



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:12 AM UTC

PDB ID : 5MOG / pdb_00005mog
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

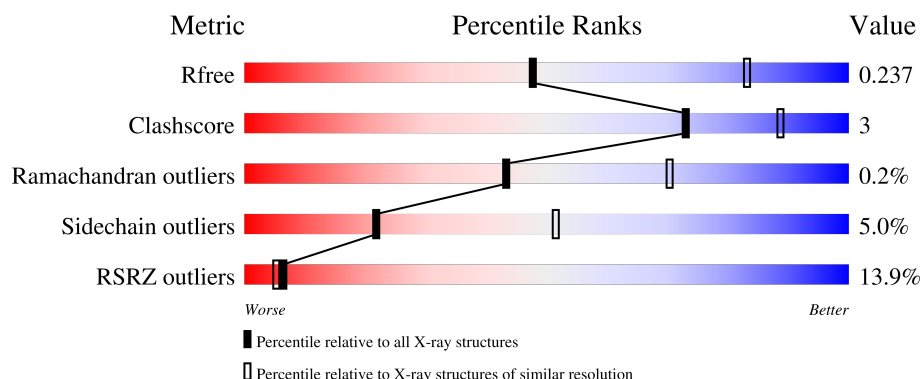
1 Overall quality at a glance

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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (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 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 $\leq 5\%$. 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	3% 82% 11% • 6%
1	B	497	3% 83% 11% • 5%
1	C	497	5% 83% 11% • 5%
1	D	497	10% 84% 10% 5%
1	E	497	44% 79% 13% • 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

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:

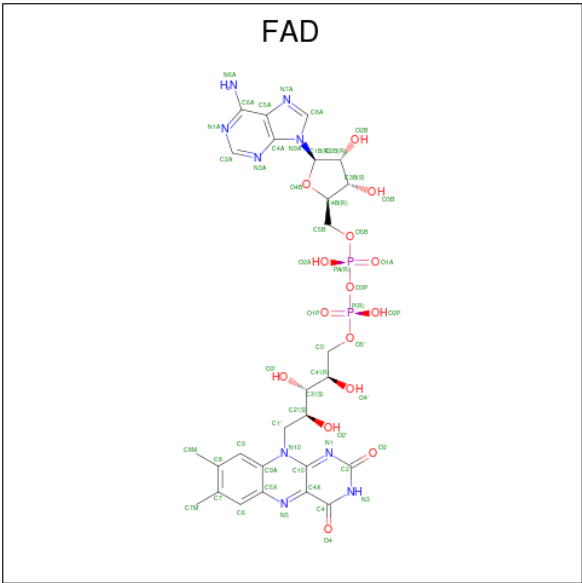
Chain	Residue	Modelled	Actual	Comment	Reference
A	579	HIS	-	expression tag	UNP A2XDA1
A	580	HIS	-	expression tag	UNP A2XDA1
A	581	HIS	-	expression tag	UNP A2XDA1
A	582	HIS	-	expression tag	UNP A2XDA1
A	583	HIS	-	expression tag	UNP A2XDA1
A	584	HIS	-	expression tag	UNP A2XDA1
B	579	HIS	-	expression tag	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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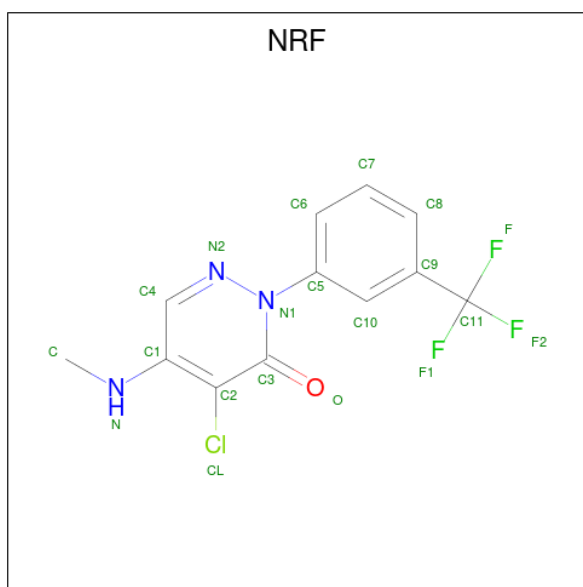
Chain	Residue	Modelled	Actual	Comment	Reference
D	580	HIS	-	expression tag	UNP A2XDA1
D	581	HIS	-	expression tag	UNP A2XDA1
D	582	HIS	-	expression tag	UNP A2XDA1
D	583	HIS	-	expression tag	UNP A2XDA1
D	584	HIS	-	expression tag	UNP A2XDA1
E	579	HIS	-	expression tag	UNP A2XDA1
E	580	HIS	-	expression tag	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 (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



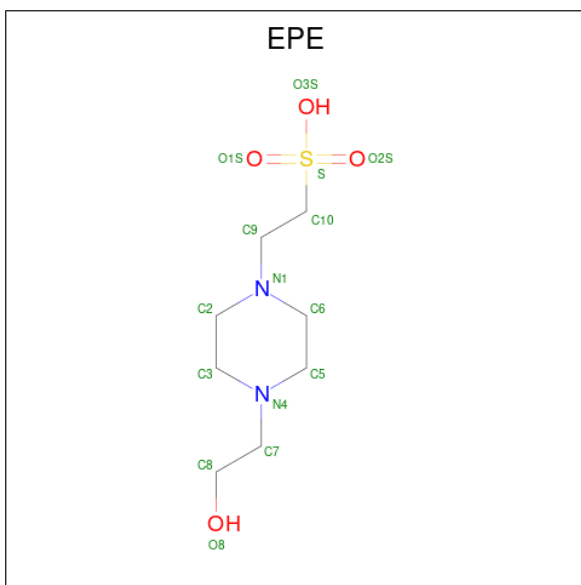
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is Norflurazon (CCD ID: NRF) (formula: C₁₂H₉ClF₃N₃O).



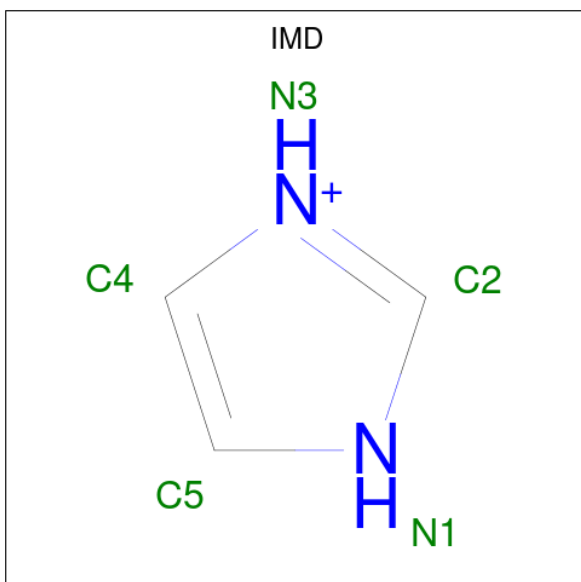
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		
3	B	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		
3	C	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		
3	D	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		
3	E	1	Total	C	Cl	F	N	O	0	0
			20	12	1	3	3	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



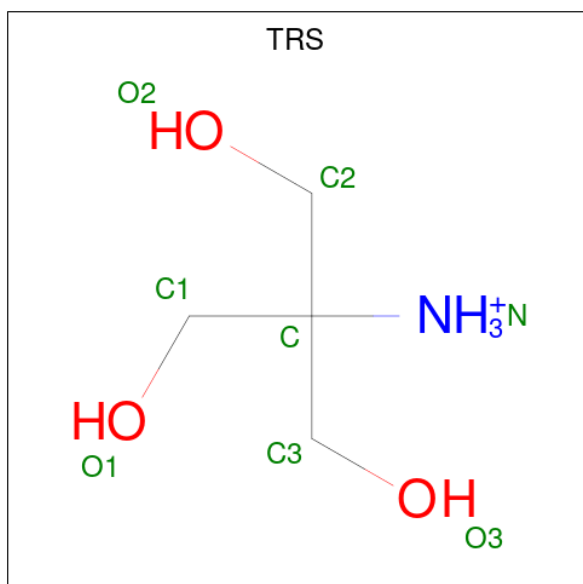
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 7 is water.

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

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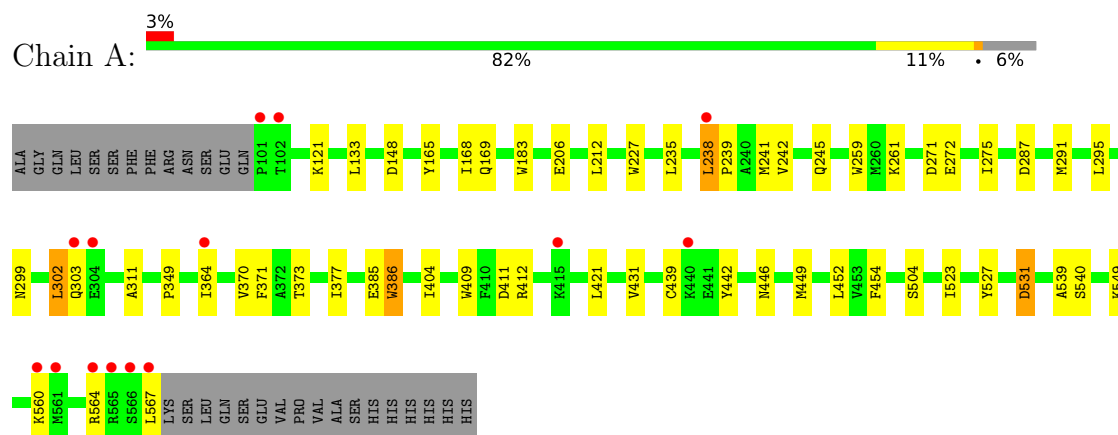
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	139	Total 139	O 139	0	0
7	C	62	Total 62	O 62	0	0
7	D	62	Total 62	O 62	0	0
7	E	11	Total 11	O 11	0	0

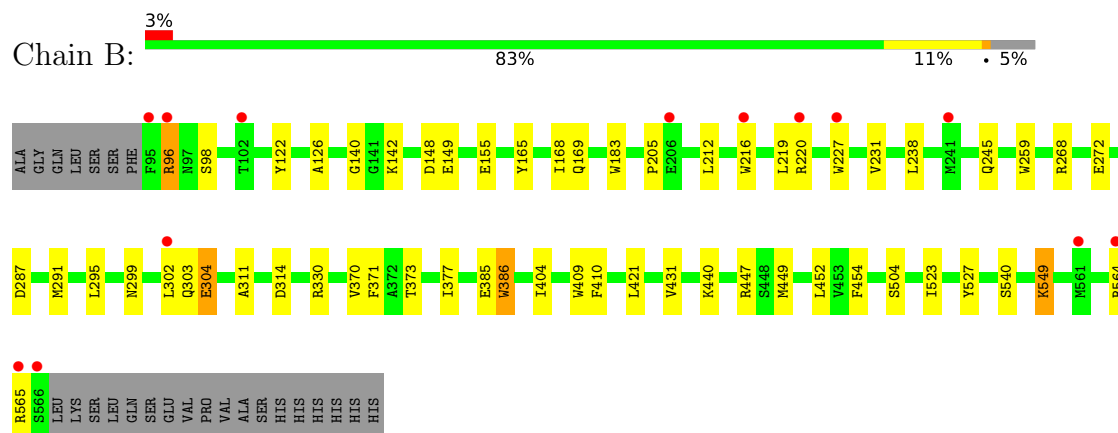
3 Residue-property plots [i](#)

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.

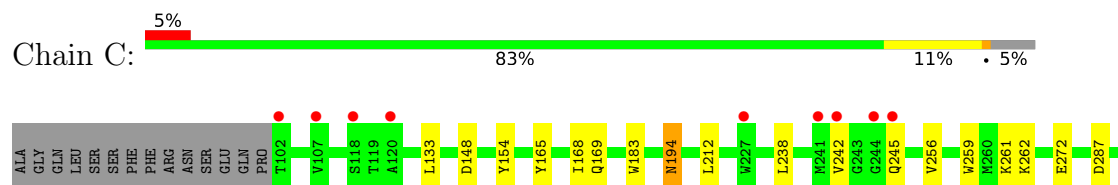
- Molecule 1: Phytoene dehydrogenase, chloroplastic/chromoplastic

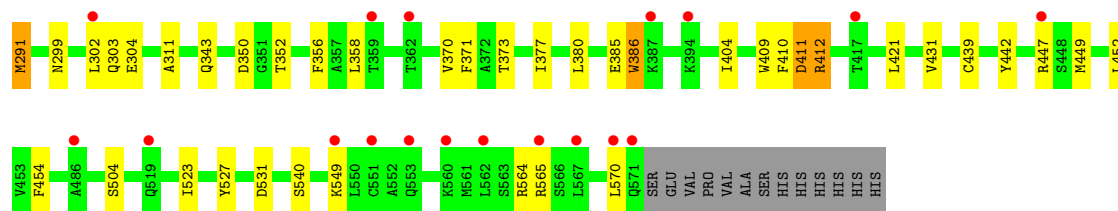


- Molecule 1: Phytoene dehydrogenase, chloroplastic/chromoplastic

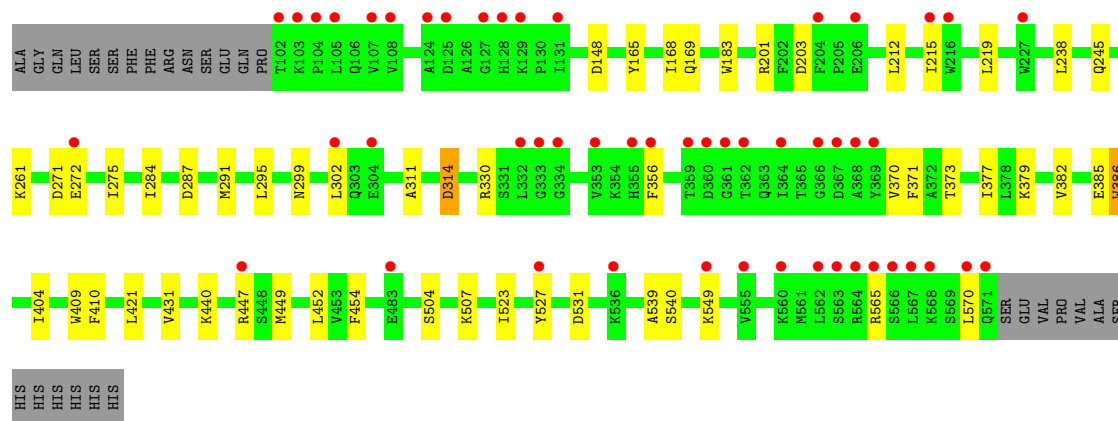
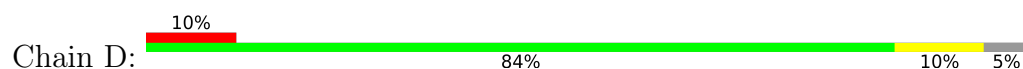


- Molecule 1: Phytoene dehydrogenase, chloroplastic/chromoplastic

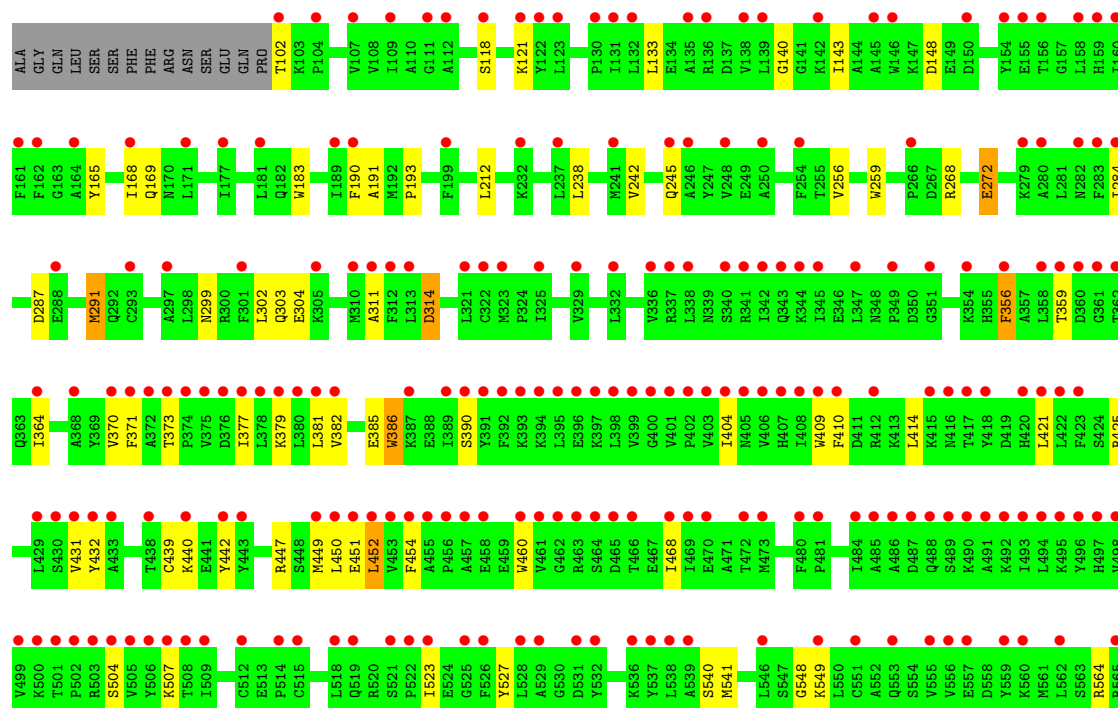
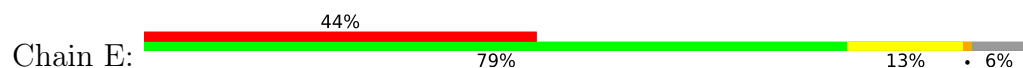




● Molecule 1: Phytoene dehydrogenase, chloroplatic/chromoplatic



● Molecule 1: Phytoene dehydrogenase, chloroplatic/chromoplatic



5566

L567

LYS
SER
LEU
GLN
SER
GLU
VAL
PRO
VAL
ALA
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

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 60.25 – 2.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.25-2.77) 100.0 (60.25-2.77)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NRF, TRS, EPE, IMD, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	0/3794	1.23	8/5141 (0.2%)
1	B	0.76	0/3852	1.23	5/5218 (0.1%)
1	C	0.76	1/3829 (0.0%)	1.22	10/5186 (0.2%)
1	D	0.75	0/3818	1.23	6/5172 (0.1%)
1	E	0.77	1/3782 (0.0%)	1.23	11/5126 (0.2%)
All	All	0.76	2/19075 (0.0%)	1.23	40/25843 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	291	MET	SD-CE	-8.54	1.58	1.79
1	C	291	MET	SD-CE	-7.99	1.59	1.79

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	ASN	CA-CB-CG	6.86	119.46	112.60
1	B	148	ASP	CA-CB-CG	6.14	118.74	112.60
1	D	148	ASP	CA-CB-CG	6.02	118.62	112.60
1	E	148	ASP	CA-CB-CG	6.00	118.60	112.60
1	C	148	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	148	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	386	TRP	CA-C-N	5.45	128.33	120.38
1	B	386	TRP	C-N-CA	5.45	128.33	120.38
1	A	242	VAL	CA-C-N	5.42	125.25	120.10
1	A	242	VAL	C-N-CA	5.42	125.25	120.10
1	D	386	TRP	CA-C-N	5.36	128.20	120.38
1	D	386	TRP	C-N-CA	5.36	128.20	120.38
1	E	386	TRP	CA-C-N	5.33	128.17	120.38
1	E	386	TRP	C-N-CA	5.33	128.17	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	356	PHE	CA-CB-CG	5.32	119.12	113.80
1	E	242	VAL	CA-C-N	5.30	125.13	120.10
1	E	242	VAL	C-N-CA	5.30	125.13	120.10
1	B	287	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	386	TRP	CA-C-N	5.21	127.99	120.38
1	C	386	TRP	C-N-CA	5.21	127.99	120.38
1	B	140	GLY	N-CA-C	5.19	119.86	113.79
1	C	531	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	242	VAL	CA-C-N	5.18	125.02	120.10
1	C	242	VAL	C-N-CA	5.18	125.02	120.10
1	C	356	PHE	CA-CB-CG	5.18	118.98	113.80
1	C	287	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	386	TRP	CA-C-N	5.16	127.91	120.38
1	A	386	TRP	C-N-CA	5.16	127.91	120.38
1	A	531	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	287	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	411	ASP	CA-CB-CG	5.11	117.71	112.60
1	E	287	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	356	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	411	ASP	CA-CB-CG	5.06	117.66	112.60
1	E	314	ASP	CA-CB-CG	5.06	117.66	112.60
1	E	390	SER	CA-C-N	5.05	127.36	120.54
1	E	390	SER	C-N-CA	5.05	127.36	120.54
1	E	140	GLY	N-CA-C	5.04	119.69	113.79
1	A	287	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	314	ASP	CA-CB-CG	5.03	117.63	112.60

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	23	0
1	B	3757	0	3766	30	0
1	C	3736	0	3760	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3728	0	3747	19	0
1	E	3692	0	3699	37	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
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	122	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 (122) 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:256:VAL:HA	1:E:291:MET:HE2	1.49	0.94
1:C:256:VAL:HA	1:C:291:MET:HE2	1.49	0.91
1:C:259:TRP:HB3	1:C:291:MET:HE3	1.56	0.87
1:E:259:TRP:HB3	1:E:291:MET:HE3	1.57	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:ILE:HG21	1:E:541:MET:HE3	1.78	0.64
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:A:560:LYS:HB3	1:C:380:LEU:HD22	1.81	0.63
1:E:191:ALA:O	1:E:425:ARG:HD3	1.99	0.62
1:E:256:VAL:HA	1:E:291:MET:CE	2.28	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:C:256:VAL:HA	1:C:291:MET:CE	2.28	0.59
1:D:330:ARG:HH12	6:D:602:TRS:H21	1.68	0.58
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:C:352:THR:HG21	1:C:565:ARG:HH12	1.72	0.55
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: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:259:TRP:HB3	1:E:291:MET:CE	2.38	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: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:219:LEU:CD2	1:B:227:TRP:CH2	2.97	0.48
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: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:E:451:GLU:C	1:E:452:LEU:HD23	2.42	0.45
1:B:370:VAL:HG22	1:B:527:TYR:HB2	1.98	0.45
1:B:291:MET:HE3	1:B:295:LEU:HG	1.98	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:D:291:MET:HE3	1:D:295:LEU:HG	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:CYS:HB3	1:A:442:TYR:HB2	2.02	0.42
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:H	1:B:304:GLU:HG2	1.70	0.41
1:C:386:TRP:CZ2	1:C:523:ILE:HG21	2.55	0.41
1:D:386:TRP:CZ2	1:D:523:ILE:HG21	2.55	0.41
1:D:421:LEU:HD11	1:D:431:VAL:HB	2.01	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:A:291:MET:HE3	1:A:295:LEU:HG	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/497 (94%)	449 (97%)	15 (3%)	1 (0%)	43	70
1	B	471/497 (95%)	455 (97%)	15 (3%)	1 (0%)	43	70
1	C	469/497 (94%)	454 (97%)	14 (3%)	1 (0%)	43	70
1	D	468/497 (94%)	452 (97%)	15 (3%)	1 (0%)	43	70
1	E	464/497 (93%)	448 (97%)	15 (3%)	1 (0%)	43	70
All	All	2337/2485 (94%)	2258 (97%)	74 (3%)	5 (0%)	43	70

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 ⓘ

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%)	379 (95%)	21 (5%)	20	49
1	B	406/427 (95%)	385 (95%)	21 (5%)	21	50
1	C	404/427 (95%)	382 (95%)	22 (5%)	20	48
1	D	403/427 (94%)	387 (96%)	16 (4%)	28	60
1	E	398/427 (93%)	377 (95%)	21 (5%)	20	49
All	All	2011/2135 (94%)	1910 (95%)	101 (5%)	22	51

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LYS
1	A	168	ILE
1	A	206	GLU
1	A	212	LEU
1	A	238	LEU
1	A	245	GLN
1	A	261	LYS
1	A	272	GLU
1	A	299	ASN
1	A	302	LEU
1	A	303	GLN
1	A	371	PHE
1	A	373	THR
1	A	377	ILE
1	A	385	GLU
1	A	412	ARG
1	A	446	ASN
1	A	452	LEU
1	A	549	LYS
1	A	564	ARG
1	A	567	LEU
1	B	96	ARG
1	B	98	SER
1	B	149	GLU
1	B	168	ILE
1	B	212	LEU
1	B	238	LEU
1	B	245	GLN
1	B	268	ARG
1	B	272	GLU
1	B	299	ASN
1	B	302	LEU
1	B	303	GLN
1	B	304	GLU
1	B	371	PHE
1	B	373	THR
1	B	377	ILE
1	B	385	GLU
1	B	452	LEU
1	B	549	LYS
1	B	564	ARG
1	B	565	ARG
1	C	168	ILE

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Mol	Chain	Res	Type
1	C	194	ASN
1	C	212	LEU
1	C	238	LEU
1	C	245	GLN
1	C	261	LYS
1	C	262	LYS
1	C	272	GLU
1	C	299	ASN
1	C	302	LEU
1	C	303	GLN
1	C	304	GLU
1	C	343	GLN
1	C	371	PHE
1	C	373	THR
1	C	377	ILE
1	C	385	GLU
1	C	412	ARG
1	C	452	LEU
1	C	549	LYS
1	C	564	ARG
1	C	570	LEU
1	D	168	ILE
1	D	212	LEU
1	D	238	LEU
1	D	245	GLN
1	D	261	LYS
1	D	272	GLU
1	D	299	ASN
1	D	302	LEU
1	D	371	PHE
1	D	373	THR
1	D	377	ILE
1	D	385	GLU
1	D	452	LEU
1	D	549	LYS
1	D	565	ARG
1	D	570	LEU
1	E	102	THR
1	E	121	LYS
1	E	168	ILE
1	E	212	LEU
1	E	238	LEU

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Mol	Chain	Res	Type
1	E	245	GLN
1	E	268	ARG
1	E	272	GLU
1	E	299	ASN
1	E	302	LEU
1	E	303	GLN
1	E	304	GLU
1	E	359	THR
1	E	371	PHE
1	E	373	THR
1	E	377	ILE
1	E	381	LEU
1	E	385	GLU
1	E	452	LEU
1	E	549	LYS
1	E	564	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	222	ASN
1	A	245	GLN
1	A	285	ASN
1	A	299	ASN
1	A	355	HIS
1	B	169	GLN
1	B	178	ASN
1	B	245	GLN
1	B	299	ASN
1	B	348	ASN
1	B	355	HIS
1	C	178	ASN
1	C	222	ASN
1	C	245	GLN
1	C	285	ASN
1	C	299	ASN
1	C	355	HIS
1	D	169	GLN
1	D	178	ASN
1	D	245	GLN
1	D	285	ASN

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Mol	Chain	Res	Type
1	D	299	ASN
1	D	348	ASN
1	D	355	HIS
1	E	178	ASN
1	E	245	GLN
1	E	285	ASN
1	E	299	ASN
1	E	348	ASN
1	E	355	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	IMD	D	605	-	5,5,5	0.32	0	5,5,5	0.55	0
4	EPE	B	603	-	15,15,15	1.16	1 (6%)	19,20,20	0.34	0
2	FAD	D	600	-	58,58,58	0.41	0	85,89,89	0.60	1 (1%)
5	IMD	B	606	-	5,5,5	0.31	0	5,5,5	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TRS	D	602	-	7,7,7	0.28	0	9,9,9	0.30	0
5	IMD	A	604	-	5,5,5	0.31	0	5,5,5	0.54	0
6	TRS	B	604	-	7,7,7	0.29	0	9,9,9	0.37	0
4	EPE	B	602	-	15,15,15	1.29	1 (6%)	19,20,20	0.45	0
3	NRF	E	601	-	19,21,21	1.19	2 (10%)	27,31,31	1.05	3 (11%)
3	NRF	B	601	-	19,21,21	1.18	2 (10%)	27,31,31	0.97	3 (11%)
4	EPE	A	602	-	15,15,15	1.08	1 (6%)	19,20,20	0.26	0
3	NRF	A	601	-	19,21,21	1.17	2 (10%)	27,31,31	1.02	3 (11%)
2	FAD	A	600	-	58,58,58	0.40	0	85,89,89	0.50	0
5	IMD	B	605	-	5,5,5	0.32	0	5,5,5	0.55	0
4	EPE	E	602	-	15,15,15	1.10	1 (6%)	19,20,20	0.47	0
2	FAD	B	600	-	58,58,58	0.42	0	85,89,89	0.56	0
2	FAD	C	600	-	58,58,58	0.43	0	85,89,89	0.59	0
4	EPE	A	603	-	15,15,15	0.66	1 (6%)	19,20,20	0.33	0
3	NRF	D	601	-	19,21,21	1.11	2 (10%)	27,31,31	1.03	4 (14%)
3	NRF	C	601	-	19,21,21	1.18	2 (10%)	27,31,31	0.98	3 (11%)
5	IMD	D	604	-	5,5,5	0.31	0	5,5,5	0.55	0
2	FAD	E	600	-	58,58,58	0.40	0	85,89,89	0.55	0
5	IMD	D	603	-	5,5,5	0.32	0	5,5,5	0.55	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
5	IMD	D	605	-	-	-	0/1/1/1
4	EPE	B	603	-	-	1/9/19/19	0/1/1/1
2	FAD	D	600	-	-	7/34/50/50	0/6/6/6
5	IMD	B	606	-	-	-	0/1/1/1
6	TRS	D	602	-	-	0/9/9/9	-
5	IMD	A	604	-	-	-	0/1/1/1
6	TRS	B	604	-	-	1/9/9/9	-
4	EPE	B	602	-	-	5/9/19/19	0/1/1/1
3	NRF	E	601	-	-	0/11/12/12	0/2/2/2
3	NRF	B	601	-	-	0/11/12/12	0/2/2/2
4	EPE	A	602	-	-	8/9/19/19	0/1/1/1
3	NRF	A	601	-	-	0/11/12/12	0/2/2/2
2	FAD	A	600	-	-	7/34/50/50	0/6/6/6
5	IMD	B	605	-	-	-	0/1/1/1

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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	-	-	7/34/50/50	0/6/6/6
2	FAD	C	600	-	-	7/34/50/50	0/6/6/6
4	EPE	A	603	-	-	4/9/19/19	0/1/1/1
3	NRF	D	601	-	-	0/11/12/12	0/2/2/2
3	NRF	C	601	-	-	0/11/12/12	0/2/2/2
5	IMD	D	604	-	-	-	0/1/1/1
2	FAD	E	600	-	-	7/34/50/50	0/6/6/6
5	IMD	D	603	-	-	-	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	EPE	C10-S	-4.86	1.70	1.77
4	B	603	EPE	C10-S	-4.45	1.71	1.77
4	A	602	EPE	C10-S	-4.15	1.71	1.77
4	E	602	EPE	C10-S	-4.13	1.71	1.77
3	C	601	NRF	C4-C1	3.90	1.48	1.43
3	B	601	NRF	C4-C1	3.77	1.48	1.43
3	E	601	NRF	C4-C1	3.73	1.48	1.43
3	A	601	NRF	C4-C1	3.66	1.48	1.43
3	D	601	NRF	C4-C1	3.50	1.47	1.43
3	E	601	NRF	C1-N	3.23	1.38	1.34
3	A	601	NRF	C1-N	3.22	1.38	1.34
3	B	601	NRF	C1-N	3.17	1.38	1.34
3	C	601	NRF	C1-N	3.01	1.38	1.34
3	D	601	NRF	C1-N	3.00	1.38	1.34
4	A	603	EPE	C10-S	-2.33	1.74	1.77

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	NRF	C2-C1-N	-3.20	122.60	129.89
3	A	601	NRF	C2-C1-N	-3.18	122.64	129.89
3	B	601	NRF	C2-C1-N	-3.17	122.67	129.89
3	D	601	NRF	C2-C1-N	-3.16	122.68	129.89
3	C	601	NRF	C2-C1-N	-3.16	122.69	129.89
3	E	601	NRF	C1-C2-C3	2.42	124.38	122.24
3	D	601	NRF	C1-C2-C3	2.23	124.21	122.24
3	A	601	NRF	C1-C2-C3	2.21	124.20	122.24
3	D	601	NRF	C4-N2-N1	2.19	120.28	115.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NRF	C4-N2-N1	2.17	120.23	115.54
3	E	601	NRF	C4-N2-N1	2.16	120.22	115.54
3	C	601	NRF	C4-N2-N1	2.12	120.13	115.54
3	B	601	NRF	C1-C2-C3	2.10	124.10	122.24
2	D	600	FAD	O2P-P-O5'	2.06	116.93	107.57
3	C	601	NRF	C1-C2-C3	2.05	124.05	122.24
3	B	601	NRF	C4-N2-N1	2.04	119.95	115.54
3	D	601	NRF	C1-C2-CL	-2.01	120.09	122.39

There are no chirality outliers.

All (59) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	B	602	EPE	C9-C10-S-O3S
4	A	602	EPE	C9-C10-S-O1S
4	B	602	EPE	C9-C10-S-O2S
4	E	602	EPE	C9-C10-S-O2S
2	D	600	FAD	C5'-O5'-P-O2P
2	D	600	FAD	C5'-O5'-P-O3P
2	E	600	FAD	C5'-O5'-P-O3P
4	B	602	EPE	C8-C7-N4-C5
4	A	602	EPE	C10-C9-N1-C6
2	A	600	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	C2'-C3'-C4'-C5'
2	E	600	FAD	C2'-C3'-C4'-C5'
2	E	600	FAD	O3'-C3'-C4'-O4'
2	B	600	FAD	O3'-C3'-C4'-O4'
2	C	600	FAD	O3'-C3'-C4'-O4'
2	D	600	FAD	O3'-C3'-C4'-O4'
2	B	600	FAD	C2'-C3'-C4'-C5'
2	C	600	FAD	C2'-C3'-C4'-C5'
2	D	600	FAD	C2'-C3'-C4'-C5'
2	A	600	FAD	O3'-C3'-C4'-C5'
2	C	600	FAD	O3'-C3'-C4'-C5'
2	D	600	FAD	O3'-C3'-C4'-C5'
2	E	600	FAD	O3'-C3'-C4'-C5'
6	B	604	TRS	C1-C-C2-O2
2	B	600	FAD	O3'-C3'-C4'-C5'
2	B	600	FAD	C2B-C1B-N9A-C8A
2	C	600	FAD	C2B-C1B-N9A-C8A
2	D	600	FAD	C2B-C1B-N9A-C8A
2	E	600	FAD	C2B-C1B-N9A-C8A
2	A	600	FAD	C2B-C1B-N9A-C8A

There are no ring outliers.

9 monomers are involved in 11 short contacts:

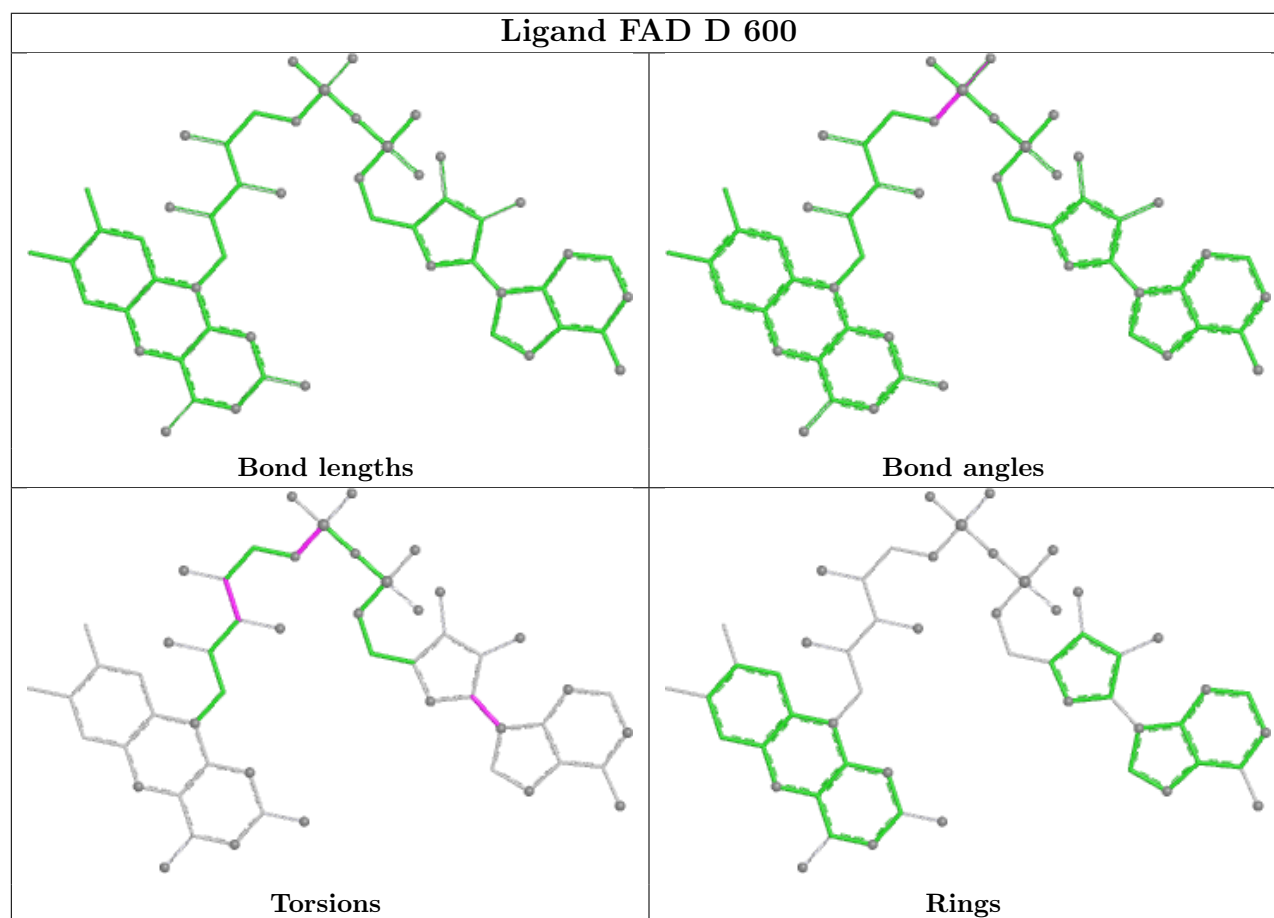
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	602	TRS	1	0
6	B	604	TRS	3	0
3	E	601	NRF	1	0
3	B	601	NRF	1	0
3	A	601	NRF	1	0
4	E	602	EPE	1	0
4	A	603	EPE	1	0

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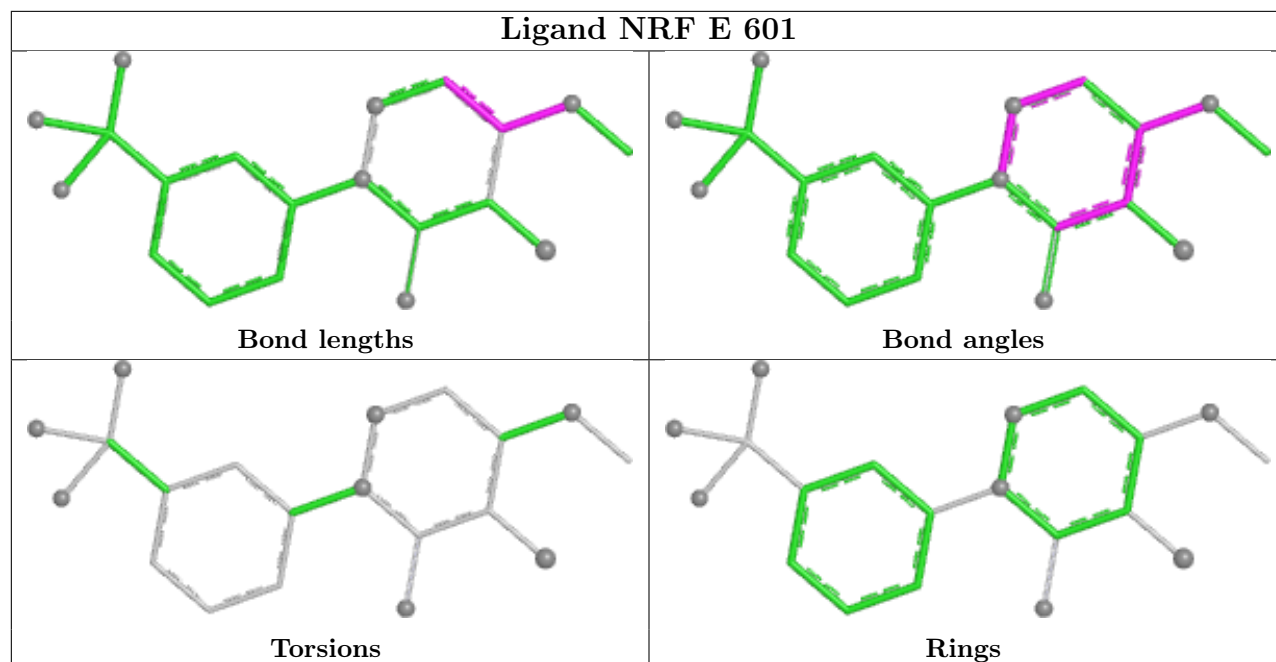
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	NRF	1	0
3	C	601	NRF	1	0

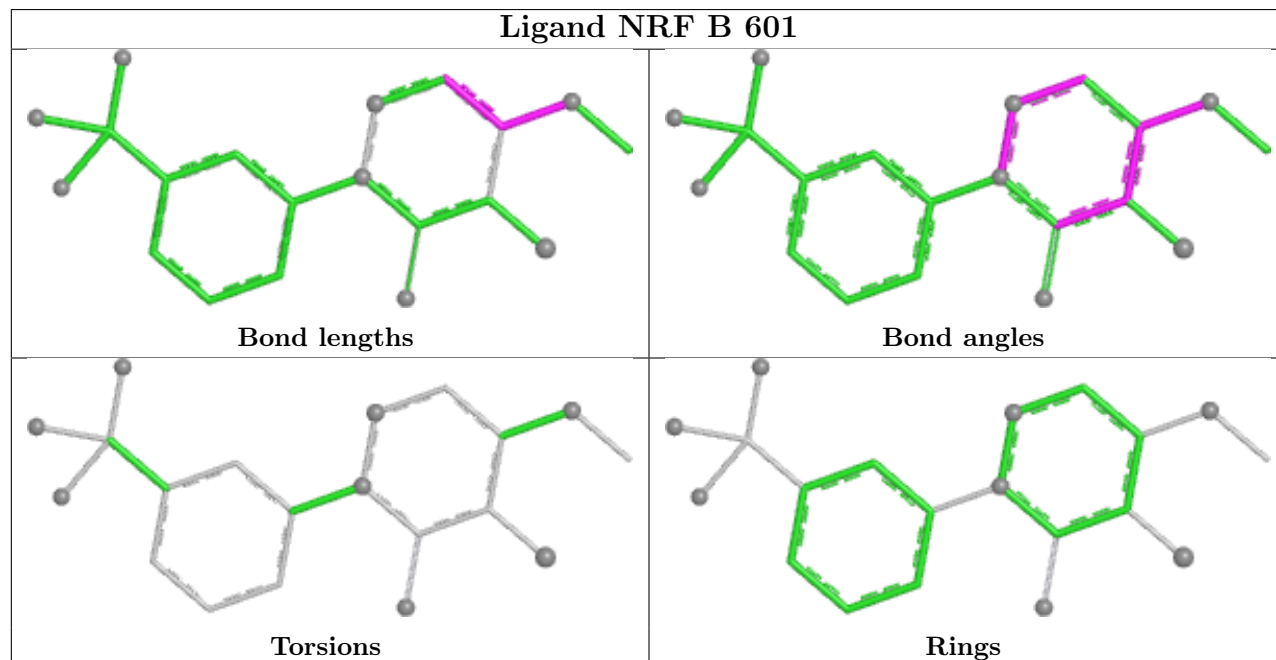
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

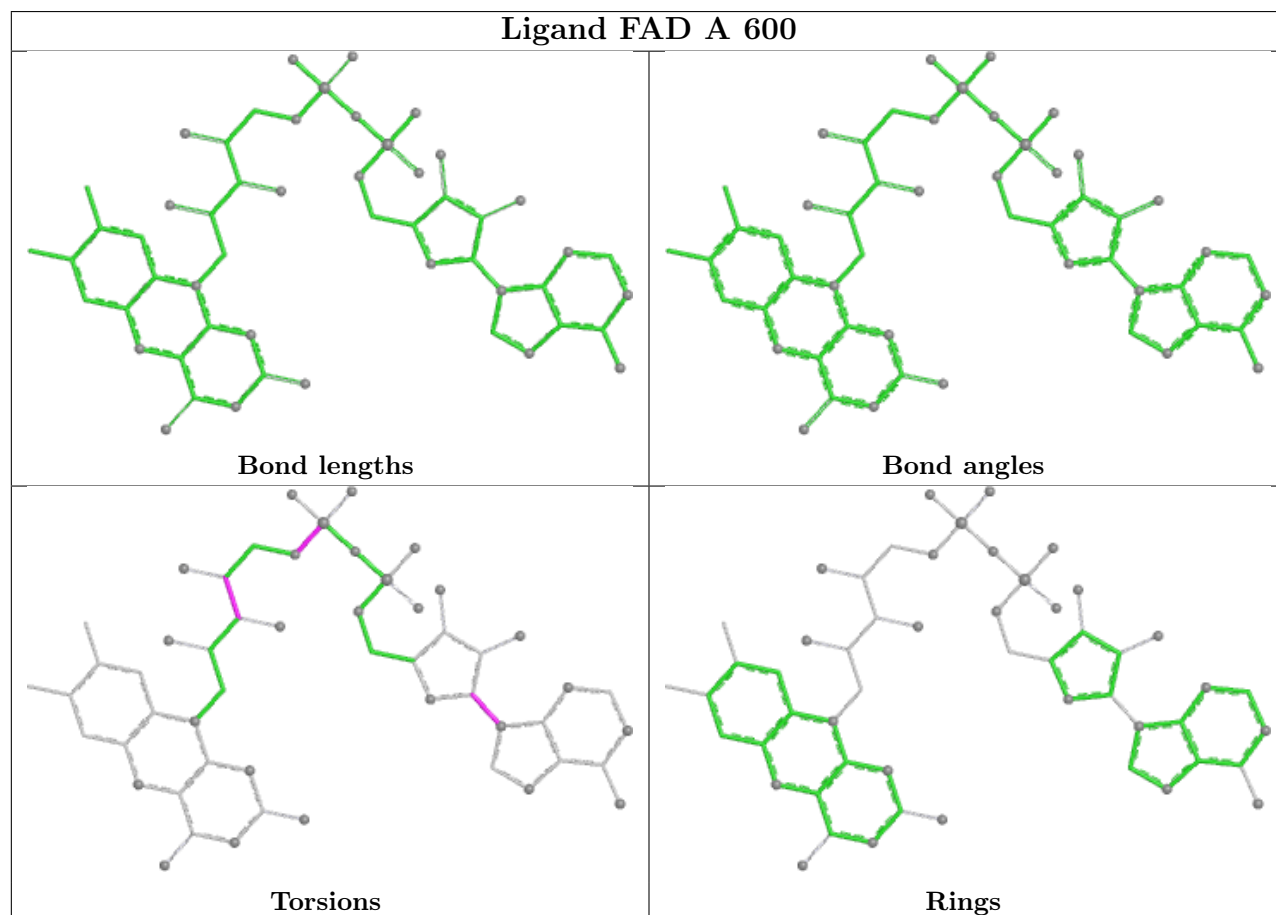
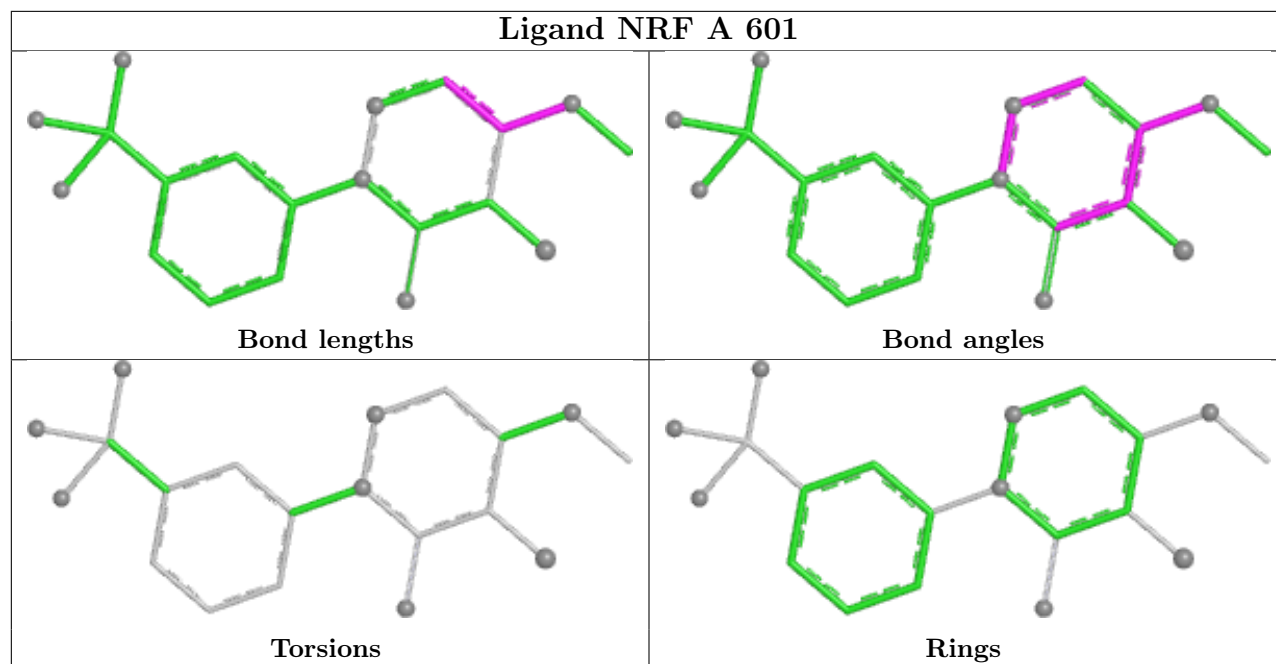


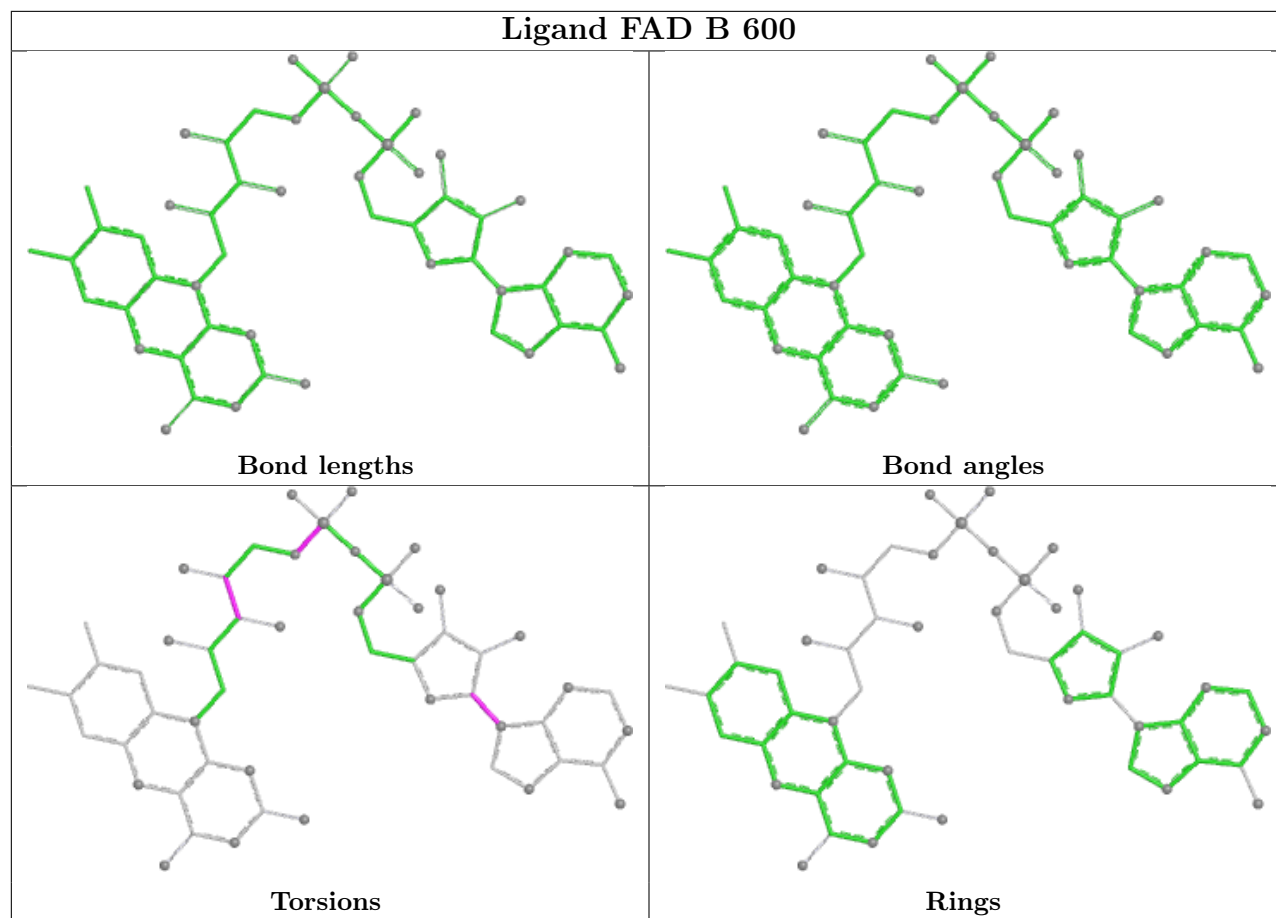
Ligand NRF E 601



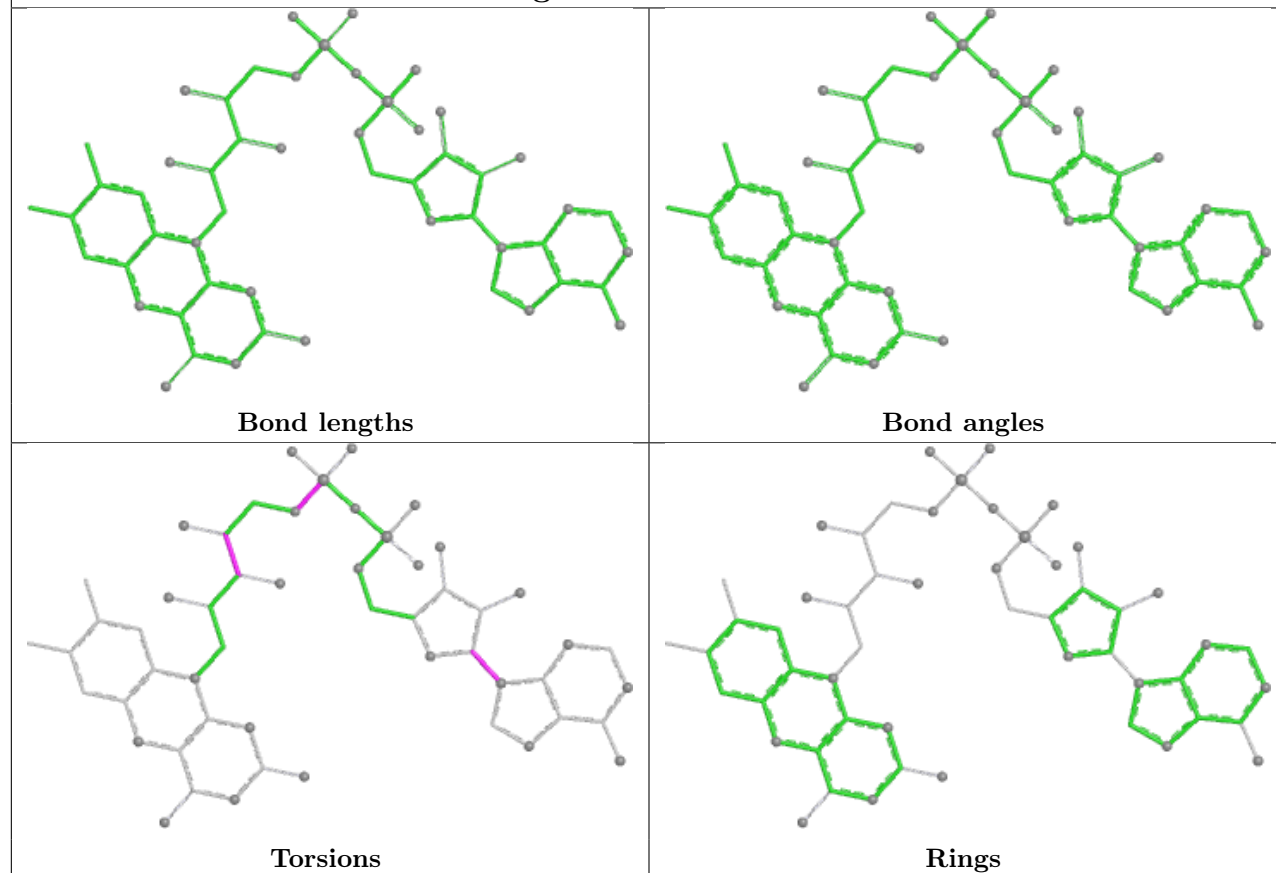
Ligand NRF B 601



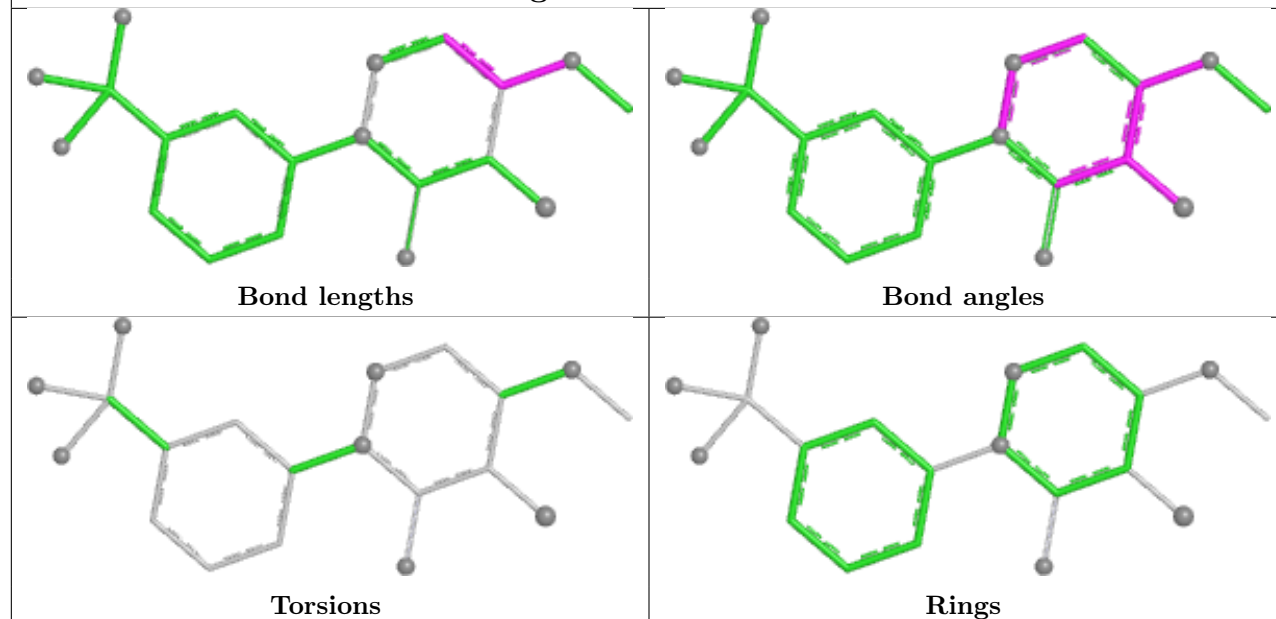


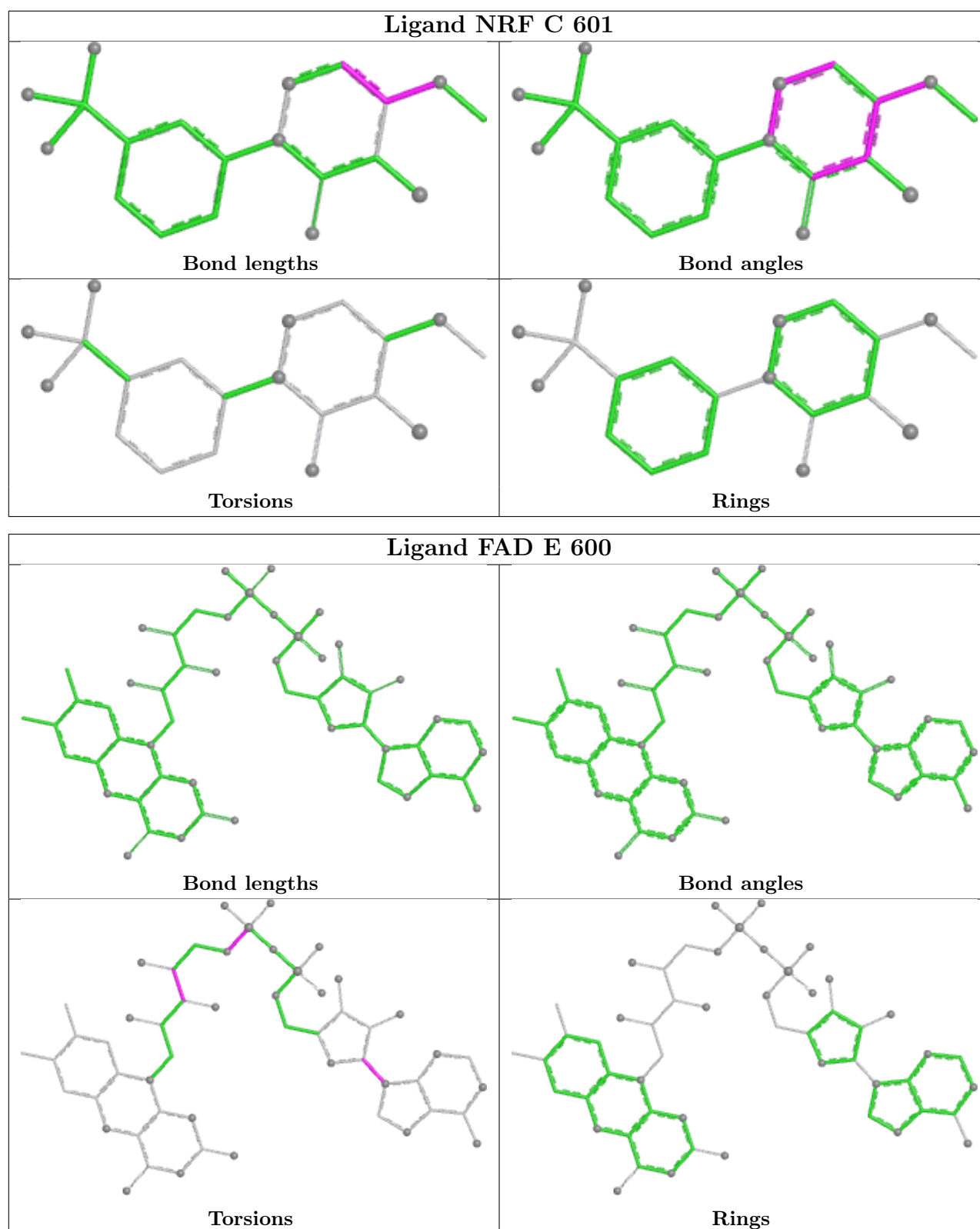


Ligand FAD C 600



Ligand NRF D 601





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	467/497 (93%)	0.21	14 (2%) 52 45	38, 58, 83, 139	0
1	B	472/497 (94%)	0.17	13 (2%) 55 47	33, 57, 89, 135	1 (0%)
1	C	470/497 (94%)	0.75	27 (5%) 29 24	47, 75, 102, 180	1 (0%)
1	D	470/497 (94%)	0.78	51 (10%) 10 8	47, 73, 105, 211	0
1	E	466/497 (93%)	2.09	221 (47%) 0 0	68, 125, 162, 215	0
All	All	2345/2485 (94%)	0.80	326 (13%) 6 5	33, 71, 142, 215	2 (0%)

All (326) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	567	LEU	11.8
1	E	567	LEU	5.7
1	E	461	VAL	5.6
1	E	499	VAL	5.6
1	E	454	PHE	5.4
1	E	494	LEU	5.1
1	E	453	VAL	4.9
1	E	382	VAL	4.8
1	E	452	LEU	4.8
1	E	377	ILE	4.8
1	E	498	VAL	4.8
1	A	564	ARG	4.8
1	E	468	ILE	4.7
1	E	374	PRO	4.6
1	E	450	LEU	4.6
1	E	493	ILE	4.6
1	A	565	ARG	4.5
1	E	406	VAL	4.5
1	E	381	LEU	4.5
1	E	344	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	431	VAL	4.4
1	D	105	LEU	4.3
1	E	518	LEU	4.3
1	E	359	THR	4.3
1	D	359	THR	4.3
1	E	485	ALA	4.2
1	E	404	ILE	4.2
1	E	486	ALA	4.2
1	E	501	THR	4.2
1	E	372	ALA	4.2
1	C	570	LEU	4.1
1	E	387	LYS	4.1
1	E	156	THR	4.1
1	E	433	ALA	4.1
1	E	371	PHE	4.1
1	D	567	LEU	4.0
1	C	549	LYS	4.0
1	E	394	LYS	4.0
1	E	376	ASP	4.0
1	E	380	LEU	4.0
1	D	570	LEU	3.9
1	E	487	ASP	3.9
1	E	503	ARG	3.9
1	E	469	ILE	3.9
1	E	142	LYS	3.8
1	E	457	ALA	3.8
1	E	502	PRO	3.8
1	B	564	ARG	3.8
1	E	403	VAL	3.8
1	E	139	LEU	3.8
1	E	473	MET	3.8
1	E	440	LYS	3.8
1	E	556	VAL	3.8
1	B	566	SER	3.7
1	E	536	LYS	3.7
1	E	345	ILE	3.7
1	E	496	TYR	3.7
1	E	358	LEU	3.6
1	E	189	ILE	3.6
1	D	102	THR	3.6
1	E	432	TYR	3.6
1	E	341	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	368	ALA	3.6
1	E	154	TYR	3.6
1	E	532	TYR	3.6
1	D	562	LEU	3.6
1	E	138	VAL	3.6
1	E	123	LEU	3.5
1	E	429	LEU	3.5
1	D	368	ALA	3.5
1	E	505	VAL	3.5
1	D	206	GLU	3.5
1	E	283	PHE	3.5
1	E	523	ILE	3.4
1	E	130	PRO	3.4
1	E	293	CYS	3.4
1	E	104	PRO	3.4
1	C	567	LEU	3.4
1	E	506	TYR	3.4
1	C	447[A]	ARG	3.3
1	D	127	GLY	3.3
1	B	565	ARG	3.3
1	E	402	PRO	3.3
1	E	451	GLU	3.3
1	E	539	ALA	3.3
1	C	562	LEU	3.3
1	E	489	SER	3.3
1	E	160	ILE	3.3
1	E	500	LYS	3.2
1	E	525	GLY	3.2
1	E	107	VAL	3.2
1	E	465	ASP	3.2
1	D	560	LYS	3.2
1	E	422	LEU	3.2
1	E	389	ILE	3.2
1	E	509	ILE	3.2
1	E	158	LEU	3.1
1	C	302	LEU	3.1
1	D	128	HIS	3.1
1	E	109	ILE	3.1
1	E	455	ALA	3.1
1	E	460	TRP	3.1
1	E	397	LYS	3.1
1	D	565	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	375	VAL	3.1
1	E	409	TRP	3.1
1	C	553	GLN	3.0
1	D	549	LYS	3.0
1	E	146	TRP	3.0
1	A	566	SER	3.0
1	E	349	PRO	3.0
1	D	129	LYS	3.0
1	C	102	THR	3.0
1	E	241	MET	3.0
1	E	462	GLY	3.0
1	E	343	GLN	3.0
1	E	102	THR	3.0
1	E	399	VAL	3.0
1	E	538	LEU	3.0
1	E	529	ALA	3.0
1	A	238	LEU	2.9
1	E	321	LEU	2.9
1	E	528	LEU	2.9
1	E	396	GLU	2.9
1	E	504	SER	2.9
1	E	364	ILE	2.9
1	E	379	LYS	2.9
1	E	122	TYR	2.9
1	D	334	GLY	2.9
1	E	329	VAL	2.9
1	C	359	THR	2.9
1	E	491	ALA	2.9
1	A	304	GLU	2.8
1	E	449	MET	2.8
1	E	342	ILE	2.8
1	D	332	LEU	2.8
1	E	464	SER	2.8
1	E	282	ASN	2.8
1	E	145	ALA	2.8
1	B	241	MET	2.8
1	E	391	TYR	2.8
1	E	430	SER	2.8
1	D	107	VAL	2.8
1	E	112	ALA	2.8
1	E	161	PHE	2.8
1	E	410	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	423	PHE	2.8
1	E	136	ARG	2.8
1	C	227	TRP	2.7
1	E	280	ALA	2.7
1	E	362	THR	2.7
1	E	466	THR	2.7
1	E	472	THR	2.7
1	C	387	LYS	2.7
1	E	312	PHE	2.7
1	D	369	TYR	2.7
1	E	495	LYS	2.7
1	E	559	TYR	2.7
1	E	497	HIS	2.7
1	D	304	GLU	2.7
1	C	107	VAL	2.7
1	D	362	THR	2.7
1	E	162	PHE	2.7
1	E	526	PHE	2.7
1	D	104	PRO	2.7
1	E	284	ILE	2.7
1	B	302	LEU	2.7
1	D	527	TYR	2.6
1	E	512	CYS	2.6
1	E	155	GLU	2.6
1	E	555	VAL	2.6
1	B	561	MET	2.6
1	C	560	LYS	2.6
1	E	400	GLY	2.6
1	D	108	VAL	2.6
1	E	370	VAL	2.6
1	D	227	TRP	2.6
1	E	323	MET	2.6
1	E	443	TYR	2.6
1	C	362	THR	2.6
1	C	571	GLN	2.6
1	D	364	ILE	2.6
1	E	232	LYS	2.6
1	E	415	LYS	2.6
1	E	490	LYS	2.6
1	D	571	GLN	2.6
1	E	405	ASN	2.6
1	E	150	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	171	LEU	2.5
1	E	412	ARG	2.5
1	E	418	TYR	2.5
1	E	246	ALA	2.5
1	E	356	PHE	2.5
1	A	101	PRO	2.5
1	E	301	PHE	2.5
1	B	102	THR	2.5
1	E	521	SER	2.5
1	E	456	PRO	2.5
1	A	303	GLN	2.5
1	D	356	PHE	2.5
1	E	392	PHE	2.5
1	E	393	LYS	2.5
1	E	131	ILE	2.5
1	E	340	SER	2.5
1	D	361	GLY	2.5
1	E	248	VAL	2.5
1	A	560	LYS	2.4
1	E	484	ILE	2.4
1	D	566	SER	2.4
1	E	416	ASN	2.4
1	C	118	SER	2.4
1	D	272	GLU	2.4
1	E	507	LYS	2.4
1	D	555	VAL	2.4
1	E	401	VAL	2.4
1	E	519	GLN	2.4
1	E	254	PHE	2.4
1	E	132	LEU	2.4
1	E	325	ILE	2.4
1	E	360	ASP	2.4
1	C	551	CYS	2.4
1	E	492	LYS	2.4
1	D	204	PHE	2.4
1	E	168	ILE	2.4
1	E	395	LEU	2.4
1	D	355	HIS	2.4
1	E	159	HIS	2.4
1	D	103	LYS	2.4
1	D	536	LYS	2.4
1	E	305	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	514	PRO	2.4
1	E	245	GLN	2.4
1	C	242	VAL	2.4
1	A	364	ILE	2.3
1	D	367	ASP	2.3
1	D	216	TRP	2.3
1	B	220[A]	ARG	2.3
1	E	313	LEU	2.3
1	E	373	THR	2.3
1	B	216	TRP	2.3
1	C	244	GLY	2.3
1	D	366	GLY	2.3
1	E	111	GLY	2.3
1	E	553	GLN	2.3
1	E	338	LEU	2.3
1	E	398	LEU	2.3
1	E	546	LEU	2.3
1	E	408	ILE	2.3
1	E	562	LEU	2.3
1	E	135	ALA	2.3
1	E	297	ALA	2.3
1	E	549	LYS	2.3
1	E	560	LYS	2.3
1	C	245	GLN	2.3
1	E	378	LEU	2.3
1	E	458	GLU	2.2
1	E	537	TYR	2.2
1	D	353	VAL	2.2
1	E	332	LEU	2.2
1	A	415	LYS	2.2
1	B	95	PHE	2.2
1	C	120	ALA	2.2
1	D	333	GLY	2.2
1	E	421	LEU	2.2
1	E	121	LYS	2.2
1	E	279	LYS	2.2
1	E	310	MET	2.2
1	E	420	HIS	2.2
1	D	124	ALA	2.2
1	A	102	THR	2.2
1	E	481	PRO	2.2
1	D	360	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	480	PHE	2.2
1	E	250	ALA	2.2
1	E	508	THR	2.2
1	B	96	ARG	2.2
1	E	551	CYS	2.2
1	E	266	PRO	2.2
1	C	394	LYS	2.2
1	D	131	ILE	2.2
1	E	177	ILE	2.2
1	B	206	GLU	2.1
1	E	288	GLU	2.1
1	E	337	ARG	2.1
1	A	561	MET	2.1
1	D	302	LEU	2.1
1	E	347	LEU	2.1
1	E	390	SER	2.1
1	B	227	TRP	2.1
1	E	522	PRO	2.1
1	E	237	LEU	2.1
1	E	442	TYR	2.1
1	D	125	ASP	2.1
1	E	190	PHE	2.1
1	E	164	ALA	2.1
1	D	564	ARG	2.1
1	E	417	THR	2.1
1	C	519	GLN	2.1
1	E	488	GLN	2.1
1	E	322	CYS	2.1
1	E	361	GLY	2.1
1	D	215	ILE	2.1
1	E	354	LYS	2.1
1	E	181	LEU	2.1
1	E	336	VAL	2.1
1	E	199	PHE	2.1
1	C	486	ALA	2.0
1	D	483	GLU	2.0
1	E	463	ARG	2.0
1	E	557	GLU	2.0
1	E	565	ARG	2.0
1	E	118	SER	2.0
1	A	440	LYS	2.0
1	E	351	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	515	CYS	2.0
1	E	470	GLU	2.0
1	D	568	LYS	2.0
1	E	311	ALA	2.0
1	E	531	ASP	2.0
1	D	563	SER	2.0
1	C	241	MET	2.0
1	C	417	THR	2.0
1	E	438	THR	2.0
1	E	407	HIS	2.0
1	C	565	ARG	2.0
1	D	447	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	IMD	D	603	5/5	0.52	0.41	122,122,123,123	0
4	EPE	E	602	15/15	0.53	0.26	143,148,161,161	0
4	EPE	A	603	15/15	0.54	0.34	140,147,160,160	0
4	EPE	B	603	15/15	0.69	0.22	100,110,131,132	0
5	IMD	B	606	5/5	0.78	0.26	94,94,95,95	0
6	TRS	B	604	8/8	0.78	0.22	102,105,107,108	0
5	IMD	D	604	5/5	0.80	0.31	114,114,114,114	0
2	FAD	E	600	53/53	0.80	0.15	93,117,145,145	0
5	IMD	D	605	5/5	0.85	0.23	98,98,98,98	0
5	IMD	B	605	5/5	0.86	0.33	112,112,113,113	0
6	TRS	D	602	8/8	0.86	0.17	100,103,104,105	0

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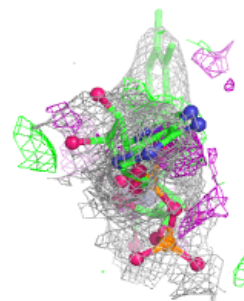
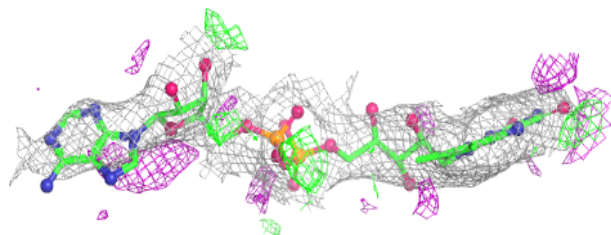
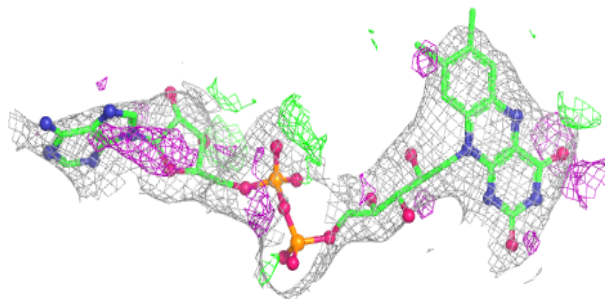
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NRF	E	601	20/20	0.87	0.14	95,100,102,102	0
5	IMD	A	604	5/5	0.88	0.24	108,108,108,108	0
4	EPE	A	602	15/15	0.90	0.17	80,84,91,92	0
4	EPE	B	602	15/15	0.90	0.16	78,85,91,91	0
2	FAD	D	600	53/53	0.95	0.08	48,56,62,63	0
2	FAD	C	600	53/53	0.95	0.08	44,57,62,63	0
3	NRF	C	601	20/20	0.96	0.08	59,66,68,68	0
3	NRF	D	601	20/20	0.96	0.09	57,63,68,68	0
2	FAD	B	600	53/53	0.97	0.07	38,45,48,49	0
2	FAD	A	600	53/53	0.97	0.06	31,39,45,47	0
3	NRF	A	601	20/20	0.97	0.07	42,48,51,52	0
3	NRF	B	601	20/20	0.97	0.07	39,48,54,58	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.

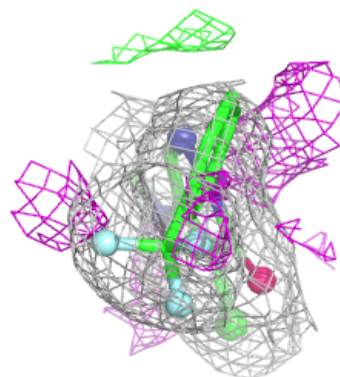
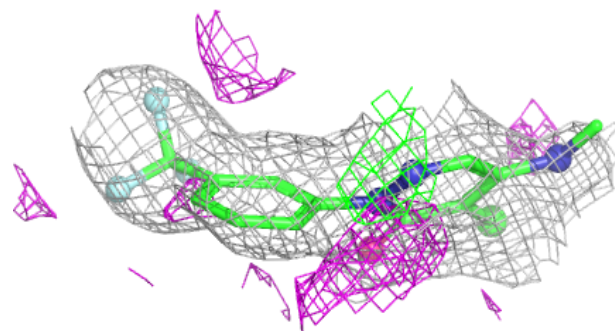
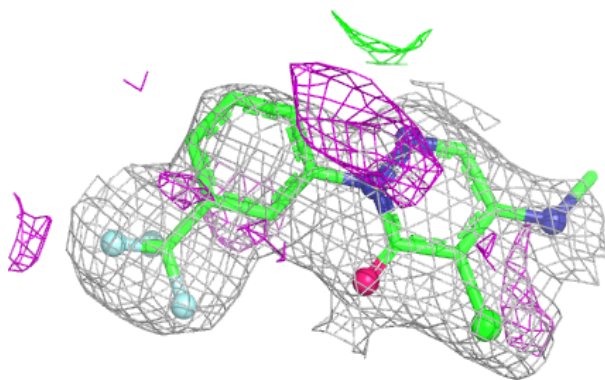
Electron density around FAD E 600:

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

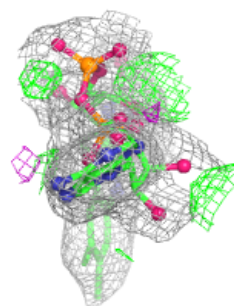
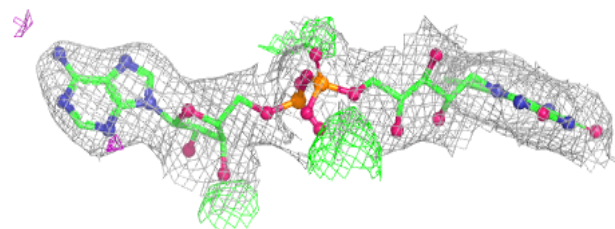
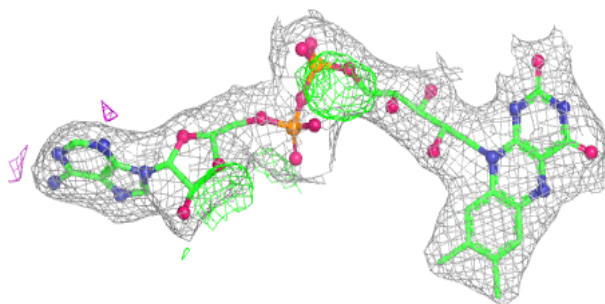


Electron density around NRF E 601:

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and green (positive)

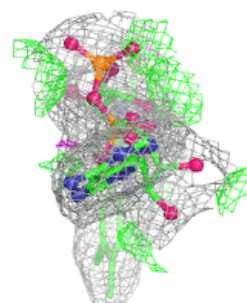
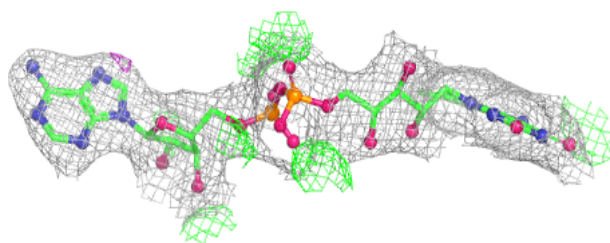
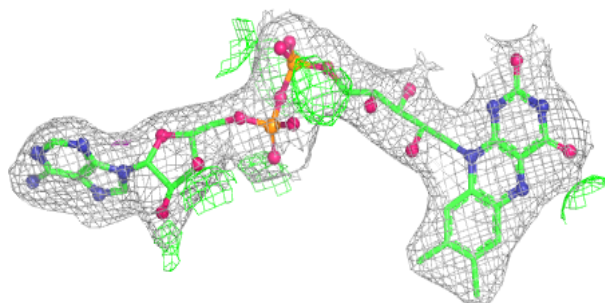
**Electron density around FAD D 600:**

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and green (positive)

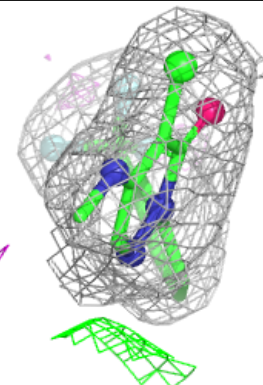
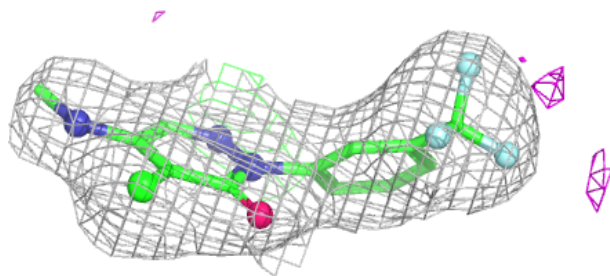
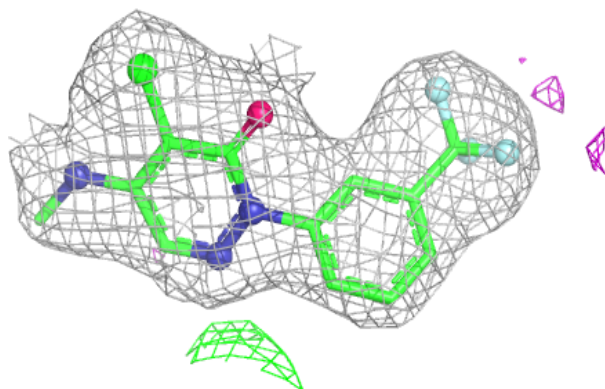


Electron density around FAD C 600:

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and green (positive)

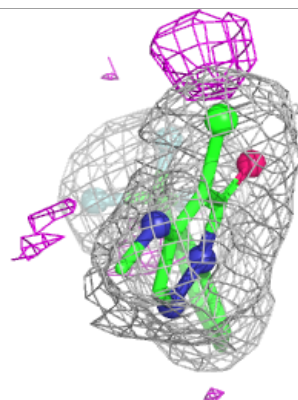
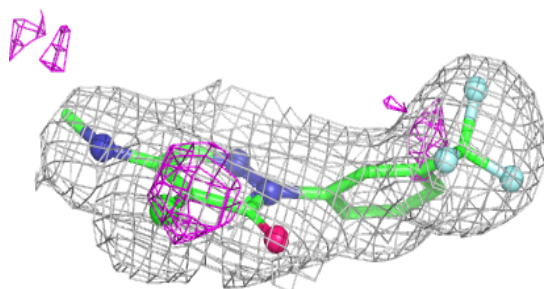
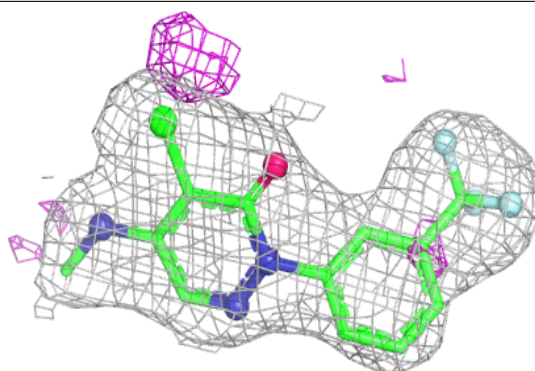
**Electron density around NRF C 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

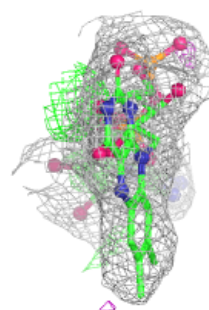
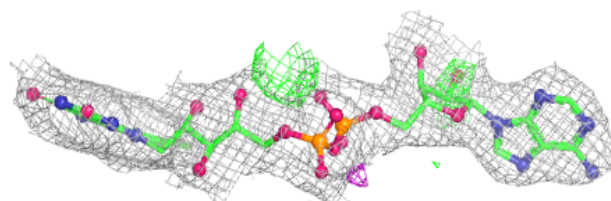
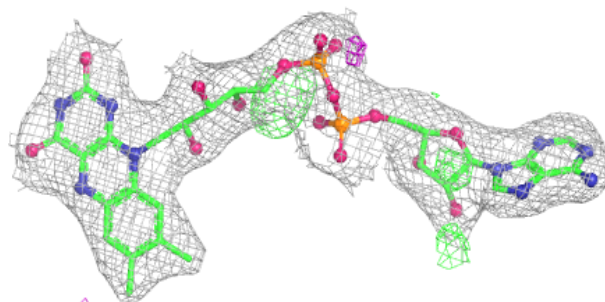


Electron density around NRF D 601:

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and green (positive)

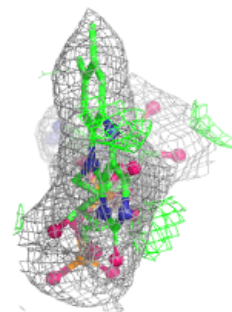
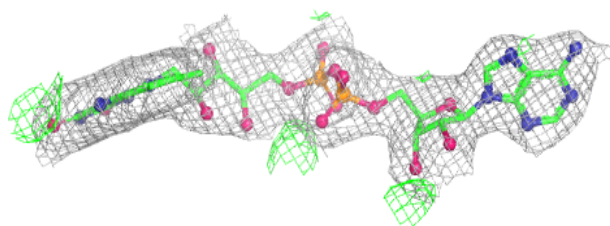
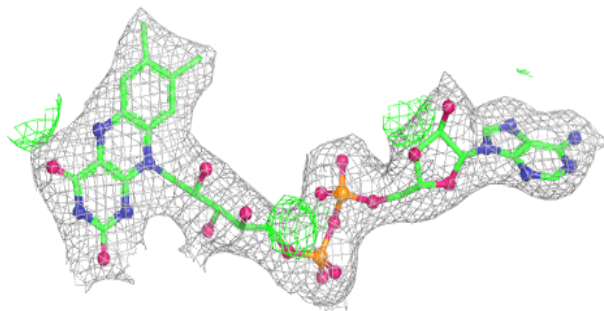
**Electron density around FAD B 600:**

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and green (positive)

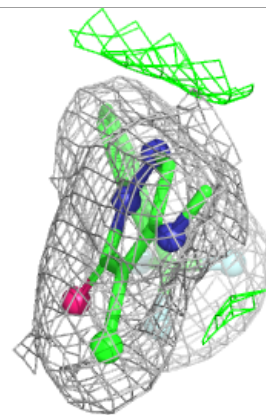
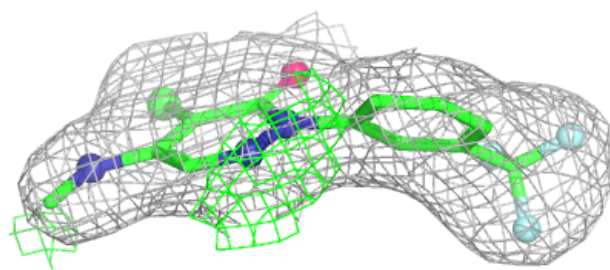
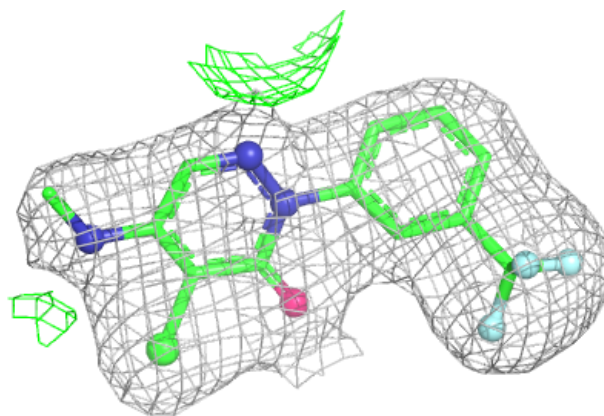


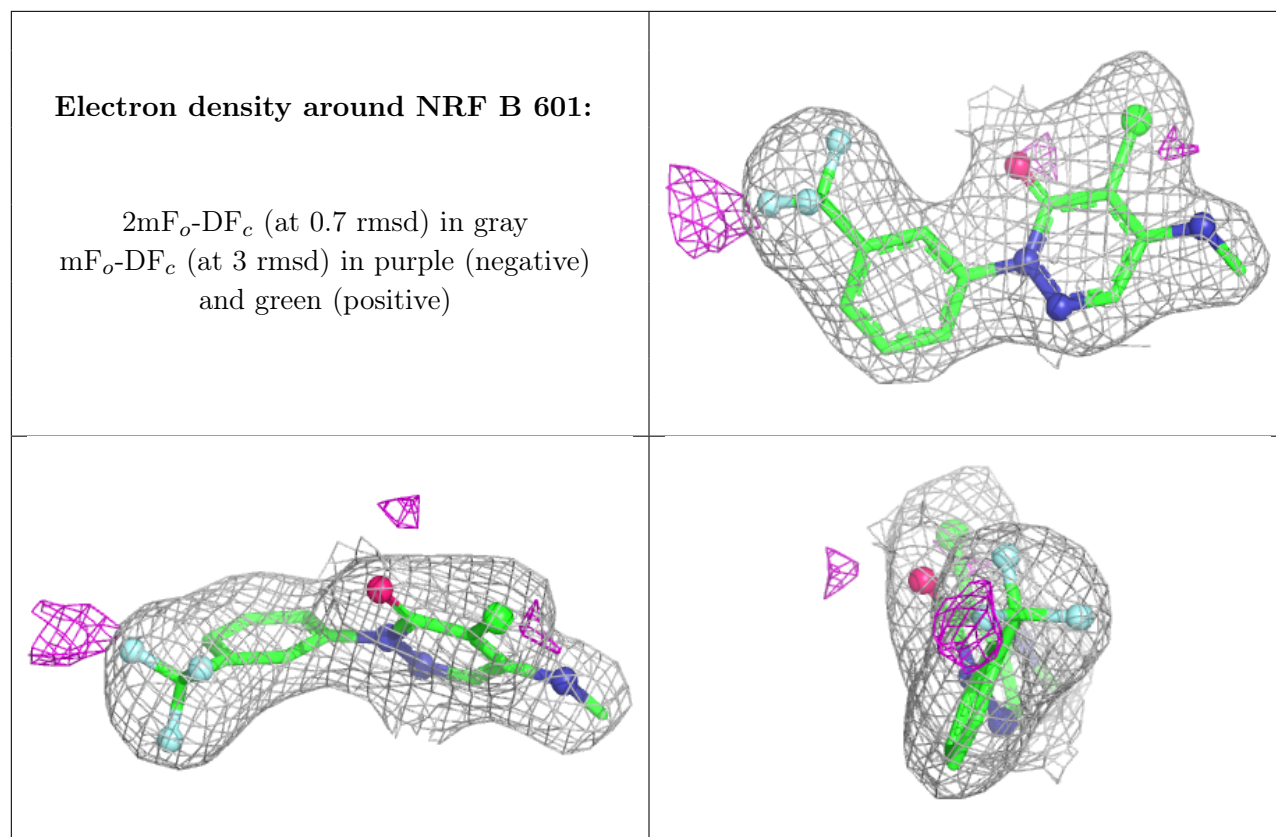
Electron density around FAD A 600:

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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.