



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:46 pm BST

PDB ID : 1H6V  
Title : Mammalian thioredoxin reductase  
Authors : Sandalova, T.; Zhong, L.; Lindqvist, Y.; Holmgren, A.; Schneider, G.  
Deposited on : 2001-06-27  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

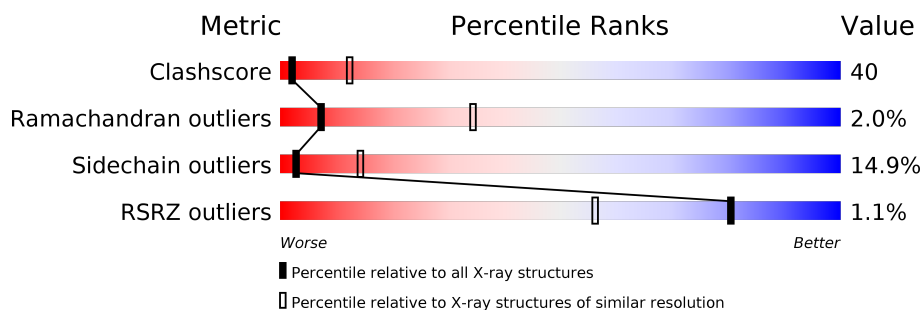
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	499	
1	B	499	
1	C	499	
1	D	499	
1	E	499	
1	F	499	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23075 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 THIOREDOXIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3764	2391	635	716	22			
1	B	487	Total	C	N	O	S	0	0	0
			3753	2387	633	713	20			
1	C	482	Total	C	N	O	S	0	0	0
			3707	2356	627	704	20			
1	D	487	Total	C	N	O	S	0	0	0
			3753	2387	633	713	20			
1	E	491	Total	C	N	O	S	0	0	0
			3773	2397	637	717	22			
1	F	490	Total	C	N	O	S	0	0	0
			3764	2391	635	716	22			

There are 11 discrepancies between the modelled and reference sequences:

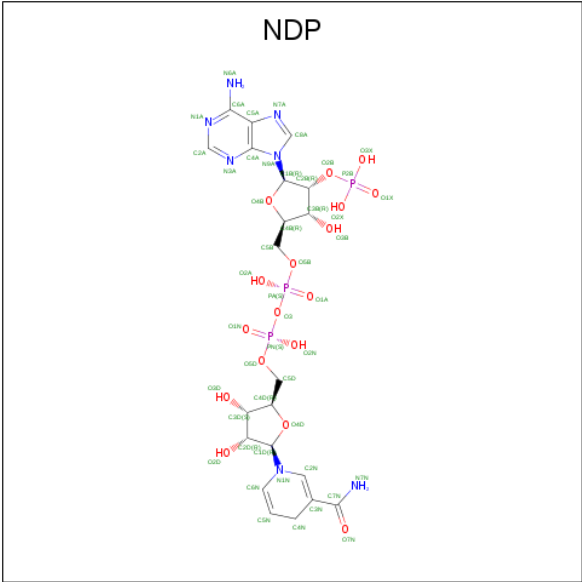
Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ASN	ARG	conflict	UNP O89049
B	52	ASN	ARG	conflict	UNP O89049
C	52	ASN	ARG	conflict	UNP O89049
D	52	ASN	ARG	conflict	UNP O89049
E	52	ASN	ARG	conflict	UNP O89049
F	52	ASN	ARG	conflict	UNP O89049
A	497	CYS	SEL	engineered mutation	UNP O89049
B	497	CYS	SEL	engineered mutation	UNP O89049
C	497	CYS	SEL	engineered mutation	UNP O89049
D	497	CYS	SEL	engineered mutation	UNP O89049
E	497	CYS	SEL	engineered mutation	UNP O89049

- 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		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	B	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	C	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	D	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	E	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	F	1	Total	C	N	O	P	0	0
			39	15	5	16	3		

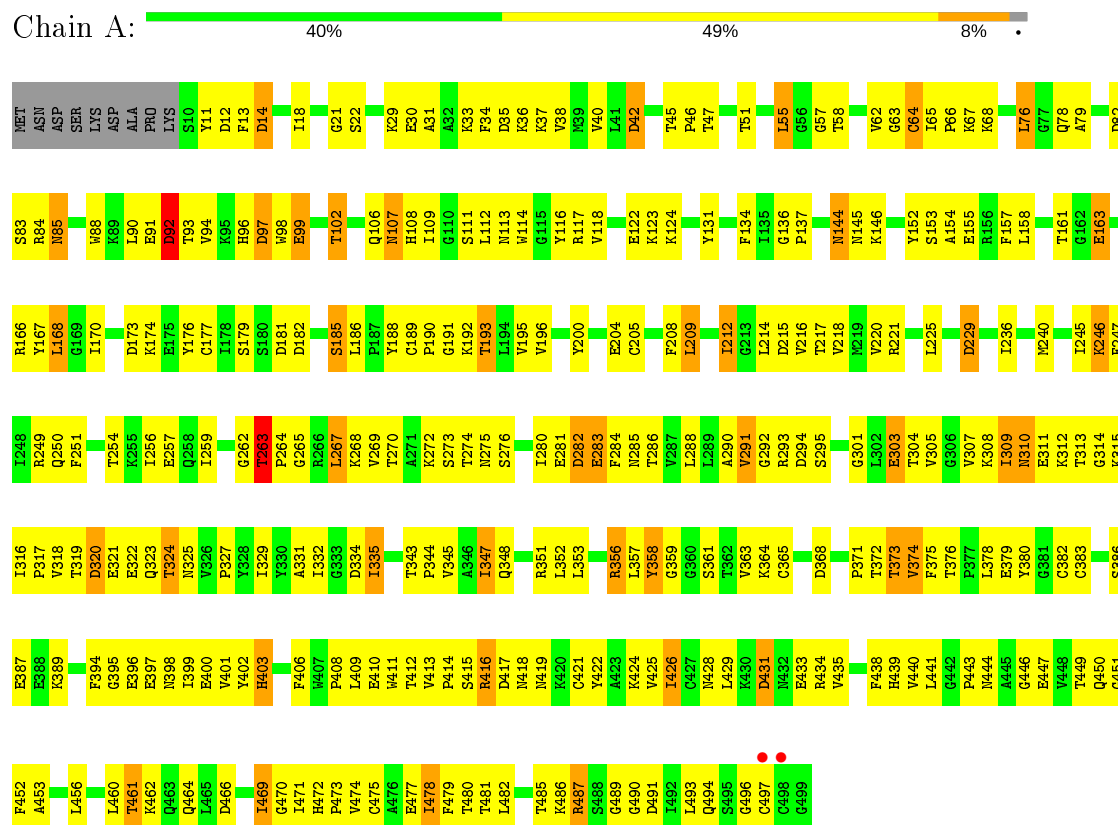
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	C	3	Total	O	0	0
			3	3		
4	D	1	Total	O	0	0
			1	1		
4	E	2	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			1	1		

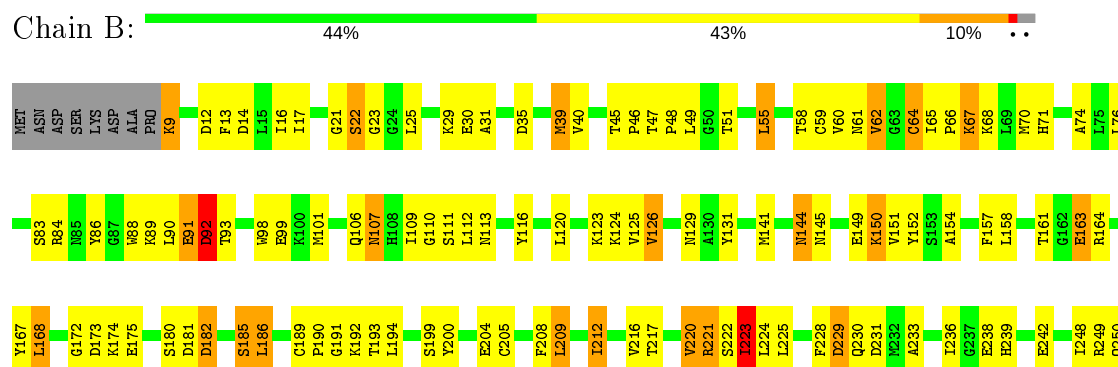
### 3 Residue-property plots

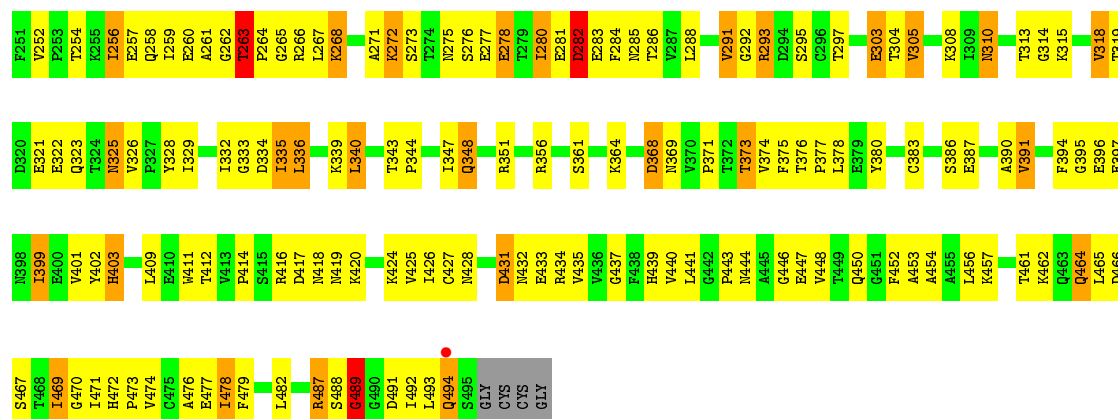
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: THIOREDOXIN REDUCTASE

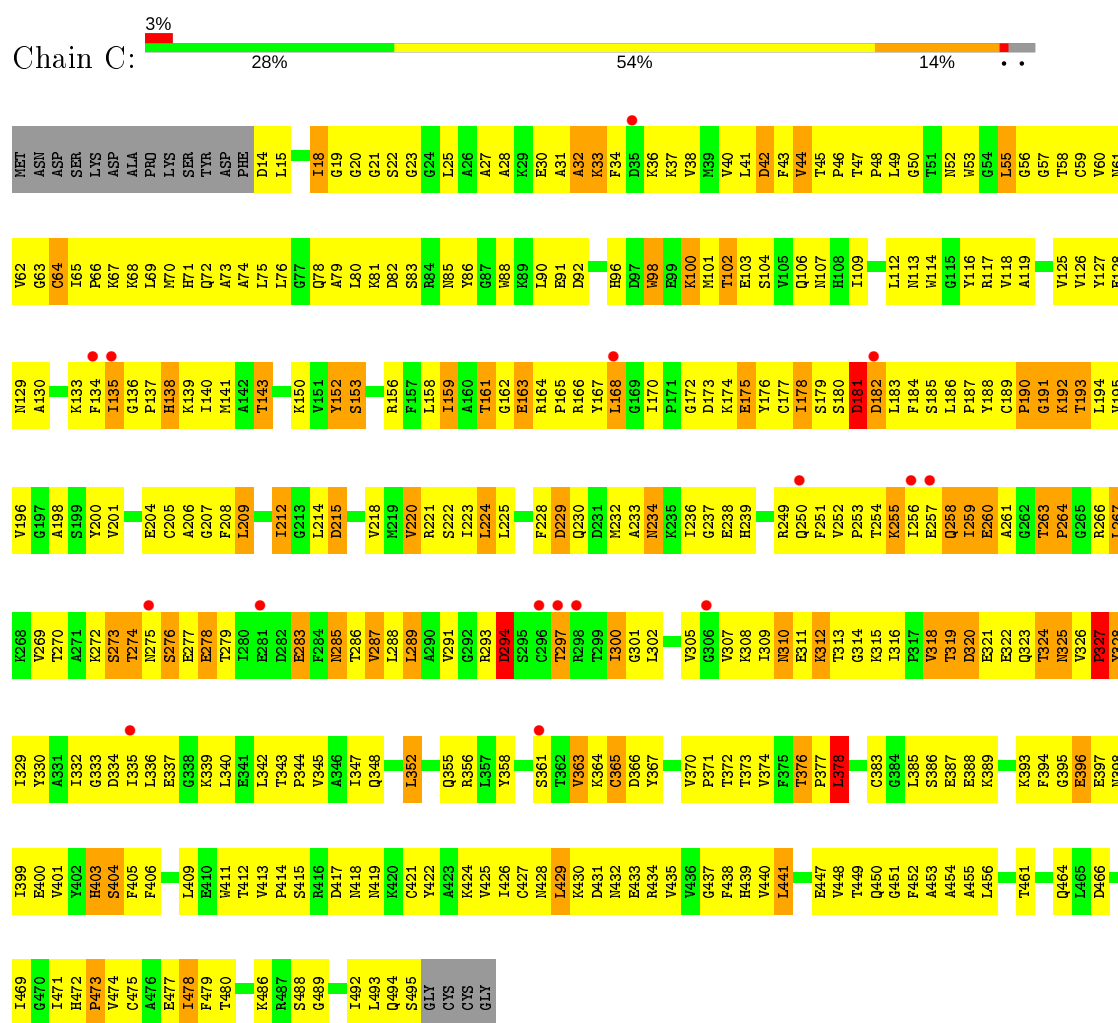


#### • Molecule 1: THIOREDOXIN REDUCTASE

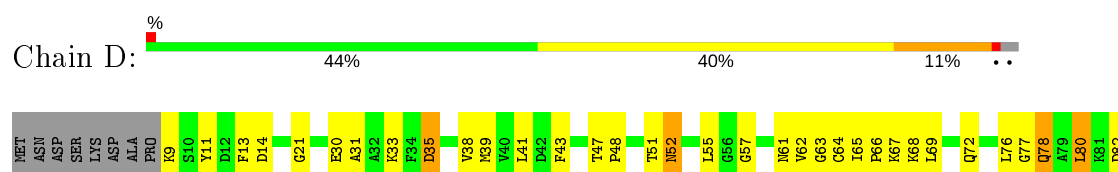


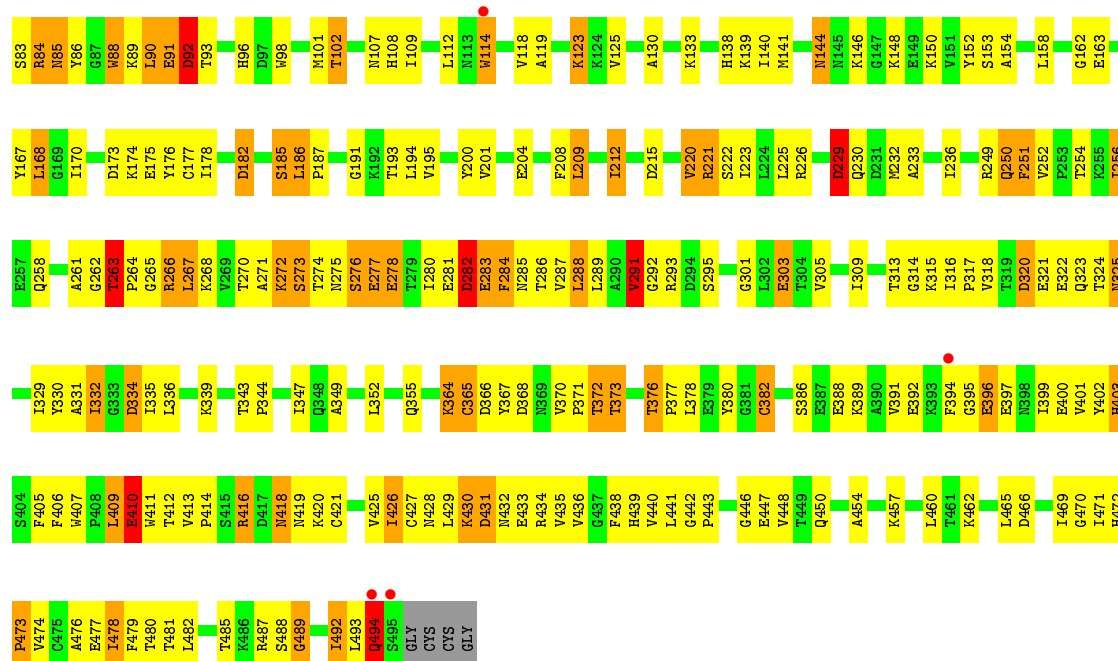


### • Molecule 1: THIOREDOXIN REDUCTASE

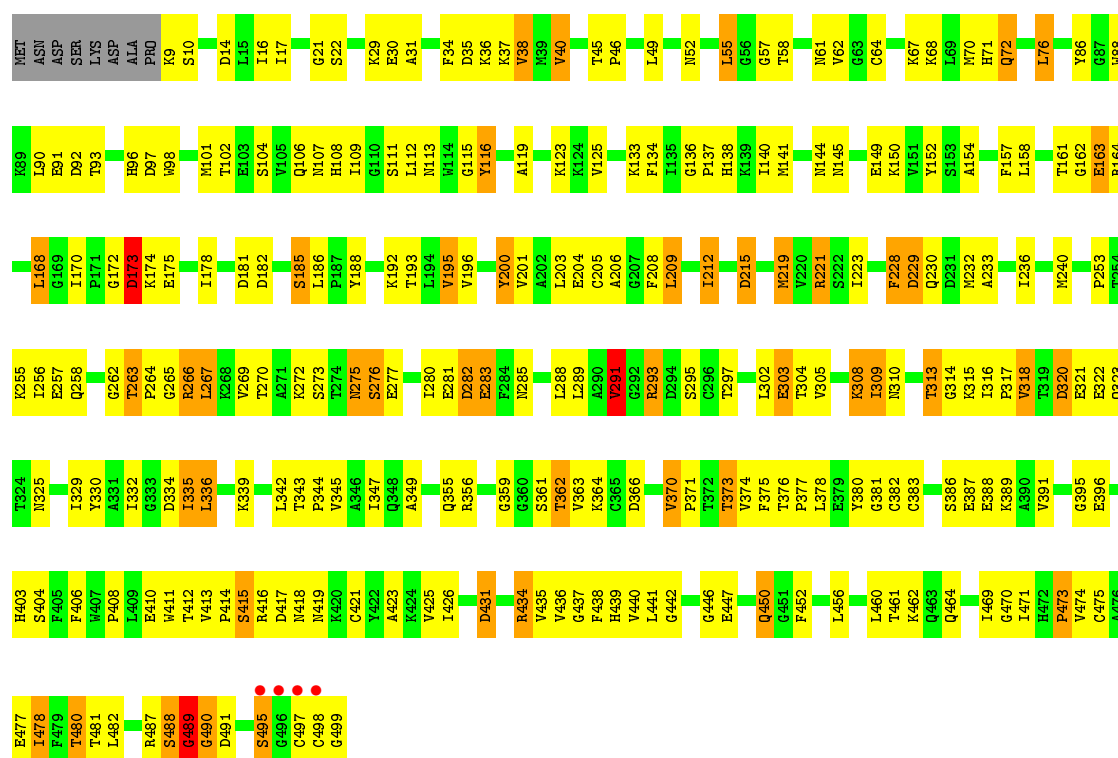


### • Molecule 1: THIOREDOXIN REDUCTASE

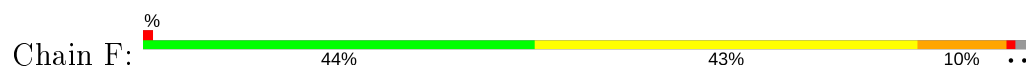




### • Molecule 1: THIOREDOXIN REDUCTASE



### • Molecule 1: THIOREDOXIN REDUCTASE





I469	V391	K345	E242	L168	D82	MET
G470	E392	V318	K246	G169	S83	ASN
I471		T319		I170	R84	ASP
H472	G395	D320	R349	P471		SER
P473	E396	E321	Q250	G172	K89	LYS
V474	E400	E322	Q250	D173	L90	ASP
C475		Q323	V252	K174	E91	ALA
A476		Q323	V252	E175	D92	PRO
I477	H403	T324	P253		T93	LYS
E478	S404	N325	T254	I178	V94	S10
F479	F405		K255	S179	G95	Y11
T480	F406	I329	I256	S180	H96	D12
		Y330	E257	D181	D97	F13
K486	W411	I332	Q258	D182	E99	D14
R487	T412	I332				L15
S488	V413	D334	A261	S185	K100	
G489	P414	I335	G262	L186	M101	G20
A490	S415	I336	T263	P187	T102	G21
D491	R416		P264	I188	E103	S22
I492	D417	K339	G265	C189	S104	
L493	N418	R266	R266	P190	V105	K29
Q494	N419	L340	L267	G191	Q106	E39
S495	K420			K192	N107	A31
G496	C421	T343	T270	T193	H108	A32
C497	Y422	P344		L194	I109	K33
C498	K423	I347	S273	V195	G110	F34
G499	V425	Q348	T274	V196	L112	D85
	I426		N275		N113	
	C427	R351	E277	L203		V38
	N428	L352			Y116	K39
		L353	I280	F208		V40
	D431	A354	E281	L209		L41
		Q355	D282	K123	K124	D42
	R434	R356	E283	I212	K123	
V435	V435		F284	G213		T47
V436		S361	N285	L214	Y131	P48
G437	F438	T362	T286	T217		L49
F438	H439	V363	V287	H138	P137	
H439	V440	K364	L288	K139	H138	L55
V440		C365	L289	R221	T140	G56
	L441		A290	G222	M141	G57
G442	G442	D368	V291	S222	A142	T58
		N369	G292	I223	C142	C59
G446	G446	V370	R293	L224	N144	V60
E447	V448	P371	D294	L225		
		T372	S295			V62
T449	Q450	T373	C296	F228	K150	G63
		V374	T297	D229	Y151	C64
		F375		Q230	S153	I65
				D231	A154	P66
	K457	L302	L302	N232	K67	
C458	C458	L378	E303	K233	K68	
		F379	T304	A233	L158	L69
T461	R462	Y380	V305	N234	I159	H70
Q463	Q464	G381	K308	K235	G162	H71
				G237	E163	Q72
L465	L465	E387	I309	E238		
D466		E388		H239	L76	
		K389	T313	N240		
		R390	C314	E240	R166	
				E240	Y165	V31

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.92Å 140.46Å 170.83Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.86 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-3.00) 92.5 (29.86-2.99)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.224 , 0.263 0.257 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 4.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	23075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NDP, 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	0.92	0/3838	1.07	15/5193 (0.3%)
1	B	0.90	0/3827	1.04	14/5178 (0.3%)
1	C	0.82	1/3779 (0.0%)	1.03	15/5114 (0.3%)
1	D	0.97	3/3827 (0.1%)	1.08	16/5178 (0.3%)
1	E	0.99	2/3847 (0.1%)	1.11	16/5204 (0.3%)
1	F	0.80	0/3838	1.03	14/5193 (0.3%)
All	All	0.90	6/22956 (0.0%)	1.06	90/31060 (0.3%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	489	GLY	C-O	-6.05	1.14	1.23
1	D	410	GLU	CD-OE1	5.80	1.32	1.25
1	D	114	TRP	CB-CG	-5.08	1.41	1.50
1	C	300	ILE	C-O	-5.07	1.13	1.23
1	D	88	TRP	CB-CG	-5.03	1.41	1.50

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ASP	CB-CG-OD2	9.47	126.82	118.30
1	F	229	ASP	CB-CG-OD2	9.21	126.59	118.30
1	F	417	ASP	CB-CG-OD2	8.16	125.65	118.30
1	E	282	ASP	CB-CG-OD2	7.91	125.42	118.30
1	F	466	ASP	CB-CG-OD2	7.83	125.35	118.30

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	3764	0	3764	309	0
1	B	3753	0	3763	287	0
1	C	3707	0	3721	463	0
1	D	3753	0	3761	294	0
1	E	3773	0	3777	257	0
1	F	3764	0	3764	300	0
2	A	53	0	31	5	0
2	B	53	0	31	10	0
2	C	53	0	31	17	0
2	D	53	0	31	4	0
2	E	53	0	31	3	0
2	F	53	0	31	5	0
3	A	39	0	18	2	0
3	B	39	0	18	8	0
3	C	39	0	18	6	0
3	D	39	0	18	6	0
3	E	39	0	18	1	0
3	F	39	0	18	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	2	0
4	D	1	0	0	0	0
4	E	2	0	0	1	0
4	F	1	0	0	0	0
All	All	23075	0	22844	1832	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 40.

The worst 5 of 1832 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:C:98:TRP:NE1	1:C:190:PRO:HD2	1.54	1.21
1:C:98:TRP:CD1	1:C:189:CYS:HA	1.76	1.20
1:D:477:GLU:O	1:D:480:THR:HG22	1.49	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LEU:HD13	1:C:441:LEU:HD11	1.13	1.12
1:C:98:TRP:CZ3	1:C:102:THR:HG23	1.85	1.12

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	488/499 (98%)	445 (91%)	36 (7%)	7 (1%)	11	43
1	B	485/499 (97%)	436 (90%)	40 (8%)	9 (2%)	8	36
1	C	480/499 (96%)	395 (82%)	70 (15%)	15 (3%)	4	23
1	D	485/499 (97%)	439 (90%)	37 (8%)	9 (2%)	8	36
1	E	489/499 (98%)	441 (90%)	39 (8%)	9 (2%)	8	37
1	F	488/499 (98%)	438 (90%)	40 (8%)	10 (2%)	7	34
All	All	2915/2994 (97%)	2594 (89%)	262 (9%)	59 (2%)	7	34

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	THR
1	A	489	GLY
1	B	92	ASP
1	B	263	THR
1	B	314	GLY

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/414 (98%)	352 (87%)	54 (13%)	4	17
1	B	405/414 (98%)	344 (85%)	61 (15%)	3	14
1	C	400/414 (97%)	325 (81%)	75 (19%)	1	8
1	D	405/414 (98%)	342 (84%)	63 (16%)	2	13
1	E	407/414 (98%)	354 (87%)	53 (13%)	4	19
1	F	406/414 (98%)	349 (86%)	57 (14%)	3	16
All	All	2429/2484 (98%)	2066 (85%)	363 (15%)	3	14

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	310	ASN
1	D	168	LEU
1	F	250	GLN
1	C	325	ASN
1	C	404	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	418	ASN
1	D	108	HIS
1	F	250	GLN
1	C	444	ASN
1	D	61	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

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NDP	E	601	-	36,42,52	1.48	6 (16%)	43,65,80	1.33	4 (9%)
2	FAD	B	600	-	51,58,58	1.46	10 (19%)	60,89,89	1.82	13 (21%)
3	NDP	C	601	-	36,42,52	1.56	8 (22%)	43,65,80	1.72	10 (23%)
2	FAD	D	600	-	51,58,58	1.59	10 (19%)	60,89,89	1.91	13 (21%)
3	NDP	A	601	-	36,42,52	1.49	5 (13%)	43,65,80	1.57	7 (16%)
2	FAD	F	600	-	51,58,58	1.31	6 (11%)	60,89,89	1.78	11 (18%)
2	FAD	A	600	-	51,58,58	1.39	5 (9%)	60,89,89	2.00	14 (23%)
2	FAD	C	600	-	51,58,58	1.49	8 (15%)	60,89,89	2.10	18 (30%)
2	FAD	E	600	-	51,58,58	1.55	8 (15%)	60,89,89	2.39	15 (25%)
3	NDP	F	601	-	36,42,52	1.55	7 (19%)	43,65,80	1.43	8 (18%)
3	NDP	D	601	-	36,42,52	1.45	5 (13%)	43,65,80	1.67	9 (20%)
3	NDP	B	601	-	36,42,52	1.77	9 (25%)	43,65,80	1.52	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	E	601	-	-	5/23/56/77	0/4/4/5
2	FAD	B	600	-	-	4/30/50/50	0/6/6/6
3	NDP	C	601	-	-	5/23/56/77	0/4/4/5
2	FAD	D	600	-	-	5/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	A	601	-	-	13/23/56/77	0/4/4/5
2	FAD	F	600	-	-	10/30/50/50	0/6/6/6
2	FAD	A	600	-	-	9/30/50/50	0/6/6/6
2	FAD	C	600	-	-	10/30/50/50	0/6/6/6
2	FAD	E	600	-	-	10/30/50/50	0/6/6/6
3	NDP	F	601	-	-	6/23/56/77	0/4/4/5
3	NDP	D	601	-	-	12/23/56/77	0/4/4/5
3	NDP	B	601	-	-	9/23/56/77	0/4/4/5

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C2A-N3A	4.49	1.39	1.32
2	E	600	FAD	C2A-N3A	4.48	1.39	1.32
2	B	600	FAD	C2A-N3A	4.41	1.39	1.32
2	D	600	FAD	C2A-N3A	4.29	1.39	1.32
3	C	601	NDP	P2B-O3X	4.17	1.70	1.54

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	FAD	C1'-N10-C10	9.86	127.24	118.41
2	E	600	FAD	C5X-C9A-N10	8.13	123.61	117.72
2	A	600	FAD	P-O3P-PA	-6.71	109.79	132.83
2	D	600	FAD	P-O3P-PA	-6.11	111.86	132.83
2	F	600	FAD	C4-N3-C2	5.78	120.02	115.14

There are no chirality outliers.

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	FAD	C2'-C1'-N10-C9A
3	C	601	NDP	O4B-C4B-C5B-O5B
3	C	601	NDP	PA-O3-PN-O5D
2	D	600	FAD	O4B-C4B-C5B-O5B
2	D	600	FAD	PA-O3P-P-O5'

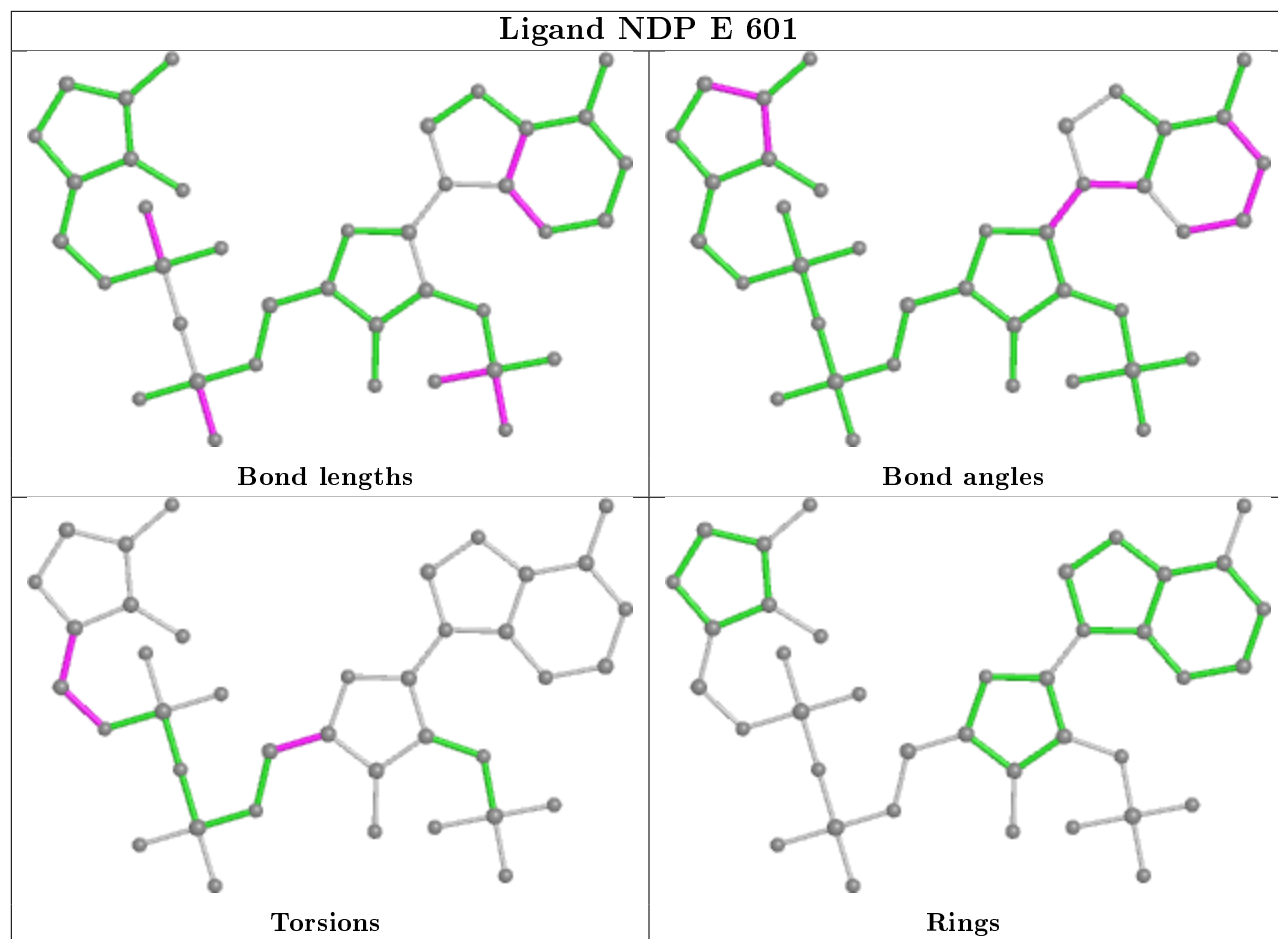
There are no ring outliers.

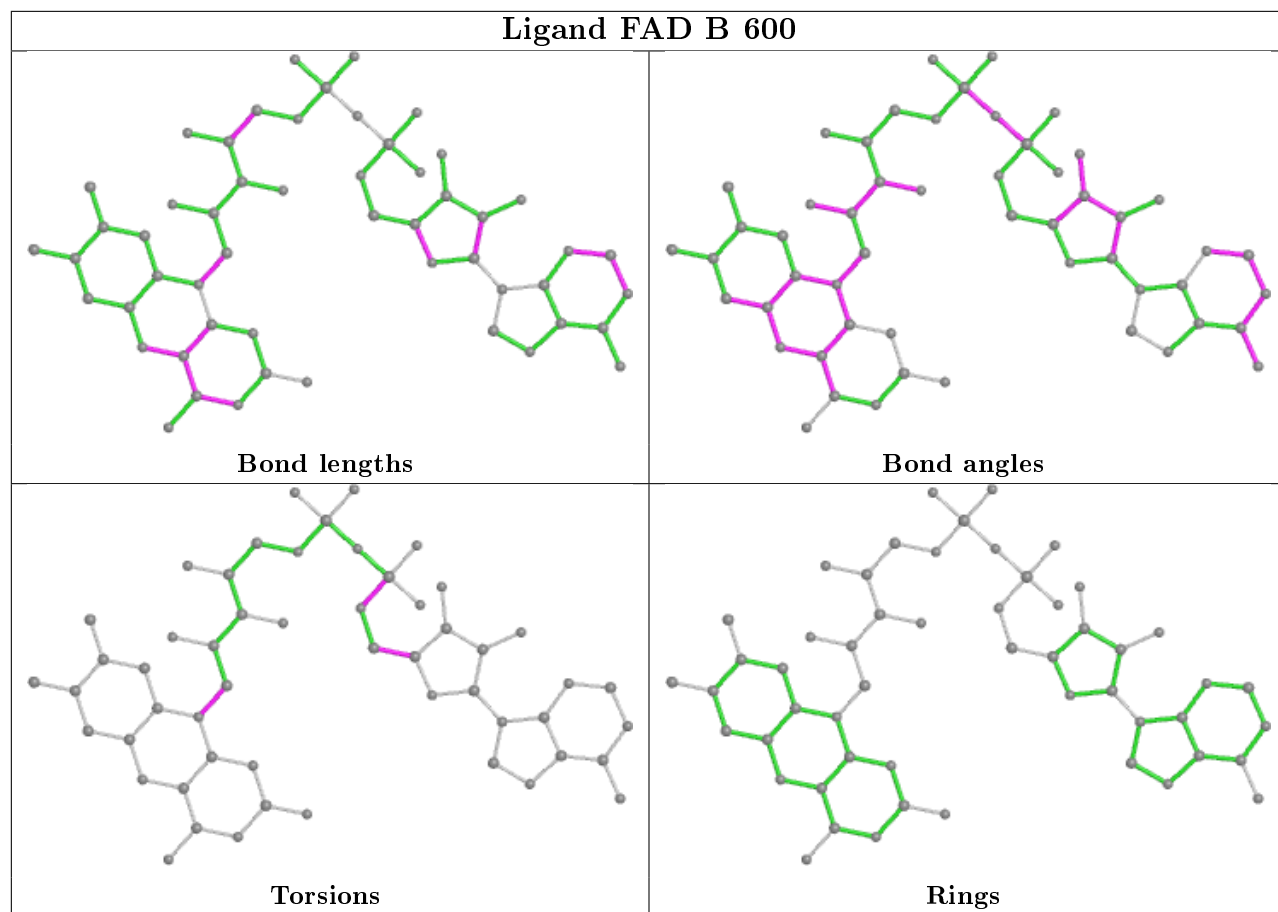
12 monomers are involved in 71 short contacts:

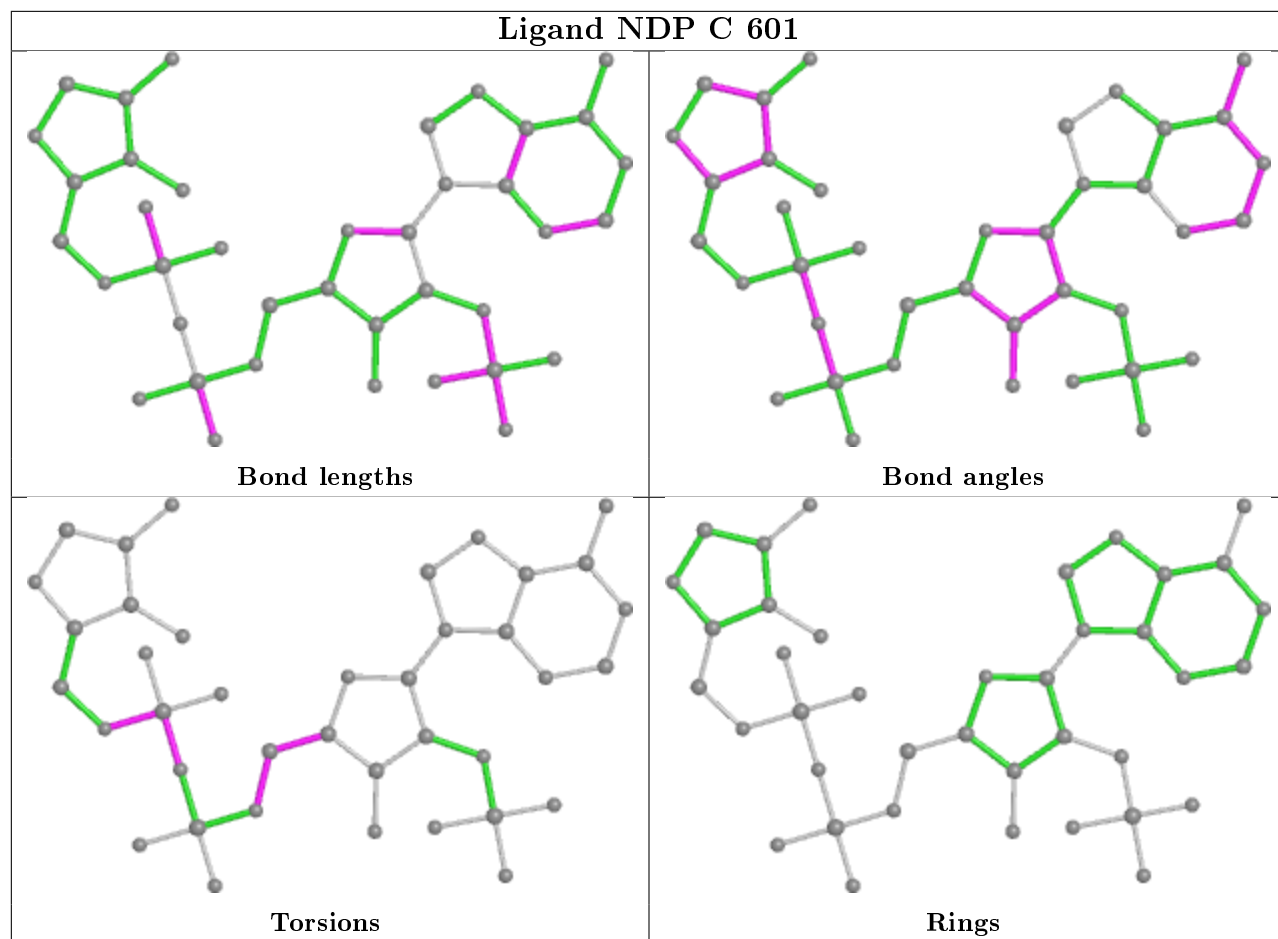


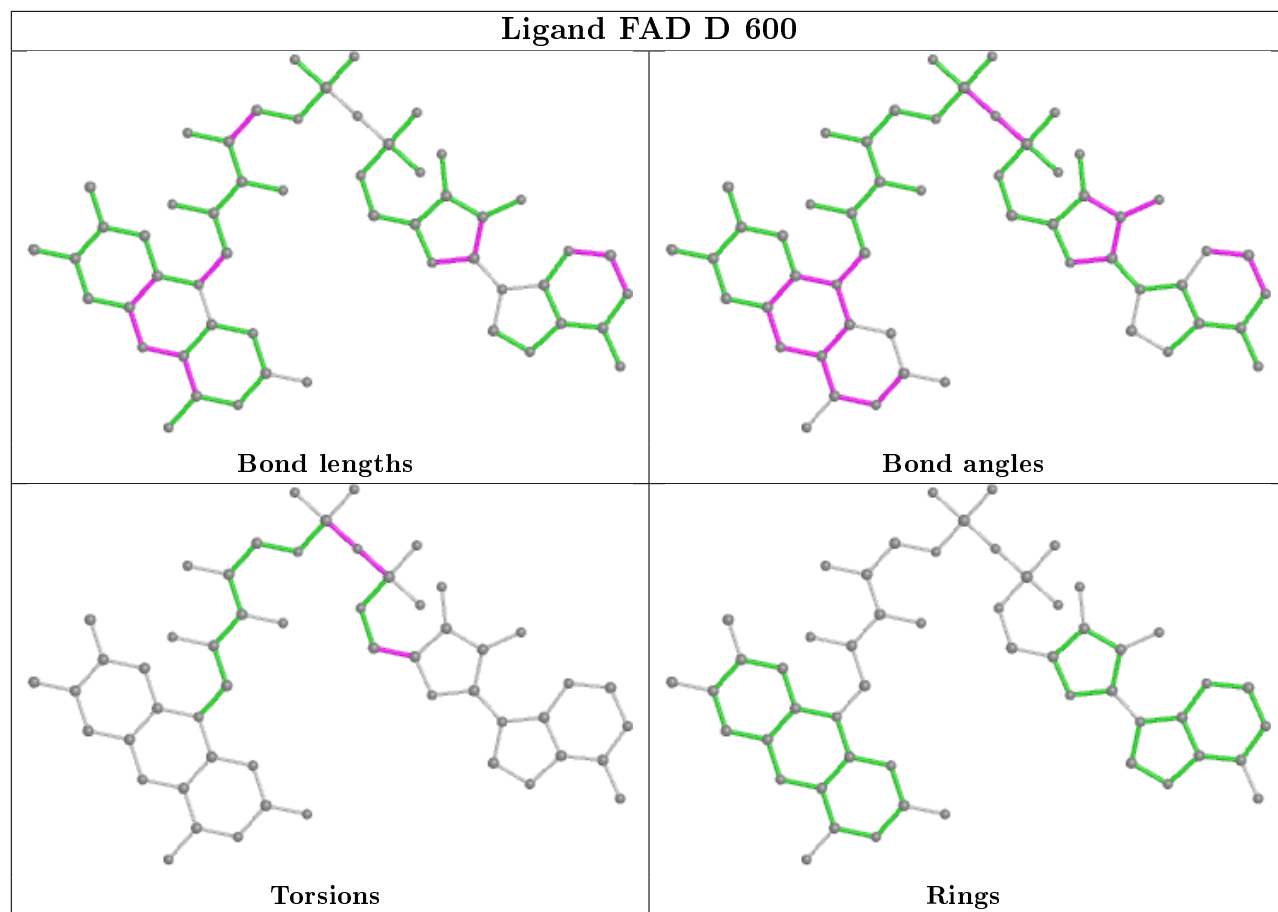
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	NDP	1	0
2	B	600	FAD	10	0
3	C	601	NDP	6	0
2	D	600	FAD	4	0
3	A	601	NDP	2	0
2	F	600	FAD	5	0
2	A	600	FAD	5	0
2	C	600	FAD	17	0
2	E	600	FAD	3	0
3	F	601	NDP	4	0
3	D	601	NDP	6	0
3	B	601	NDP	8	0

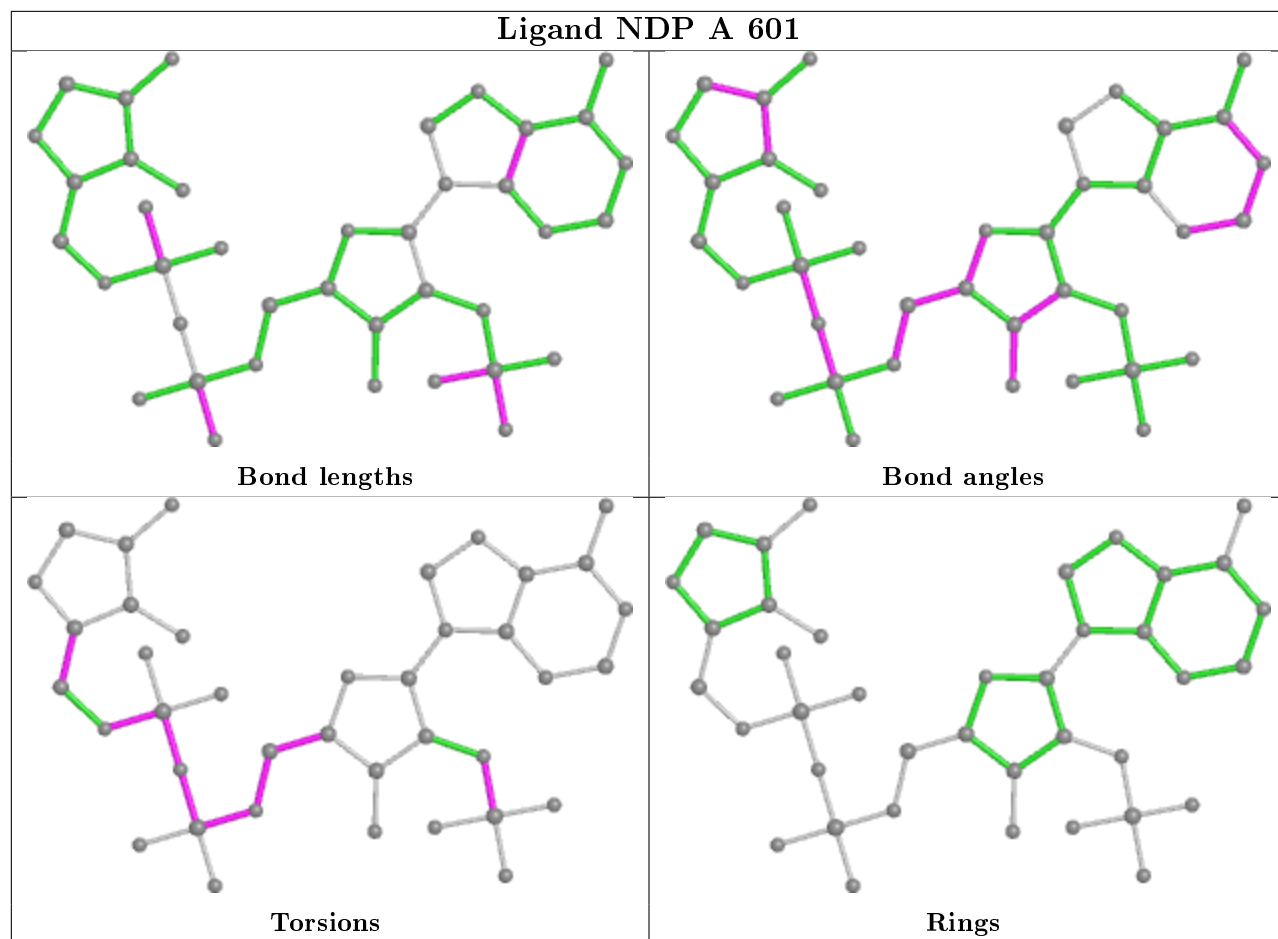
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

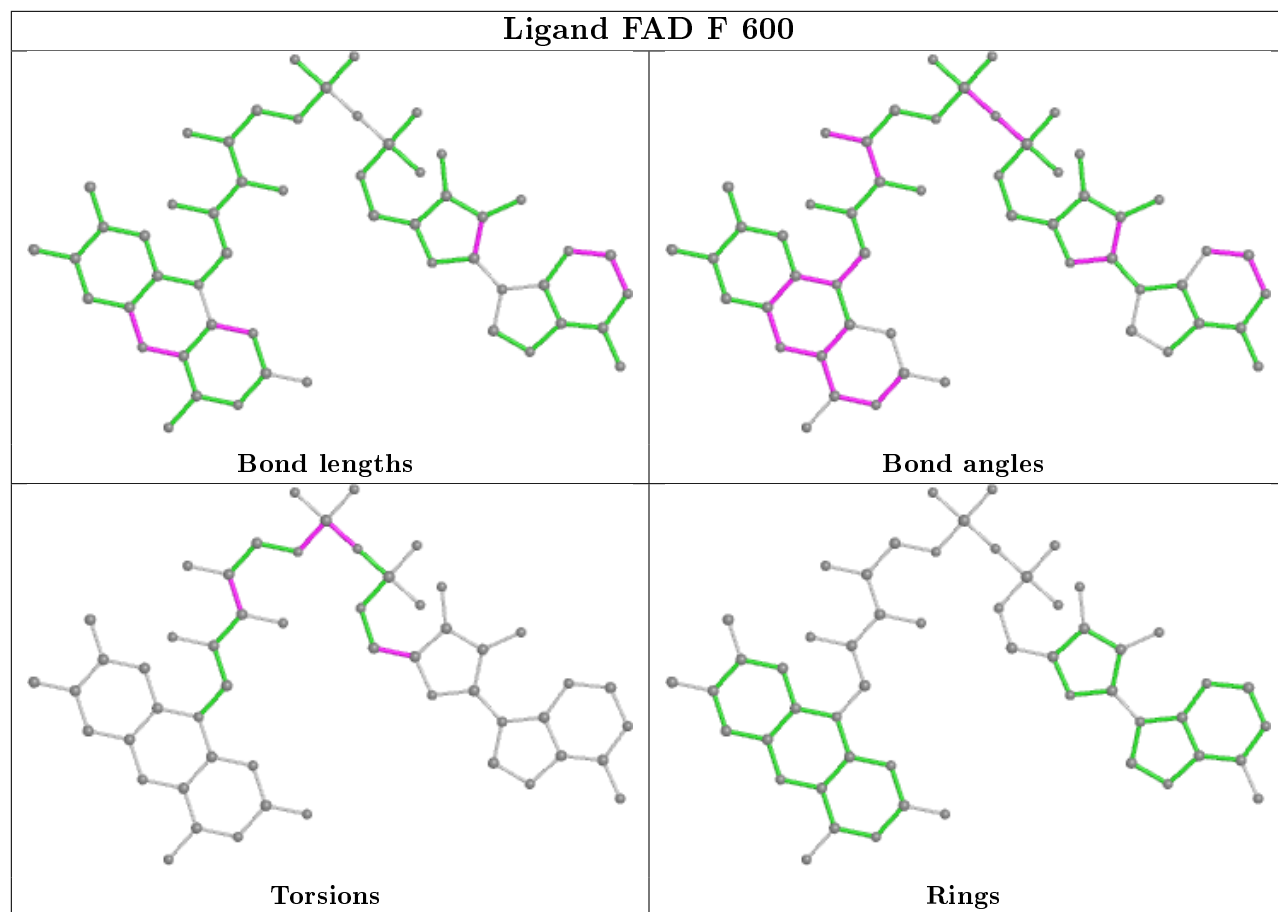


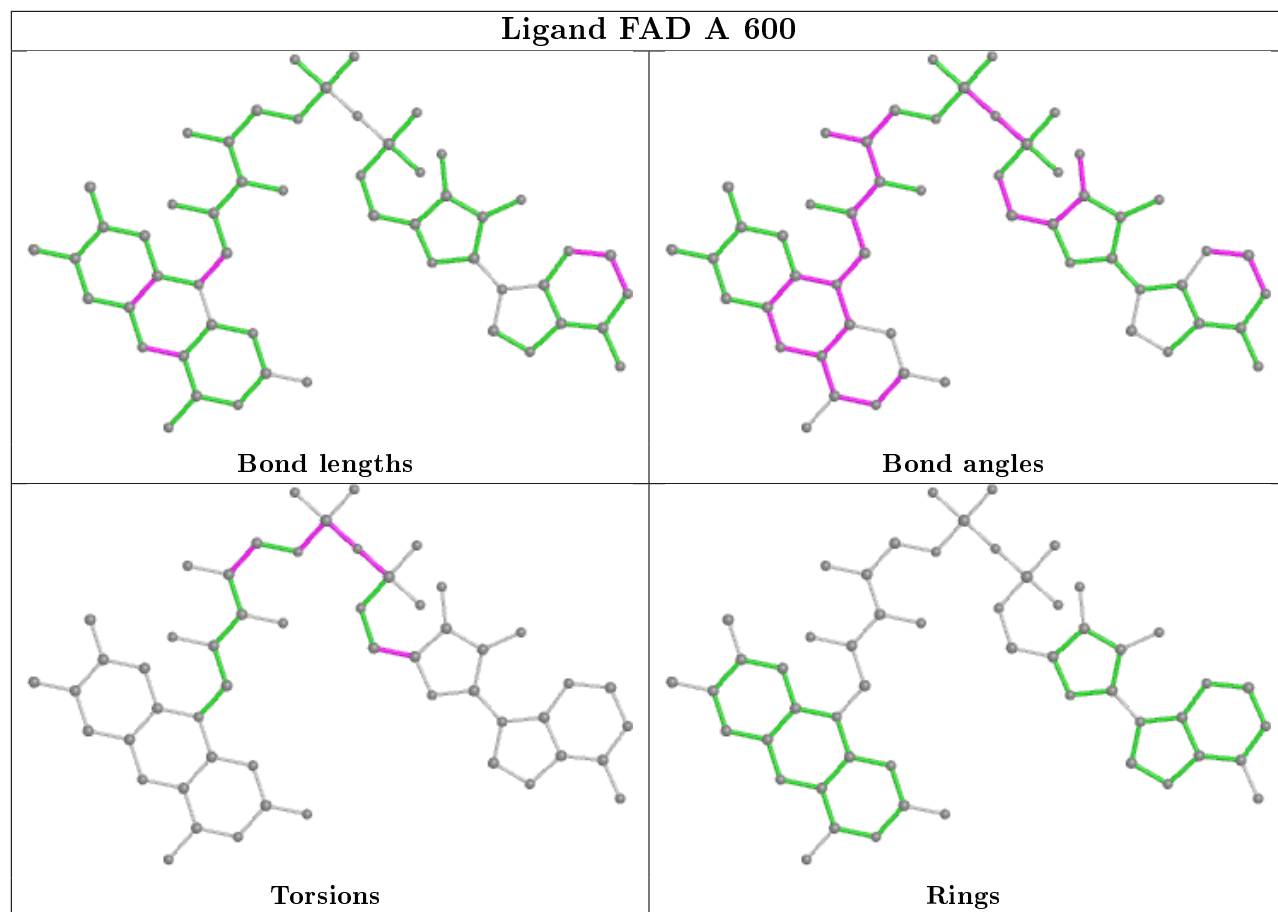




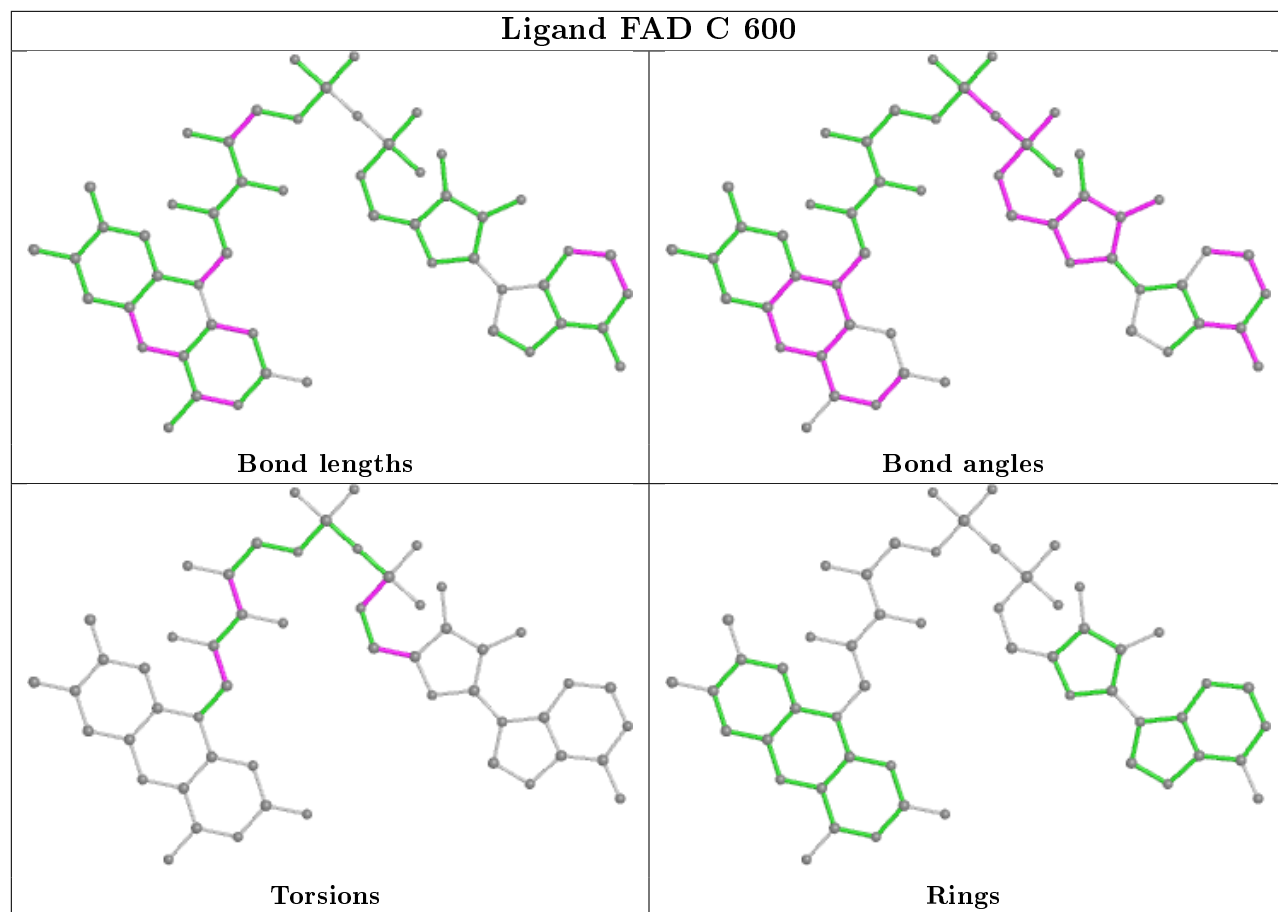


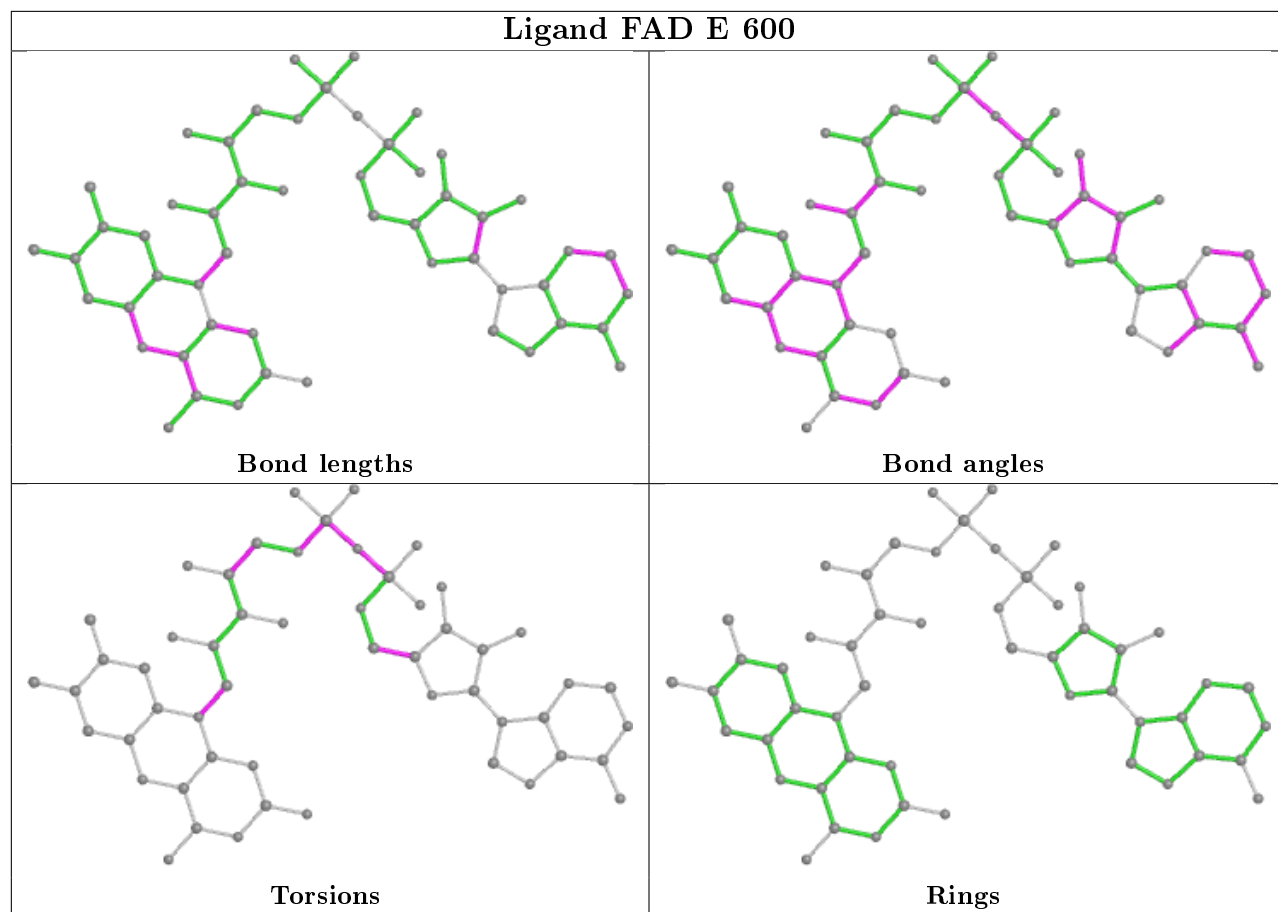


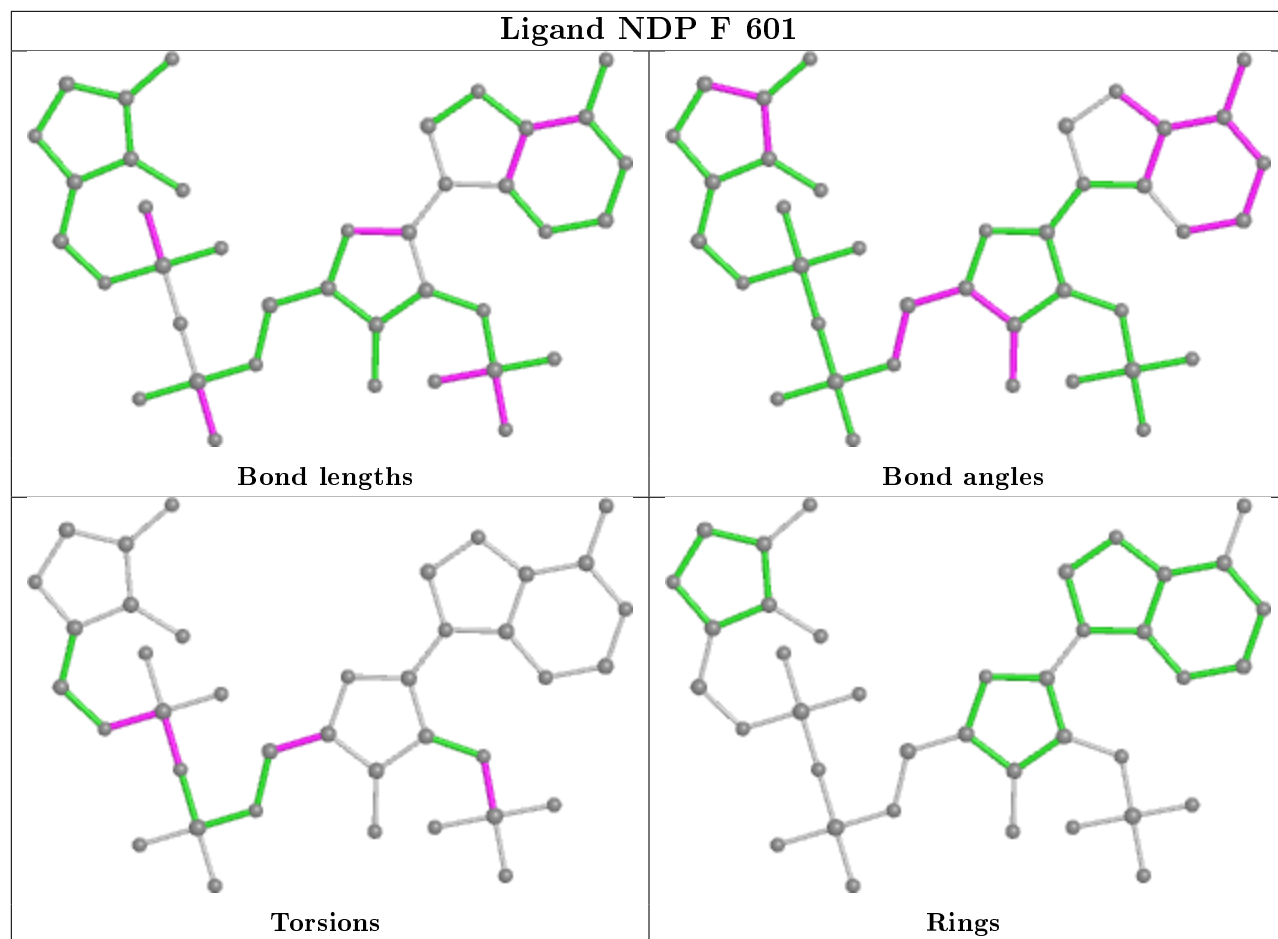


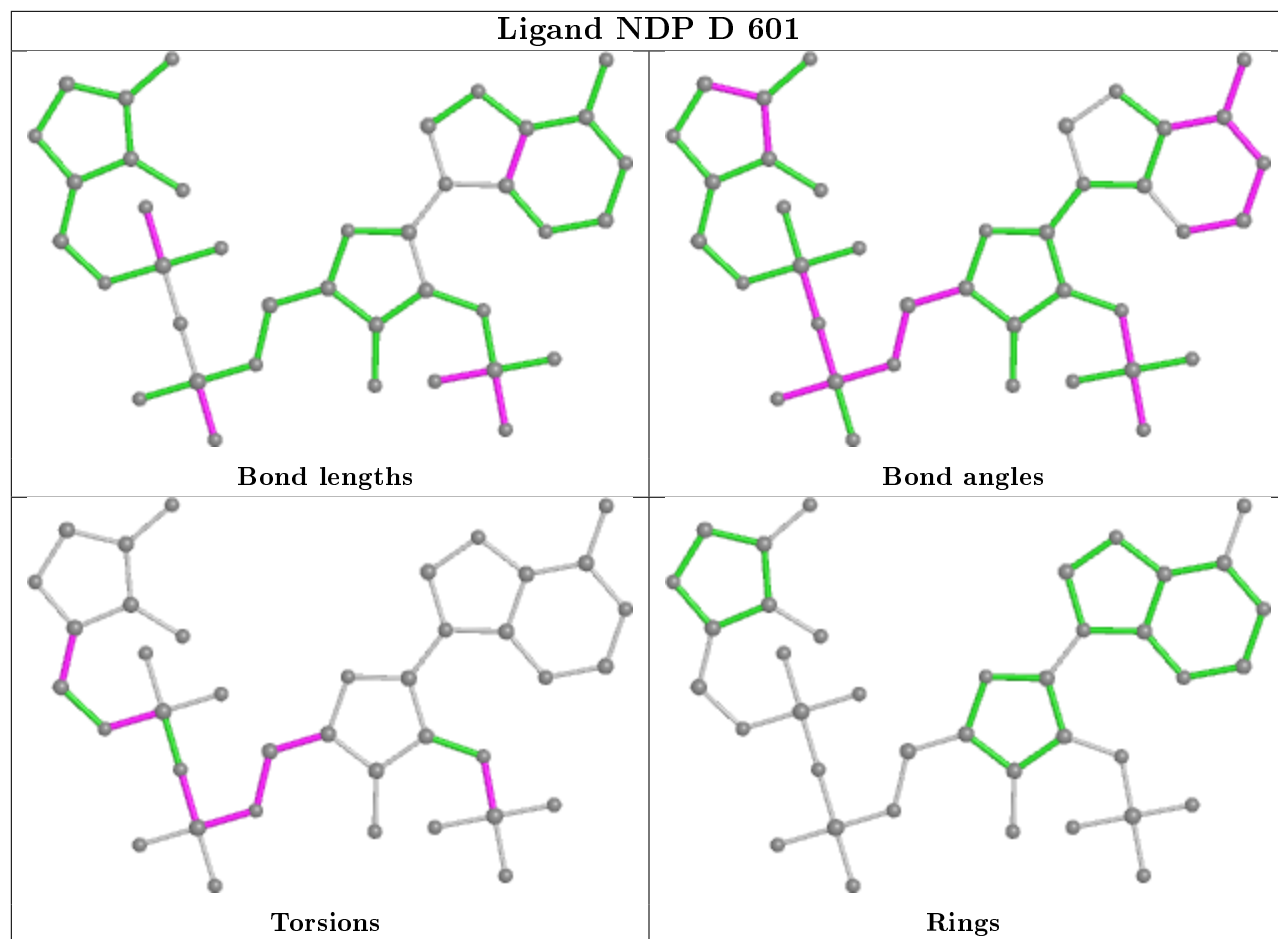


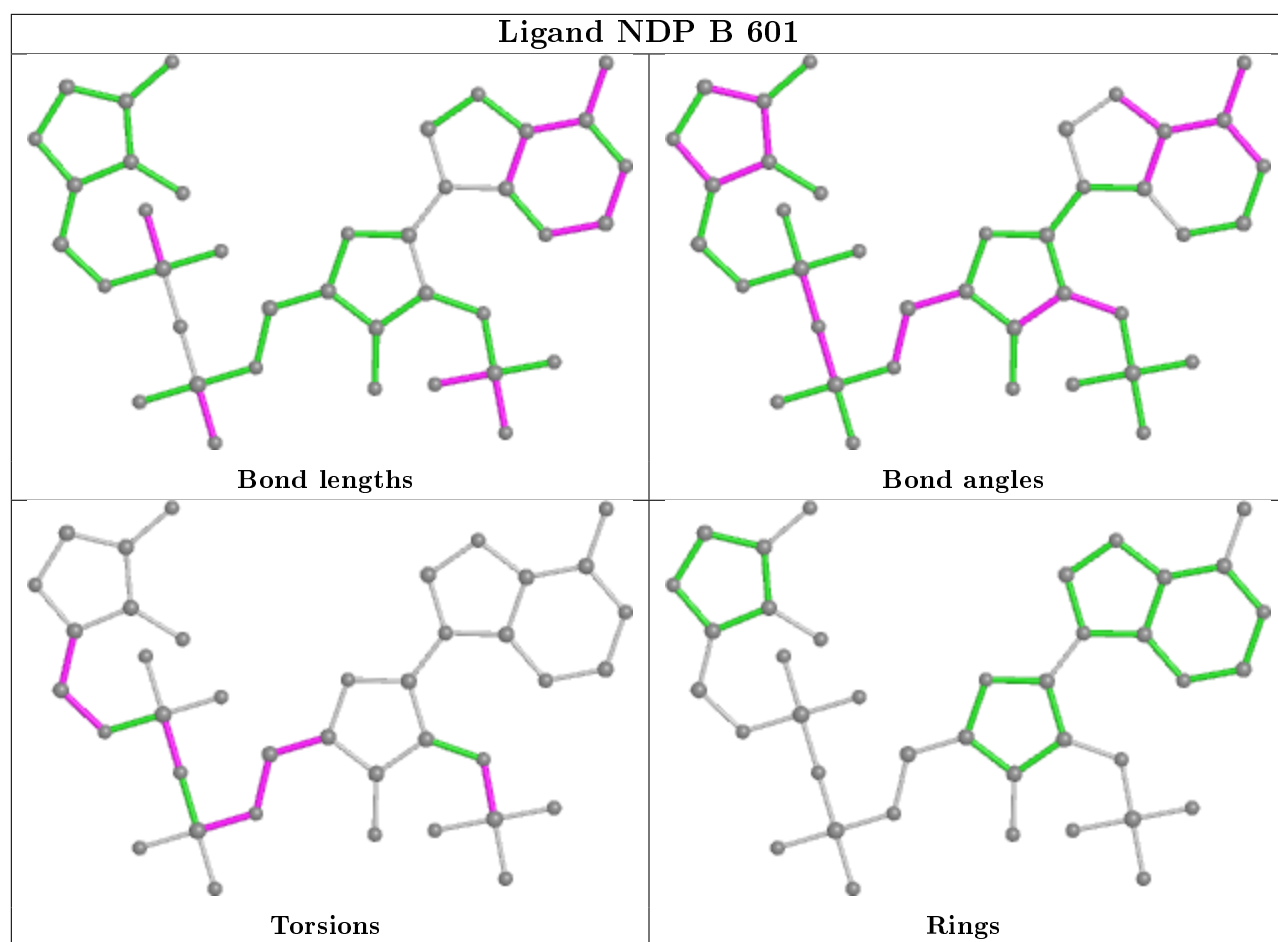












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	490/499 (98%)	-0.38	2 (0%) 92 79	7, 13, 20, 49	0
1	B	487/499 (97%)	-0.48	1 (0%) 95 87	6, 13, 20, 39	0
1	C	482/499 (96%)	0.11	16 (3%) 46 20	6, 13, 19, 44	0
1	D	487/499 (97%)	-0.33	4 (0%) 86 65	6, 12, 19, 38	0
1	E	491/499 (98%)	-0.39	4 (0%) 86 65	7, 13, 20, 48	0
1	F	490/499 (98%)	-0.24	6 (1%) 79 54	6, 13, 20, 48	0
All	All	2927/2994 (97%)	-0.29	33 (1%) 80 56	6, 13, 20, 49	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	497	CYS	6.9
1	E	495	SER	5.5
1	C	297	THR	5.1
1	F	495	SER	5.1
1	A	498	CYS	3.6

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

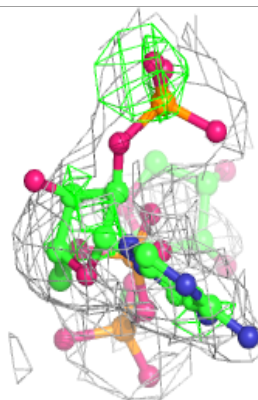
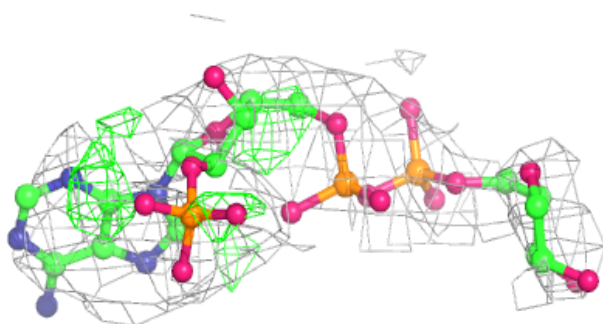
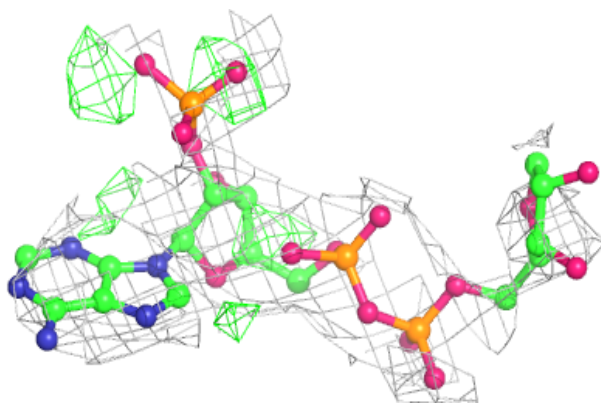
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NDP	C	601	39/48	0.77	0.26	82,92,100,101	0
3	NDP	F	601	39/48	0.78	0.29	72,95,112,112	0
3	NDP	A	601	39/48	0.85	0.22	41,49,78,78	0
3	NDP	D	601	39/48	0.85	0.20	44,55,77,77	0
2	FAD	C	600	53/53	0.86	0.28	34,45,49,51	0
3	NDP	B	601	39/48	0.89	0.22	31,50,69,71	0
3	NDP	E	601	39/48	0.91	0.21	45,52,76,79	0
2	FAD	F	600	53/53	0.92	0.26	27,33,53,55	0
2	FAD	E	600	53/53	0.94	0.28	10,17,54,56	0
2	FAD	A	600	53/53	0.94	0.22	14,24,36,36	0
2	FAD	B	600	53/53	0.95	0.25	18,26,42,46	0
2	FAD	D	600	53/53	0.95	0.29	20,29,40,47	0

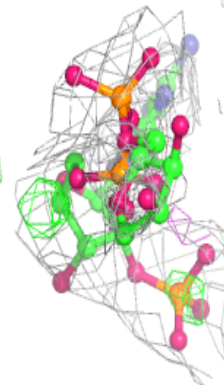
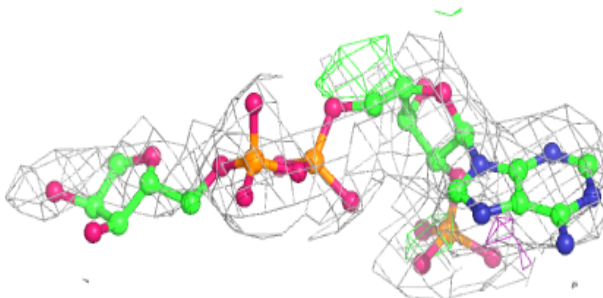
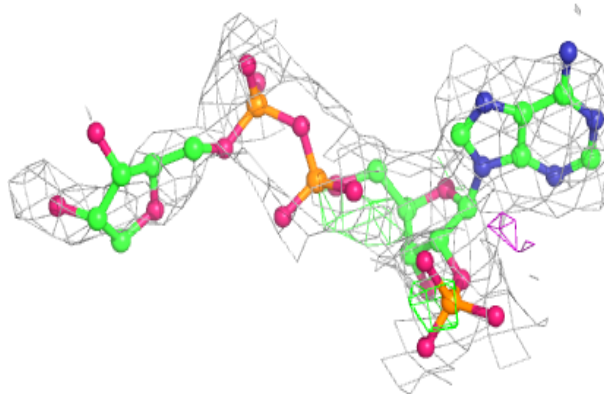
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NDP 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 NDP F 601:**

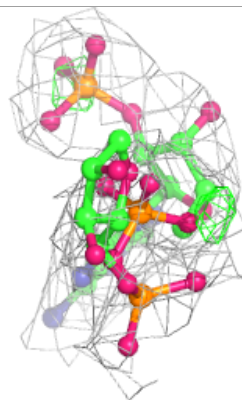
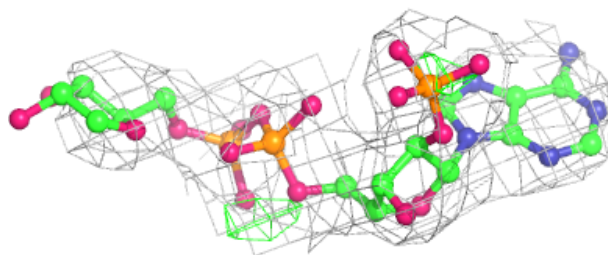
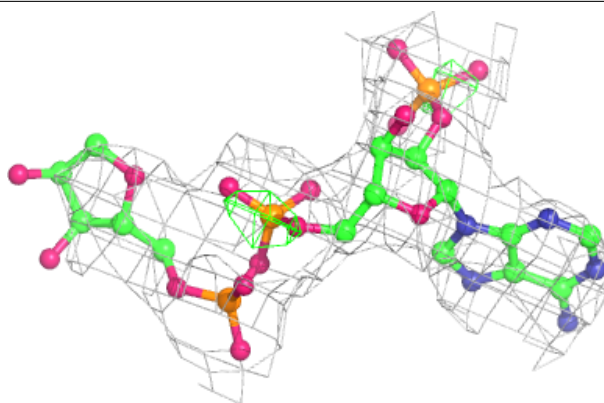
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



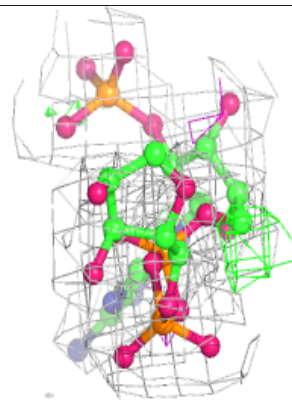
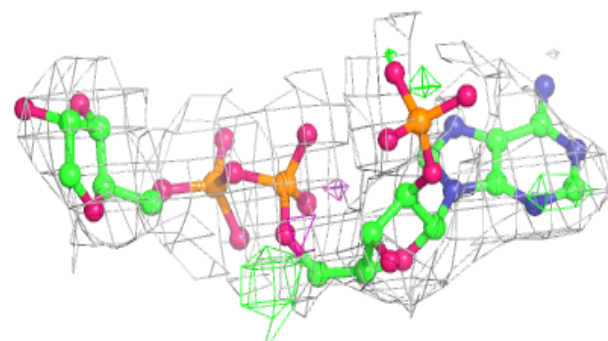
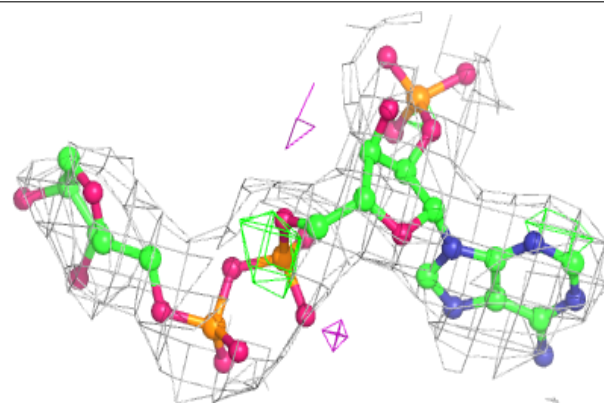


**Electron density around NDP A 601:**

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

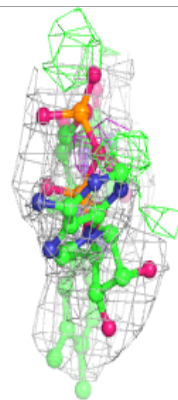
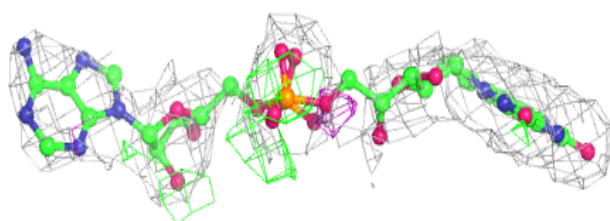
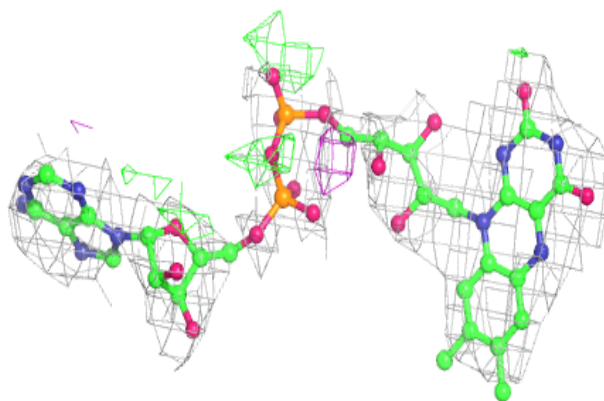
**Electron density around NDP D 601:**

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

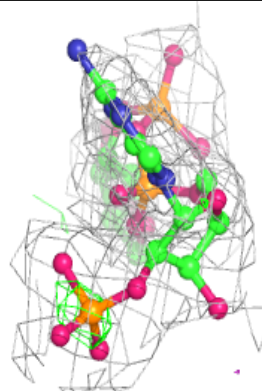
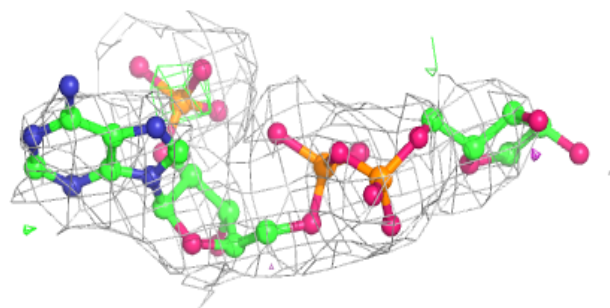
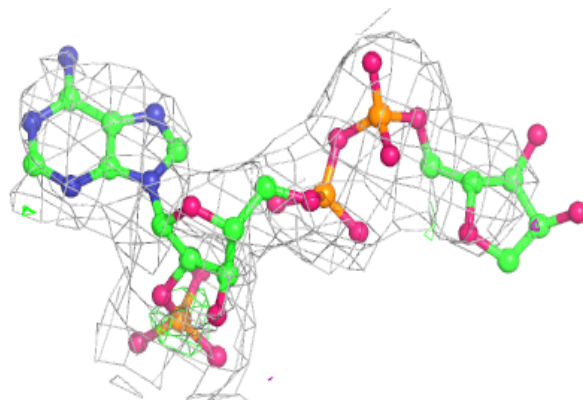


**Electron density around FAD C 600:**

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

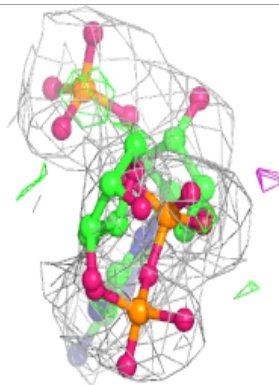
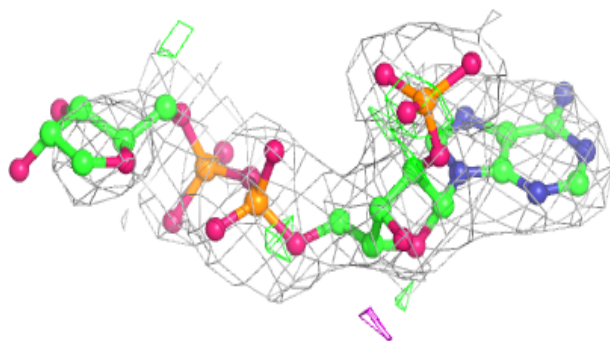
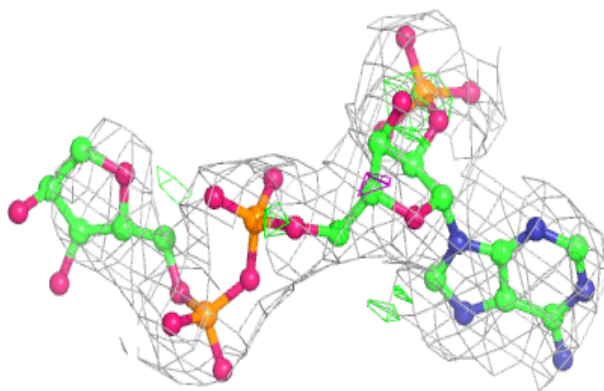
**Electron density around NDP B 601:**

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

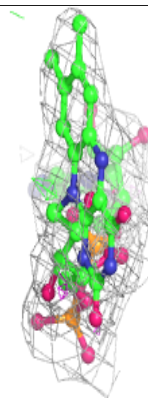
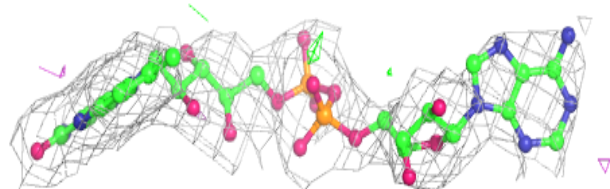
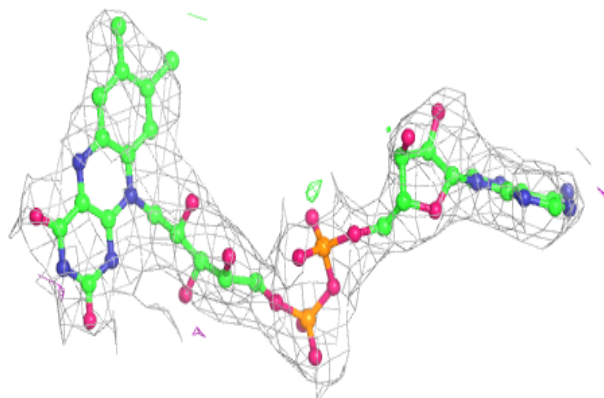


**Electron density around NDP E 601:**

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

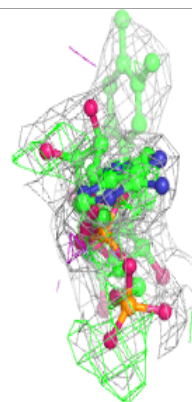
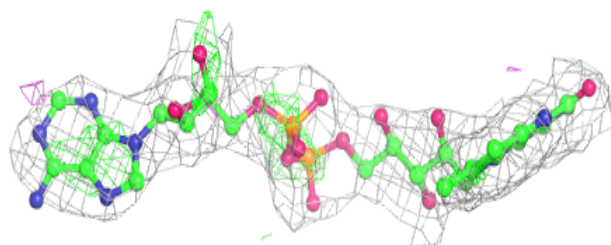
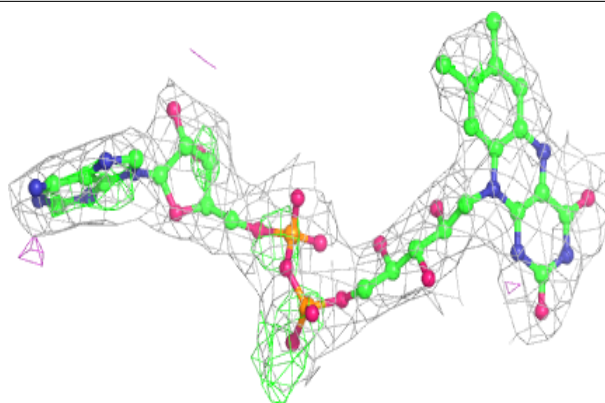
**Electron density around FAD F 600:**

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

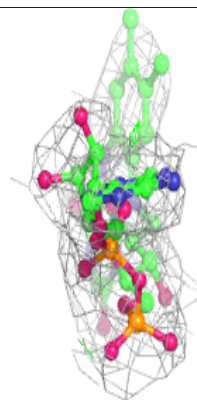
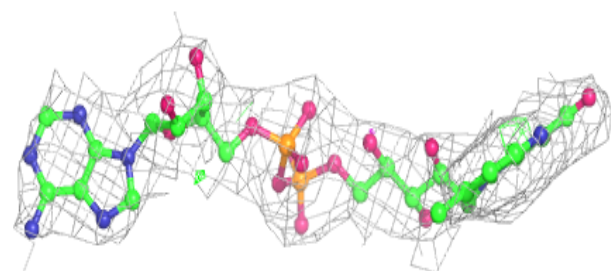
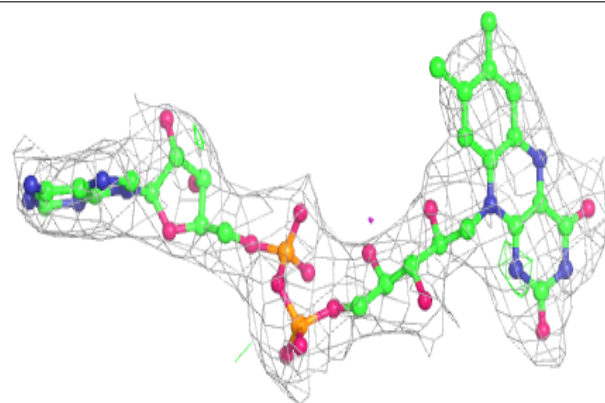


**Electron density around FAD E 600:**

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

**Electron density around FAD A 600:**

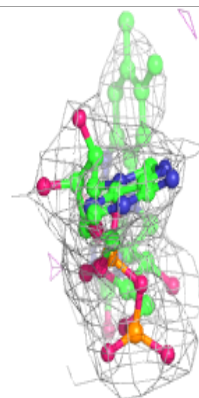
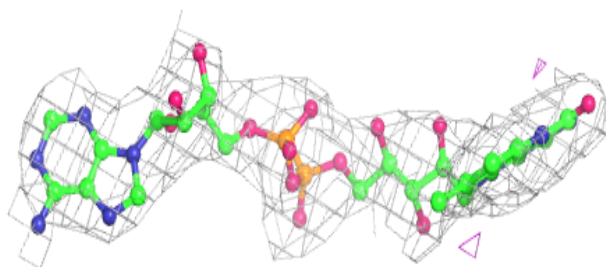
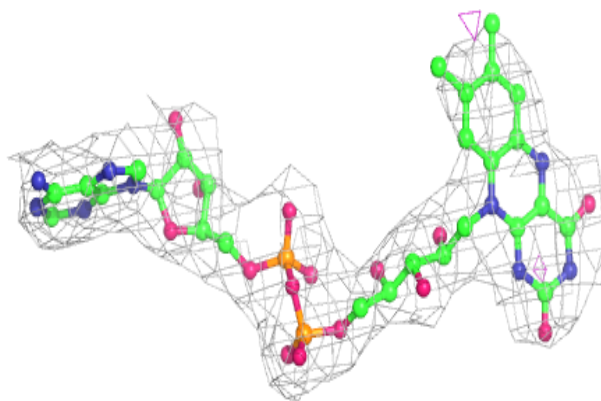
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



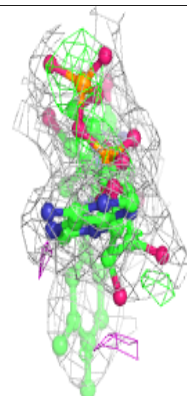
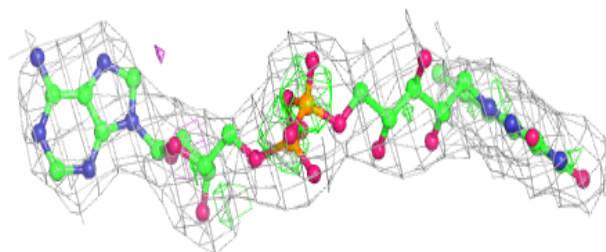
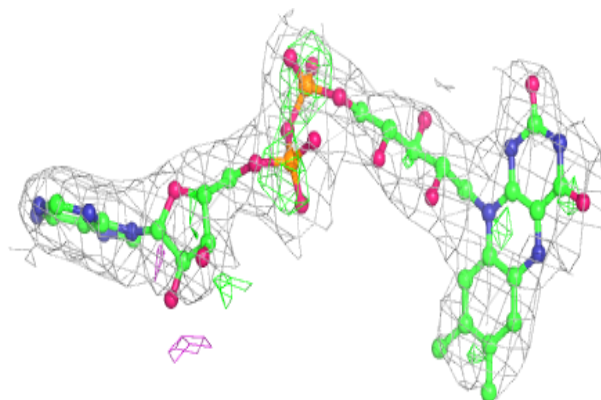


**Electron density around FAD B 600:**

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

**Electron density around 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.