	118.23
2	A	301	FAD	C4A-C5A-N7A	-2.69	106.59	109.40
2	C	301	FAD	C4A-C5A-N7A	-2.69	106.59	109.40
2	D	301	FAD	C4A-C5A-N7A	-2.69	106.60	109.40
2	B	301	FAD	C4A-C5A-N7A	-2.67	106.61	109.40
2	C	301	FAD	C4X-C10-N1	-2.65	118.59	124.73
2	A	301	FAD	C4X-C10-N1	-2.64	118.60	124.73
2	B	301	FAD	C4X-C10-N1	-2.63	118.62	124.73
2	D	301	FAD	C4X-C10-N1	-2.62	118.64	124.73
2	C	301	FAD	C10-N1-C2	2.24	121.39	116.90
2	B	301	FAD	C10-N1-C2	2.24	121.38	116.90
2	A	301	FAD	C10-N1-C2	2.22	121.35	116.90
2	D	301	FAD	C10-N1-C2	2.21	121.32	116.90
2	B	301	FAD	O4-C4-C4X	-2.20	120.77	126.60
2	C	301	FAD	O4-C4-C4X	-2.20	120.77	126.60
2	A	301	FAD	O4-C4-C4X	-2.19	120.78	126.60
2	D	301	FAD	O4-C4-C4X	-2.18	120.81	126.60
2	C	301	FAD	C4X-C4-N3	2.08	118.48	113.19
2	A	301	FAD	C4X-C10-N10	2.07	119.50	116.48
2	D	301	FAD	C4X-C4-N3	2.07	118.44	113.19
2	B	301	FAD	C4X-C4-N3	2.07	118.44	113.19
2	A	301	FAD	C4X-C4-N3	2.06	118.43	113.19
2	D	301	FAD	C4X-C10-N10	2.06	119.49	116.48
2	C	301	FAD	C4X-C10-N10	2.04	119.47	116.48
2	B	301	FAD	C4X-C10-N10	2.04	119.46	116.48

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FAD	C5B-O5B-PA-O2A
2	A	301	FAD	C1'-C2'-C3'-O3'
2	A	301	FAD	C1'-C2'-C3'-C4'
2	B	301	FAD	C5B-O5B-PA-O1A
2	B	301	FAD	C1'-C2'-C3'-C4'
2	B	301	FAD	C5'-O5'-P-O2P
2	B	301	FAD	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
2	C	301	FAD	C4B-C5B-O5B-PA
2	C	301	FAD	C5'-O5'-P-O3P
2	D	301	FAD	C5B-O5B-PA-O1A
2	D	301	FAD	C5B-O5B-PA-O2A
2	D	301	FAD	C4B-C5B-O5B-PA
2	D	301	FAD	C3'-C4'-C5'-O5'
2	D	301	FAD	O4'-C4'-C5'-O5'
2	A	301	FAD	O4B-C4B-C5B-O5B
2	B	301	FAD	O4B-C4B-C5B-O5B
2	C	301	FAD	C3B-C4B-C5B-O5B
2	A	301	FAD	C3B-C4B-C5B-O5B
2	B	301	FAD	O3'-C3'-C4'-C5'
2	B	301	FAD	C2'-C3'-C4'-C5'
2	A	301	FAD	O2'-C2'-C3'-O3'
2	B	301	FAD	O3'-C3'-C4'-O4'
2	A	301	FAD	O2'-C2'-C3'-C4'
2	B	301	FAD	C2'-C3'-C4'-O4'
2	B	301	FAD	C3B-C4B-C5B-O5B
2	A	301	FAD	O3'-C3'-C4'-C5'
2	C	301	FAD	O4B-C4B-C5B-O5B
2	A	301	FAD	C2'-C3'-C4'-O4'
2	A	301	FAD	C2'-C3'-C4'-C5'
2	A	301	FAD	O3'-C3'-C4'-O4'
2	C	301	FAD	PA-O3P-P-O5'
2	D	301	FAD	PA-O3P-P-O5'
2	C	301	FAD	C5'-O5'-P-O1P
2	B	301	FAD	C1'-C2'-C3'-O3'
2	D	301	FAD	C3B-C4B-C5B-O5B
2	B	301	FAD	C4B-C5B-O5B-PA
2	D	301	FAD	O4B-C4B-C5B-O5B
2	B	301	FAD	O4'-C4'-C5'-O5'
2	B	301	FAD	O2'-C2'-C3'-C4'
2	D	301	FAD	P-O3P-PA-O2A
2	A	301	FAD	C5B-O5B-PA-O3P
2	B	301	FAD	C5B-O5B-PA-O3P
2	D	301	FAD	C5B-O5B-PA-O3P
2	B	301	FAD	O2'-C2'-C3'-O3'
2	A	301	FAD	C5B-O5B-PA-O1A
2	C	301	FAD	C5B-O5B-PA-O1A
2	A	301	FAD	C2'-C1'-N10-C10

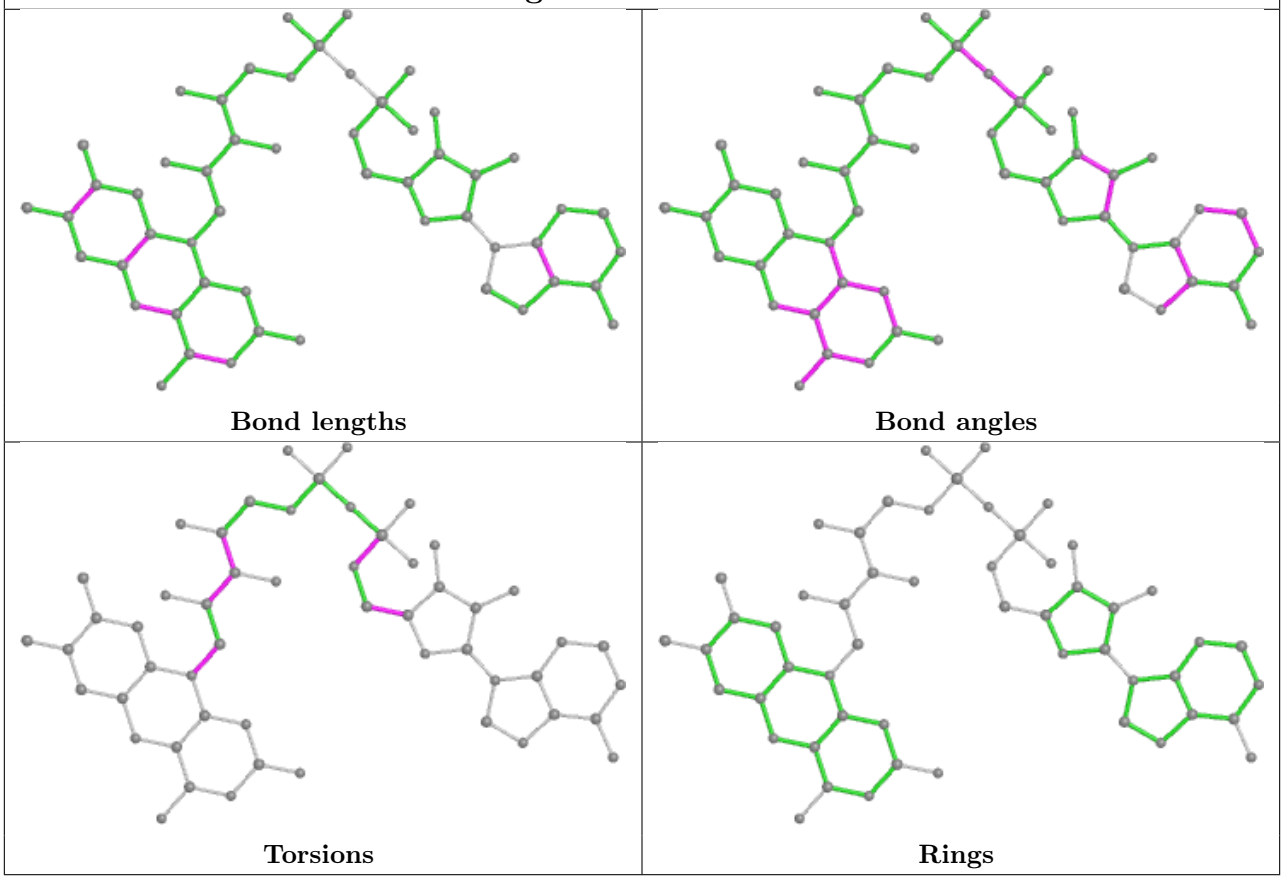
There are no ring outliers.

4 monomers are involved in 18 short contacts:

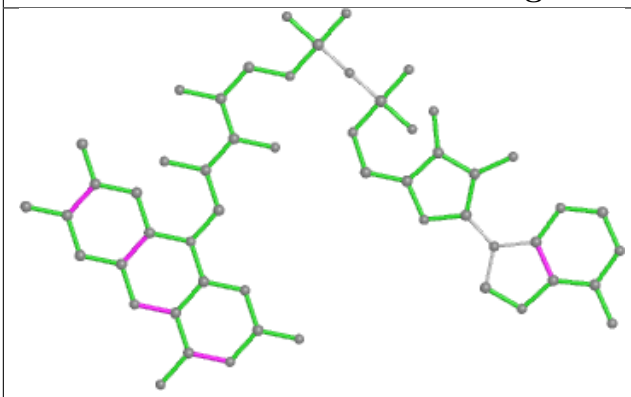
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	FAD	10	0
2	C	301	FAD	5	0
2	D	301	FAD	4	0
2	B	301	FAD	4	0

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.

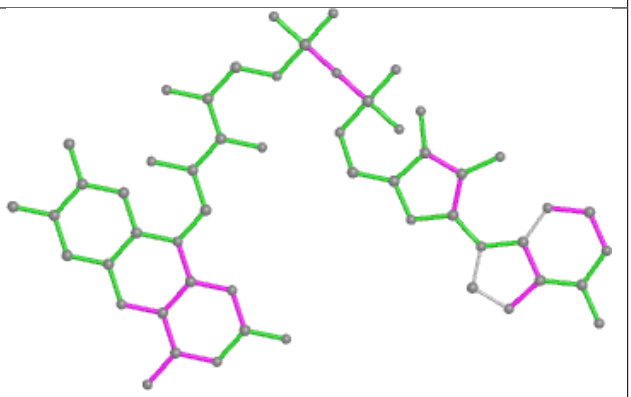
Ligand FAD A 301



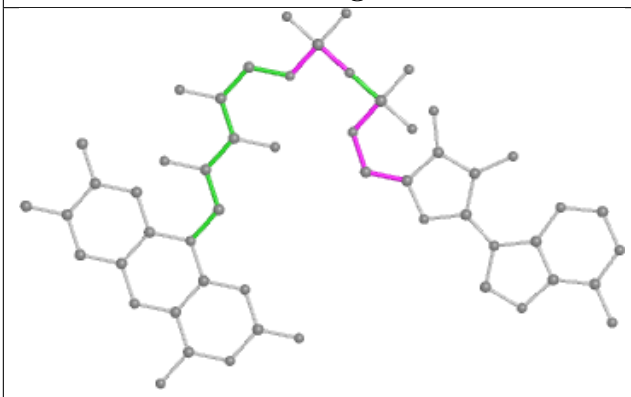
Ligand FAD C 301



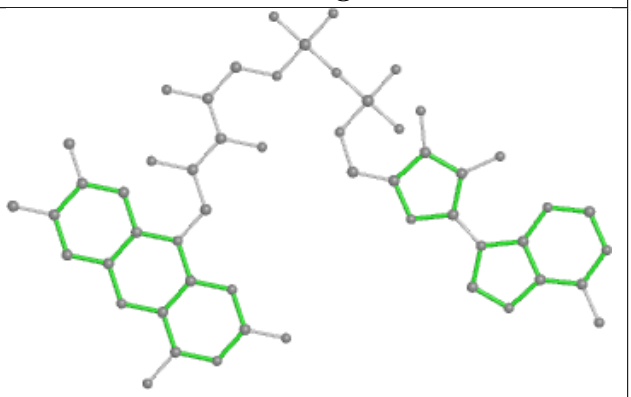
Bond lengths



Bond angles

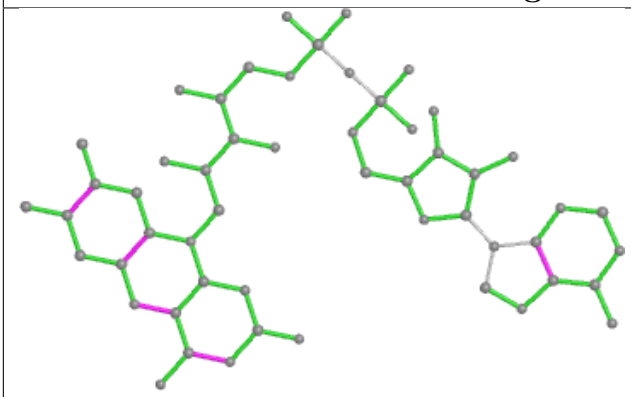


Torsions

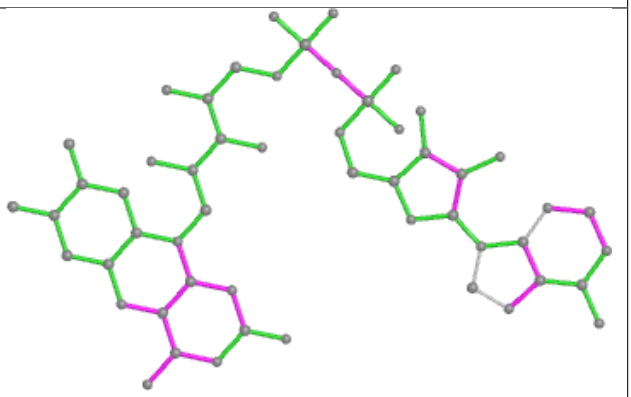


Rings

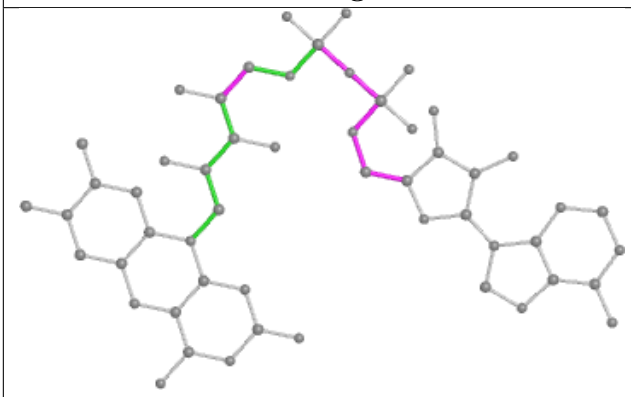
Ligand FAD D 301



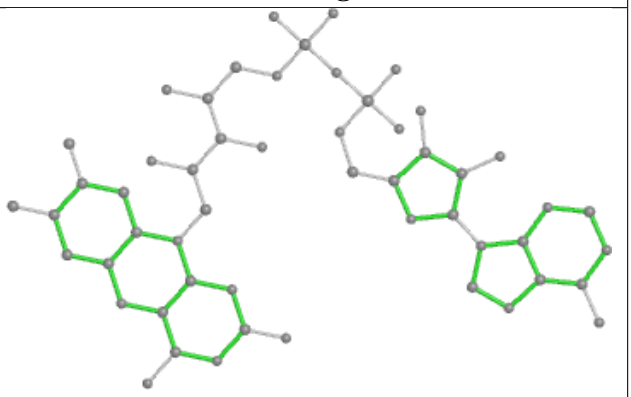
Bond lengths



Bond angles

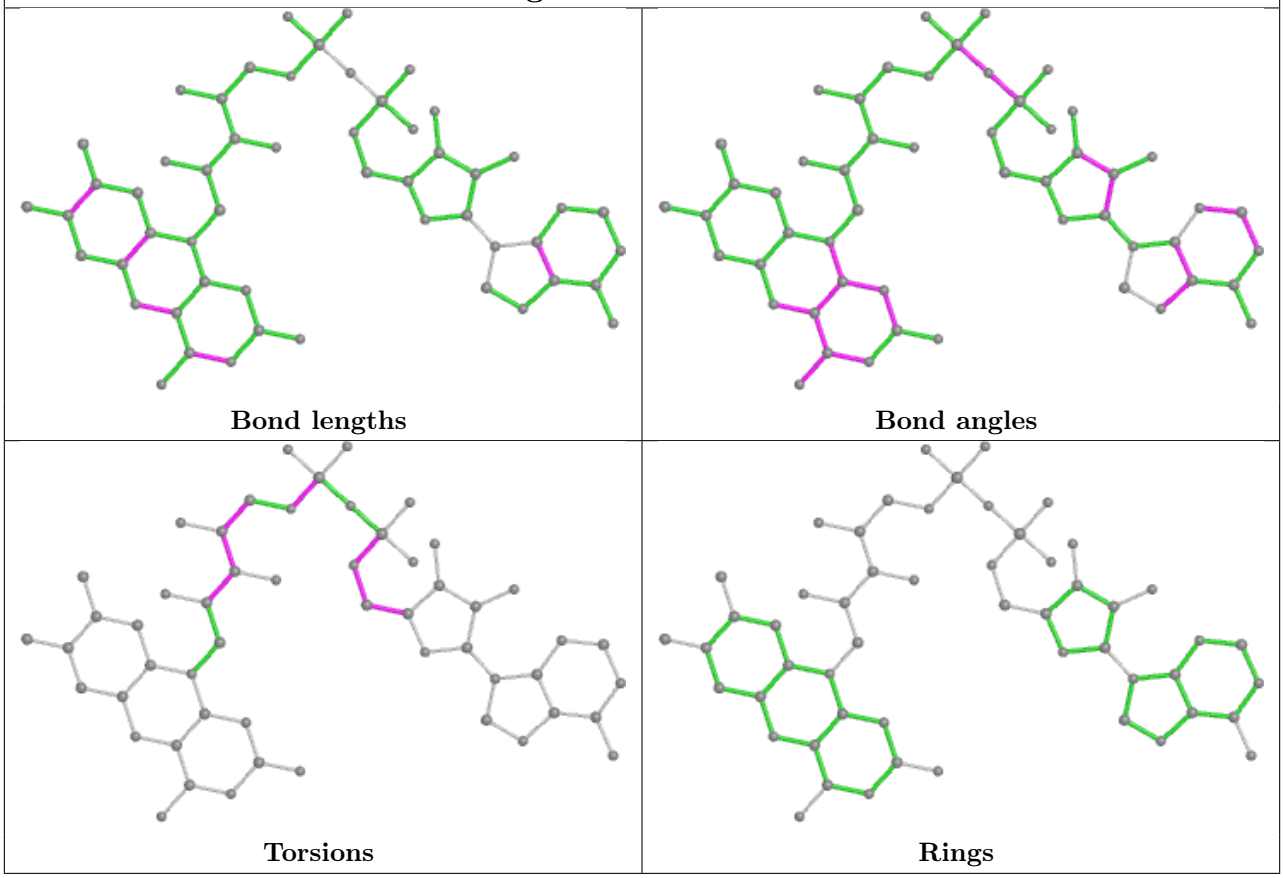


Torsions



Rings

Ligand FAD B 301



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	212/238 (89%)	1.17	47 (22%)	0	0	68, 105, 212, 232	0
1	B	200/238 (84%)	0.81	34 (17%)	1	1	69, 96, 174, 191	0
1	C	202/238 (84%)	0.78	37 (18%)	1	1	52, 89, 207, 232	0
1	D	225/238 (94%)	0.34	14 (6%)	20	23	48, 74, 120, 134	0
All	All	839/952 (88%)	0.77	132 (15%)	2	2	48, 92, 198, 232	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	ALA	13.0
1	A	192	LEU	10.4
1	A	229	ALA	9.1
1	B	229	ALA	8.8
1	A	199	GLN	8.3
1	C	227	ALA	8.3
1	A	203	PHE	7.5
1	A	193	PRO	7.2
1	A	194	ASN	7.0
1	A	228	GLN	6.9
1	B	224	LEU	6.0
1	C	226	ASP	5.9
1	A	221	ALA	5.9
1	A	222	LYS	5.8
1	A	223	LYS	5.6
1	C	197	GLU	5.5
1	B	153	GLU	5.4
1	C	222	LYS	5.4
1	C	211	PRO	5.3
1	C	203	PHE	5.3
1	A	198	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	207	LEU	5.3
1	A	220	GLU	5.2
1	C	198	GLU	5.2
1	A	216	ASN	5.2
1	B	197	GLU	5.0
1	B	198	GLU	5.0
1	C	223	LYS	5.0
1	B	223	LYS	4.9
1	B	194	ASN	4.8
1	C	154	ILE	4.8
1	C	193	PRO	4.7
1	B	228	GLN	4.7
1	B	192	LEU	4.6
1	B	195	LEU	4.6
1	B	154	ILE	4.5
1	B	221	ALA	4.5
1	C	199	GLN	4.5
1	A	191	HIS	4.4
1	A	204	ILE	4.4
1	B	225	ASN	4.4
1	A	195	LEU	4.3
1	B	220	GLU	4.3
1	B	196	ASN	4.2
1	B	208	LYS	4.2
1	C	229	ALA	4.2
1	A	210	ASP	4.2
1	B	227	ALA	4.2
1	A	197	GLU	4.0
1	C	228	GLN	4.0
1	A	200	ARG	3.9
1	C	200	ARG	3.9
1	A	226	ASP	3.9
1	A	219	ALA	3.9
1	C	194	ASN	3.8
1	C	195	LEU	3.8
1	D	227	ALA	3.8
1	B	222	LYS	3.7
1	C	221	ALA	3.7
1	B	199	GLN	3.7
1	C	215	ALA	3.7
1	A	211	PRO	3.6
1	A	157	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	224	LEU	3.6
1	B	200	ARG	3.6
1	D	163	THR	3.5
1	A	218	LEU	3.4
1	D	154	ILE	3.4
1	A	77	GLU	3.4
1	C	224	LEU	3.4
1	C	220	GLU	3.4
1	C	219	ALA	3.3
1	A	214	SER	3.3
1	A	139	GLU	3.2
1	A	189	ILE	3.2
1	B	86	CYS	3.2
1	A	209	ASP	3.2
1	B	126	ASP	3.1
1	C	214	SER	3.1
1	A	86	CYS	3.1
1	A	104	MET	3.1
1	D	86	CYS	3.1
1	C	209	ASP	3.1
1	B	226	ASP	3.0
1	C	218	LEU	3.0
1	B	152	VAL	2.9
1	A	202	ALA	2.9
1	B	193	PRO	2.9
1	D	226	ASP	2.9
1	C	153	GLU	2.9
1	C	216	ASN	2.9
1	C	66	HIS	2.9
1	D	155	MET	2.9
1	A	161	THR	2.8
1	B	66	HIS	2.8
1	C	225	ASN	2.8
1	A	143	LYS	2.8
1	C	207	LEU	2.8
1	A	196	ASN	2.8
1	A	66	HIS	2.8
1	C	152	VAL	2.7
1	D	192	LEU	2.6
1	A	213	GLN	2.6
1	B	189	ILE	2.6
1	B	218	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	212	SER	2.5
1	A	201	ASN	2.5
1	A	163	THR	2.5
1	D	197	GLU	2.5
1	A	212	SER	2.5
1	B	87	ILE	2.4
1	A	81	TRP	2.4
1	A	225	ASN	2.4
1	B	36	LYS	2.3
1	B	209	ASP	2.3
1	B	204	ILE	2.3
1	D	-3	GLY	2.3
1	C	86	CYS	2.3
1	B	202	ALA	2.3
1	C	168	ARG	2.2
1	C	206	SER	2.2
1	D	153	GLU	2.2
1	C	104	MET	2.2
1	D	66	HIS	2.2
1	C	118	THR	2.2
1	D	166	PRO	2.1
1	C	210	ASP	2.1
1	D	7	LYS	2.1
1	D	223	LYS	2.1
1	A	97	GLN	2.1
1	B	119	ILE	2.0
1	A	178	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

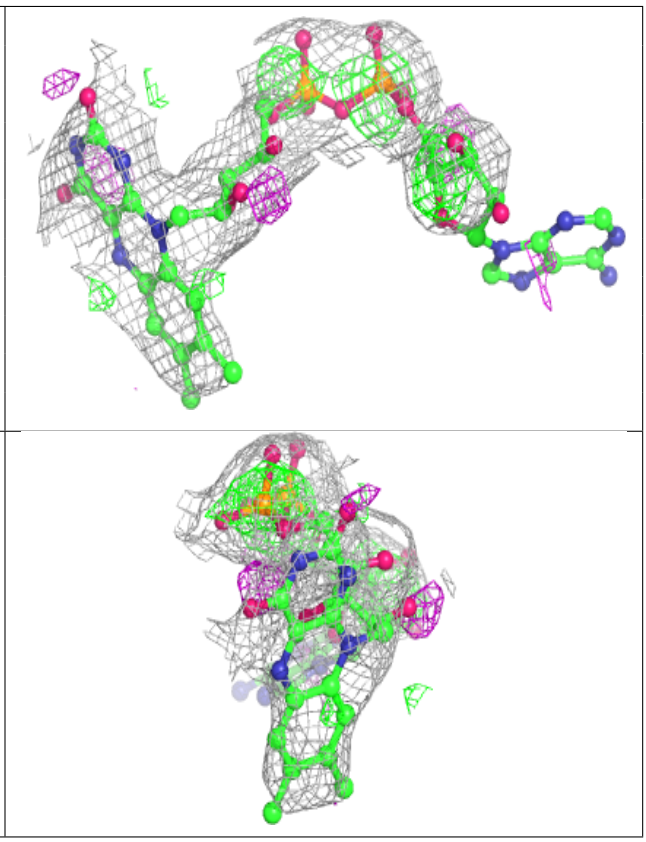
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	A	301	53/53	0.72	0.39	99,133,252,255	0
2	FAD	C	301	53/53	0.85	0.33	83,128,271,273	0
2	FAD	B	301	53/53	0.90	0.30	105,153,227,228	0
2	FAD	D	301	53/53	0.91	0.25	64,81,245,254	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.

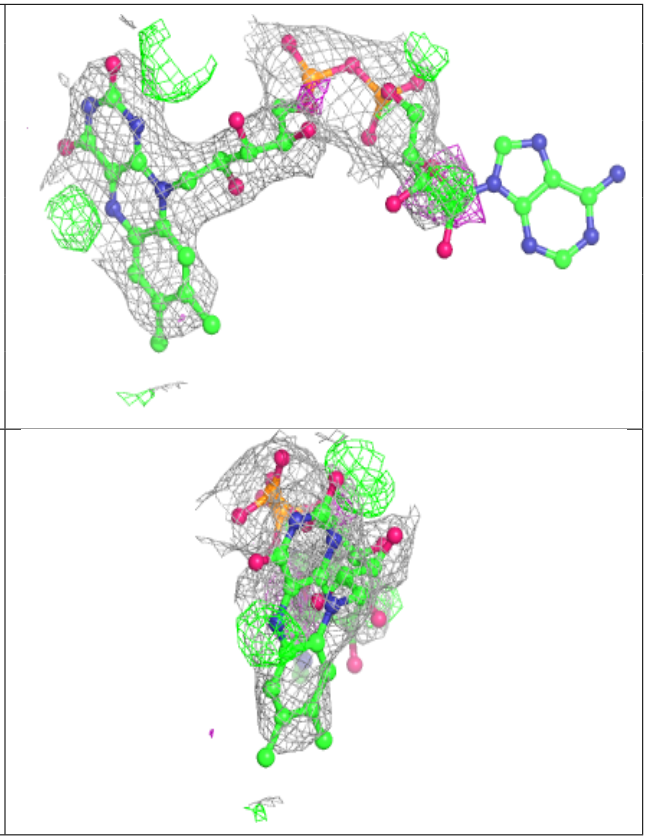
Electron density around FAD A 301:

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



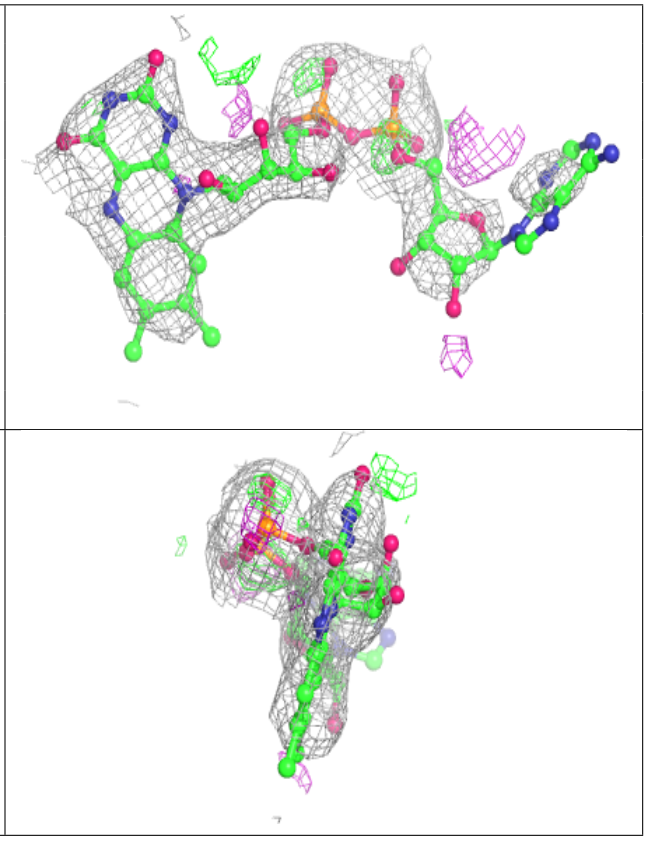
Electron density around FAD C 301:

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



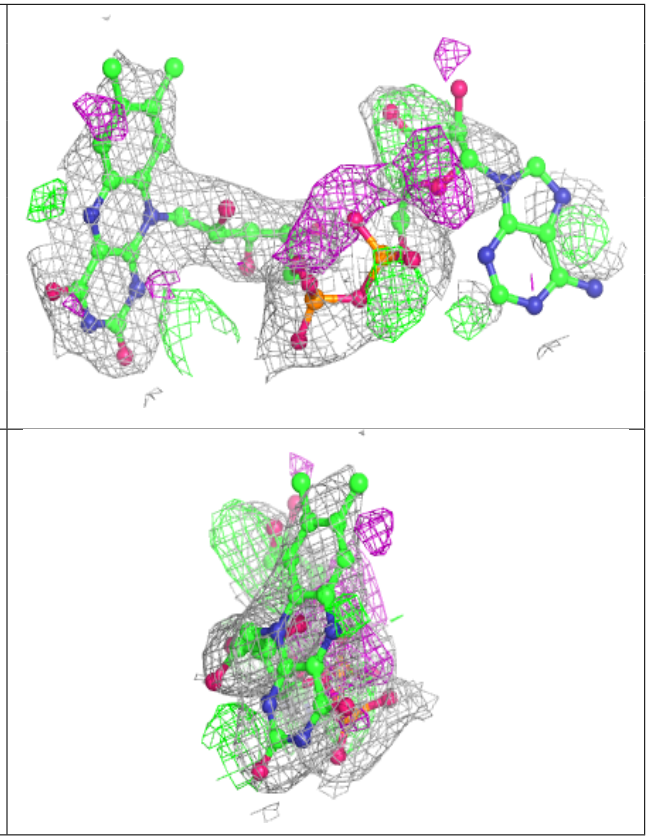
Electron density around FAD B 301:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.