Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:23 am BST

PDB ID	:	5MOG
Title	:	Oryza sativa phytoene desaturase inhibited by norflurazon
Authors	:	Brausemann, A.; Gemmecker, S.; Koschmieder, J.; Beyer, P.; Einsle, O.
Deposited on	:	2016-12-14
Resolution	:	2.77 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 following versions of software and data (see references ⓘ) were used in the production of this report:

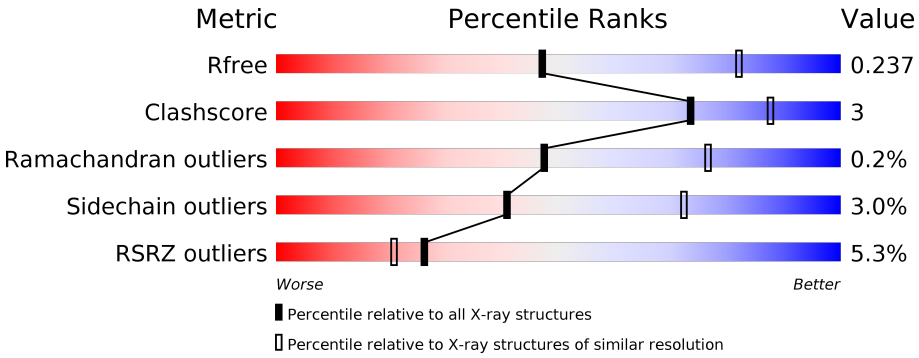
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 on 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	497	85% 9% 6%
1	B	497	% 86% 9% • 5%
1	C	497	% 86% 8% 5%
1	D	497	2% 86% 8% 5%
1	E	497	21% 82% 11% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IMD	D	603	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19520 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 Phytoene dehydrogenase, chloroplastic/chromoplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3703	2388	618	677	20			
1	B	472	Total	C	N	O	S	0	1	0
			3757	2419	631	687	20			
1	C	470	Total	C	N	O	S	0	1	0
			3736	2408	626	682	20			
1	D	470	Total	C	N	O	S	0	0	0
			3728	2403	623	682	20			
1	E	466	Total	C	N	O	S	0	0	0
			3692	2380	616	676	20			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	579	HIS	-	expression tag	UNP A2XDA1
A	580	HIS	-	expression tag	UNP A2XDA1
A	581	HIS	-	expression tag	UNP A2XDA1
A	582	HIS	-	expression tag	UNP A2XDA1
A	583	HIS	-	expression tag	UNP A2XDA1
A	584	HIS	-	expression tag	UNP A2XDA1
B	579	HIS	-	expression tag	UNP A2XDA1
B	580	HIS	-	expression tag	UNP A2XDA1
B	581	HIS	-	expression tag	UNP A2XDA1
B	582	HIS	-	expression tag	UNP A2XDA1
B	583	HIS	-	expression tag	UNP A2XDA1
B	584	HIS	-	expression tag	UNP A2XDA1
C	579	HIS	-	expression tag	UNP A2XDA1
C	580	HIS	-	expression tag	UNP A2XDA1
C	581	HIS	-	expression tag	UNP A2XDA1
C	582	HIS	-	expression tag	UNP A2XDA1
C	583	HIS	-	expression tag	UNP A2XDA1
C	584	HIS	-	expression tag	UNP A2XDA1
D	579	HIS	-	expression tag	UNP A2XDA1

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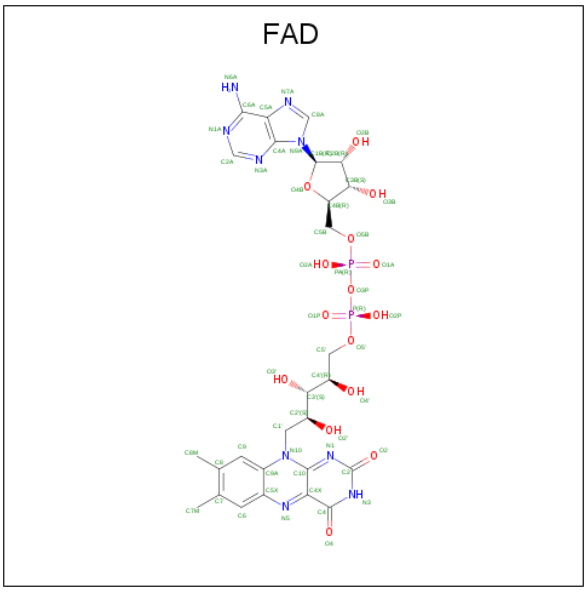
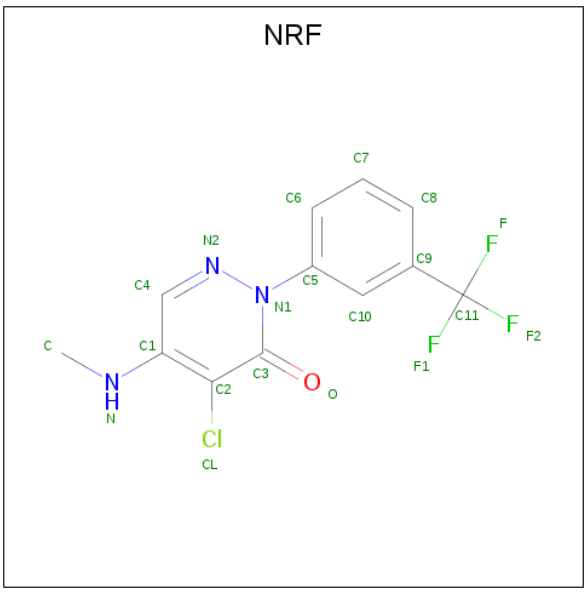
Chain	Residue	Modelled	Actual	Comment	Reference
D	580	HIS	-	expression tag	UNP A2XDA1
D	581	HIS	-	expression tag	UNP A2XDA1
D	582	HIS	-	expression tag	UNP A2XDA1
D	583	HIS	-	expression tag	UNP A2XDA1
D	584	HIS	-	expression tag	UNP A2XDA1
E	579	HIS	-	expression tag	UNP A2XDA1
E	580	HIS	-	expression tag	UNP A2XDA1
E	581	HIS	-	expression tag	UNP A2XDA1
E	582	HIS	-	expression tag	UNP A2XDA1
E	583	HIS	-	expression tag	UNP A2XDA1
E	584	HIS	-	expression tag	UNP A2XDA1

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



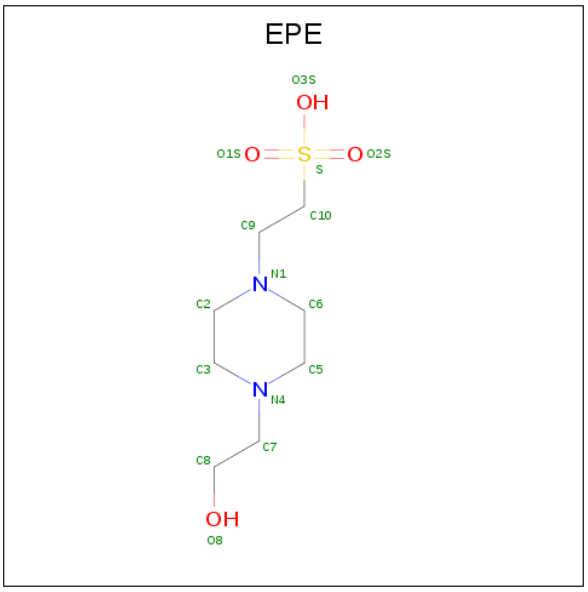
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is Norflurazon (three-letter code: NRF) (formula: $C_{12}H_9ClF_3N_3O$).



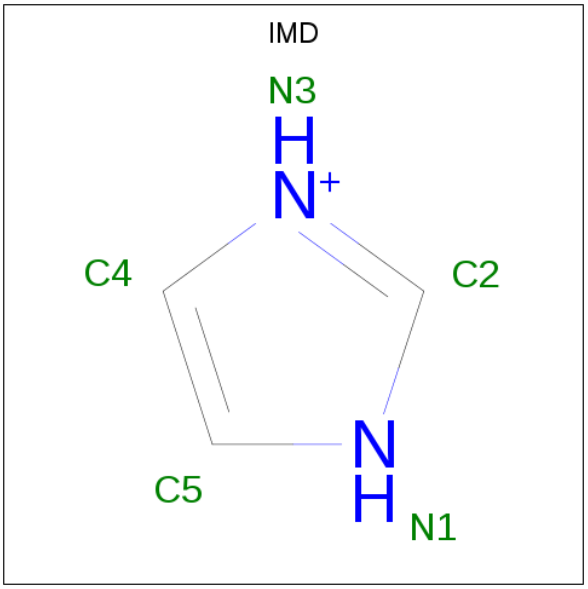
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		
3	B	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		
3	C	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		
3	D	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		
3	E	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



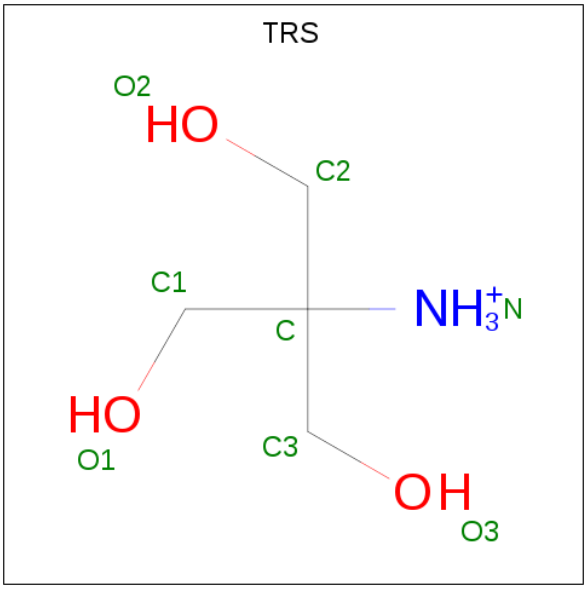
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 8 4 1 3	0	0
6	D	1	Total C N O 8 4 1 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	144	Total O 144 144	0	0

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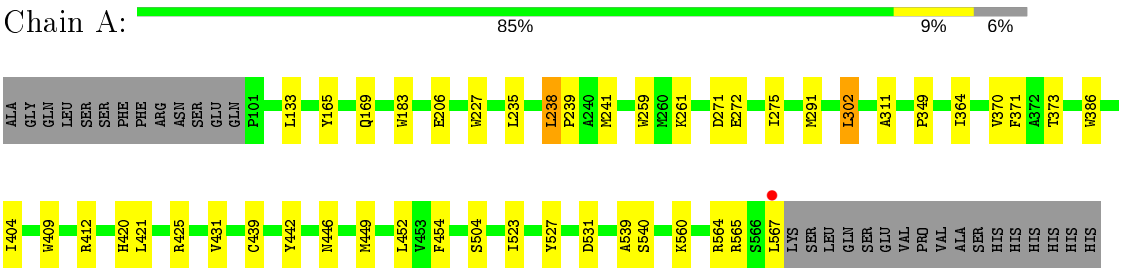
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	139	Total O 139 139	0	0
7	C	62	Total O 62 62	0	0
7	D	62	Total O 62 62	0	0
7	E	11	Total O 11 11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

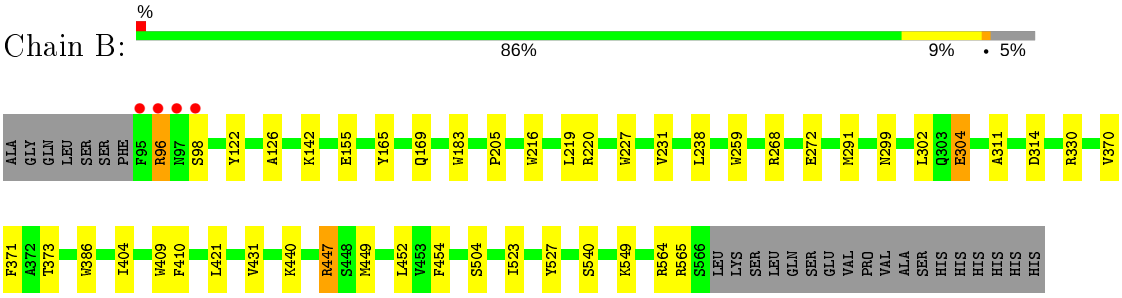
- Molecule 1: Phytoene dehydrogenase, chloroplastic/chromoplastic

Chain A:



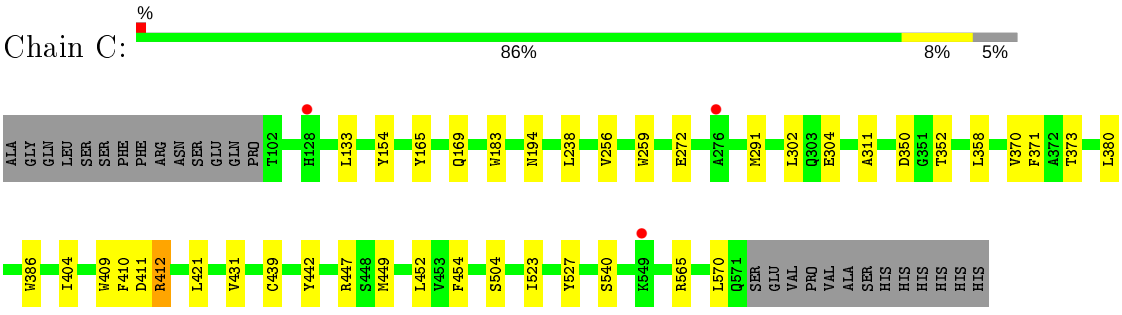
- Molecule 1: Phytoene dehydrogenase, chloroplastic/chromoplastic

Chain B:



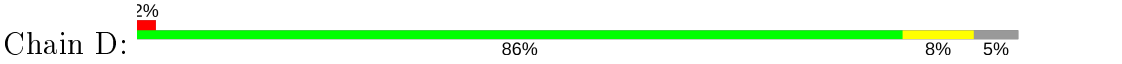
- Molecule 1: Phytoene dehydrogenase, chloroplastic/chromoplastic

Chain C:



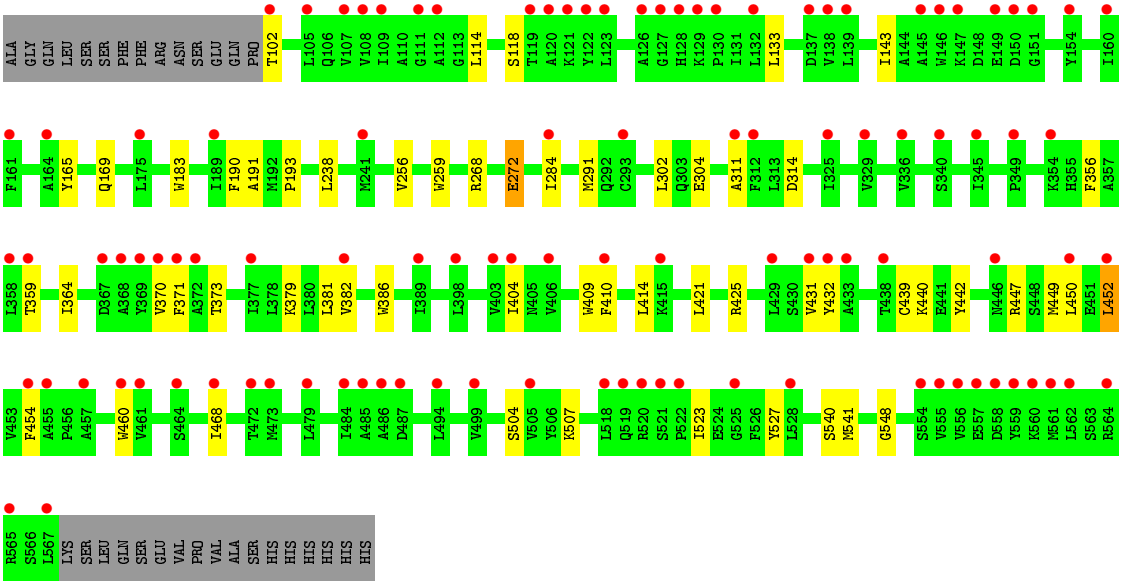
- Molecule 1: Phytoene dehydrogenase, chloroplastic/chromoplastic

Chain D:



• Molecule 1: Phytoene dehydrogenase, chloroplastic/chromoplastic

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	230.21Å 230.21Å 179.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.25 – 2.77 60.15 – 2.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.25-2.77) 100.0 (60.15-2.77)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.77Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.209 , 0.224 0.217 , 0.237	Depositor DCC
R_{free} test set	5852 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19520	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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: TRS, EPE, IMD, FAD, NRF

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	0.41	0/3794	0.62	0/5141
1	B	0.42	0/3852	0.62	0/5218
1	C	0.42	0/3829	0.61	0/5186
1	D	0.41	0/3818	0.62	0/5172
1	E	0.42	0/3782	0.62	0/5126
All	All	0.41	0/19075	0.62	0/25843

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	3703	0	3718	22	0
1	B	3757	0	3766	29	0
1	C	3736	0	3760	24	0
1	D	3728	0	3747	18	0
1	E	3692	0	3699	39	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	53	0	31	0	0
2	E	53	0	31	0	0
3	A	20	0	0	1	0
3	B	20	0	0	1	0
3	C	20	0	0	1	0
3	D	20	0	0	1	0
3	E	20	0	0	1	0
4	A	30	0	34	1	0
4	B	30	0	34	0	0
4	E	15	0	17	1	0
5	A	5	0	5	0	0
5	B	10	0	10	0	0
5	D	15	0	15	0	0
6	B	8	0	12	3	0
6	D	8	0	12	1	0
7	A	144	0	0	0	0
7	B	139	0	0	2	0
7	C	62	0	0	0	0
7	D	62	0	0	0	0
7	E	11	0	0	0	0
All	All	19520	0	18984	125	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 3.

All (125) 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:432:TYR:HB2	1:E:452:LEU:HD22	1.46	0.96
1:E:193:PRO:HD3	1:E:425:ARG:HH11	1.47	0.79
1:B:330:ARG:HH12	6:B:604:TRS:H12	1.47	0.78
1:A:238:LEU:HD22	1:B:216:TRP:CH2	2.23	0.73
1:E:272:GLU:HG3	1:E:425:ARG:NH2	2.05	0.72
1:E:432:TYR:HB2	1:E:452:LEU:CD2	2.22	0.69
1:E:193:PRO:HD3	1:E:425:ARG:NH1	2.08	0.67
1:E:450:LEU:HB3	1:E:452:LEU:HD21	1.77	0.67
1:E:256:VAL:HA	1:E:291:MET:HE1	1.79	0.65
1:D:215:ILE:O	1:D:219:LEU:HD13	1.98	0.63
1:B:219:LEU:HD22	1:B:227:TRP:HH2	1.64	0.63
1:C:256:VAL:HA	1:C:291:MET:CE	2.28	0.63
1:A:560:LYS:HB3	1:C:380:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:VAL:HA	1:E:291:MET:CE	2.28	0.63
1:E:191:ALA:O	1:E:425:ARG:HD3	1.99	0.62
1:E:114:LEU:HD11	1:E:541:MET:HE3	1.82	0.61
1:C:256:VAL:HG13	1:C:291:MET:HE1	1.82	0.60
1:E:190:PHE:HB3	1:E:425:ARG:HD2	1.84	0.60
1:B:330:ARG:HH22	6:B:604:TRS:H31	1.68	0.59
1:E:432:TYR:CB	1:E:452:LEU:HD22	2.27	0.59
1:D:330:ARG:HH12	6:D:602:TRS:H21	1.68	0.58
1:E:256:VAL:HG13	1:E:291:MET:HE1	1.86	0.57
1:B:96:ARG:HG2	1:B:122:TYR:O	2.04	0.56
1:B:142:LYS:HE3	7:B:726:HOH:O	2.06	0.56
1:E:143:ILE:HG21	1:E:541:MET:HE3	1.88	0.56
1:E:259:TRP:HB3	1:E:291:MET:HE2	1.88	0.56
1:C:352:THR:HG21	1:C:565:ARG:HH12	1.72	0.55
1:C:256:VAL:HA	1:C:291:MET:HE1	1.88	0.55
1:E:259:TRP:HB3	1:E:291:MET:CE	2.38	0.54
1:C:259:TRP:HB3	1:C:291:MET:CE	2.38	0.53
1:D:201:ARG:HD2	1:D:203:ASP:OD1	2.08	0.53
1:B:165:TYR:O	1:B:169:GLN:HG2	2.09	0.53
1:A:349:PRO:HB3	1:C:154:TYR:CE1	2.44	0.52
1:B:231:VAL:HG11	4:E:602:EPE:H71	1.91	0.52
1:B:96:ARG:HG3	1:B:126:ALA:HB2	1.92	0.52
1:B:219:LEU:HD22	1:B:227:TRP:CH2	2.45	0.51
1:B:410:PHE:O	1:B:447:ARG:HG2	2.10	0.51
1:A:239:PRO:HG2	1:B:220[A]:ARG:HH22	1.75	0.51
1:D:410:PHE:O	1:D:447:ARG:HG2	2.10	0.51
1:E:118:SER:OG	1:E:548:GLY:HA3	2.10	0.51
1:D:165:TYR:O	1:D:169:GLN:HG2	2.10	0.51
1:C:256:VAL:HA	1:C:291:MET:HE2	1.92	0.51
1:A:165:TYR:O	1:A:169:GLN:HG2	2.11	0.51
1:C:350:ASP:OD1	1:C:352:THR:HG22	2.10	0.50
1:C:165:TYR:O	1:C:169:GLN:HG2	2.11	0.50
1:E:460:TRP:HB3	1:E:468:ILE:HD11	1.94	0.50
1:E:165:TYR:O	1:E:169:GLN:HG2	2.11	0.50
1:A:227:TRP:HB2	4:A:603:EPE:H92	1.94	0.49
1:A:238:LEU:HB3	1:B:216:TRP:CZ2	2.49	0.48
1:E:414:LEU:CD1	1:E:450:LEU:HD11	2.42	0.48
1:A:133:LEU:HD11	1:A:364:ILE:HG21	1.95	0.48
1:A:404:ILE:HB	1:A:454:PHE:HB3	1.96	0.48
1:B:219:LEU:CD2	1:B:227:TRP:CH2	2.97	0.48
1:B:96:ARG:HH22	1:B:549:LYS:HG2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ARG:NH1	6:B:604:TRS:H12	2.24	0.48
1:E:314:ASP:HB2	1:E:440:LYS:HE2	1.96	0.47
1:E:404:ILE:HB	1:E:454:PHE:HB3	1.96	0.47
1:B:404:ILE:HB	1:B:454:PHE:HB3	1.95	0.47
1:E:193:PRO:CD	1:E:425:ARG:NH1	2.76	0.47
1:B:314:ASP:HB2	1:B:440:LYS:HE2	1.97	0.47
1:D:404:ILE:HB	1:D:454:PHE:HB3	1.96	0.47
1:C:409:TRP:CE2	1:C:449:MET:HG3	2.50	0.47
1:D:314:ASP:HB2	1:D:440:LYS:HE2	1.97	0.46
1:E:379:LYS:O	1:E:382:VAL:HG22	2.14	0.46
1:C:259:TRP:HB3	1:C:291:MET:HE2	1.97	0.46
1:D:409:TRP:CE2	1:D:449:MET:HG3	2.51	0.46
1:B:409:TRP:CE2	1:B:449:MET:HG3	2.51	0.46
1:C:404:ILE:HB	1:C:454:PHE:HB3	1.96	0.46
1:E:370:VAL:HG22	1:E:527:TYR:HB2	1.97	0.46
1:D:379:LYS:O	1:D:382:VAL:HG22	2.15	0.46
1:E:409:TRP:CE2	1:E:449:MET:HG3	2.51	0.46
1:C:370:VAL:HG22	1:C:527:TYR:HB2	1.98	0.45
1:A:241:MET:HB3	1:A:302:LEU:HD22	1.97	0.45
1:A:409:TRP:CE2	1:A:449:MET:HG3	2.51	0.45
1:D:370:VAL:HG22	1:D:527:TYR:HB2	1.98	0.45
1:B:370:VAL:HG22	1:B:527:TYR:HB2	1.98	0.45
1:C:259:TRP:HB3	1:C:291:MET:HE3	2.00	0.44
1:A:239:PRO:HB3	1:B:205:PRO:HB3	2.00	0.44
1:E:133:LEU:HD11	1:E:364:ILE:HG21	2.00	0.44
1:A:370:VAL:HG22	1:A:527:TYR:HB2	1.99	0.44
1:A:386:TRP:CZ2	1:A:523:ILE:HG21	2.53	0.43
1:B:386:TRP:CZ2	1:B:523:ILE:HG21	2.54	0.43
1:A:183:TRP:CE3	1:A:311:ALA:HB2	2.53	0.43
1:E:183:TRP:CE3	1:E:311:ALA:HB2	2.53	0.43
1:A:421:LEU:HD11	1:A:431:VAL:HB	2.01	0.42
1:C:421:LEU:HD11	1:C:431:VAL:HB	2.01	0.42
1:E:386:TRP:CZ2	1:E:523:ILE:HG21	2.54	0.42
1:C:183:TRP:CE3	1:C:311:ALA:HB2	2.54	0.42
1:A:235:LEU:HD23	1:B:216:TRP:CZ2	2.54	0.42
1:C:259:TRP:CG	1:C:291:MET:HG2	2.55	0.42
1:D:201:ARG:CD	1:D:203:ASP:OD1	2.66	0.42
1:D:540:SER:HB3	3:D:601:NRF:CL	2.56	0.42
1:C:540:SER:HB3	3:C:601:NRF:CL	2.56	0.42
1:E:256:VAL:HA	1:E:291:MET:HE2	2.01	0.42
1:A:439:CYS:HB3	1:A:442:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:540:SER:HB3	3:E:601:NRF:CL	2.57	0.42
1:E:272:GLU:CG	1:E:425:ARG:NH2	2.80	0.42
1:E:410:PHE:O	1:E:447:ARG:HG3	2.20	0.42
1:A:540:SER:HB3	3:A:601:NRF:CL	2.57	0.41
1:B:304:GLU:HG2	1:B:304:GLU:H	1.70	0.41
1:C:386:TRP:CZ2	1:C:523:ILE:HG21	2.55	0.41
1:D:421:LEU:HD11	1:D:431:VAL:HB	2.01	0.41
1:D:386:TRP:CZ2	1:D:523:ILE:HG21	2.55	0.41
1:B:155:GLU:HB3	7:B:758:HOH:O	2.19	0.41
1:B:183:TRP:CE3	1:B:311:ALA:HB2	2.54	0.41
1:D:531:ASP:HB2	1:D:539:ALA:HA	2.02	0.41
1:E:460:TRP:CE3	1:E:468:ILE:HD13	2.55	0.41
1:E:259:TRP:CG	1:E:291:MET:HG2	2.55	0.41
1:E:284:ILE:HG21	1:E:507:LYS:HE3	2.02	0.41
1:E:421:LEU:HD11	1:E:431:VAL:HB	2.01	0.41
1:B:540:SER:HB3	3:B:601:NRF:CL	2.58	0.41
1:D:271:ASP:HA	1:D:275:ILE:HG13	2.03	0.41
1:B:421:LEU:HD11	1:B:431:VAL:HB	2.01	0.41
1:E:439:CYS:HB3	1:E:442:TYR:HB2	2.03	0.41
1:A:531:ASP:HB2	1:A:539:ALA:HA	2.03	0.41
1:A:259:TRP:CG	1:A:291:MET:HG2	2.56	0.41
1:C:439:CYS:HB3	1:C:442:TYR:HB2	2.03	0.41
1:B:259:TRP:CG	1:B:291:MET:HG2	2.55	0.41
1:D:183:TRP:CE3	1:D:311:ALA:HB2	2.56	0.41
1:C:133:LEU:HD13	1:C:358:LEU:HD21	2.04	0.40
1:C:410:PHE:O	1:C:447[A]:ARG:HG3	2.21	0.40
1:C:411:ASP:OD1	1:C:412:ARG:HG2	2.21	0.40
1:D:284:ILE:HG21	1:D:507:LYS:HE3	2.03	0.40
1:A:271:ASP:HA	1:A:275:ILE:HG13	2.04	0.40
1:E:356:PHE:HB2	1:E:364:ILE:HG23	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	465/497 (94%)	449 (97%)	15 (3%)	1 (0%)	47	76
1	B	471/497 (95%)	455 (97%)	15 (3%)	1 (0%)	47	76
1	C	469/497 (94%)	454 (97%)	14 (3%)	1 (0%)	47	76
1	D	468/497 (94%)	452 (97%)	15 (3%)	1 (0%)	47	76
1	E	464/497 (93%)	448 (97%)	15 (3%)	1 (0%)	47	76
All	All	2337/2485 (94%)	2258 (97%)	74 (3%)	5 (0%)	47	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	SER
1	B	504	SER
1	C	504	SER
1	E	504	SER
1	D	504	SER

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	400/427 (94%)	385 (96%)	15 (4%)	33	64
1	B	406/427 (95%)	392 (97%)	14 (3%)	37	68
1	C	404/427 (95%)	394 (98%)	10 (2%)	47	77
1	D	403/427 (94%)	392 (97%)	11 (3%)	44	75
1	E	398/427 (93%)	387 (97%)	11 (3%)	43	74
All	All	2011/2135 (94%)	1950 (97%)	61 (3%)	41	72

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	GLU
1	A	238	LEU
1	A	261	LYS
1	A	272	GLU
1	A	302	LEU
1	A	371	PHE
1	A	373	THR
1	A	412	ARG
1	A	420	HIS
1	A	425	ARG
1	A	446	ASN
1	A	452	LEU
1	A	564	ARG
1	A	565	ARG
1	A	567	LEU
1	B	96	ARG
1	B	98	SER
1	B	238	LEU
1	B	268	ARG
1	B	272	GLU
1	B	299	ASN
1	B	302	LEU
1	B	304	GLU
1	B	371	PHE
1	B	373	THR
1	B	447	ARG
1	B	452	LEU
1	B	564	ARG
1	B	565	ARG
1	C	194	ASN
1	C	238	LEU
1	C	272	GLU
1	C	302	LEU
1	C	304	GLU
1	C	371	PHE
1	C	373	THR
1	C	412	ARG
1	C	452	LEU
1	C	570	LEU
1	D	238	LEU
1	D	272	GLU
1	D	302	LEU
1	D	371	PHE

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Mol	Chain	Res	Type
1	D	373	THR
1	D	385	GLU
1	D	425	ARG
1	D	447	ARG
1	D	452	LEU
1	D	565	ARG
1	D	570	LEU
1	E	102	THR
1	E	238	LEU
1	E	268	ARG
1	E	272	GLU
1	E	302	LEU
1	E	304	GLU
1	E	359	THR
1	E	371	PHE
1	E	373	THR
1	E	381	LEU
1	E	452	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	299	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

23 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	$\#\|Z\| > 2$
6	TRS	D	602	-	7,7,7	0.23	0	9,9,9	0.23	0
4	EPE	E	602	-	15,15,15	1.08	1 (6%)	18,20,20	0.56	0
2	FAD	B	600	-	51,58,58	1.52	5 (9%)	60,89,89	2.17	7 (11%)
5	IMD	D	605	-	3,5,5	0.38	0	4,5,5	0.72	0
3	NRF	C	601	-	19,21,21	1.37	1 (5%)	24,31,31	1.31	3 (12%)
3	NRF	A	601	-	19,21,21	1.32	1 (5%)	24,31,31	1.28	3 (12%)
3	NRF	E	601	-	19,21,21	1.34	1 (5%)	24,31,31	1.29	3 (12%)
4	EPE	A	602	-	15,15,15	1.06	1 (6%)	18,20,20	0.25	0
4	EPE	B	602	-	15,15,15	1.26	1 (6%)	18,20,20	0.44	0
5	IMD	D	603	-	3,5,5	0.37	0	4,5,5	0.72	0
2	FAD	D	600	-	51,58,58	1.53	5 (9%)	60,89,89	2.18	7 (11%)
3	NRF	B	601	-	19,21,21	1.33	1 (5%)	24,31,31	1.35	3 (12%)
5	IMD	A	604	-	3,5,5	0.38	0	4,5,5	0.71	0
5	IMD	B	605	-	3,5,5	0.38	0	4,5,5	0.71	0
2	FAD	C	600	-	51,58,58	1.56	5 (9%)	60,89,89	2.18	7 (11%)
5	IMD	D	604	-	3,5,5	0.38	0	4,5,5	0.71	0
4	EPE	A	603	-	15,15,15	0.65	1 (6%)	18,20,20	0.32	0
5	IMD	B	606	-	3,5,5	0.39	0	4,5,5	0.70	0
2	FAD	A	600	-	51,58,58	1.49	5 (9%)	60,89,89	2.15	7 (11%)
4	EPE	B	603	-	15,15,15	1.13	1 (6%)	18,20,20	0.31	0
2	FAD	E	600	-	51,58,58	1.51	5 (9%)	60,89,89	2.17	7 (11%)
3	NRF	D	601	-	19,21,21	1.29	1 (5%)	24,31,31	1.29	3 (12%)
6	TRS	B	604	-	7,7,7	0.23	0	9,9,9	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TRS	D	602	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	E	602	-	-	5/9/19/19	0/1/1/1
2	FAD	B	600	-	-	6/30/50/50	0/6/6/6
5	IMD	D	605	-	-	-	0/1/1/1
3	NRF	C	601	-	-	0/12/12/12	0/2/2/2
3	NRF	A	601	-	-	0/12/12/12	0/2/2/2
3	NRF	E	601	-	-	0/12/12/12	0/2/2/2
4	EPE	A	602	-	-	8/9/19/19	0/1/1/1
4	EPE	B	602	-	-	5/9/19/19	0/1/1/1
5	IMD	D	603	-	-	-	0/1/1/1
5	IMD	A	604	-	-	-	0/1/1/1
3	NRF	B	601	-	-	0/12/12/12	0/2/2/2
2	FAD	D	600	-	-	7/30/50/50	0/6/6/6
5	IMD	B	605	-	-	-	0/1/1/1
2	FAD	C	600	-	-	8/30/50/50	0/6/6/6
5	IMD	D	604	-	-	-	0/1/1/1
4	EPE	A	603	-	-	4/9/19/19	0/1/1/1
5	IMD	B	606	-	-	-	0/1/1/1
2	FAD	A	600	-	-	7/30/50/50	0/6/6/6
4	EPE	B	603	-	-	1/9/19/19	0/1/1/1
2	FAD	E	600	-	-	7/30/50/50	0/6/6/6
3	NRF	D	601	-	-	0/12/12/12	0/2/2/2
6	TRS	B	604	-	-	0/9/9/9	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	FAD	C4X-C10	7.97	1.46	1.38
2	E	600	FAD	C4X-C10	7.70	1.46	1.38
2	D	600	FAD	C4X-C10	7.57	1.46	1.38
2	B	600	FAD	C4X-C10	7.56	1.46	1.38
2	A	600	FAD	C4X-C10	7.40	1.46	1.38
3	C	601	NRF	C4-C1	5.45	1.48	1.39
3	B	601	NRF	C4-C1	5.34	1.48	1.39
3	E	601	NRF	C4-C1	5.31	1.48	1.39
3	A	601	NRF	C4-C1	5.26	1.48	1.39
3	D	601	NRF	C4-C1	5.12	1.47	1.39
4	B	602	EPE	C10-S	-4.74	1.70	1.77
4	B	603	EPE	C10-S	-4.34	1.71	1.77
4	A	602	EPE	C10-S	-4.04	1.71	1.77
4	E	602	EPE	C10-S	-4.02	1.71	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	C4-C4X	3.49	1.47	1.41
2	B	600	FAD	C4-N3	3.46	1.39	1.33
2	C	600	FAD	C4-N3	3.43	1.39	1.33
2	D	600	FAD	C9A-N10	3.42	1.43	1.38
2	C	600	FAD	C4-C4X	3.42	1.47	1.41
2	B	600	FAD	C9A-N10	3.41	1.43	1.38
2	A	600	FAD	C4-N3	3.40	1.39	1.33
2	A	600	FAD	C9A-N10	3.39	1.43	1.38
2	D	600	FAD	C4-N3	3.38	1.38	1.33
2	E	600	FAD	C4-N3	3.37	1.38	1.33
2	E	600	FAD	C4-C4X	3.37	1.47	1.41
2	C	600	FAD	C9A-N10	3.32	1.43	1.38
2	A	600	FAD	C4-C4X	3.18	1.46	1.41
2	E	600	FAD	C9A-N10	3.02	1.42	1.38
2	B	600	FAD	C4-C4X	3.02	1.46	1.41
2	D	600	FAD	C5X-N5	2.66	1.39	1.35
2	B	600	FAD	C5X-N5	2.59	1.39	1.35
2	A	600	FAD	C5X-N5	2.55	1.39	1.35
2	C	600	FAD	C5X-N5	2.53	1.39	1.35
2	E	600	FAD	C5X-N5	2.40	1.39	1.35
4	A	603	EPE	C10-S	-2.25	1.74	1.77

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	FAD	C4-N3-C2	12.65	125.83	115.14
2	C	600	FAD	C4-N3-C2	12.63	125.80	115.14
2	E	600	FAD	C4-N3-C2	12.61	125.79	115.14
2	A	600	FAD	C4-N3-C2	12.61	125.79	115.14
2	D	600	FAD	C4-N3-C2	12.60	125.78	115.14
2	D	600	FAD	C4X-C4-N3	-6.95	113.93	123.43
2	E	600	FAD	C4X-C4-N3	-6.93	113.95	123.43
2	A	600	FAD	C4X-C4-N3	-6.92	113.97	123.43
2	C	600	FAD	C4X-C4-N3	-6.87	114.04	123.43
2	B	600	FAD	C4X-C4-N3	-6.81	114.12	123.43
3	B	601	NRF	C3-C2-CL	-4.45	115.15	120.65
3	C	601	NRF	C3-C2-CL	-4.34	115.29	120.65
3	E	601	NRF	C3-C2-CL	-4.26	115.39	120.65
3	A	601	NRF	C3-C2-CL	-4.25	115.41	120.65
2	D	600	FAD	C10-C4X-N5	4.22	124.17	121.26
2	B	600	FAD	C10-C4X-N5	4.21	124.17	121.26
2	C	600	FAD	C10-C4X-N5	4.18	124.15	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAD	C10-C4X-N5	4.07	124.08	121.26
3	D	601	NRF	C3-C2-CL	-4.06	115.64	120.65
2	E	600	FAD	C10-C4X-N5	4.03	124.04	121.26
2	B	600	FAD	C4-C4X-C10	-3.51	117.63	119.95
2	D	600	FAD	C4-C4X-C10	-3.49	117.64	119.95
2	C	600	FAD	C4-C4X-C10	-3.49	117.64	119.95
2	E	600	FAD	C4-C4X-C10	-3.39	117.71	119.95
2	A	600	FAD	C4-C4X-C10	-3.36	117.73	119.95
2	C	600	FAD	C4X-C10-N10	-3.20	117.01	120.30
2	E	600	FAD	C4X-C10-N10	-3.14	117.08	120.30
2	D	600	FAD	C4X-C10-N10	-3.05	117.16	120.30
2	B	600	FAD	C4X-C10-N10	-3.03	117.19	120.30
2	A	600	FAD	C4X-C10-N10	-2.97	117.25	120.30
3	C	601	NRF	C2-C1-N	2.97	122.69	120.46
3	D	601	NRF	C2-C1-N	2.96	122.68	120.46
3	B	601	NRF	C2-C1-N	2.94	122.67	120.46
3	A	601	NRF	C2-C1-N	2.91	122.64	120.46
2	A	600	FAD	C1'-N10-C10	2.90	121.01	118.41
2	B	600	FAD	C1'-N10-C10	2.90	121.00	118.41
2	C	600	FAD	C1'-N10-C10	2.89	121.00	118.41
2	E	600	FAD	C1'-N10-C10	2.86	120.97	118.41
3	E	601	NRF	C2-C1-N	2.85	122.60	120.46
2	D	600	FAD	C1'-N10-C10	2.67	120.80	118.41
2	C	600	FAD	C5A-C6A-N6A	2.33	123.90	120.35
2	D	600	FAD	C5A-C6A-N6A	2.31	123.86	120.35
3	D	601	NRF	C4-C1-C2	-2.26	114.37	117.45
3	C	601	NRF	C4-C1-C2	-2.25	114.39	117.45
3	B	601	NRF	C4-C1-C2	-2.25	114.39	117.45
2	A	600	FAD	C5A-C6A-N6A	2.24	123.76	120.35
2	E	600	FAD	C5A-C6A-N6A	2.21	123.71	120.35
3	E	601	NRF	C4-C1-C2	-2.21	114.45	117.45
2	B	600	FAD	C5A-C6A-N6A	2.14	123.60	120.35
3	A	601	NRF	C4-C1-C2	-2.13	114.55	117.45

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	602	EPE	C10-C9-N1-C6
4	E	602	EPE	C9-C10-S-O1S
4	E	602	EPE	C9-C10-S-O3S
2	B	600	FAD	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
2	B	600	FAD	C5'-O5'-P-O3P
4	A	602	EPE	C9-C10-S-O2S
4	A	602	EPE	C9-C10-S-O3S
4	B	602	EPE	C8-C7-N4-C3
4	B	602	EPE	C9-C10-S-O1S
2	C	600	FAD	C5'-O5'-P-O3P
4	A	603	EPE	S-C10-C9-N1
4	A	603	EPE	C9-C10-S-O1S
4	A	603	EPE	C9-C10-S-O2S
4	A	603	EPE	C9-C10-S-O3S
2	A	600	FAD	C5'-O5'-P-O1P
2	A	600	FAD	C5'-O5'-P-O3P
4	B	603	EPE	C10-C9-N1-C6
4	A	602	EPE	N4-C7-C8-O8
2	B	600	FAD	C2'-C3'-C4'-O4'
2	D	600	FAD	C2'-C3'-C4'-O4'
2	C	600	FAD	C2'-C3'-C4'-O4'
2	A	600	FAD	C2'-C3'-C4'-O4'
2	E	600	FAD	C2'-C3'-C4'-O4'
4	A	602	EPE	C8-C7-N4-C5
4	A	602	EPE	C8-C7-N4-C3
4	E	602	EPE	C10-C9-N1-C2
4	A	602	EPE	C10-C9-N1-C2
2	D	600	FAD	C5'-O5'-P-O3P
2	E	600	FAD	C5'-O5'-P-O3P
2	D	600	FAD	C5'-O5'-P-O2P
2	C	600	FAD	C5'-O5'-P-O2P
2	E	600	FAD	C5'-O5'-P-O2P
4	B	602	EPE	C9-C10-S-O3S
4	E	602	EPE	C9-C10-S-O2S
4	A	602	EPE	C9-C10-S-O1S
4	B	602	EPE	C9-C10-S-O2S
4	B	602	EPE	C8-C7-N4-C5
4	A	602	EPE	C10-C9-N1-C6
2	A	600	FAD	C2'-C3'-C4'-C5'
2	E	600	FAD	C2'-C3'-C4'-C5'
2	A	600	FAD	O3'-C3'-C4'-O4'
2	E	600	FAD	O3'-C3'-C4'-O4'
2	B	600	FAD	O3'-C3'-C4'-O4'
2	D	600	FAD	O3'-C3'-C4'-O4'
2	C	600	FAD	O3'-C3'-C4'-O4'
2	B	600	FAD	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
2	D	600	FAD	C2'-C3'-C4'-C5'
2	C	600	FAD	C2'-C3'-C4'-C5'
2	C	600	FAD	C5'-O5'-P-O1P
2	B	600	FAD	O4B-C4B-C5B-O5B
2	D	600	FAD	O4B-C4B-C5B-O5B
2	C	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	O4B-C4B-C5B-O5B
2	E	600	FAD	O4B-C4B-C5B-O5B
2	D	600	FAD	O3'-C3'-C4'-C5'
2	C	600	FAD	O3'-C3'-C4'-C5'
2	A	600	FAD	O3'-C3'-C4'-C5'
2	E	600	FAD	O3'-C3'-C4'-C5'

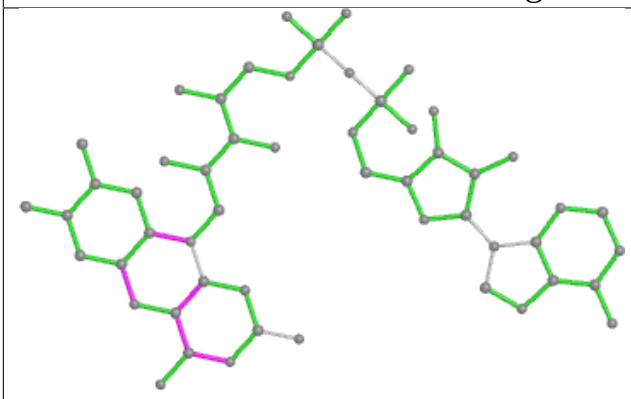
There are no ring outliers.

9 monomers are involved in 11 short contacts:

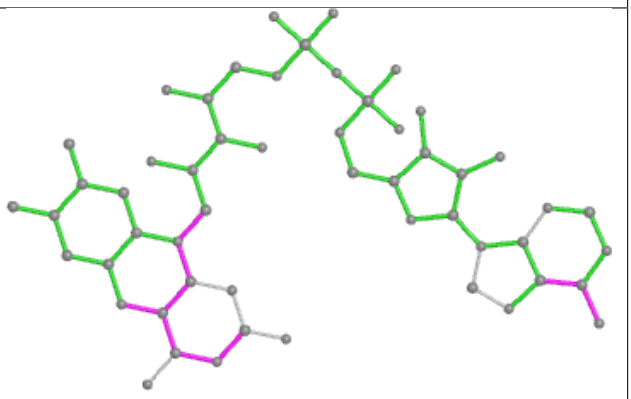
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	602	TRS	1	0
4	E	602	EPE	1	0
3	C	601	NRF	1	0
3	A	601	NRF	1	0
3	E	601	NRF	1	0
3	B	601	NRF	1	0
4	A	603	EPE	1	0
3	D	601	NRF	1	0
6	B	604	TRS	3	0

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.

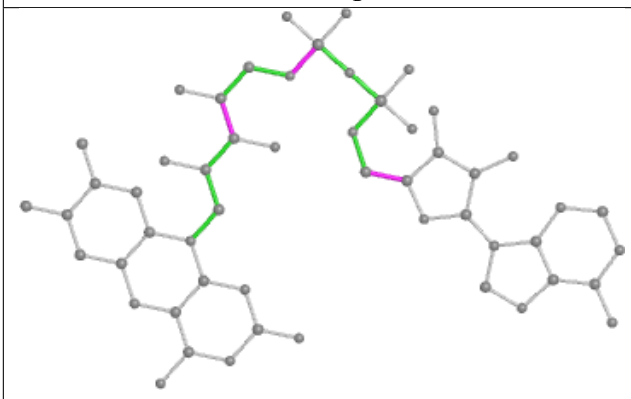
Ligand FAD B 600



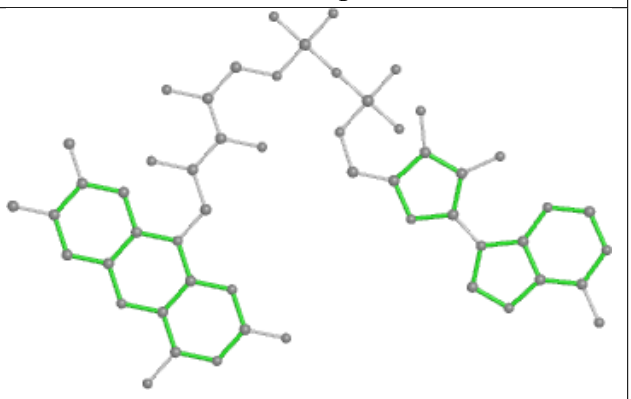
Bond lengths



Bond angles

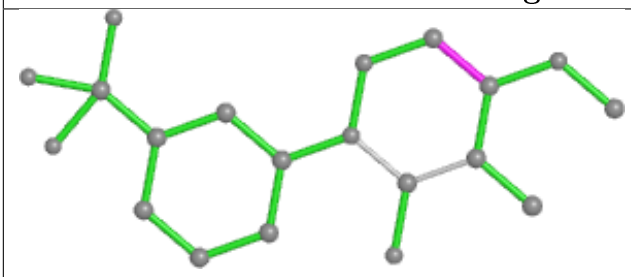


Torsions

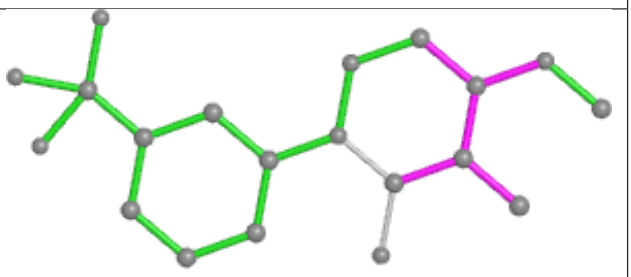


Rings

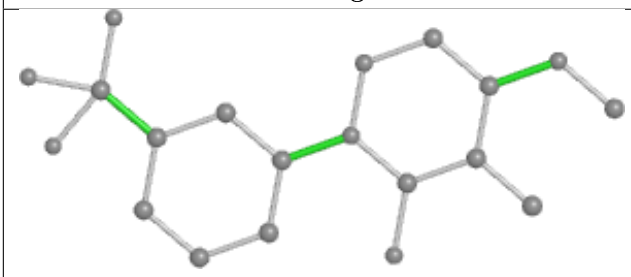
Ligand NRF C 601



Bond lengths



Bond angles



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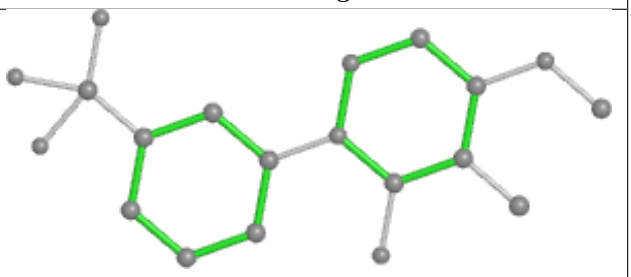
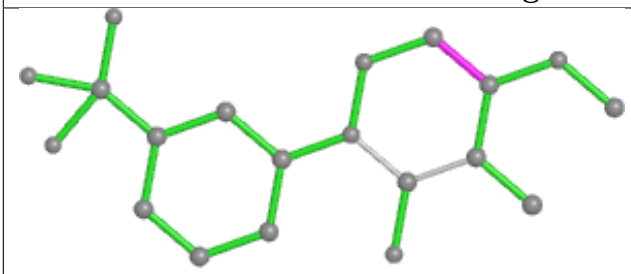
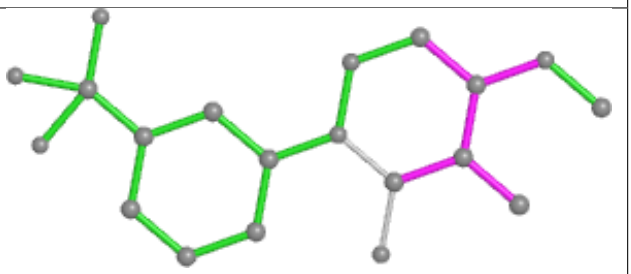


Rings

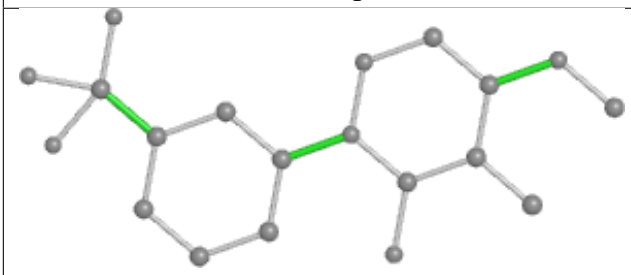
Ligand NRF A 601



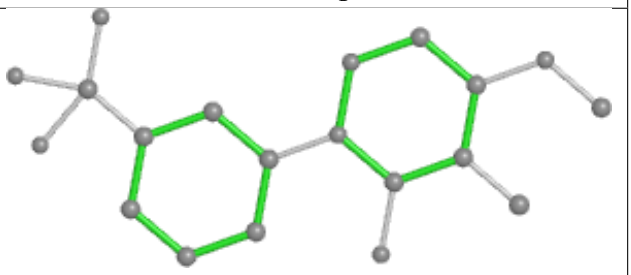
Bond lengths



Bond angles

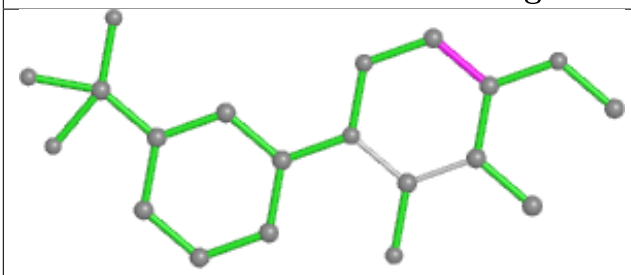


Torsions

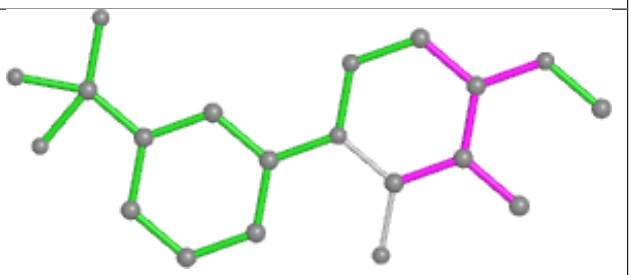


Rings

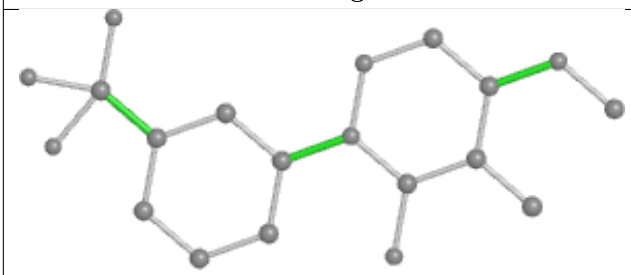
Ligand NRF E 601



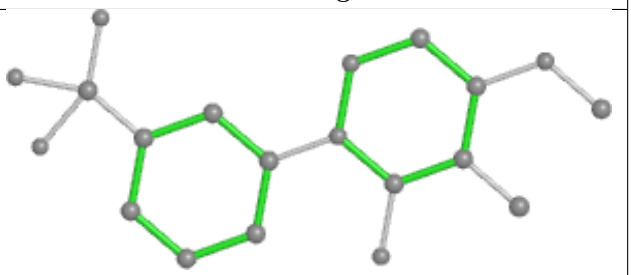
Bond lengths



Bond angles

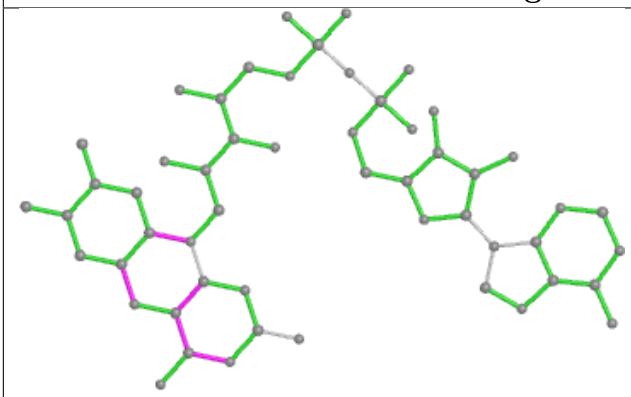


Torsions

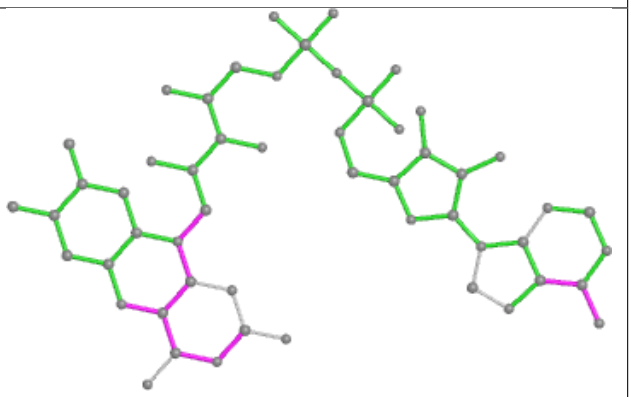


Rings

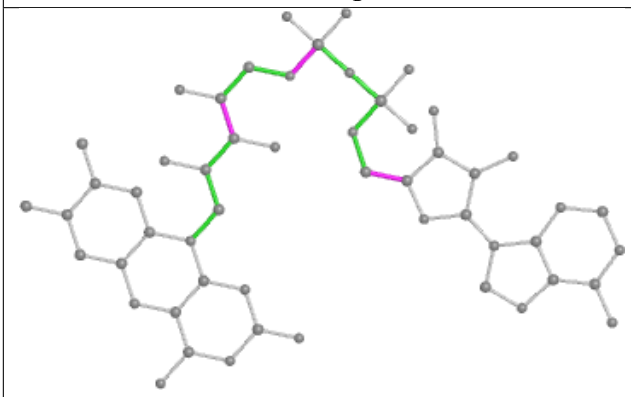
Ligand FAD D 600



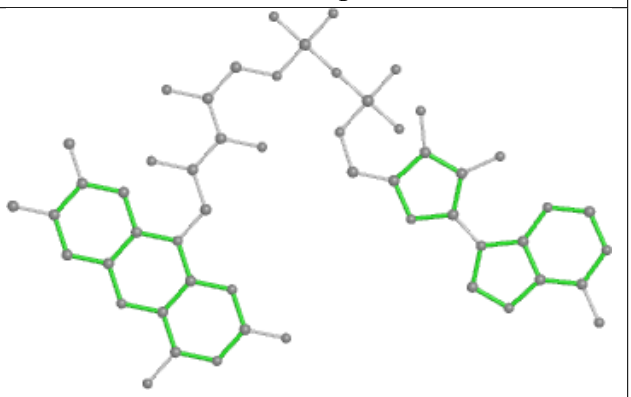
Bond lengths



Bond angles

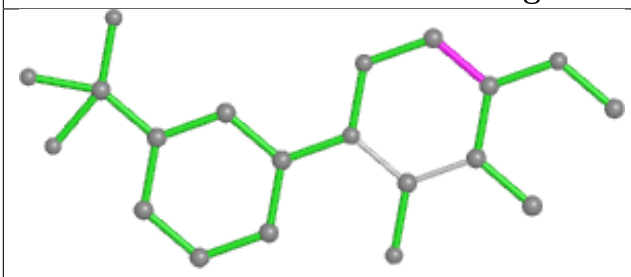


Torsions

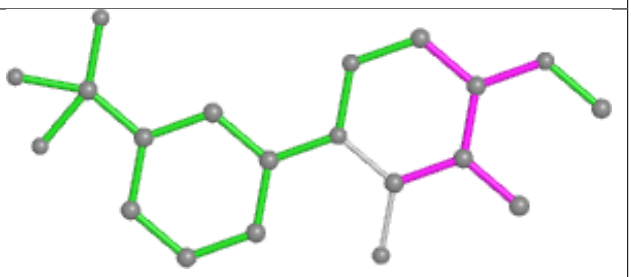


Rings

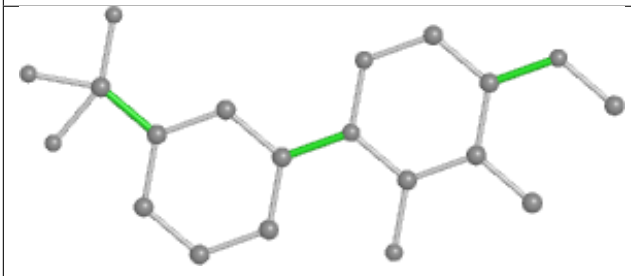
Ligand NRF B 601



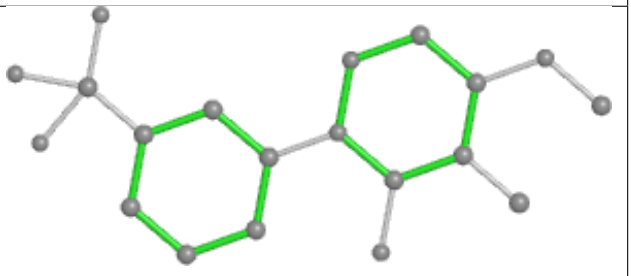
Bond lengths



Bond angles

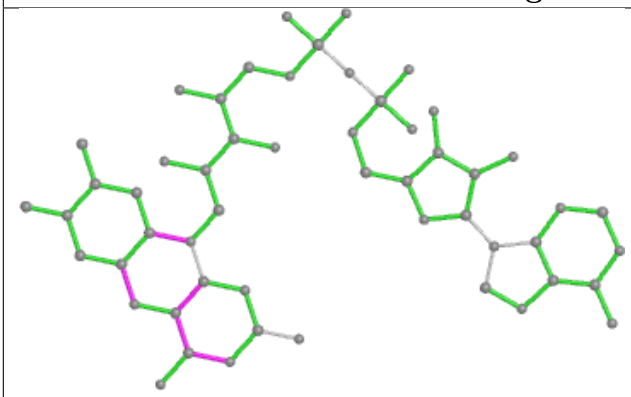


Torsions

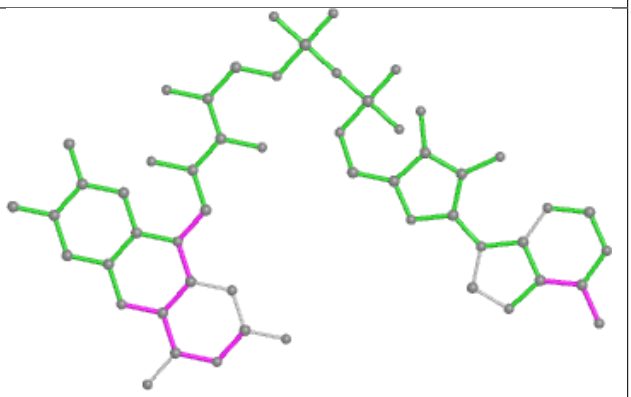


Rings

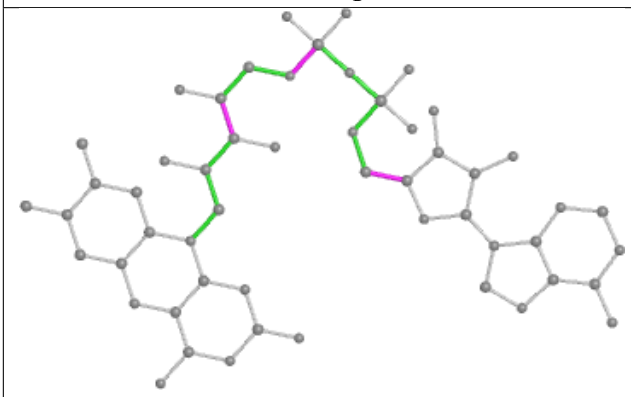
Ligand FAD C 600



Bond lengths



Bond angles



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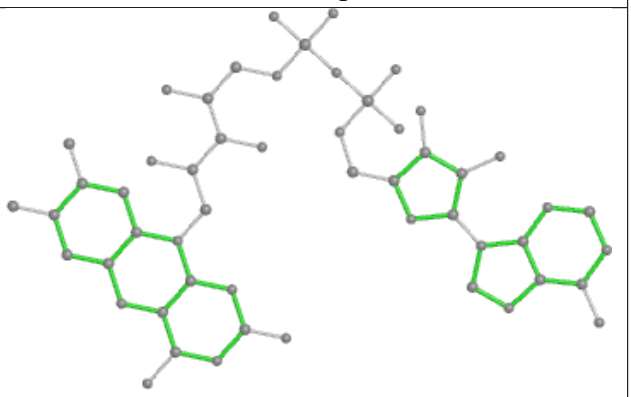
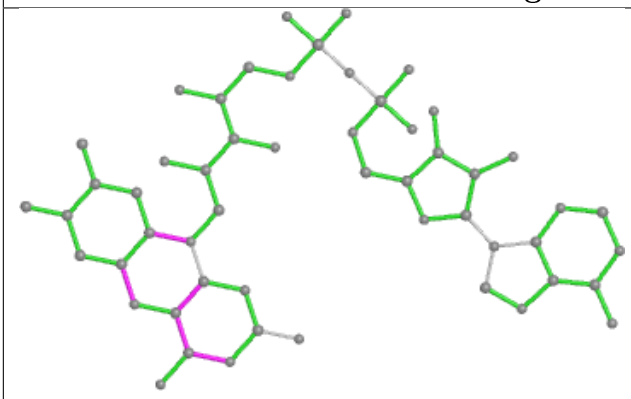
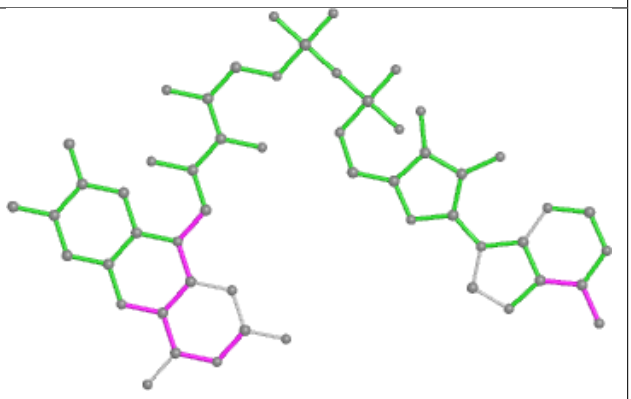


Rings

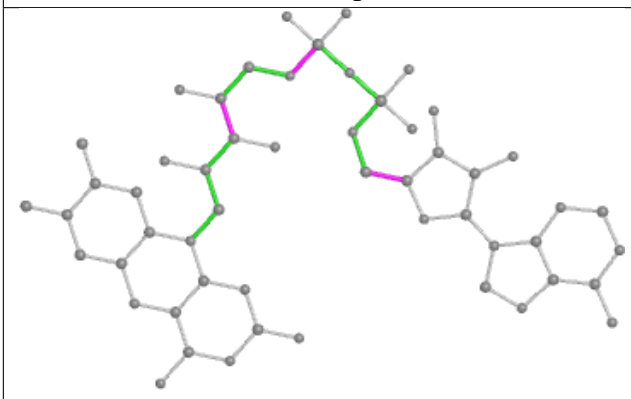
Ligand FAD A 600



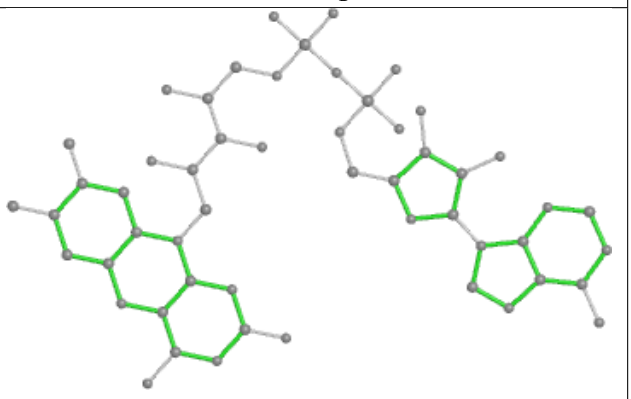
Bond lengths



Bond angles

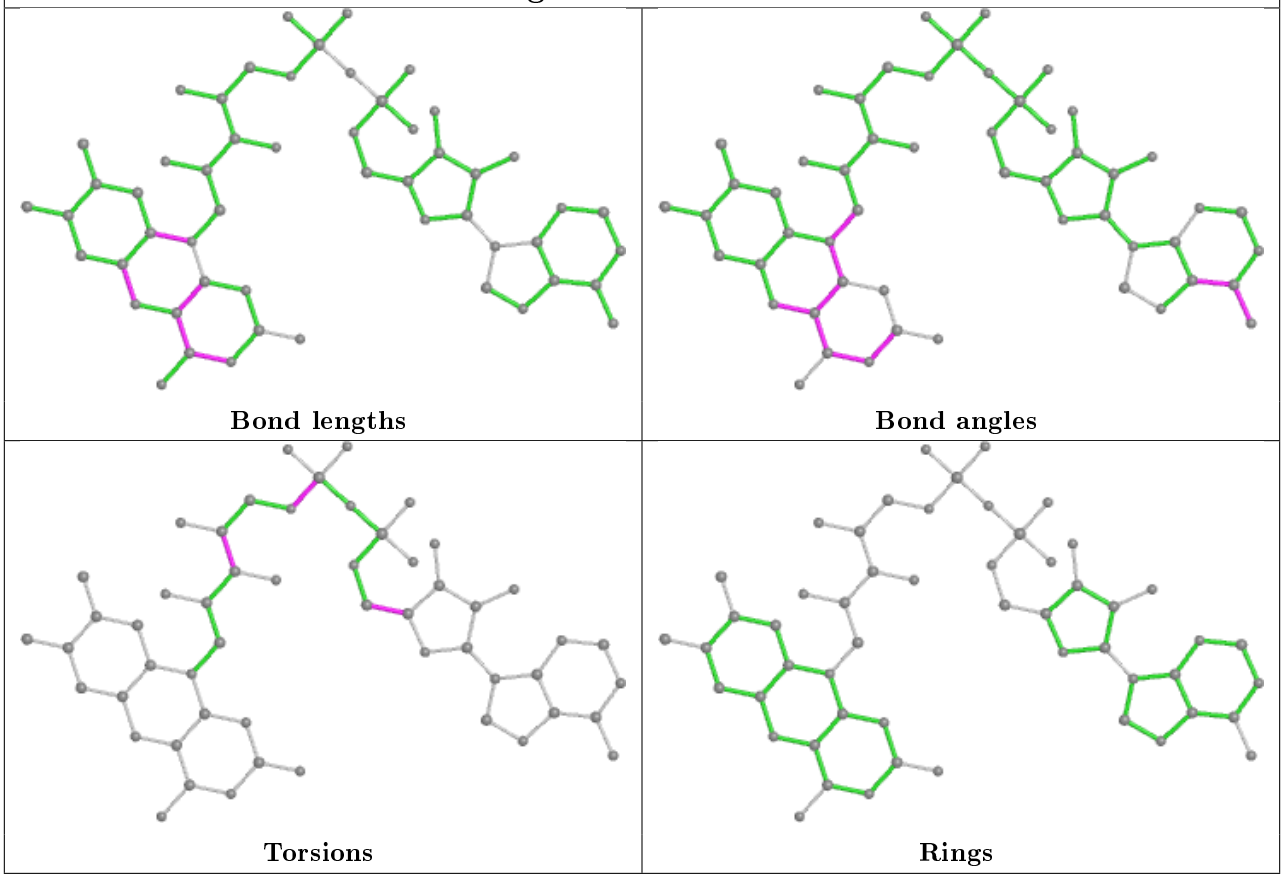


Torsions

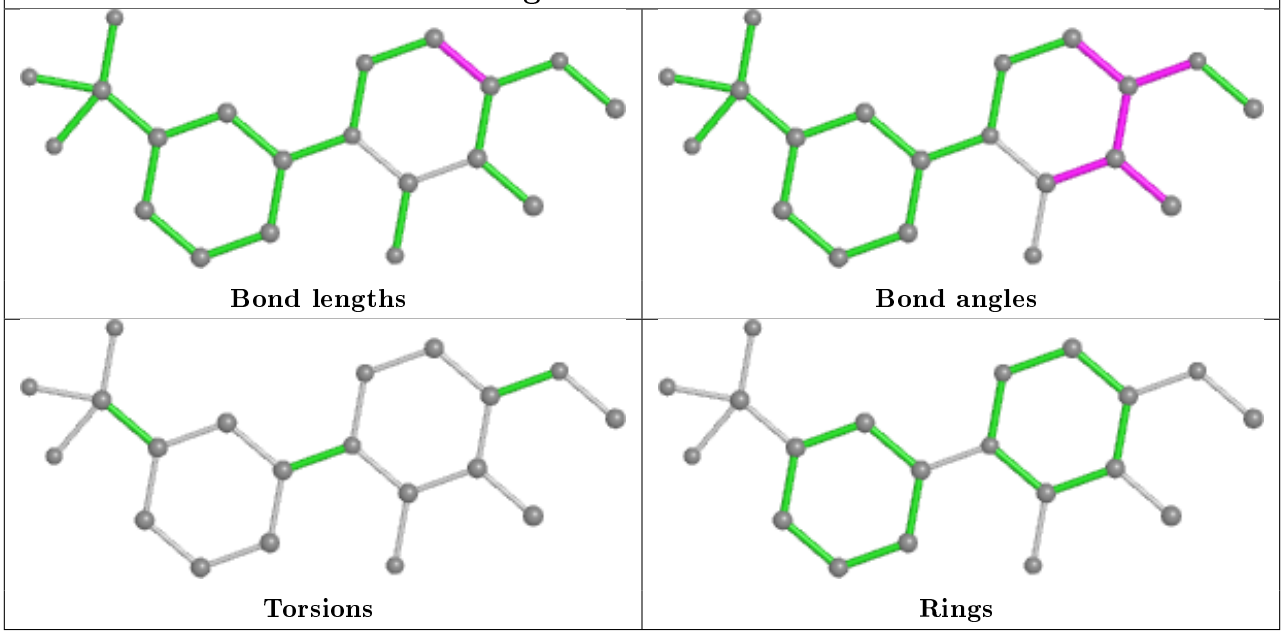


Rings

Ligand FAD E 600



Ligand NRF D 601



5.7 Other polymers (i)

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	467/497 (93%)	-0.12	1 (0%) 95 95	38, 58, 83, 139	0
1	B	472/497 (94%)	-0.09	4 (0%) 86 84	40, 57, 89, 135	0
1	C	470/497 (94%)	-0.03	3 (0%) 89 88	51, 75, 102, 180	0
1	D	470/497 (94%)	0.11	10 (2%) 63 59	47, 73, 105, 211	0
1	E	466/497 (93%)	1.07	106 (22%) 0 0	69, 125, 162, 215	0
All	All	2345/2485 (94%)	0.19	124 (5%) 26 21	38, 71, 142, 215	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	123	LEU	6.2
1	E	107	VAL	5.4
1	E	368	ALA	5.3
1	E	329	VAL	5.0
1	E	450	LEU	4.9
1	E	559	TYR	4.8
1	E	433	ALA	4.8
1	E	473	MET	4.7
1	E	454	PHE	4.6
1	E	404	ILE	4.5
1	E	349	PRO	4.5
1	E	108	VAL	4.4
1	E	567	LEU	4.4
1	E	151	GLY	4.3
1	E	149	GLU	4.2
1	E	468	ILE	4.0
1	E	150	ASP	4.0
1	D	105	LEU	3.9
1	E	494	LEU	3.9
1	E	403	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	522	PRO	3.8
1	E	345	ILE	3.7
1	E	556	VAL	3.6
1	B	97	ASN	3.6
1	D	567	LEU	3.6
1	E	130	PRO	3.6
1	E	154	TYR	3.4
1	E	112	ALA	3.4
1	E	429	LEU	3.4
1	E	120	ALA	3.3
1	E	452	LEU	3.3
1	E	525	GLY	3.3
1	E	146	TRP	3.3
1	E	485	ALA	3.3
1	E	102	THR	3.3
1	E	139	LEU	3.3
1	E	561	MET	3.3
1	E	528	LEU	3.2
1	E	486	ALA	3.2
1	B	96	ARG	3.2
1	D	569	SER	3.2
1	E	521	SER	3.2
1	E	109	ILE	3.2
1	E	479	LEU	3.1
1	E	370	VAL	3.1
1	E	128	HIS	3.1
1	E	129	LYS	3.1
1	E	484	ILE	3.0
1	E	145	ALA	3.0
1	B	98	SER	2.9
1	E	382	VAL	2.9
1	E	372	ALA	2.9
1	E	554	SER	2.8
1	E	122	TYR	2.8
1	E	311	ALA	2.8
1	E	557	GLU	2.7
1	E	432	TYR	2.7
1	E	160	ILE	2.7
1	D	555	VAL	2.7
1	E	111	GLY	2.7
1	E	359	THR	2.7
1	E	126	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	562	LEU	2.6
1	E	137	ASP	2.6
1	E	505	VAL	2.5
1	E	518	LEU	2.5
1	E	189	ILE	2.5
1	E	132	LEU	2.5
1	E	377	ILE	2.5
1	E	457	ALA	2.5
1	E	354	LYS	2.5
1	E	487	ASP	2.5
1	E	460	TRP	2.5
1	E	371	PHE	2.5
1	E	147	LYS	2.4
1	E	564	ARG	2.4
1	E	406	VAL	2.4
1	E	367	ASP	2.4
1	E	293	CYS	2.4
1	E	284	ILE	2.3
1	E	410	PHE	2.3
1	C	276	ALA	2.3
1	D	332	LEU	2.3
1	E	472	THR	2.3
1	E	431	VAL	2.3
1	E	127	GLY	2.3
1	A	567	LEU	2.3
1	E	558	ASP	2.3
1	E	312	PHE	2.2
1	E	105	LEU	2.2
1	E	175	LEU	2.2
1	E	438	THR	2.2
1	E	121	LYS	2.2
1	E	336	VAL	2.2
1	E	164	ALA	2.2
1	E	464	SER	2.2
1	E	340	SER	2.2
1	E	446	ASN	2.2
1	E	461	VAL	2.2
1	C	128	HIS	2.2
1	E	415	LYS	2.2
1	E	499	VAL	2.1
1	D	128	HIS	2.1
1	D	129	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	325	ILE	2.1
1	E	560	LYS	2.1
1	D	527	TYR	2.1
1	E	555	VAL	2.1
1	E	520	ARG	2.1
1	E	241	MET	2.1
1	C	549	LYS	2.1
1	E	138	VAL	2.1
1	E	389	ILE	2.1
1	E	398	LEU	2.1
1	E	519	GLN	2.1
1	B	95	PHE	2.1
1	E	369	TYR	2.1
1	E	562	LEU	2.0
1	E	455	ALA	2.0
1	E	119	THR	2.0
1	E	161	PHE	2.0
1	D	571	GLN	2.0
1	E	358	LEU	2.0
1	E	565	ARG	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 carbohydrates 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
5	IMD	D	603	5/5	0.58	0.74	122,122,123,123	0
4	EPE	A	603	15/15	0.59	0.40	140,147,160,160	0
4	EPE	E	602	15/15	0.68	0.27	143,148,161,161	0

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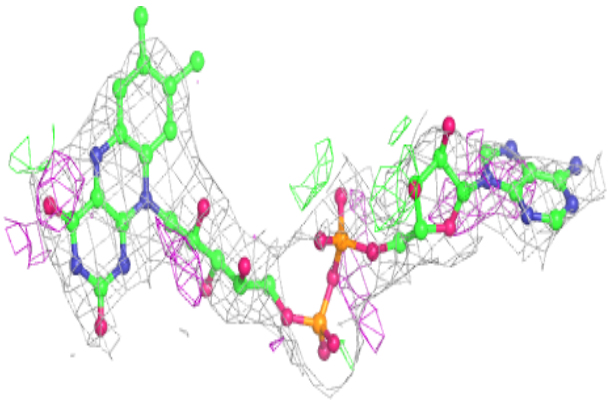
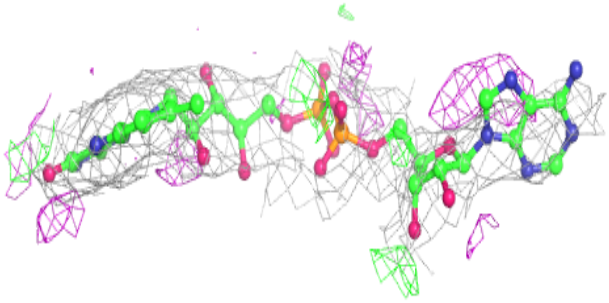
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EPE	B	603	15/15	0.74	0.24	100,110,131,132	0
5	IMD	A	604	5/5	0.80	0.23	108,108,108,108	0
5	IMD	D	604	5/5	0.83	0.19	114,114,114,114	0
6	TRS	B	604	8/8	0.85	0.32	102,105,107,108	0
5	IMD	B	605	5/5	0.88	0.34	112,112,113,113	0
2	FAD	E	600	53/53	0.88	0.25	93,117,145,145	0
5	IMD	B	606	5/5	0.88	0.19	94,94,95,95	0
5	IMD	D	605	5/5	0.90	0.22	98,98,98,98	0
6	TRS	D	602	8/8	0.90	0.30	100,103,104,105	0
3	NRF	E	601	20/20	0.91	0.25	95,100,102,102	0
4	EPE	B	602	15/15	0.95	0.20	78,85,91,91	0
4	EPE	A	602	15/15	0.96	0.17	80,84,91,92	0
3	NRF	D	601	20/20	0.97	0.18	57,63,68,68	0
2	FAD	C	600	53/53	0.97	0.14	44,57,62,63	0
2	FAD	A	600	53/53	0.98	0.18	31,39,45,47	0
2	FAD	D	600	53/53	0.98	0.16	48,56,62,63	0
3	NRF	B	601	20/20	0.98	0.15	39,48,54,58	0
2	FAD	B	600	53/53	0.98	0.18	38,45,48,49	0
3	NRF	C	601	20/20	0.98	0.16	59,66,68,68	0
3	NRF	A	601	20/20	0.99	0.16	42,48,51,52	0

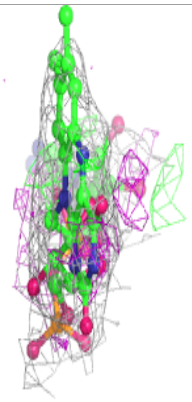
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD E 600:

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

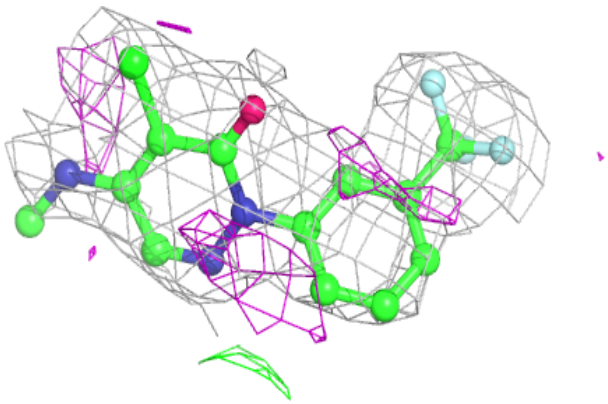


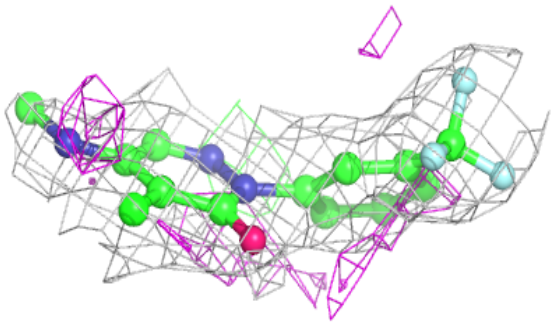


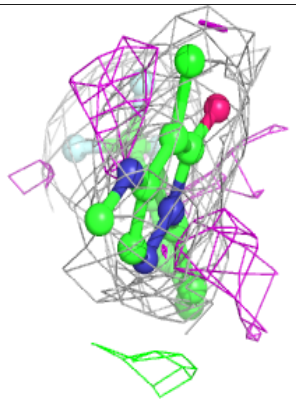


Electron density around NRF E 601:

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

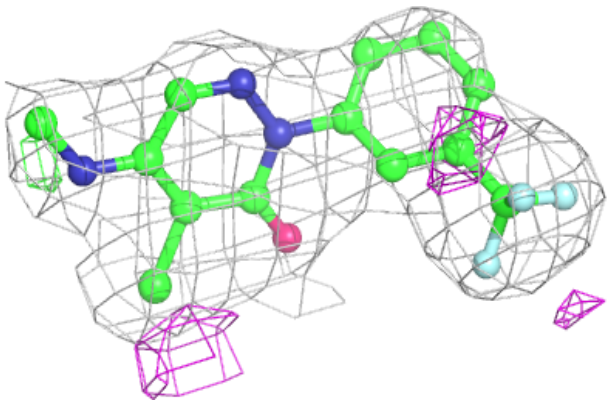


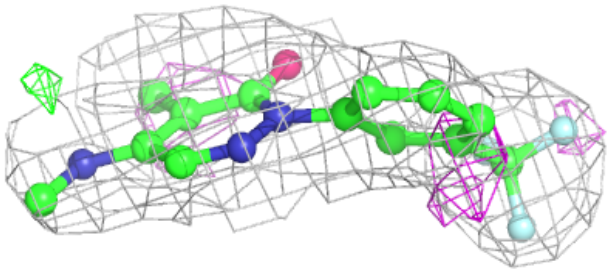


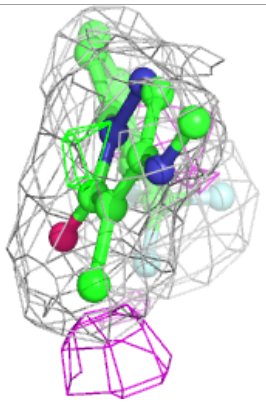


Electron density around NRF D 601:

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

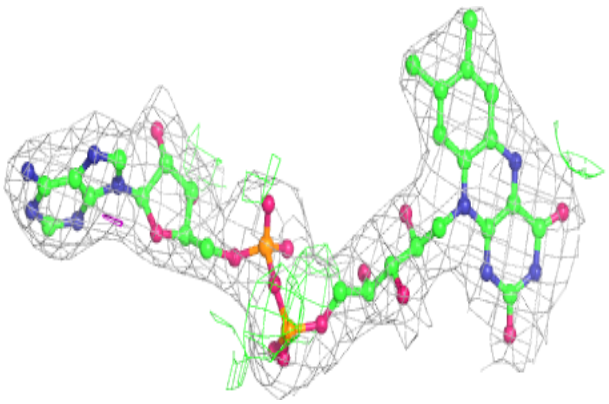


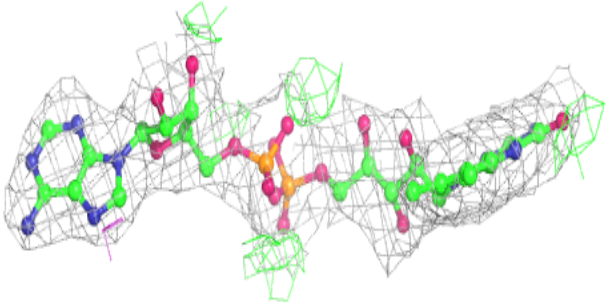


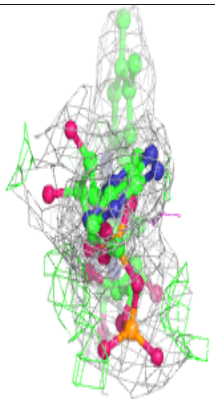


Electron density around FAD C 600:

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

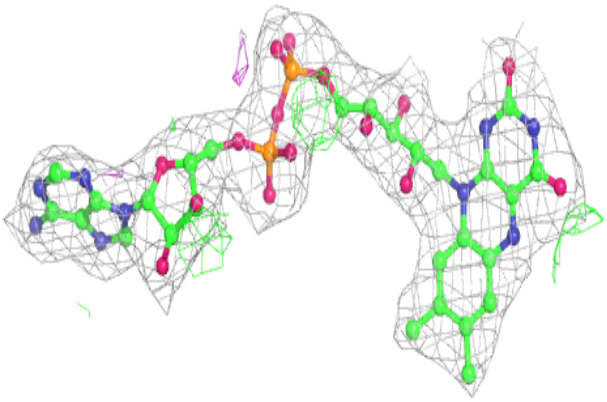


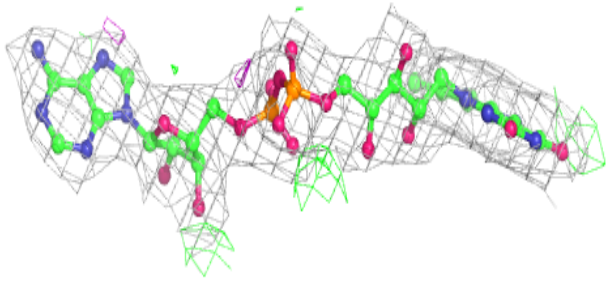


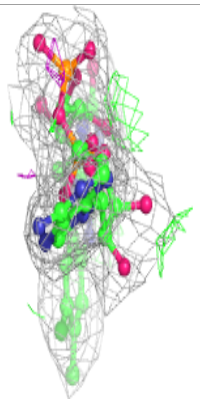


Electron density around FAD A 600:

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

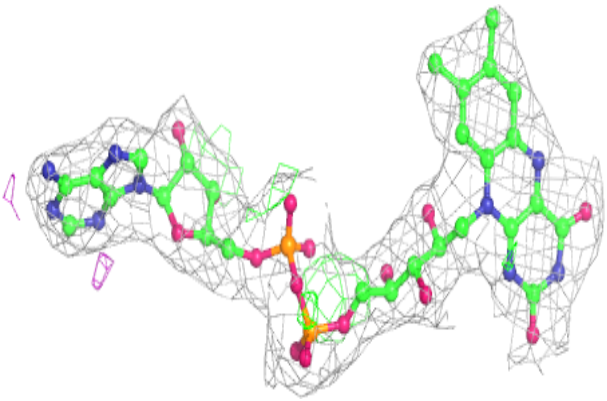


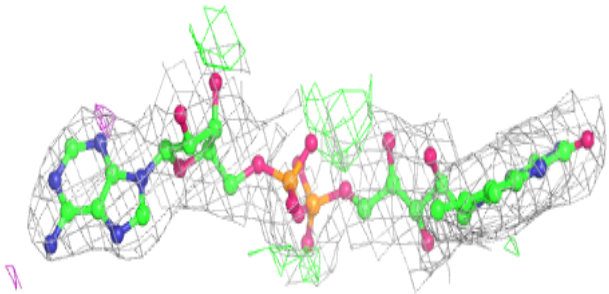


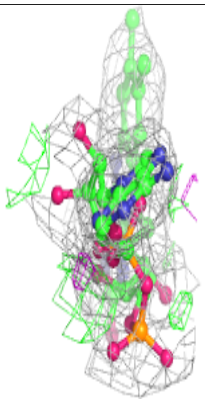


Electron density around FAD D 600:

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

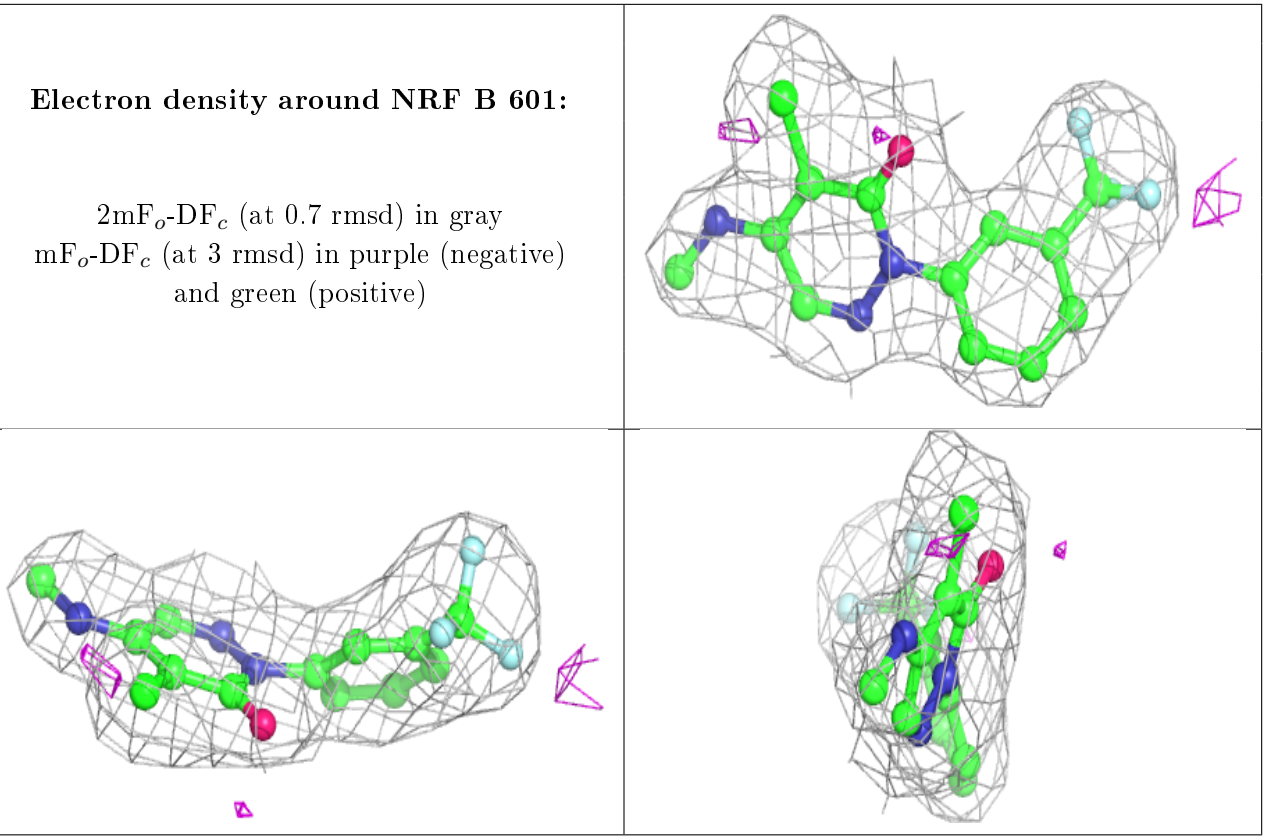






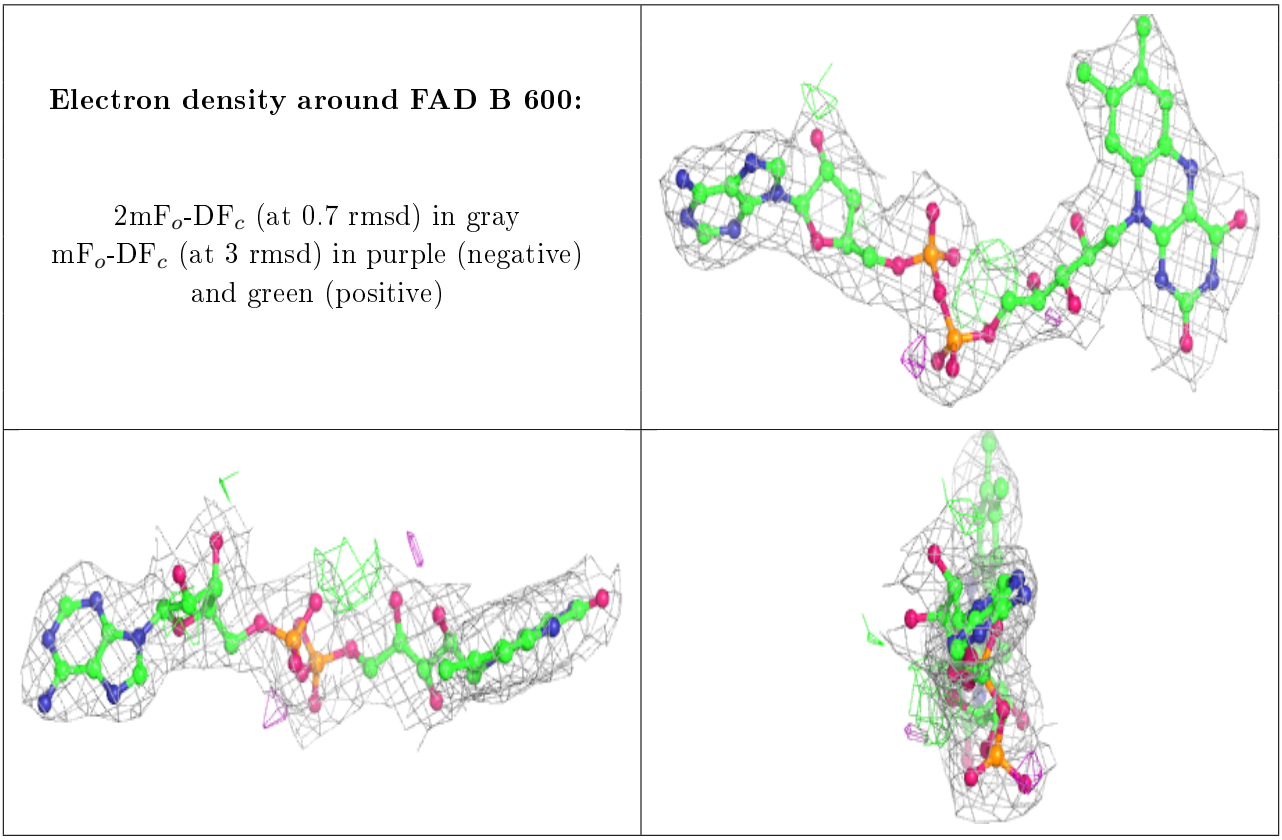
Electron density around NRF B 601:

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



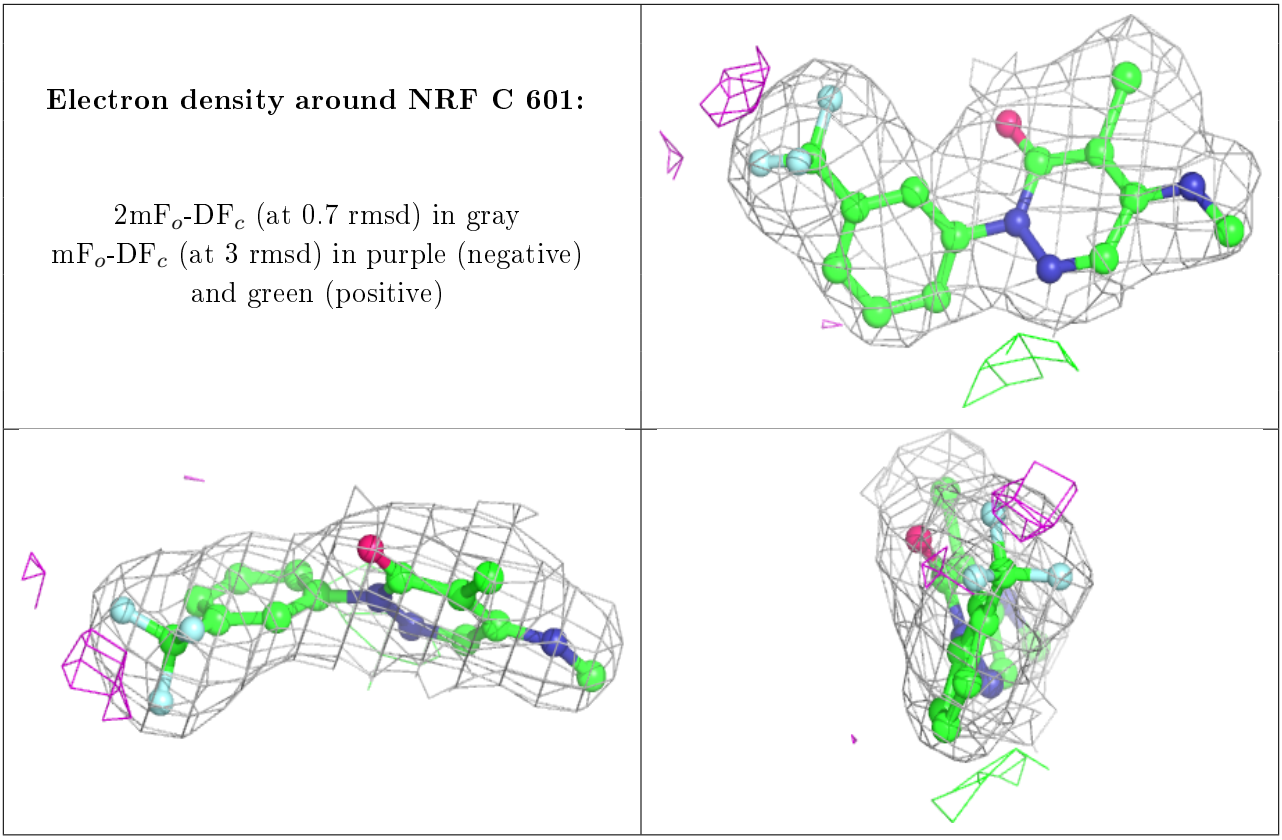
Electron density around FAD B 600:

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



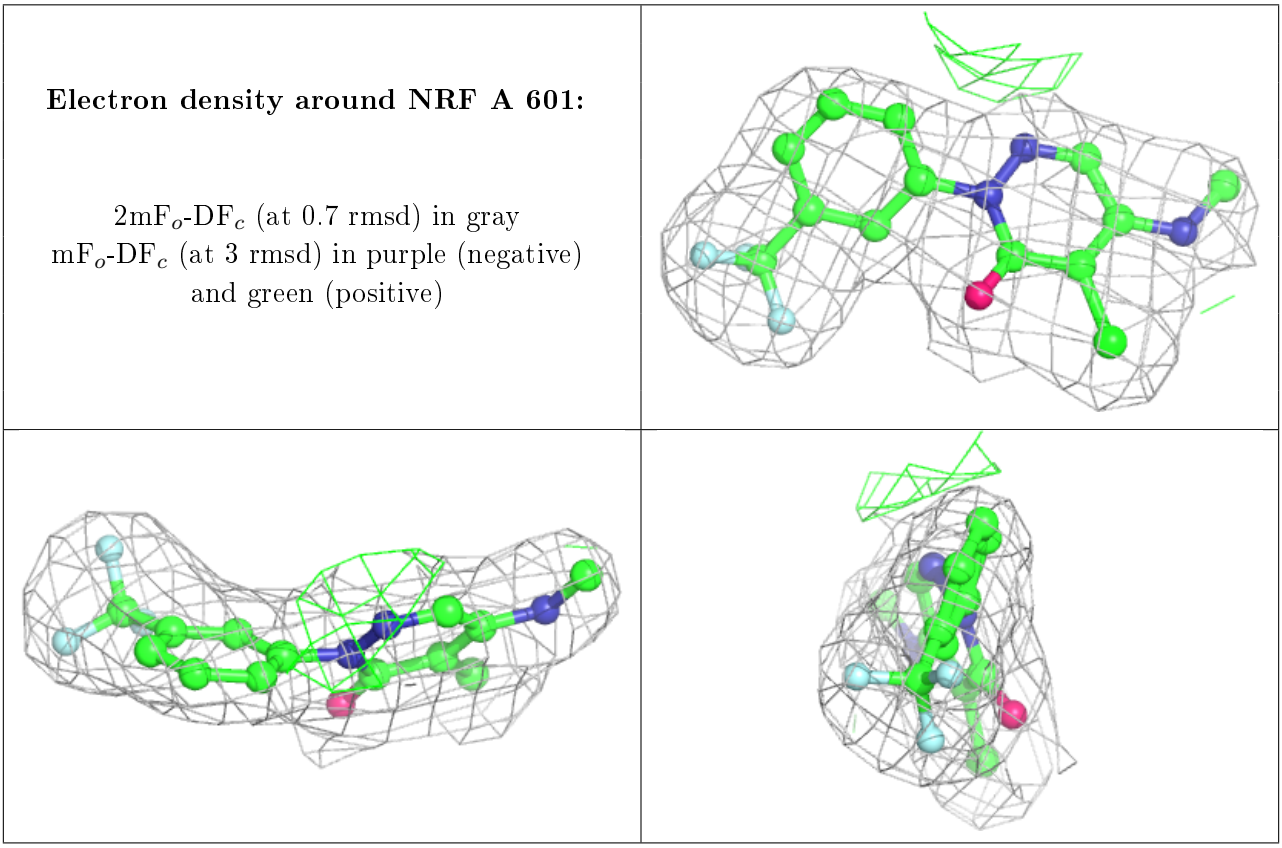
Electron density around NRF C 601:

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



Electron density around NRF A 601:

$2mF_o$-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.