Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:22 am BST

PDB ID	:	8RPH
Title	:	JanthE from Janthinobacterium sp. HH01,ketobutyryl-ThDP
Authors	:	Lanza, L.; Leogrande, C.; Rabe von Pappenheim, F.; Tittmann, K.; Mueller, M.
Deposited on	:	2024-01-16
Resolution	:	2.96 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

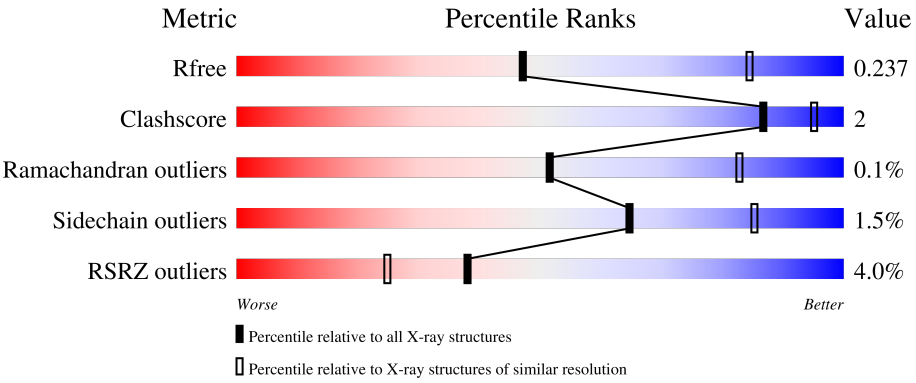
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.96 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.



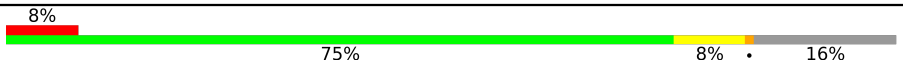
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	619	3% 93%
1	B	619	3% 93%
1	C	619	3% 94%
1	D	619	3% 93% 5%
1	E	619	3% 93% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	619	

2 Entry composition (i)

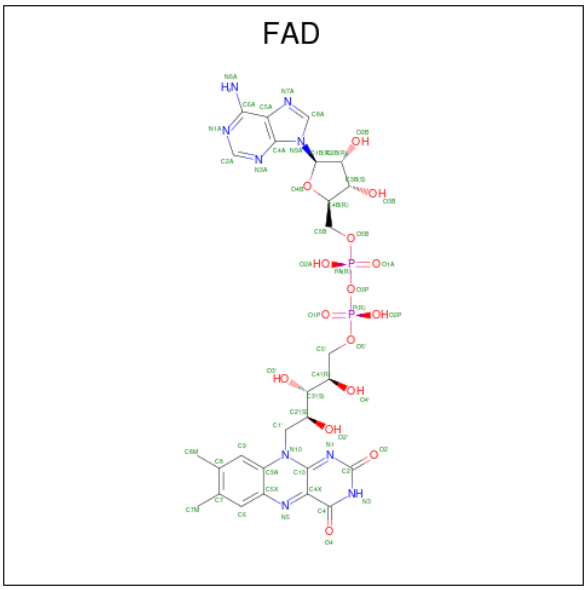
There are 6 unique types of molecules in this entry. The entry contains 55155 atoms, of which 27279 are hydrogens and 0 are deuteriums.

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 Thiamine pyrophosphate-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	605	Total	C	H	N	O	S	0	4	0
			9296	2959	4629	814	862	32			
1	B	599	Total	C	H	N	O	S	0	5	0
			9198	2930	4576	806	855	31			
1	C	605	Total	C	H	N	O	S	0	4	0
			9296	2959	4629	814	862	32			
1	D	608	Total	C	H	N	O	S	0	6	0
			9351	2974	4655	822	869	31			
1	E	605	Total	C	H	N	O	S	0	4	0
			9296	2959	4629	814	862	32			
1	F	520	Total	C	H	N	O	S	0	6	0
			7984	2542	3961	703	748	30			

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

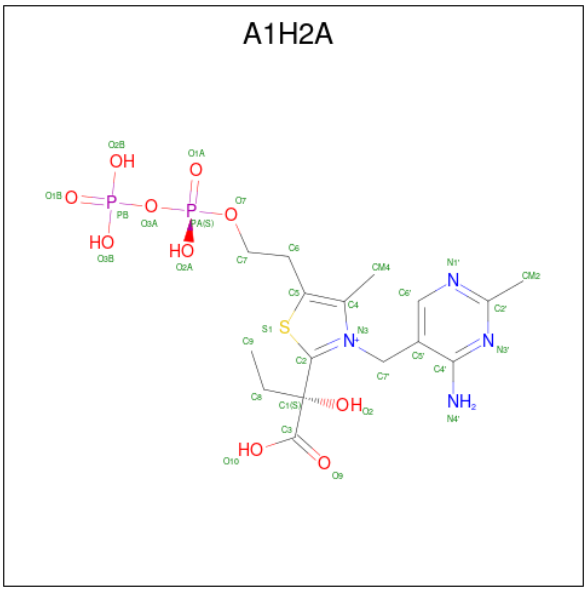


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	E	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	F	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

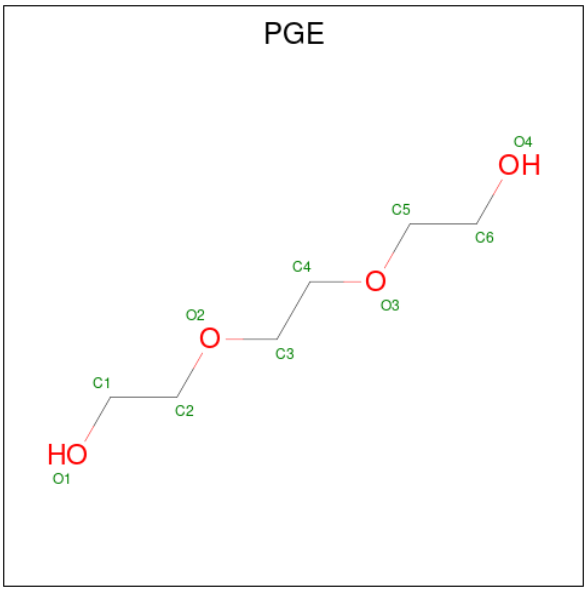
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (2 {S})-2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-5-[2-[oxidanyl(phosphonooxy)phosphoryl]oxyethyl]-1,3-thiazol-2-yl]-2-oxidanyl-butanoic acid (three-letter code: A1H2A) (formula: $C_{16}H_{25}N_4O_{10}P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	C	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	D	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	E	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	F	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C H O 24 6 14 4	0	0

- Molecule 6 is water.

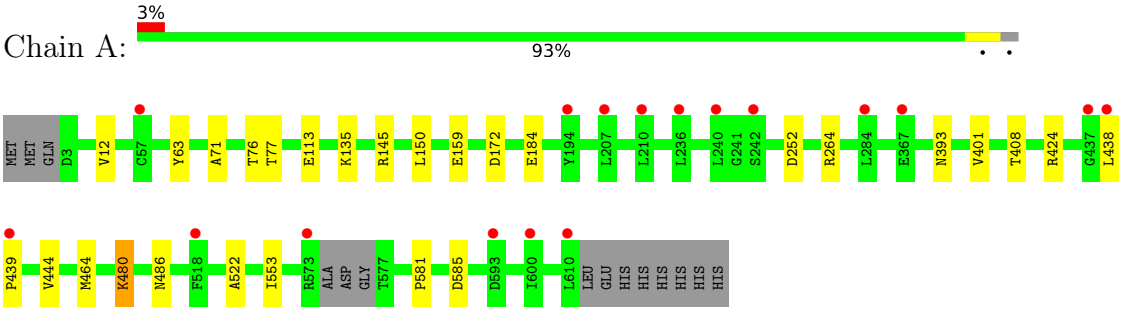
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 1 1	0	0
6	C	1	Total O 1 1	0	0

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.

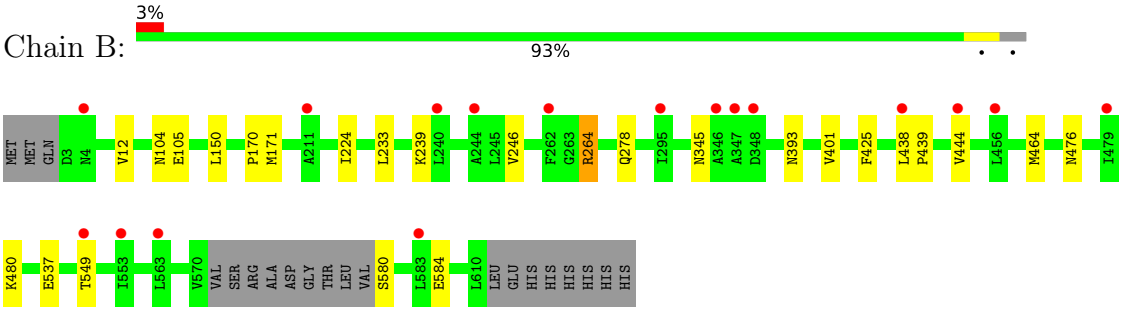
• Molecule 1: Thiamine pyrophosphate-binding protein

Chain A:



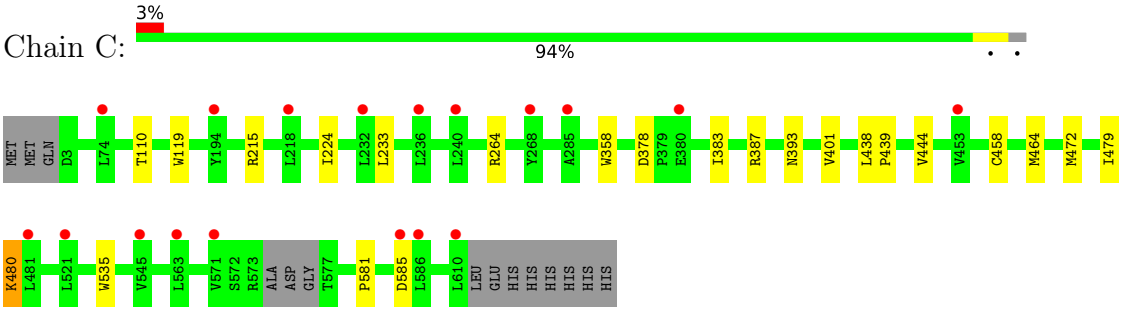
• Molecule 1: Thiamine pyrophosphate-binding protein

Chain B:



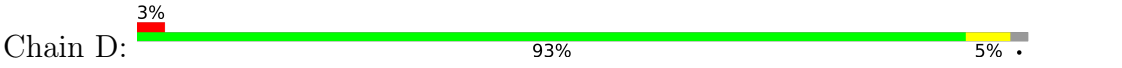
• Molecule 1: Thiamine pyrophosphate-binding protein

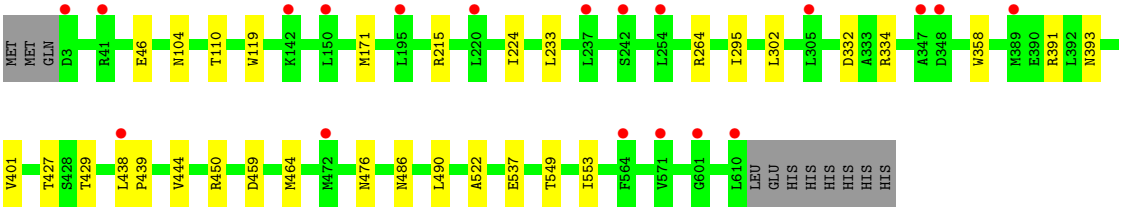
Chain C:



• Molecule 1: Thiamine pyrophosphate-binding protein

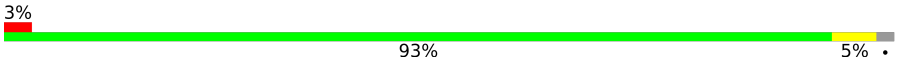
Chain D:

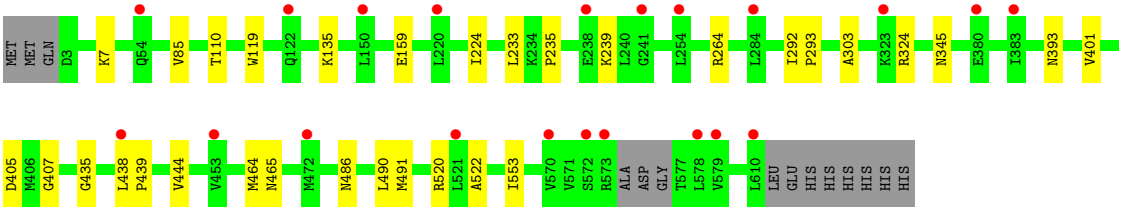




• Molecule 1: Thiamine pyrophosphate-binding protein

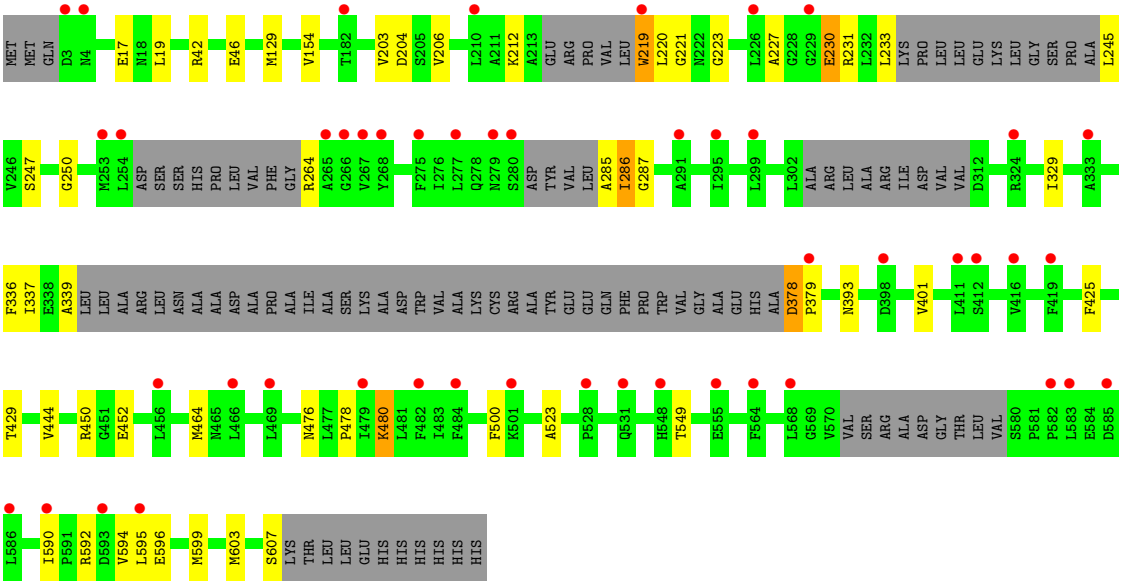
Chain E:





• Molecule 1: Thiamine pyrophosphate-binding protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.33Å 118.19Å 201.17Å 90.00° 97.06° 90.00°	Depositor
Resolution (Å)	99.82 – 2.96 99.82 – 2.96	Depositor EDS
% Data completeness (in resolution range)	94.5 (99.82-2.96) 94.5 (99.82-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.240 0.205 , 0.237	Depositor DCC
R_{free} test set	3860 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 35.9	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	0.93	EDS
Total number of atoms	55155	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: A1H2A, FAD, PGE, MG

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	0.25	0/4779	0.48	0/6483
1	B	0.27	0/4739	0.49	0/6428
1	C	0.25	0/4779	0.49	0/6483
1	D	0.25	0/4814	0.49	0/6531
1	E	0.26	0/4779	0.49	0/6483
1	F	0.29	0/4118	0.52	0/5569
All	All	0.26	0/28008	0.49	0/37977

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

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	4667	4629	4629	15	0
1	B	4622	4576	4569	11	0
1	C	4667	4629	4629	11	0
1	D	4696	4655	4649	17	0
1	E	4667	4629	4629	18	0
1	F	4023	3961	3953	39	0
2	A	53	31	31	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	31	31	1	0
2	C	53	31	31	0	0
2	D	53	31	31	0	0
2	E	53	31	31	0	0
2	F	53	31	31	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	33	0	0	3	0
4	B	33	0	0	1	0
4	C	33	0	0	2	0
4	D	33	0	0	3	0
4	E	33	0	0	4	0
4	F	33	0	0	1	0
5	D	10	14	14	2	0
6	B	1	0	0	0	0
6	C	1	0	0	1	0
All	All	27876	27279	27258	116	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 2.

All (116) 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:E:239:LYS:HE2	1:E:345:ASN:OD1	1.60	0.99
1:F:595:LEU:CD2	1:F:607:SER:HB3	1.98	0.94
1:F:595:LEU:HD23	1:F:607:SER:HB3	1.52	0.90
4:E:703:A1H2A:O2	4:E:703:A1H2A:N4'	2.06	0.88
4:B:703:A1H2A:N4'	4:B:703:A1H2A:O2	2.07	0.87
4:D:704:A1H2A:O2	4:D:704:A1H2A:N4'	2.10	0.85
1:F:595:LEU:HD21	1:F:607:SER:OG	1.80	0.80
1:F:595:LEU:HD21	1:F:607:SER:CB	2.13	0.78
1:E:490:LEU:N	4:E:703:A1H2A:O2B	2.19	0.76
1:E:239:LYS:CE	1:E:345:ASN:OD1	2.33	0.75
4:A:703:A1H2A:O2	4:A:703:A1H2A:N4'	2.19	0.74
1:F:595:LEU:CD2	1:F:607:SER:CB	2.67	0.73
1:D:490:LEU:N	4:D:704:A1H2A:O2B	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:CYS:HB3	6:C:801:HOH:O	1.90	0.71
1:F:378:ASP:N	1:F:378:ASP:OD1	2.25	0.68
1:F:595:LEU:HD21	1:F:607:SER:HB3	1.75	0.68
4:F:703:A1H2A:N4'	4:F:703:A1H2A:O2	2.27	0.68
4:C:703:A1H2A:N4'	4:C:703:A1H2A:O2	2.27	0.67
1:F:285:ALA:HB2	1:F:329:ILE:H	1.66	0.60
1:F:221:GLY:HA3	1:F:287:GLY:O	2.03	0.58
1:B:401:VAL:HG11	1:B:444:VAL:HG11	1.85	0.58
1:F:219:TRP:O	1:F:286:ILE:HG21	2.05	0.57
1:A:408:THR:N	4:A:703:A1H2A:O1B	2.37	0.57
1:A:486:ASN:ND2	4:A:703:A1H2A:O3B	2.36	0.56
1:D:537:GLU:N	1:D:537:GLU:OE1	2.36	0.56
1:F:203:VAL:O	1:F:206:VAL:N	2.39	0.56
1:F:401:VAL:HG11	1:F:444:VAL:HG11	1.88	0.56
1:F:219:TRP:O	1:F:220:LEU:HD23	2.07	0.54
1:D:401:VAL:HG11	1:D:444:VAL:HG11	1.89	0.54
1:A:438:LEU:HB2	1:A:439:PRO:HD3	1.91	0.53
1:F:247:SER:O	1:F:250:GLY:N	2.41	0.52
1:E:401:VAL:HG11	1:E:444:VAL:HG11	1.92	0.52
1:C:438:LEU:HB2	1:C:439:PRO:HD3	1.93	0.51
1:C:401:VAL:HG11	1:C:444:VAL:HG11	1.92	0.51
1:F:596:GLU:HA	1:F:596:GLU:OE1	2.10	0.51
1:F:594:VAL:HG12	1:F:594:VAL:O	2.11	0.50
1:F:46:GLU:OE2	1:F:450[B]:ARG:NH2	2.42	0.50
1:F:336:PHE:CD1	1:F:336:PHE:C	2.84	0.49
1:A:522:ALA:HB2	1:A:553:ILE:HD12	1.95	0.49
1:F:203:VAL:HG11	1:F:339:ALA:CB	2.42	0.49
1:F:592:ARG:HG2	1:F:592:ARG:O	2.12	0.49
1:A:135:LYS:NZ	1:A:159:GLU:O	2.46	0.48
1:B:438:LEU:HB2	1:B:439:PRO:HD3	1.95	0.48
1:B:224:ILE:HD13	1:B:233:LEU:HD21	1.94	0.48
1:D:46:GLU:OE2	1:D:450[B]:ARG:NH2	2.44	0.48
1:F:286:ILE:O	1:F:286:ILE:HG22	2.13	0.48
1:F:223:GLY:O	1:F:227:ALA:N	2.41	0.47
1:B:104:ASN:O	1:B:171:MET:HG3	2.14	0.47
1:B:239:LYS:NZ	1:B:345:ASN:OD1	2.48	0.47
1:D:438:LEU:HB2	1:D:439:PRO:HD3	1.96	0.47
1:E:407:GLY:HA3	4:E:703:A1H2A:O3B	2.14	0.47
1:A:401:VAL:HG11	1:A:444:VAL:HG11	1.95	0.47
1:B:105:GLU:O	1:B:170:PRO:HB3	2.15	0.47
1:F:203:VAL:O	1:F:204:ASP:C	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ASP:OD1	1:D:334:ARG:N	2.46	0.47
1:F:203:VAL:HG11	1:F:339:ALA:HB1	1.95	0.47
1:F:219:TRP:O	1:F:286:ILE:CG2	2.63	0.47
1:F:17:GLU:OE1	1:F:42:ARG:NE	2.46	0.46
1:B:246:VAL:O	1:B:264:ARG:HG3	2.16	0.46
1:E:522:ALA:HB2	1:E:553:ILE:HD12	1.98	0.46
1:B:12:VAL:HG13	1:B:150:LEU:CD1	2.46	0.46
1:A:252:ASP:OD2	1:A:424:ARG:NE	2.38	0.45
1:D:110:THR:HA	1:D:119:TRP:CE3	2.51	0.45
1:F:336:PHE:CD1	1:F:336:PHE:O	2.70	0.45
1:C:224:ILE:HD13	1:C:233:LEU:HD21	1.98	0.45
1:A:63:TYR:CD1	1:A:71:ALA:HB2	2.52	0.45
1:E:303:ALA:O	1:E:324:ARG:NH2	2.50	0.45
1:E:438:LEU:HB2	1:E:439:PRO:HD3	1.99	0.44
1:A:113:GLU:OE1	1:A:113:GLU:N	2.48	0.44
1:D:215:ARG:HA	1:D:358:TRP:CG	2.53	0.44
1:D:459:ASP:N	1:D:459:ASP:OD1	2.50	0.44
1:E:486:ASN:ND2	4:E:703:A1H2A:O1B	2.36	0.44
1:F:221:GLY:HA3	1:F:287:GLY:C	2.38	0.44
1:E:224:ILE:HD13	1:E:233:LEU:HD21	1.99	0.44
1:E:110:THR:HA	1:E:119:TRP:CE3	2.53	0.43
1:F:599:MET:HG3	1:F:603:MET:HA	2.00	0.43
1:A:480:LYS:N	1:A:480:LYS:HD2	2.34	0.43
1:F:336:PHE:O	1:F:336:PHE:CG	2.70	0.43
1:A:145:ARG:NH1	1:A:184:GLU:OE1	2.47	0.43
1:B:278:GLN:HG3	1:B:584:GLU:HB3	2.00	0.43
1:D:522:ALA:HB2	1:D:553:ILE:HD12	2.00	0.43
1:C:110:THR:HA	1:C:119:TRP:CE3	2.54	0.43
1:D:224:ILE:HD13	1:D:233:LEU:HD21	2.00	0.42
1:A:172:ASP:N	1:A:172:ASP:OD1	2.52	0.42
1:F:19:LEU:HD13	1:F:154:VAL:HG21	2.01	0.42
1:A:581:PRO:HB2	1:A:585:ASP:HB3	2.01	0.42
1:E:135:LYS:NZ	1:E:159:GLU:O	2.52	0.42
1:D:104:ASN:O	1:D:171:MET:HG3	2.20	0.42
1:F:285:ALA:CB	1:F:329:ILE:H	2.32	0.42
1:F:452:GLU:HA	1:F:478:PRO:HG2	2.01	0.42
1:F:480:LYS:N	1:F:480:LYS:HD2	2.35	0.42
1:B:12:VAL:HG13	1:B:150:LEU:HD11	2.01	0.42
1:C:472[A]:MET:HG2	1:C:479:ILE:HD12	2.01	0.42
1:F:429:THR:HB	2:F:701:FAD:O3'	2.20	0.42
1:D:391:ARG:HD3	5:D:703:PGE:H62	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:703:A1H2A:C9	4:C:703:A1H2A:S1	3.08	0.41
1:A:76:THR:OG1	1:A:77:THR:N	2.53	0.41
1:B:537:GLU:OE1	1:B:537:GLU:N	2.53	0.41
2:B:701:FAD:H9	2:B:701:FAD:H1'1	1.89	0.41
1:D:391:ARG:HA	5:D:703:PGE:H62	2.03	0.41
1:E:235:PRO:O	1:E:239:LYS:HB2	2.21	0.41
1:C:378:ASP:OD2	1:C:387:ARG:NH1	2.53	0.41
1:E:7:LYS:NZ	1:F:500:PHE:HE1	2.19	0.41
1:A:12:VAL:HG13	1:A:150:LEU:CD1	2.50	0.41
1:D:486:ASN:ND2	4:D:704:A1H2A:O3B	2.46	0.41
1:E:520:ARG:NH2	1:F:523:ALA:O	2.52	0.41
1:C:383:ILE:HG23	1:C:535:TRP:CZ2	2.55	0.41
1:D:295:ILE:HB	1:D:302:LEU:HD22	2.03	0.41
1:D:427:THR:HG23	1:D:429:THR:HG23	2.03	0.41
1:E:435:GLY:O	1:E:465:ASN:ND2	2.44	0.41
1:C:581:PRO:HB2	1:C:585:ASP:HB3	2.03	0.40
1:E:85:VAL:HG11	1:F:129:MET:SD	2.62	0.40
1:F:230:GLU:H	1:F:230:GLU:HG3	1.69	0.40
1:C:215:ARG:HA	1:C:358:TRP:CG	2.56	0.40
1:C:480:LYS:HD2	1:C:480:LYS:N	2.35	0.40
1:E:292:ILE:HB	1:E:293:PRO:HD3	2.03	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	605/619 (98%)	590 (98%)	15 (2%)	0	100	100
1	B	600/619 (97%)	583 (97%)	17 (3%)	0	100	100
1	C	605/619 (98%)	588 (97%)	17 (3%)	0	100	100
1	D	612/619 (99%)	590 (96%)	22 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	605/619 (98%)	587 (97%)	17 (3%)	1 (0%)	47 79
1	F	510/619 (82%)	487 (96%)	22 (4%)	1 (0%)	47 79
All	All	3537/3714 (95%)	3425 (97%)	110 (3%)	2 (0%)	51 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	405	ASP
1	F	379	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	492/500 (98%)	488 (99%)	4 (1%)	81 92
1	B	486/500 (97%)	478 (98%)	8 (2%)	62 84
1	C	492/500 (98%)	488 (99%)	4 (1%)	81 92
1	D	494/500 (99%)	489 (99%)	5 (1%)	76 90
1	E	492/500 (98%)	488 (99%)	4 (1%)	81 92
1	F	425/500 (85%)	408 (96%)	17 (4%)	31 64
All	All	2881/3000 (96%)	2839 (98%)	42 (2%)	65 85

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ARG
1	A	393	ASN
1	A	464	MET
1	A	480	LYS
1	B	264	ARG
1	B	393	ASN
1	B	425	PHE
1	B	464	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	476	ASN
1	B	480	LYS
1	B	549	THR
1	B	580	SER
1	C	264	ARG
1	C	393	ASN
1	C	464	MET
1	C	480	LYS
1	D	264	ARG
1	D	393	ASN
1	D	464	MET
1	D	476	ASN
1	D	549	THR
1	E	264	ARG
1	E	393	ASN
1	E	464	MET
1	E	491	MET
1	F	212	LYS
1	F	219	TRP
1	F	230	GLU
1	F	231	ARG
1	F	233	LEU
1	F	245	LEU
1	F	264	ARG
1	F	286	ILE
1	F	337	ILE
1	F	378	ASP
1	F	393	ASN
1	F	425	PHE
1	F	464	MET
1	F	476	ASN
1	F	480	LYS
1	F	549	THR
1	F	590	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	A1H2A	F	703	3	28,34,34	0.78	0	31,52,52	0.93	2 (6%)
4	A1H2A	E	703	3	28,34,34	0.82	0	31,52,52	0.96	2 (6%)
2	FAD	D	701	-	53,58,58	0.48	0	68,89,89	0.52	1 (1%)
4	A1H2A	D	704	3	28,34,34	0.80	0	31,52,52	0.94	2 (6%)
4	A1H2A	C	703	3	28,34,34	0.82	0	31,52,52	1.09	2 (6%)
4	A1H2A	B	703	3	28,34,34	1.15	1 (3%)	31,52,52	1.07	1 (3%)
5	PGE	D	703	-	9,9,9	0.11	0	8,8,8	0.21	0
2	FAD	F	701	-	53,58,58	0.47	0	68,89,89	0.56	2 (2%)
2	FAD	E	701	-	53,58,58	0.47	0	68,89,89	0.52	2 (2%)
2	FAD	A	701	-	53,58,58	0.46	0	68,89,89	0.56	2 (2%)
2	FAD	B	701	-	53,58,58	0.48	0	68,89,89	0.53	2 (2%)
4	A1H2A	A	703	3	28,34,34	0.79	0	31,52,52	0.85	1 (3%)
2	FAD	C	701	-	53,58,58	0.46	0	68,89,89	0.51	1 (1%)

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
4	A1H2A	F	703	3	-	10/25/32/32	0/2/2/2
4	A1H2A	E	703	3	-	8/25/32/32	0/2/2/2
2	FAD	D	701	-	-	8/30/50/50	0/6/6/6
4	A1H2A	D	704	3	-	8/25/32/32	0/2/2/2
4	A1H2A	C	703	3	-	8/25/32/32	0/2/2/2
4	A1H2A	B	703	3	-	10/25/32/32	0/2/2/2
5	PGE	D	703	-	-	0/7/7/7	-
2	FAD	F	701	-	-	9/30/50/50	0/6/6/6
2	FAD	E	701	-	-	8/30/50/50	0/6/6/6
2	FAD	A	701	-	-	7/30/50/50	0/6/6/6
2	FAD	B	701	-	-	8/30/50/50	0/6/6/6
4	A1H2A	A	703	3	-	4/25/32/32	0/2/2/2
2	FAD	C	701	-	-	7/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	A1H2A	C5-S1	-3.38	1.67	1.74

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	703	A1H2A	C6-C5-C4	2.95	129.80	127.43
4	E	703	A1H2A	C6-C5-C4	2.84	129.71	127.43
4	C	703	A1H2A	C5-C4-N3	2.76	113.43	107.66
4	D	704	A1H2A	C6-C5-C4	2.72	129.62	127.43
4	B	703	A1H2A	C5-C4-N3	2.72	113.34	107.66
4	A	703	A1H2A	C5-C4-N3	2.71	113.32	107.66
4	F	703	A1H2A	C5-C4-N3	2.69	113.29	107.66
2	F	701	FAD	P-O3P-PA	-2.63	123.80	132.83
4	E	703	A1H2A	C5-C4-N3	2.61	113.11	107.66
4	D	704	A1H2A	C5-C4-N3	2.60	113.10	107.66
2	A	701	FAD	P-O3P-PA	-2.48	124.33	132.83
2	D	701	FAD	C5A-C6A-N6A	2.31	123.86	120.35
2	A	701	FAD	C5A-C6A-N6A	2.30	123.84	120.35
2	B	701	FAD	C5A-C6A-N6A	2.29	123.83	120.35
2	E	701	FAD	C5A-C6A-N6A	2.28	123.82	120.35
2	F	701	FAD	C5A-C6A-N6A	2.28	123.81	120.35
2	C	701	FAD	C5A-C6A-N6A	2.23	123.75	120.35
4	F	703	A1H2A	C6-C5-C4	2.15	129.16	127.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	701	FAD	P-O3P-PA	-2.06	125.75	132.83
2	B	701	FAD	P-O3P-PA	-2.01	125.92	132.83

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C5B-O5B-PA-O1A
2	A	701	FAD	C5B-O5B-PA-O2A
2	B	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5B-O5B-PA-O2A
2	C	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	C5B-O5B-PA-O2A
2	D	701	FAD	C5B-O5B-PA-O1A
2	D	701	FAD	O4B-C4B-C5B-O5B
2	E	701	FAD	C5B-O5B-PA-O1A
2	E	701	FAD	C5B-O5B-PA-O2A
2	F	701	FAD	C5B-O5B-PA-O1A
2	F	701	FAD	C5B-O5B-PA-O2A
4	A	703	A1H2A	O2-C1-C3-O10
4	A	703	A1H2A	C8-C1-C3-O10
4	A	703	A1H2A	C8-C1-C3-O9
4	B	703	A1H2A	O2-C1-C8-C9
4	B	703	A1H2A	C3-C1-C8-C9
4	B	703	A1H2A	C2-C1-C8-C9
4	B	703	A1H2A	O2-C1-C3-O10
4	B	703	A1H2A	C8-C1-C3-O10
4	B	703	A1H2A	C8-C1-C3-O9
4	B	703	A1H2A	C7-O7-PA-O1A
4	C	703	A1H2A	C5-C6-C7-O7
4	C	703	A1H2A	C4-C5-C6-C7
4	C	703	A1H2A	O2-C1-C3-O10
4	C	703	A1H2A	C8-C1-C3-O10
4	C	703	A1H2A	O2-C1-C3-O9
4	C	703	A1H2A	C8-C1-C3-O9
4	C	703	A1H2A	C4'-C5'-C7'-N3
4	D	704	A1H2A	C5-C6-C7-O7
4	D	704	A1H2A	O2-C1-C3-O10
4	D	704	A1H2A	C8-C1-C3-O10
4	D	704	A1H2A	O2-C1-C3-O9
4	D	704	A1H2A	C8-C1-C3-O9
4	D	704	A1H2A	C7-O7-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	703	A1H2A	C5-C6-C7-O7
4	E	703	A1H2A	O2-C1-C3-O10
4	E	703	A1H2A	C8-C1-C3-O10
4	E	703	A1H2A	C8-C1-C3-O9
4	F	703	A1H2A	C5-C6-C7-O7
4	F	703	A1H2A	O2-C1-C3-O10
4	F	703	A1H2A	C8-C1-C3-O10
4	F	703	A1H2A	C8-C1-C3-O9
4	F	703	A1H2A	C4'-C5'-C7'-N3
4	F	703	A1H2A	PB-O3A-PA-O7
4	F	703	A1H2A	C7-O7-PA-O2A
4	F	703	A1H2A	C7-O7-PA-O3A
2	A	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	C3B-C4B-C5B-O5B
2	B	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	C3B-C4B-C5B-O5B
2	E	701	FAD	O4B-C4B-C5B-O5B
2	E	701	FAD	C3B-C4B-C5B-O5B
2	F	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	C3B-C4B-C5B-O5B
2	B	701	FAD	C3B-C4B-C5B-O5B
2	D	701	FAD	C3B-C4B-C5B-O5B
2	B	701	FAD	P-O3P-PA-O1A
2	A	701	FAD	C4'-C5'-O5'-P
2	B	701	FAD	C4'-C5'-O5'-P
2	C	701	FAD	C4'-C5'-O5'-P
2	D	701	FAD	C4'-C5'-O5'-P
2	E	701	FAD	C4'-C5'-O5'-P
2	F	701	FAD	C4'-C5'-O5'-P
2	A	701	FAD	P-O3P-PA-O5B
2	C	701	FAD	P-O3P-PA-O5B
2	D	701	FAD	P-O3P-PA-O5B
2	E	701	FAD	P-O3P-PA-O5B
4	D	704	A1H2A	PB-O3A-PA-O7
4	E	703	A1H2A	PB-O3A-PA-O7
4	B	703	A1H2A	C7-O7-PA-O3A
4	E	703	A1H2A	C7-O7-PA-O3A
2	F	701	FAD	P-O3P-PA-O1A
2	D	701	FAD	C5B-O5B-PA-O2A
4	A	703	A1H2A	O2-C1-C3-O9
4	B	703	A1H2A	O2-C1-C3-O9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	703	A1H2A	C6'-C5'-C7'-N3
4	D	704	A1H2A	C7-O7-PA-O2A
4	E	703	A1H2A	O2-C1-C3-O9
4	E	703	A1H2A	C7-O7-PA-O2A
2	E	701	FAD	P-O3P-PA-O1A
4	B	703	A1H2A	C2-C1-C3-O10
2	D	701	FAD	P-O3P-PA-O1A
2	B	701	FAD	P-O3P-PA-O5B
2	F	701	FAD	P-O3P-PA-O5B
2	A	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	C5B-O5B-PA-O3P
2	C	701	FAD	C5B-O5B-PA-O3P
2	D	701	FAD	C5B-O5B-PA-O3P
2	E	701	FAD	C5B-O5B-PA-O3P
2	F	701	FAD	C5B-O5B-PA-O3P
4	F	703	A1H2A	O2-C1-C3-O9
4	F	703	A1H2A	C6'-C5'-C7'-N3
2	F	701	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

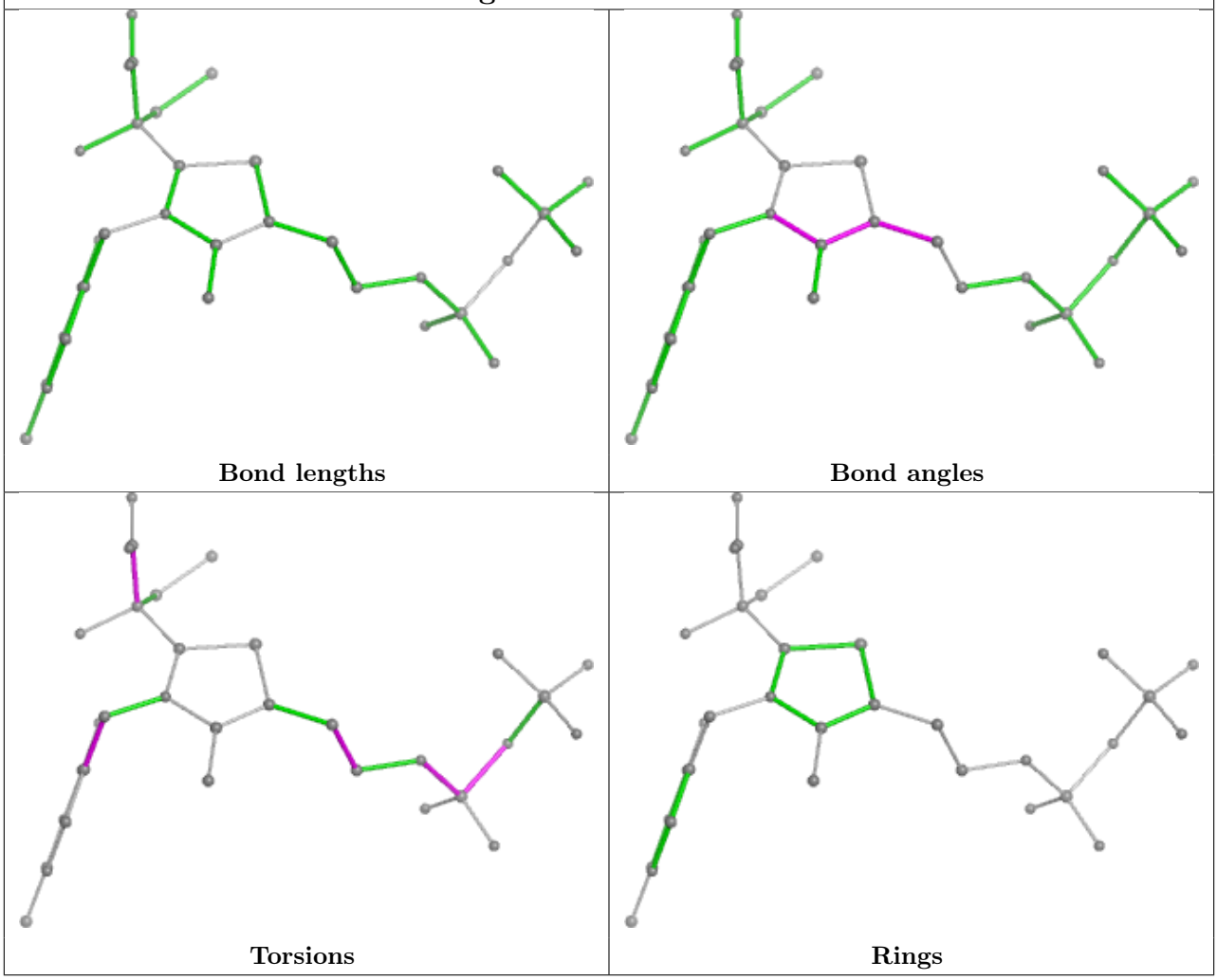
9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	703	A1H2A	1	0
4	E	703	A1H2A	4	0
4	D	704	A1H2A	3	0
4	C	703	A1H2A	2	0
4	B	703	A1H2A	1	0
5	D	703	PGE	2	0
2	F	701	FAD	1	0
2	B	701	FAD	1	0
4	A	703	A1H2A	3	0

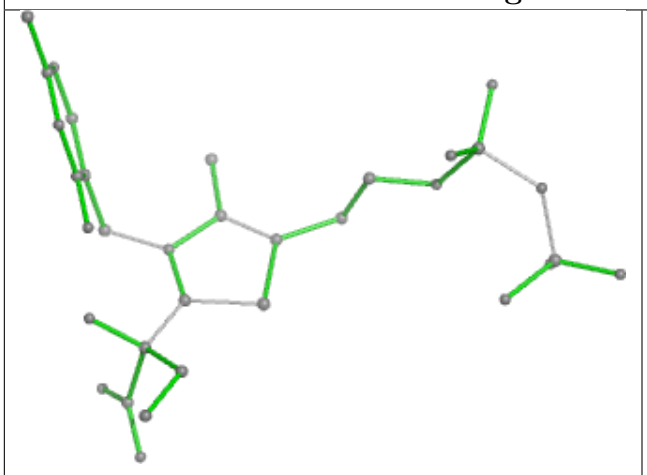
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

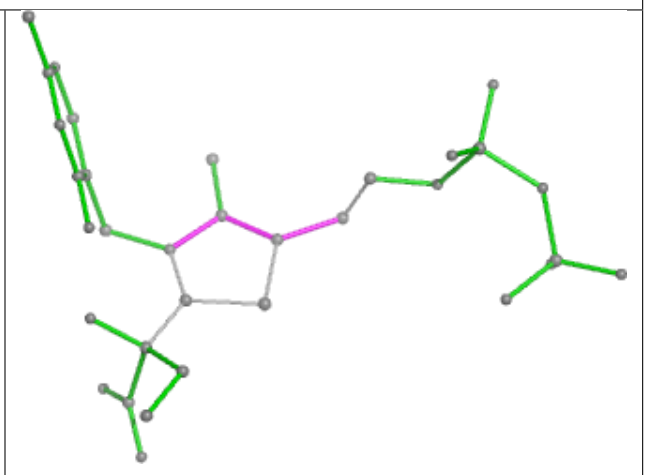
Ligand A1H2A F 703



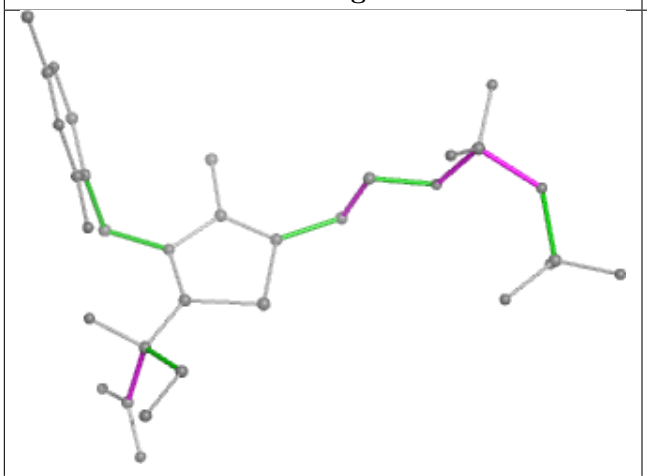
Ligand A1H2A E 703



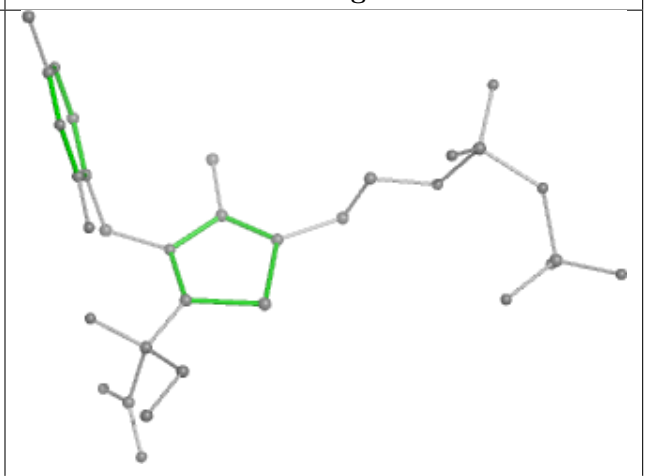
Bond lengths



Bond angles

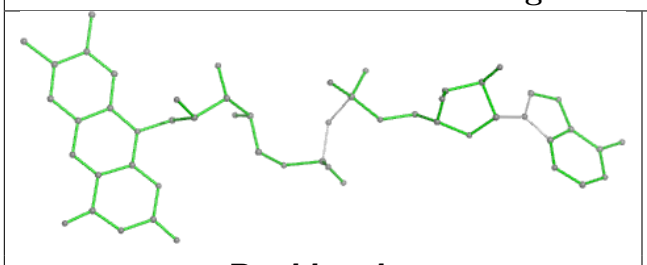


Torsions

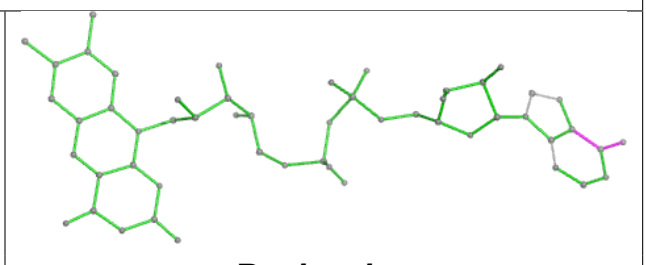


Rings

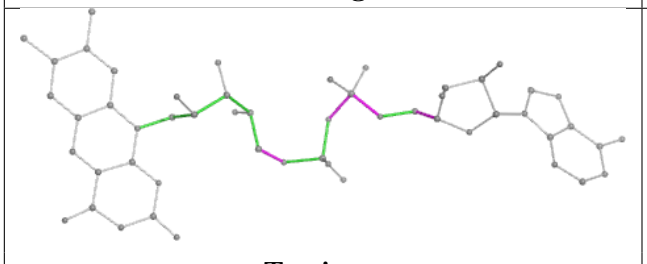
Ligand FAD D 701



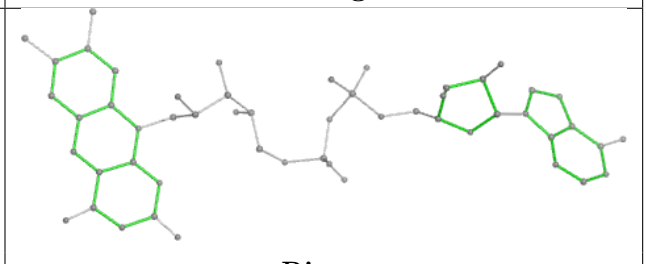
Bond lengths



Bond angles

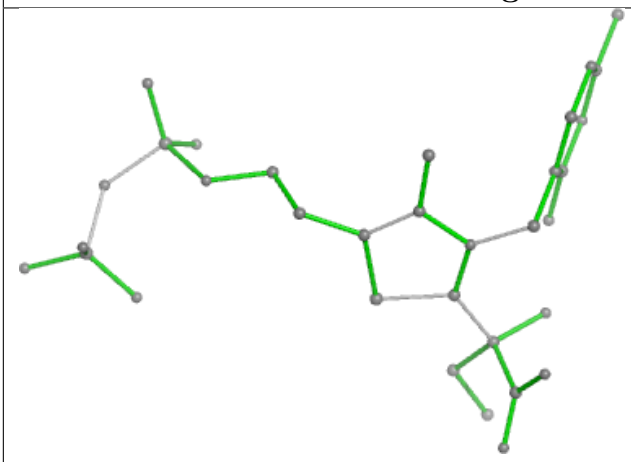


Torsions

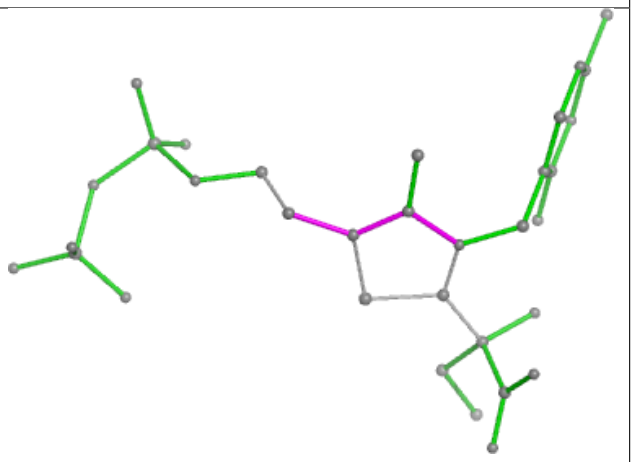


Rings

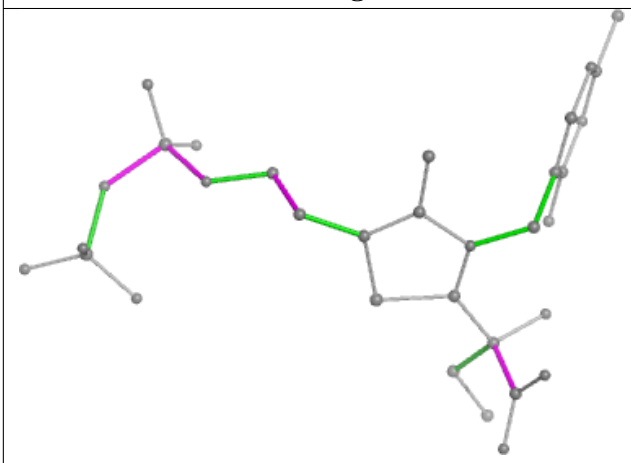
Ligand A1H2A D 704



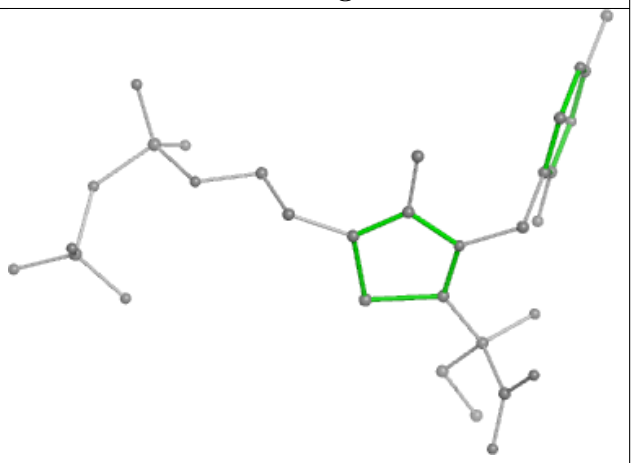
Bond lengths



Bond angles

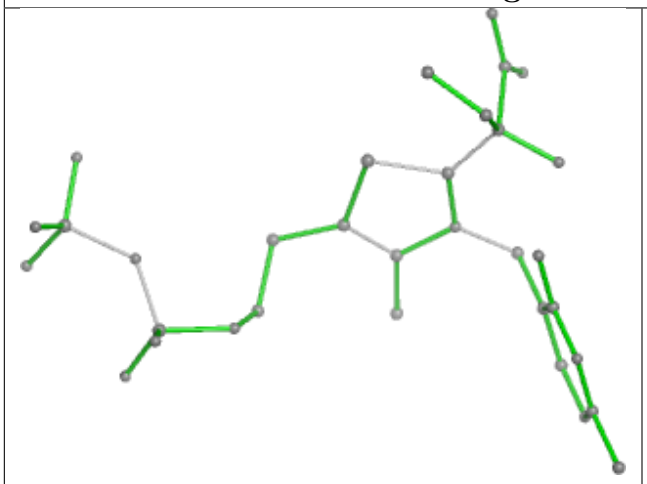


Torsions

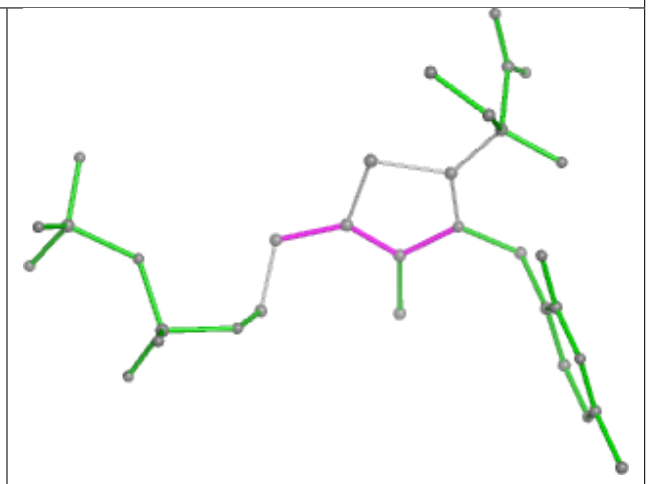


Rings

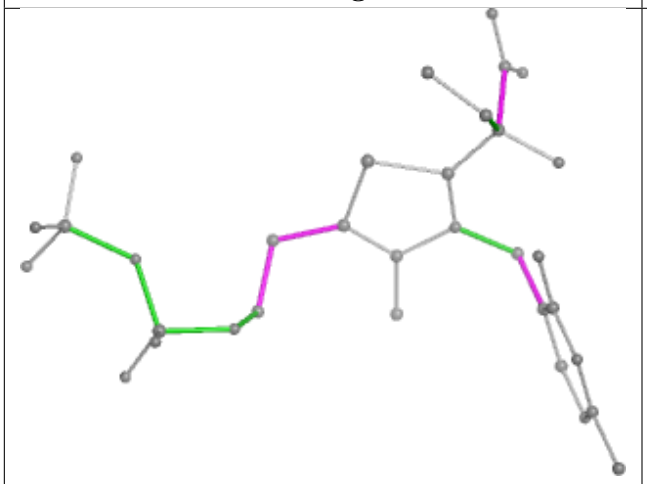
Ligand A1H2A C 703



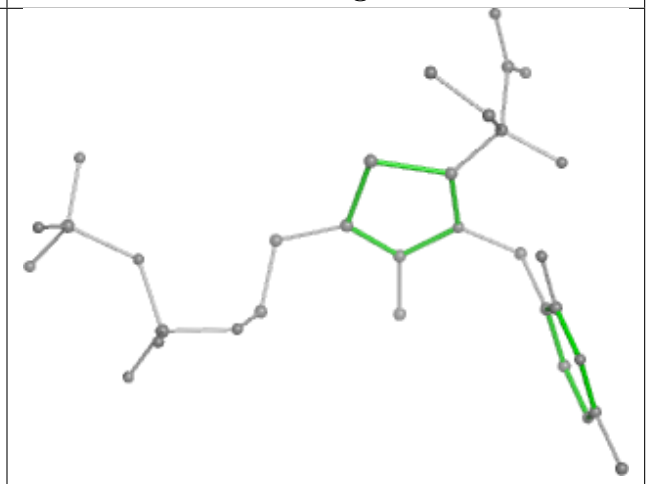
Bond lengths



Bond angles

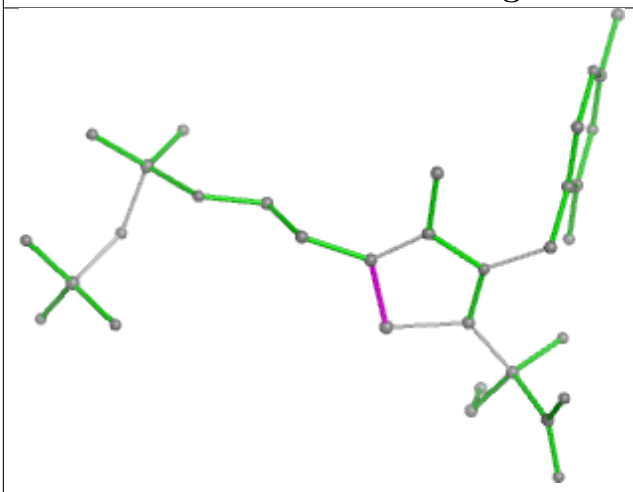


Torsions

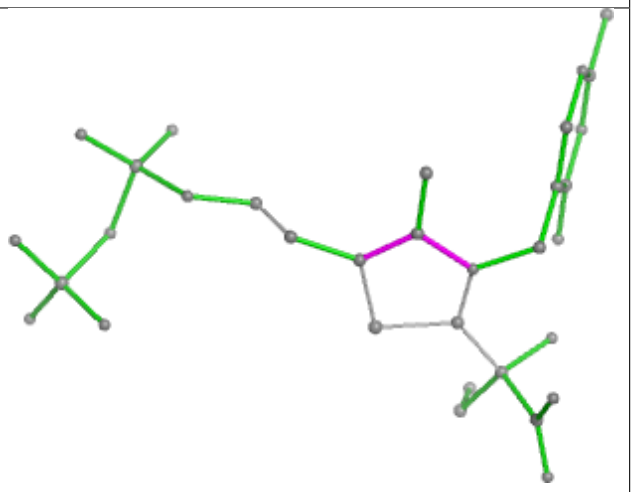


Rings

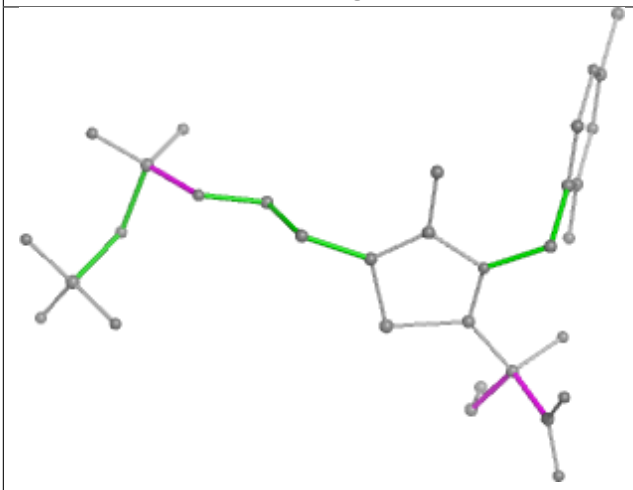
Ligand A1H2A B 703



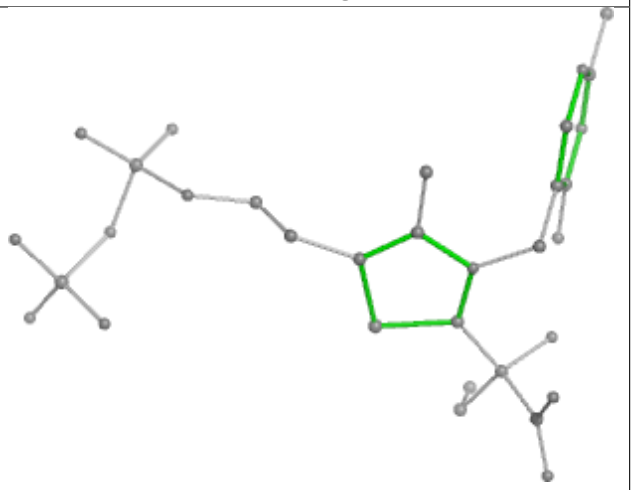
Bond lengths



Bond angles

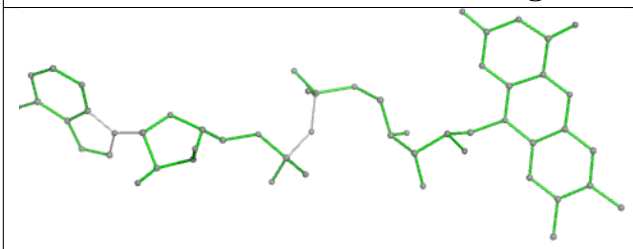


Torsions

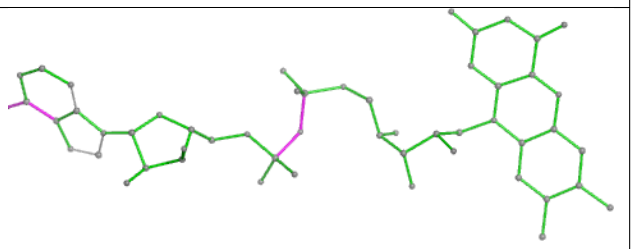


Rings

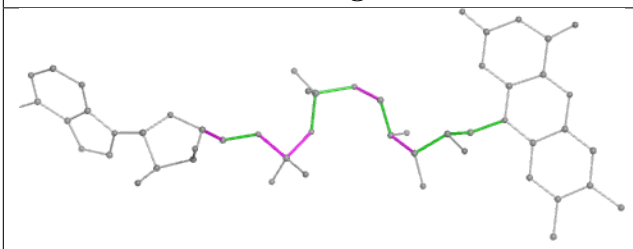
Ligand FAD F 701



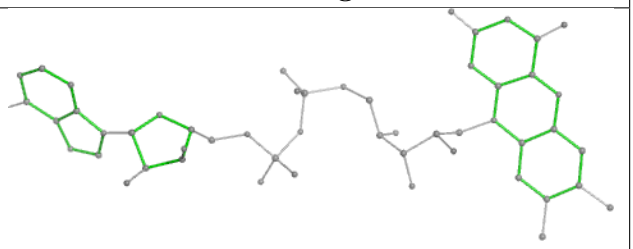
Bond lengths



Bond angles

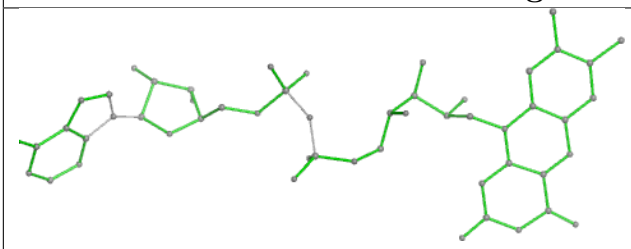


Torsions

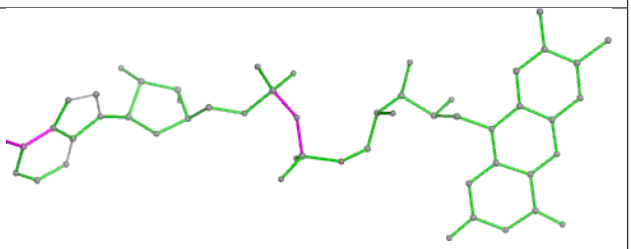


Rings

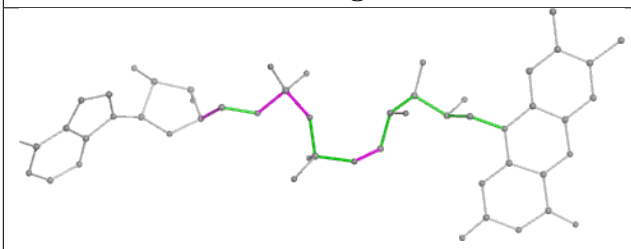
Ligand FAD E 701



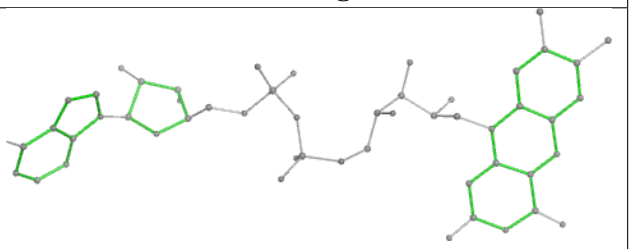
Bond lengths



Bond angles

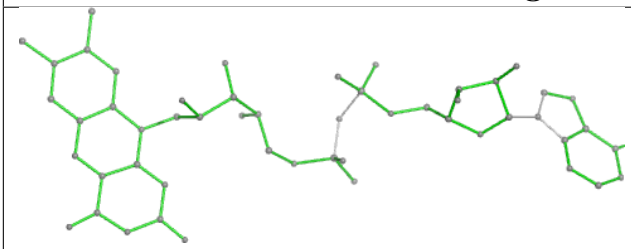


Torsions

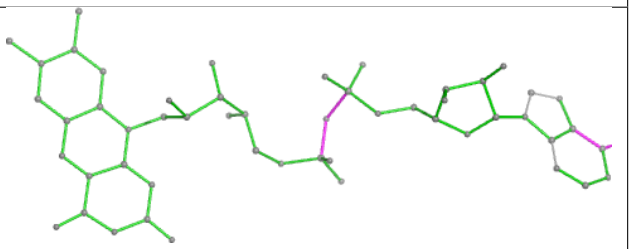


Rings

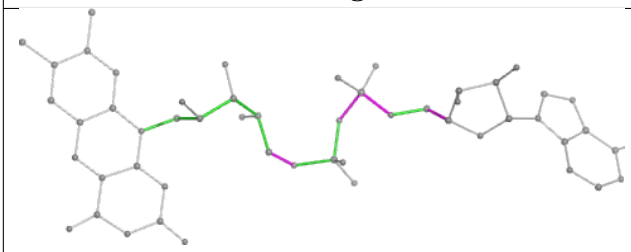
Ligand FAD A 701



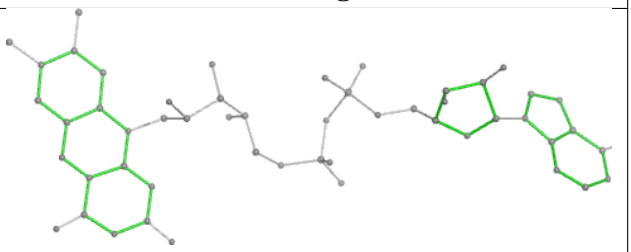
Bond lengths



Bond angles

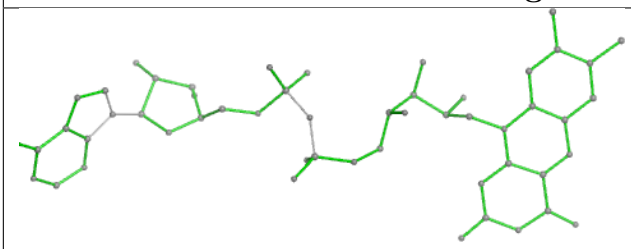


Torsions

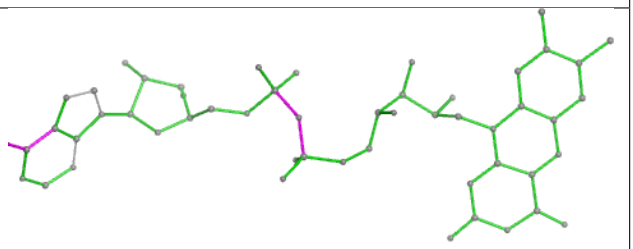


Rings

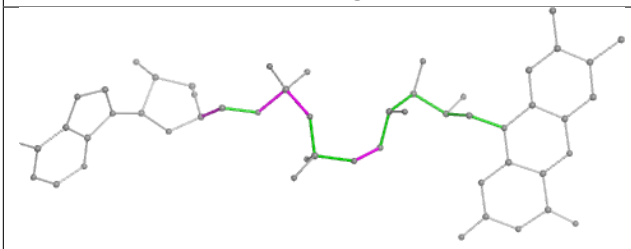
Ligand FAD B 701



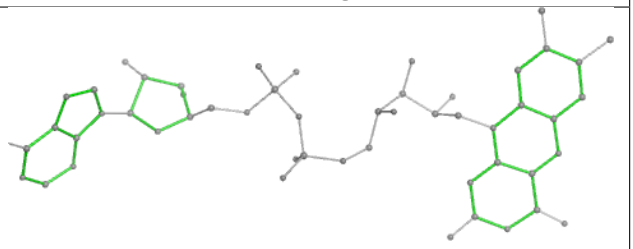
Bond lengths



Bond angles

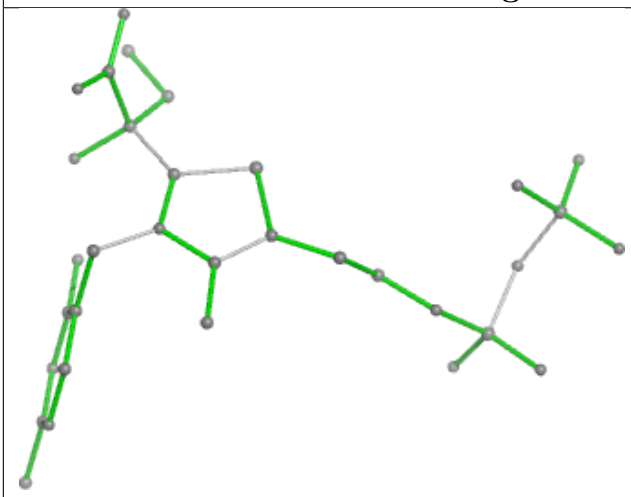


Torsions

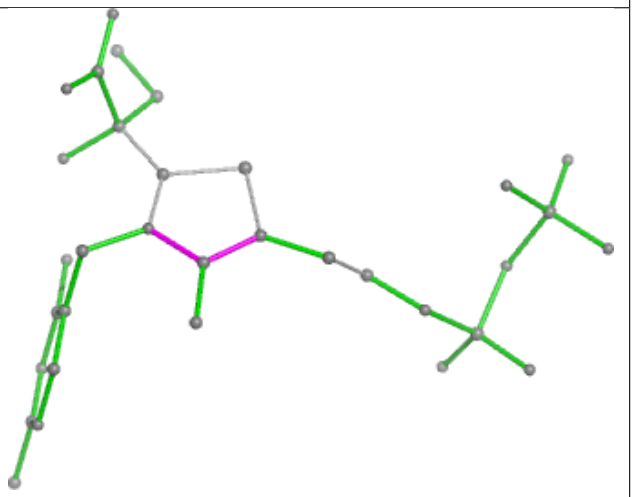


Rings

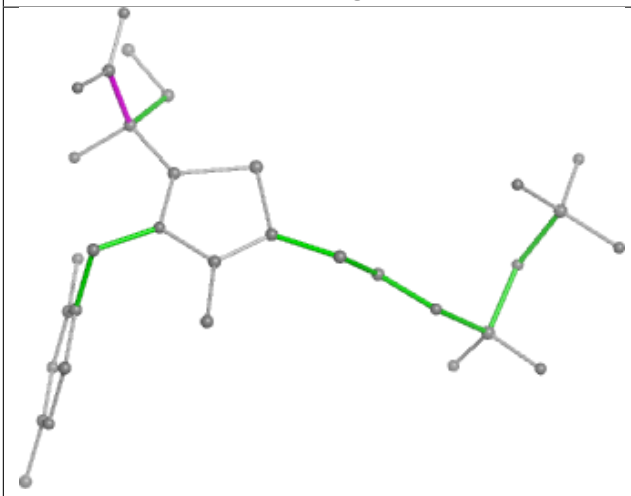
Ligand A1H2A A 703



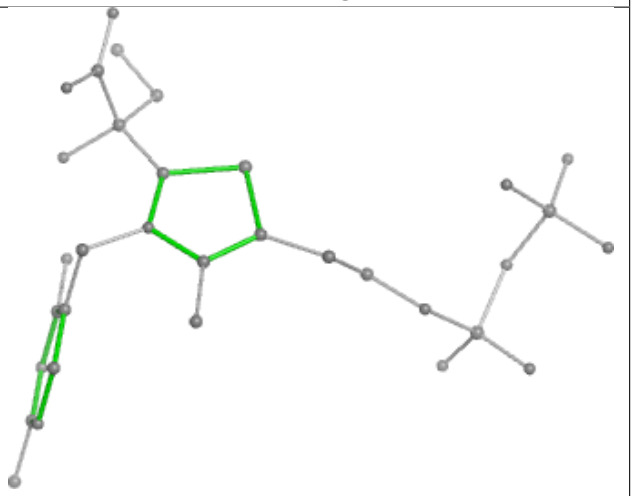
Bond lengths



Bond angles

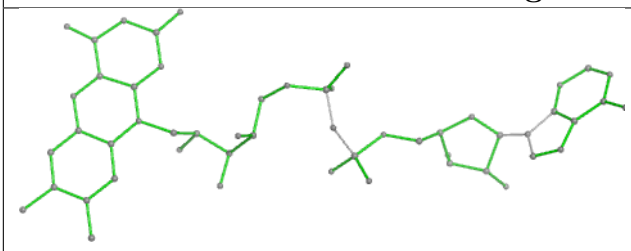


Torsions

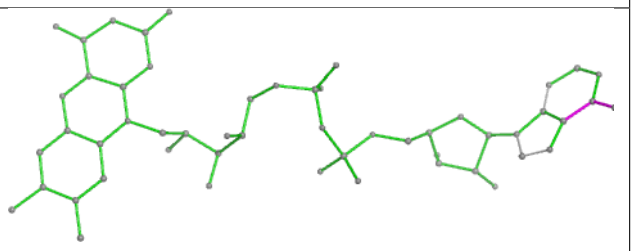


Rings

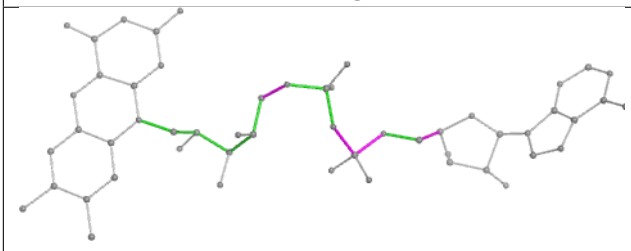
Ligand FAD C 701



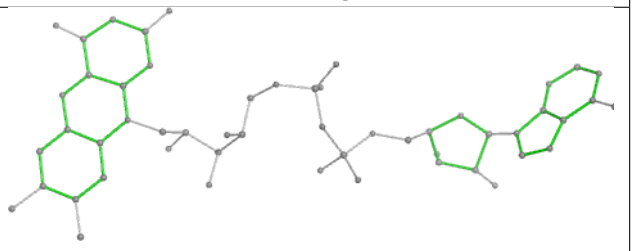
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	605/619 (97%)	0.58	17 (2%)	53	36	46, 66, 96, 124	0
1	B	599/619 (96%)	0.54	17 (2%)	53	36	50, 67, 89, 148	0
1	C	605/619 (97%)	0.54	18 (2%)	50	34	52, 66, 90, 135	0
1	D	608/619 (98%)	0.53	19 (3%)	49	32	49, 65, 92, 140	0
1	E	605/619 (97%)	0.53	21 (3%)	44	29	50, 67, 95, 151	0
1	F	520/619 (84%)	0.78	48 (9%)	9	5	54, 84, 121, 146	0
All	All	3542/3714 (95%)	0.58	140 (3%)	38	25	46, 68, 103, 151	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	590	ILE	6.0
1	F	254	LEU	5.0
1	F	267	VAL	4.7
1	E	572	SER	4.5
1	F	275	PHE	4.1
1	F	419	PHE	4.1
1	F	583	LEU	4.1
1	F	593	ASP	3.9
1	E	610	LEU	3.8
1	F	398	ASP	3.8
1	D	347	ALA	3.8
1	B	348	ASP	3.7
1	F	299	LEU	3.6
1	F	3	ASP	3.5
1	F	482	PHE	3.5
1	F	253	MET	3.4
1	A	207	LEU	3.4
1	F	586	LEU	3.4
1	E	573	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	564	PHE	3.4
1	A	236	LEU	3.3
1	A	600	ILE	3.3
1	F	324	ARG	3.3
1	C	610	LEU	3.3
1	F	585	ASP	3.2
1	D	242	SER	3.2
1	A	610	LEU	3.2
1	F	265	ALA	3.2
1	F	582	PRO	3.2
1	A	593	ASP	3.1
1	F	291	ALA	3.1
1	C	585	ASP	3.0
1	F	295	ILE	3.0
1	F	595	LEU	3.0
1	F	416	VAL	3.0
1	F	568	LEU	2.9
1	D	571	VAL	2.9
1	D	305	LEU	2.9
1	D	348	ASP	2.9
1	C	232	LEU	2.9
1	B	4	ASN	2.8
1	D	438	LEU	2.8
1	A	242	SER	2.8
1	B	346	ALA	2.8
1	F	411	LEU	2.7
1	B	549	THR	2.7
1	F	219	TRP	2.7
1	F	266	GLY	2.7
1	C	453	VAL	2.7
1	F	279	ASN	2.7
1	C	521	LEU	2.7
1	E	453	VAL	2.7
1	A	210	LEU	2.6
1	F	484	PHE	2.6
1	E	380	GLU	2.6
1	B	211	ALA	2.6
1	E	238	GLU	2.6
1	B	262	PHE	2.6
1	F	456	LEU	2.5
1	F	548	HIS	2.5
1	B	244	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	439	PRO	2.5
1	C	285	ALA	2.5
1	F	501	LYS	2.5
1	D	472	MET	2.5
1	A	284	LEU	2.5
1	E	438	LEU	2.5
1	E	578	LEU	2.4
1	F	210	LEU	2.4
1	C	545	VAL	2.4
1	E	579	VAL	2.4
1	E	241	GLY	2.4
1	A	438	LEU	2.4
1	E	570	VAL	2.3
1	E	54	GLN	2.3
1	B	563	LEU	2.3
1	A	518	PHE	2.3
1	D	142	LYS	2.3
1	A	194	TYR	2.3
1	D	237	LEU	2.3
1	A	240	LEU	2.3
1	F	379	PRO	2.3
1	D	41	ARG	2.3
1	B	553	ILE	2.3
1	A	367	GLU	2.3
1	F	182	THR	2.3
1	B	347	ALA	2.3
1	D	601	GLY	2.3
1	F	277	LEU	2.3
1	B	438	LEU	2.2
1	E	472[A]	MET	2.2
1	F	4	ASN	2.2
1	D	150	LEU	2.2
1	D	254	LEU	2.2
1	B	295	ILE	2.2
1	C	481	LEU	2.2
1	F	466	LEU	2.2
1	C	218	LEU	2.2
1	C	236	LEU	2.2
1	A	573	ARG	2.2
1	D	389	MET	2.2
1	C	563	LEU	2.2
1	F	479	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	284	LEU	2.2
1	B	444	VAL	2.2
1	C	194	TYR	2.2
1	D	220	LEU	2.2
1	E	150	LEU	2.2
1	F	531[A]	GLN	2.2
1	F	528	PRO	2.1
1	A	57	CYS	2.1
1	C	380	GLU	2.1
1	F	280	SER	2.1
1	F	412	SER	2.1
1	B	456	LEU	2.1
1	C	74	LEU	2.1
1	E	220	LEU	2.1
1	D	610	LEU	2.1
1	F	469	LEU	2.1
1	B	479	ILE	2.1
1	E	383	ILE	2.1
1	C	586	LEU	2.1
1	D	195	LEU	2.1
1	E	521	LEU	2.1
1	F	333	ALA	2.1
1	D	564	PHE	2.1
1	E	323	LYS	2.1
1	F	268	TYR	2.1
1	E	254	LEU	2.1
1	A	437	GLY	2.1
1	F	226	LEU	2.0
1	C	571	VAL	2.0
1	B	583	LEU	2.0
1	E	122	GLN	2.0
1	F	229	GLY	2.0
1	C	240	LEU	2.0
1	F	555	GLU	2.0
1	D	3	ASP	2.0
1	C	268	TYR	2.0
1	B	240	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)

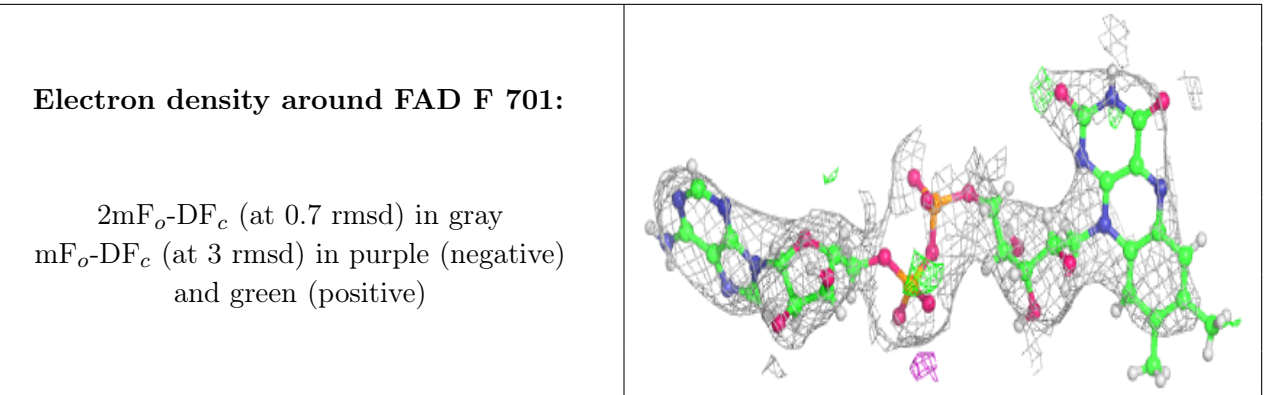
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MG	F	702	1/1	0.78	0.21	85,85,85,85	0
3	MG	C	702	1/1	0.85	0.16	60,60,60,60	0
5	PGE	D	703	10/10	0.86	0.23	78,94,97,100	0
3	MG	A	702	1/1	0.89	0.21	71,71,71,71	0
3	MG	D	702	1/1	0.90	0.29	68,68,68,68	0
2	FAD	F	701	53/53	0.93	0.26	80,94,111,115	0
3	MG	E	702	1/1	0.94	0.28	75,75,75,75	0
4	A1H2A	D	704	33/33	0.95	0.22	59,61,66,67	0
4	A1H2A	F	703	33/33	0.95	0.21	68,77,83,86	0
4	A1H2A	C	703	33/33	0.95	0.21	60,64,69,70	0
4	A1H2A	B	703	33/33	0.96	0.22	61,65,67,68	0
2	FAD	C	701	53/53	0.96	0.23	55,61,73,76	0
3	MG	B	702	1/1	0.96	0.18	67,67,67,67	0
4	A1H2A	E	703	33/33	0.96	0.21	62,65,69,71	0
2	FAD	B	701	53/53	0.96	0.21	57,60,72,76	0
4	A1H2A	A	703	33/33	0.96	0.20	61,66,68,69	0
2	FAD	E	701	53/53	0.97	0.23	55,58,71,73	0
2	FAD	A	701	53/53	0.97	0.21	54,57,69,71	0
2	FAD	D	701	53/53	0.97	0.23	56,60,71,73	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.

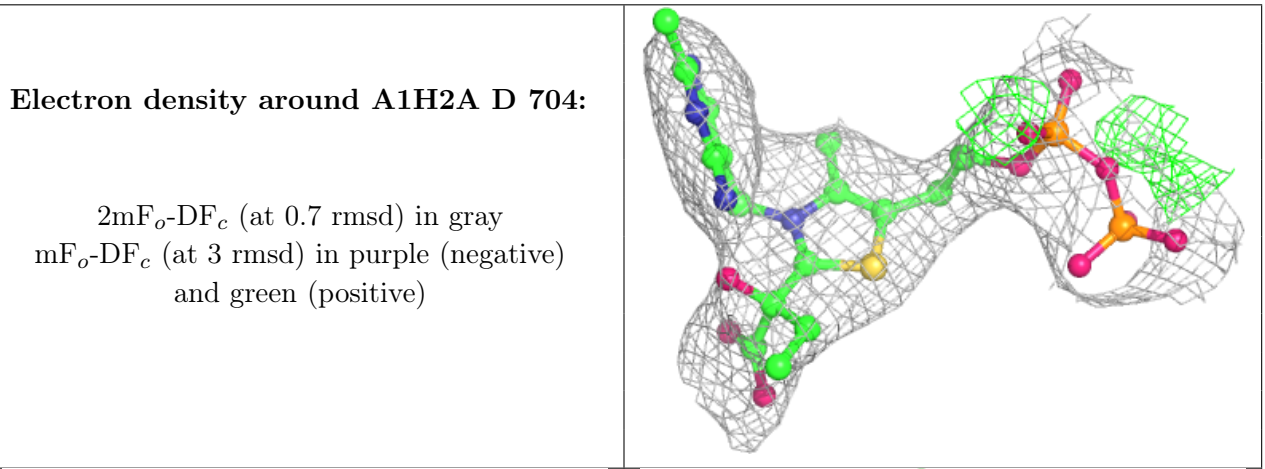
Electron density around FAD F 701:

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



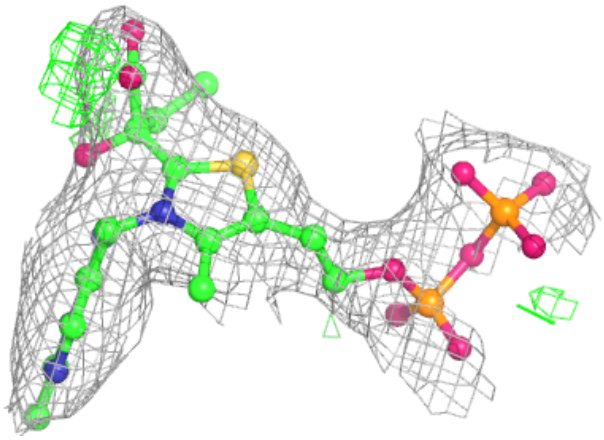
Electron density around A1H2A D 704:

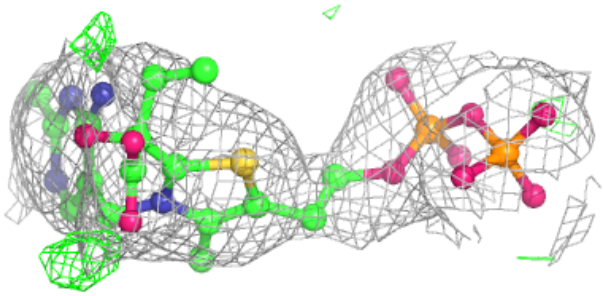
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

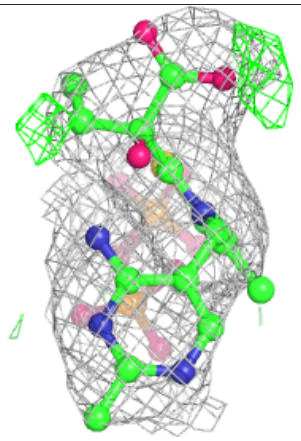


Electron density around A1H2A F 703:

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

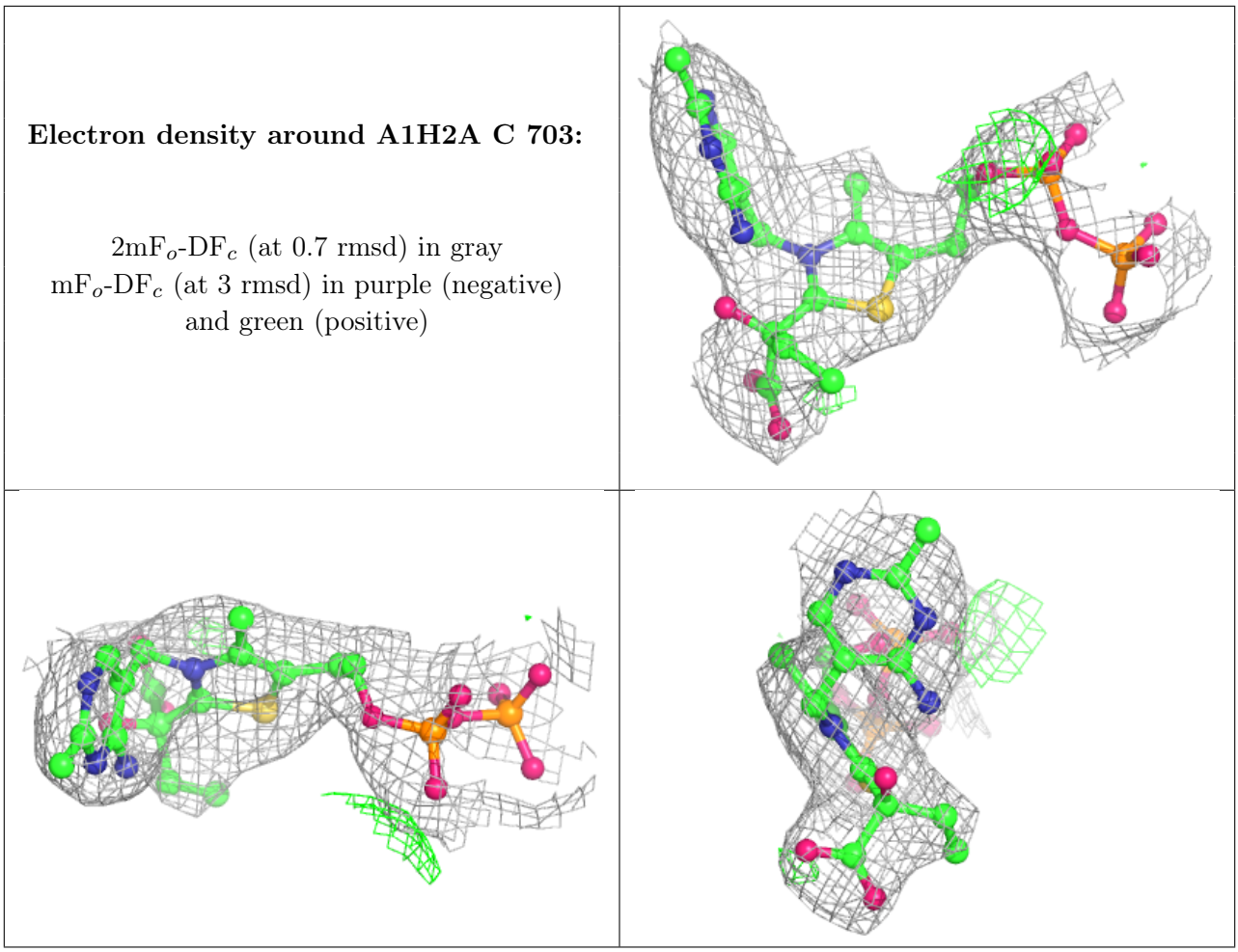






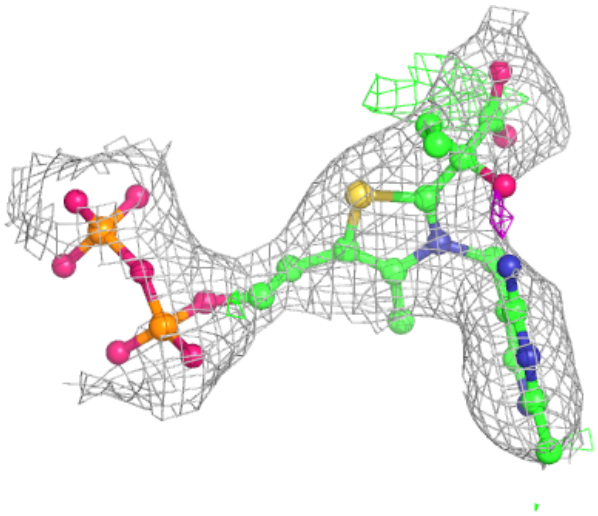
Electron density around A1H2A C 703:

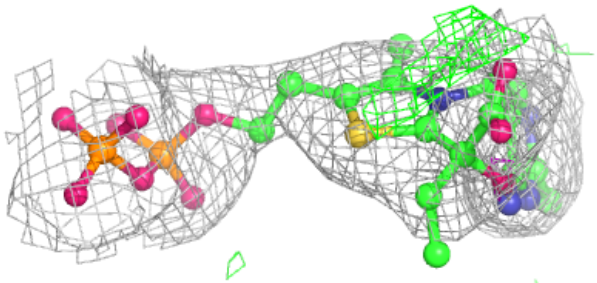
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

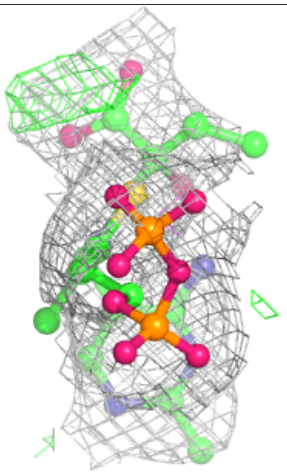


Electron density around A1H2A B 703:

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

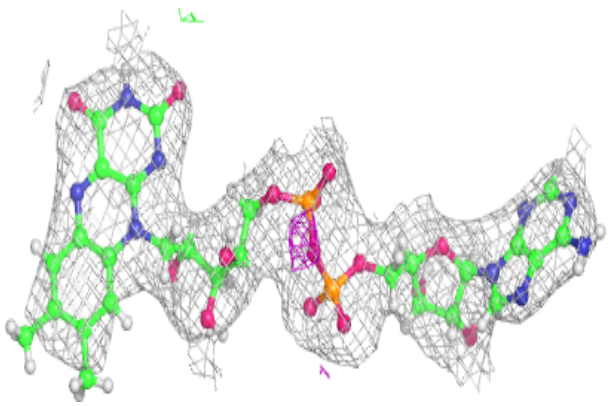


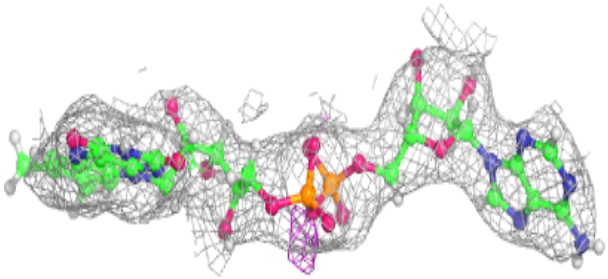


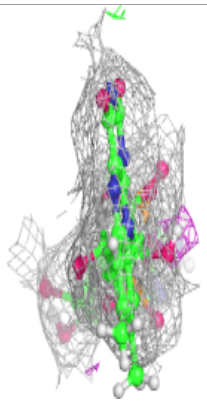


Electron density around FAD C 701:

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

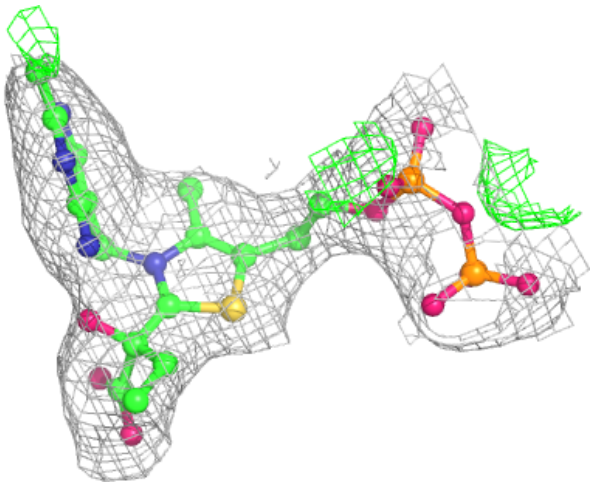


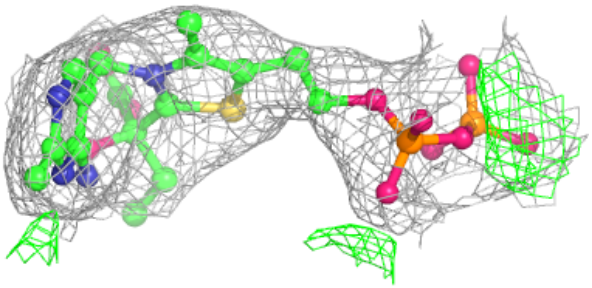


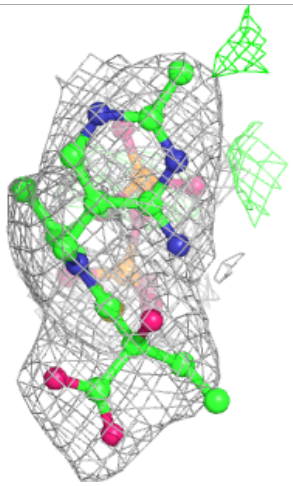


Electron density around A1H2A E 703:

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

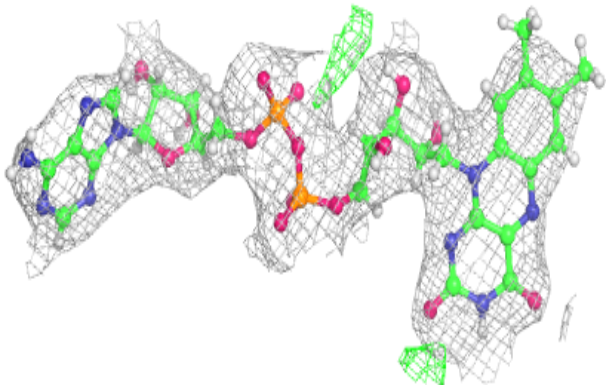


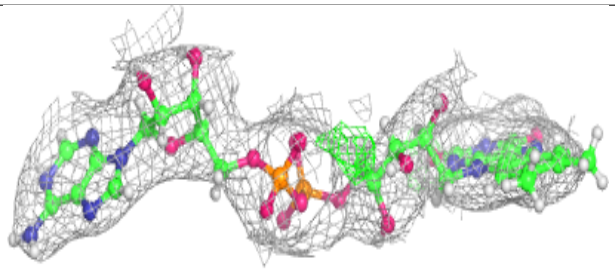


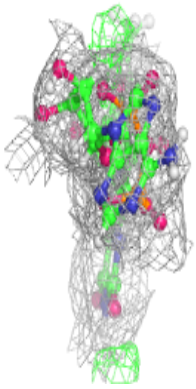


Electron density around FAD B 701:

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

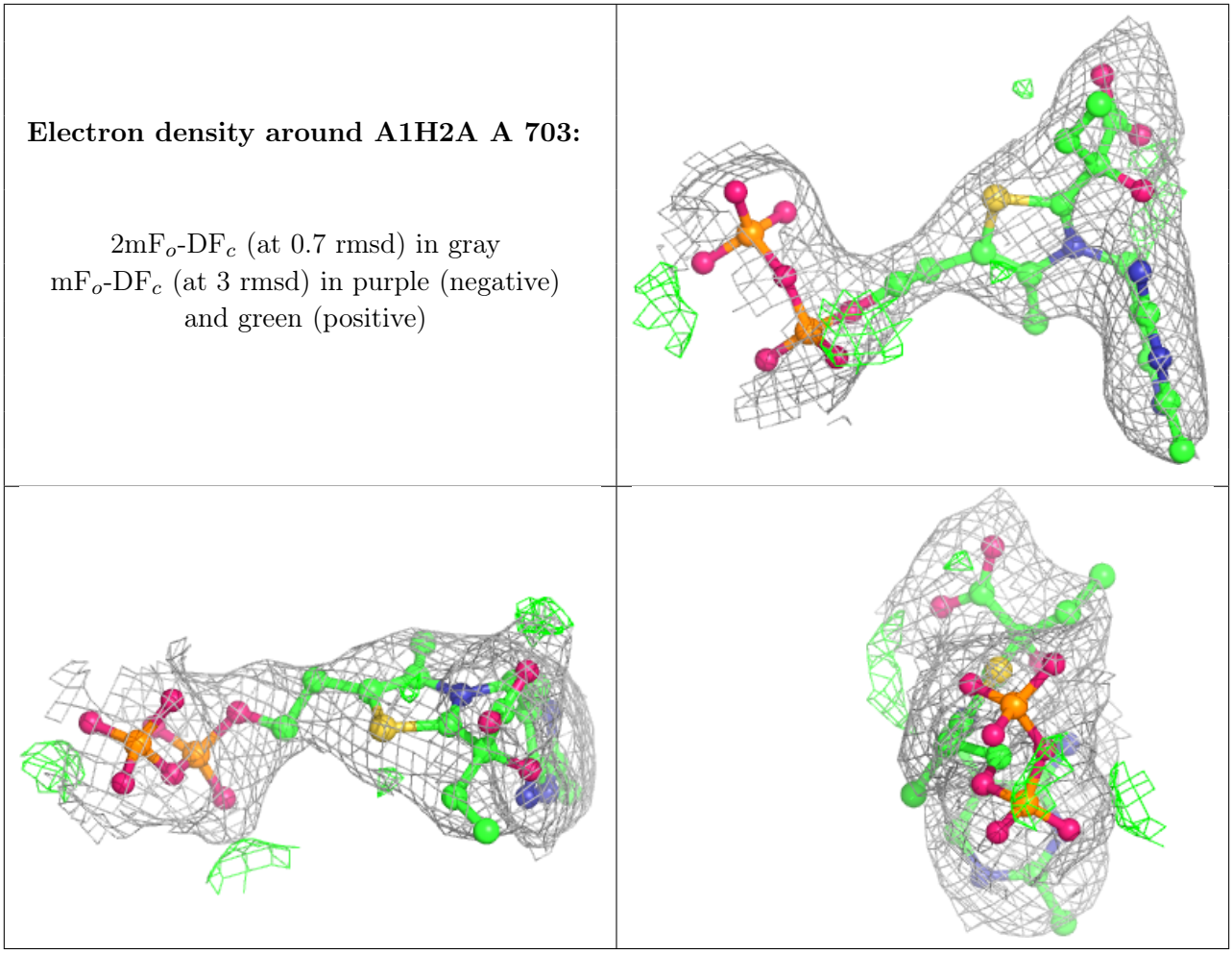






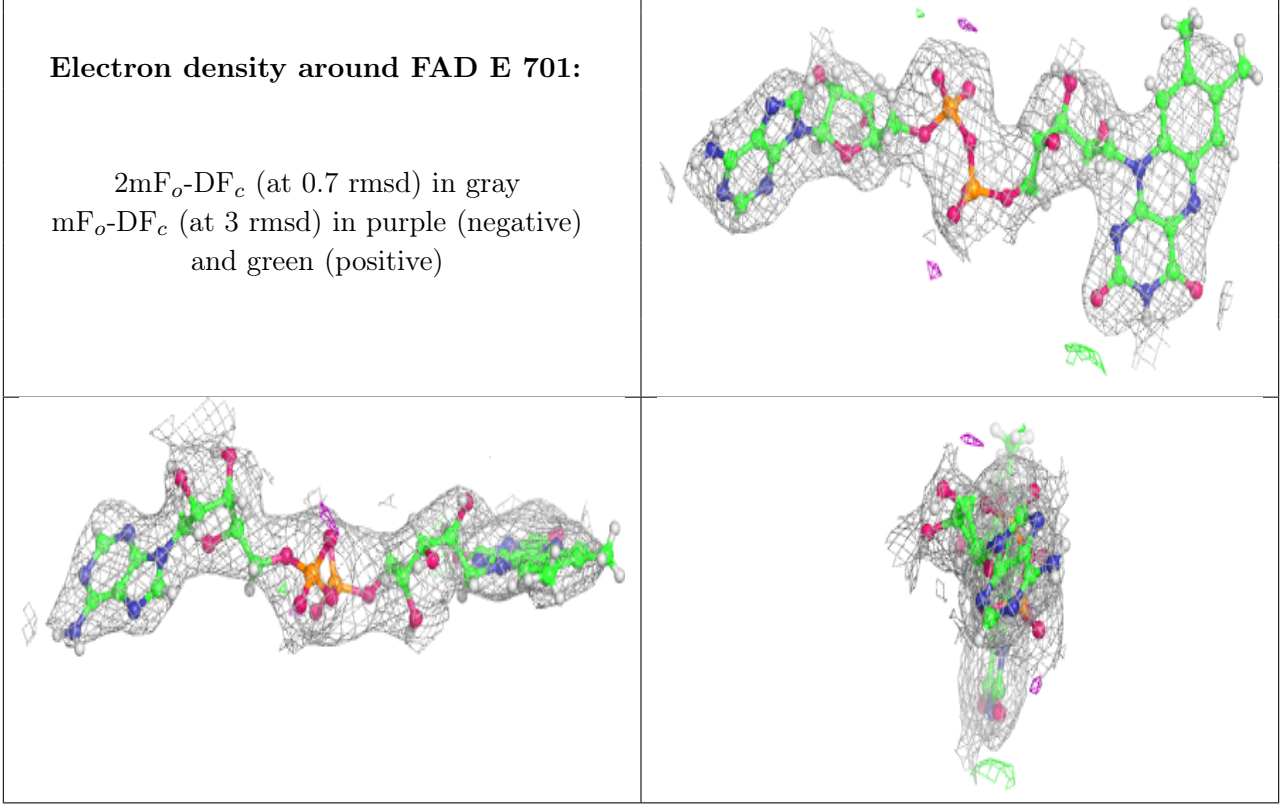
Electron density around A1H2A A 703:

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



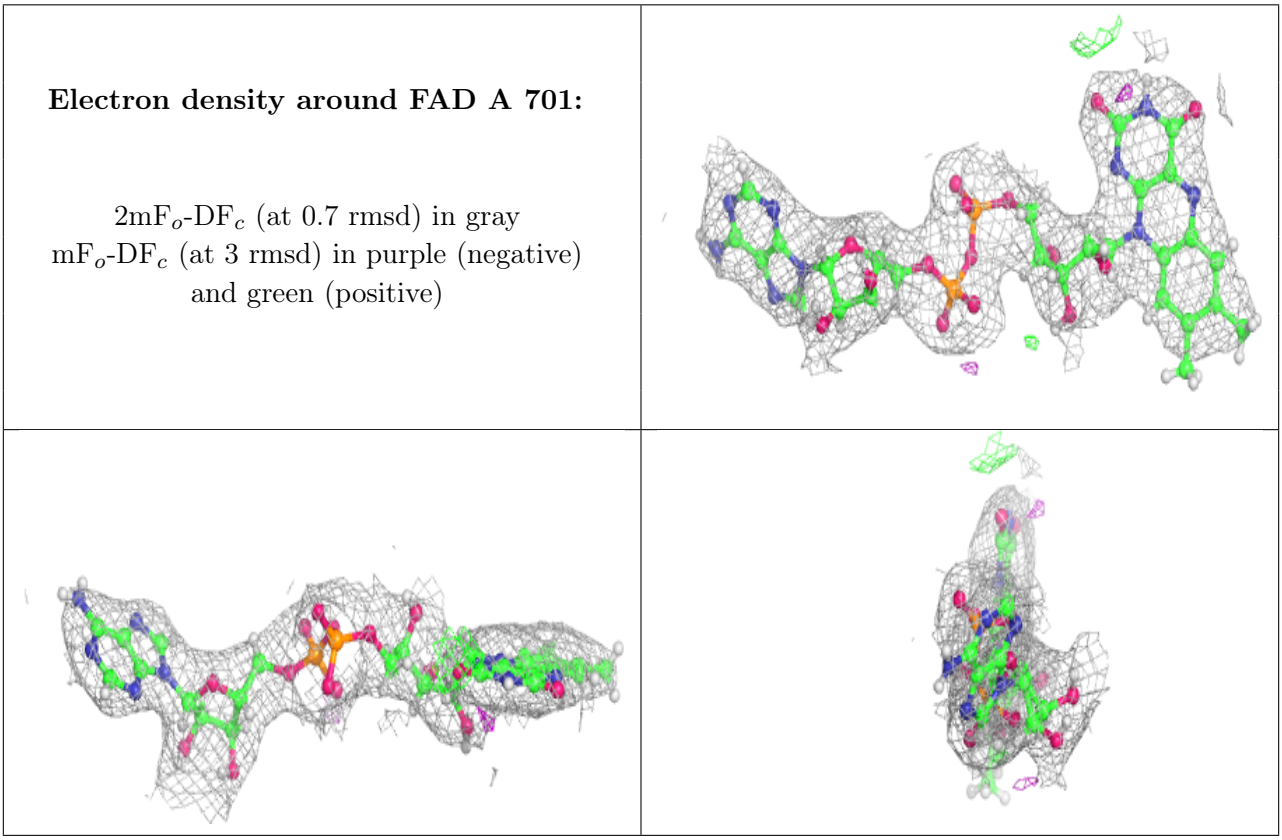
Electron density around FAD E 701:

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



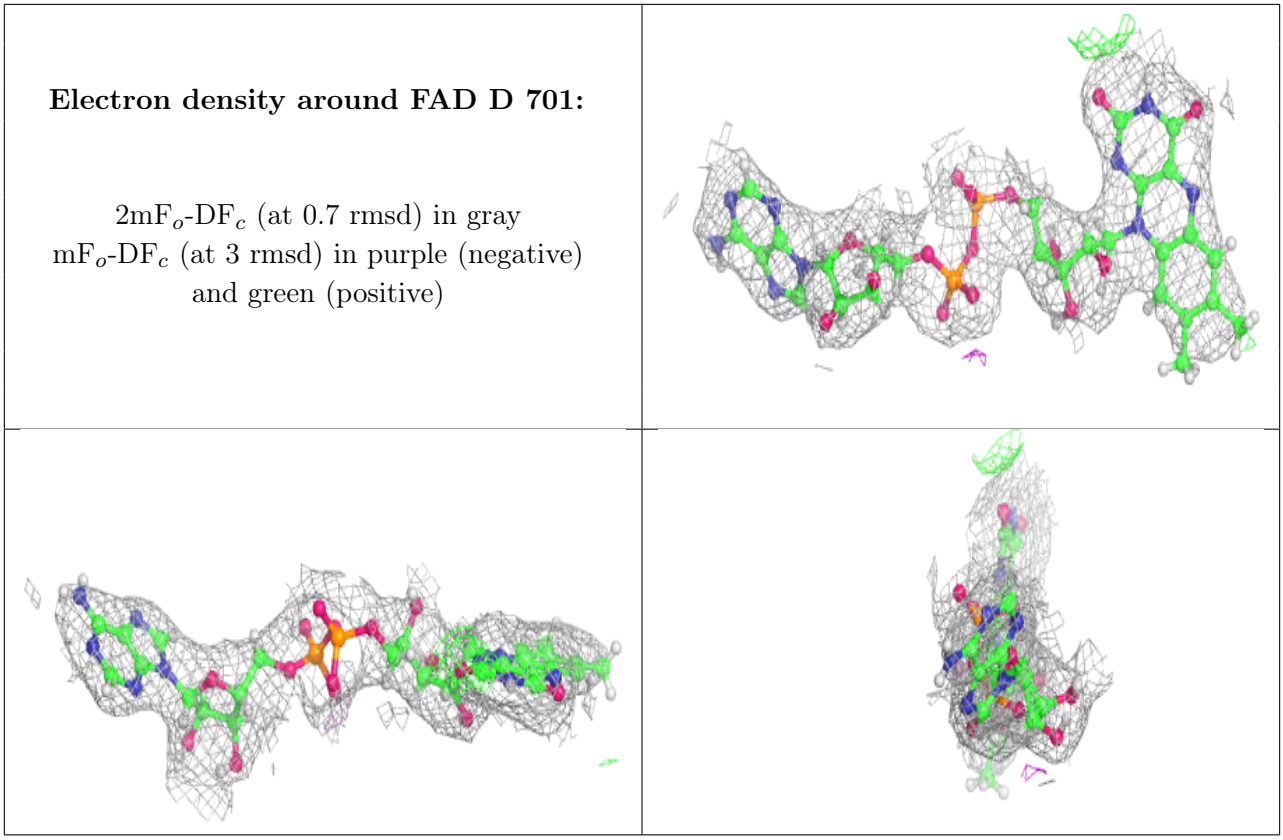
Electron density around FAD A 701:

$2mF_o$-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 701:

$2mF_o$-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.