



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:31 AM UTC

PDB ID : 2J3N / pdb_00002j3n
Title : X-ray structure of human thioredoxin reductase 1
Authors : Fritz-Wolf, K.; Urig, S.; Becker, K.
Deposited on : 2006-08-22
Resolution : 2.80 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

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

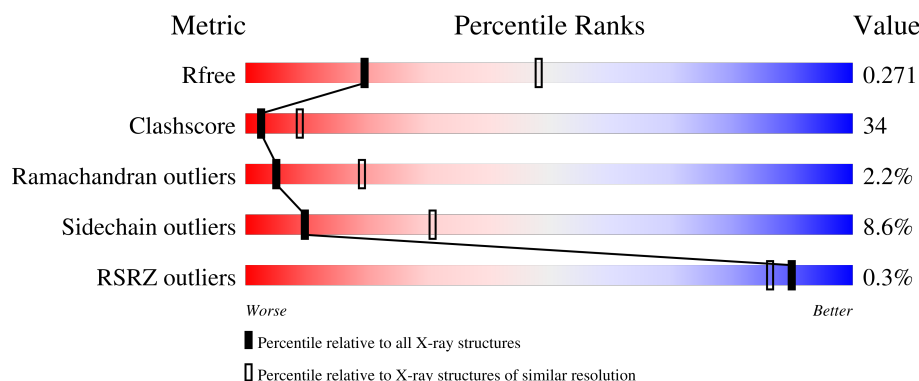
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	519	48% 39% 7% 6%
1	B	519	47% 40% 6% 6%
1	C	519	% 44% 43% 7% 6%
1	D	519	47% 39% 8% 5%
1	E	519	% 44% 41% 8% 6%

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Mol	Chain	Length	Quality of chain
1	F	519	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (43%), yellow (44%), orange (7%), and grey (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
3	NAP	A	601	X	-	-	-
3	NAP	B	601	X	-	-	-
3	NAP	C	601	X	-	-	-

2 Entry composition [i](#)

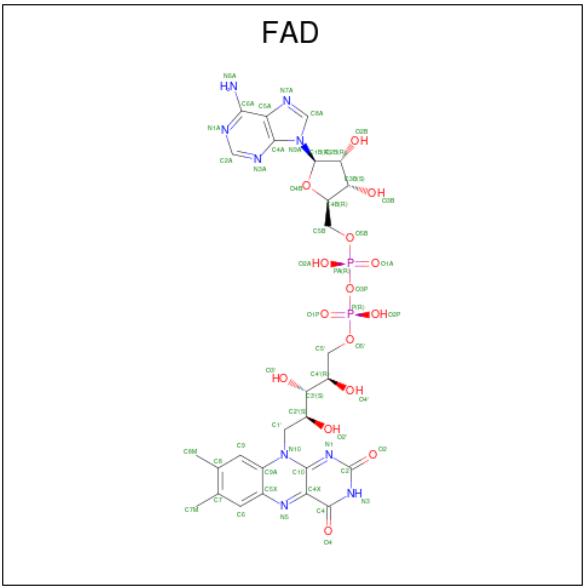
There are 5 unique types of molecules in this entry. The entry contains 23294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1.

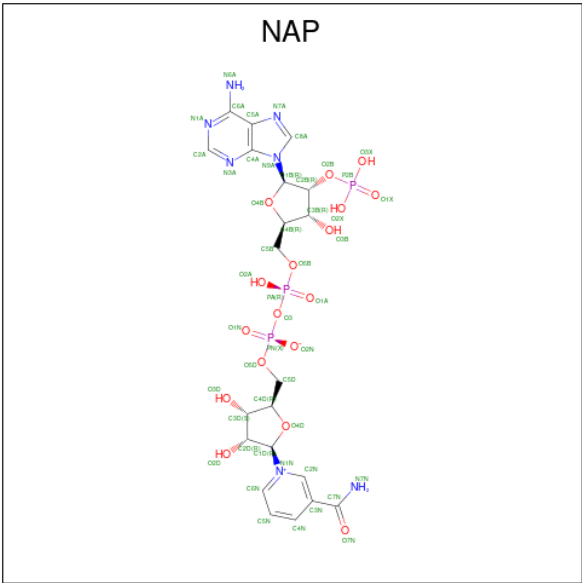
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	1
			3756	2387	642	708	19			
1	B	487	Total	C	N	O	S	0	0	1
			3760	2390	643	708	19			
1	C	490	Total	C	N	O	S	0	0	0
			3776	2397	645	713	21			
1	D	491	Total	C	N	O	S	0	0	0
			3785	2403	647	714	21			
1	E	490	Total	C	N	O	S	0	0	0
			3776	2397	645	713	21			
1	F	486	Total	C	N	O	S	0	0	1
			3751	2385	641	706	19			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



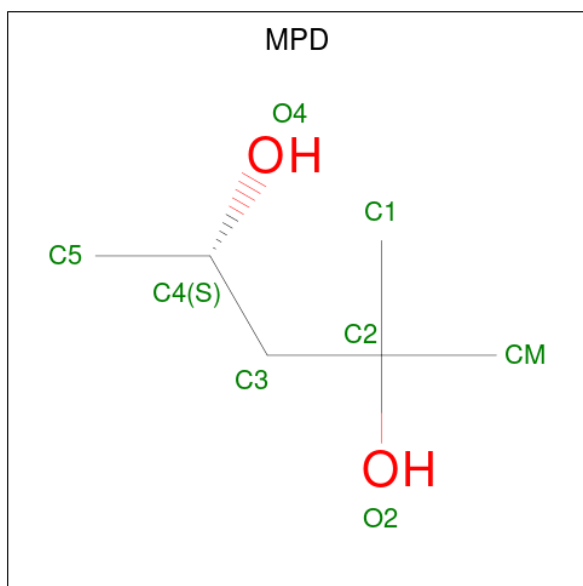
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	9	Total	O	0	0
			9	9		
5	C	7	Total	O	0	0
			7	7		

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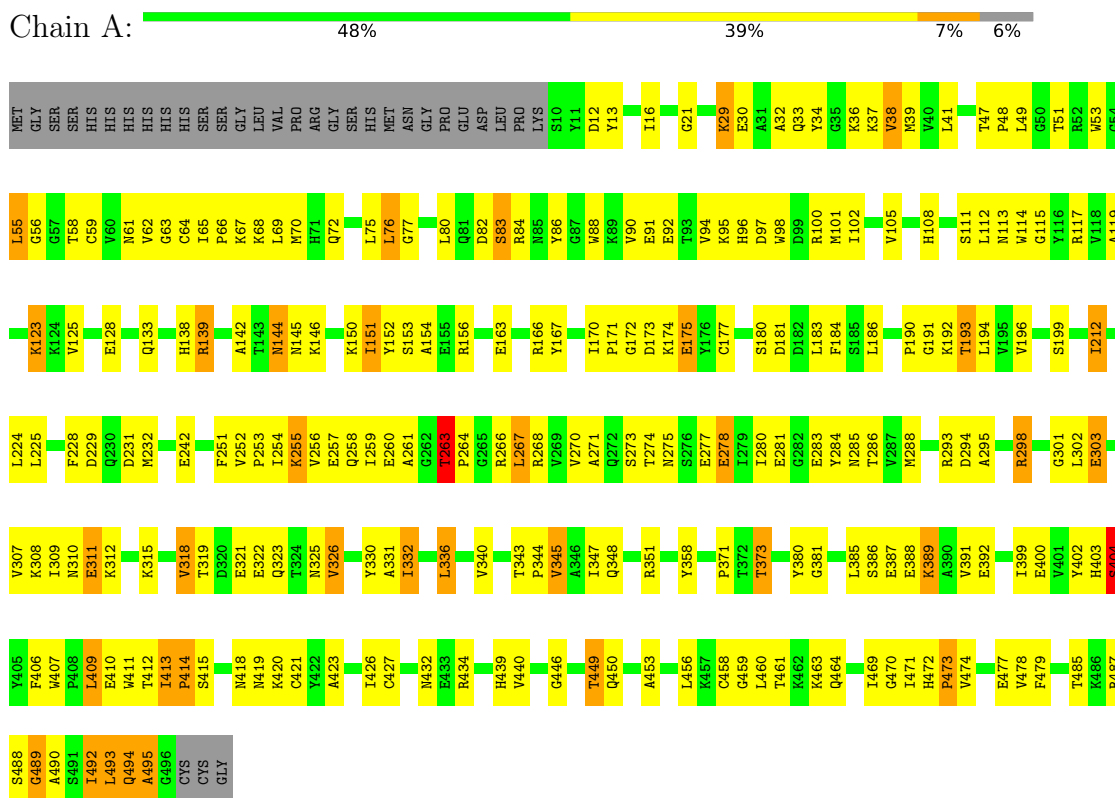
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		
5	E	4	Total	O	0	0
			4	4		
5	F	7	Total	O	0	0
			7	7		

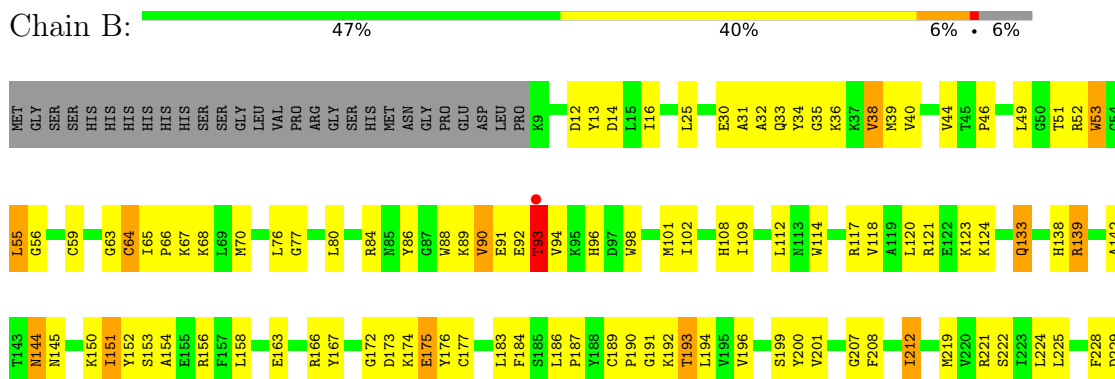
3 Residue-property plots

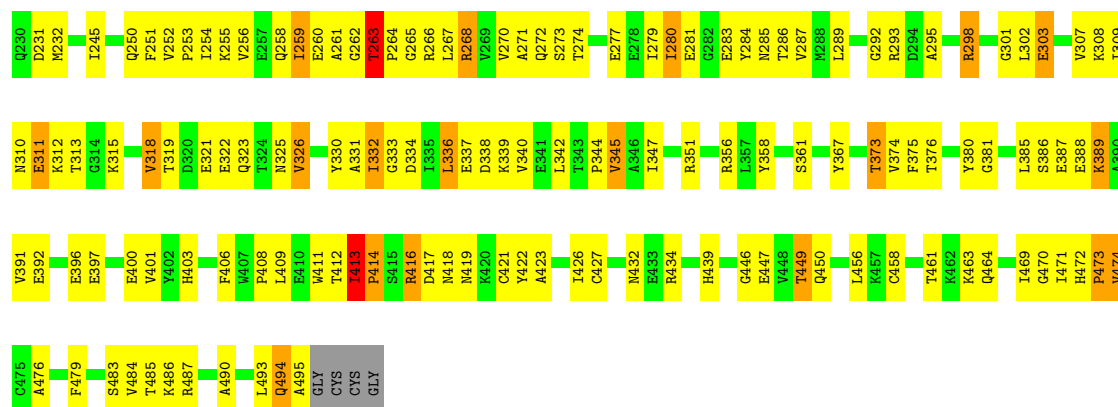
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: THIOREDOXIN REDUCTASE 1

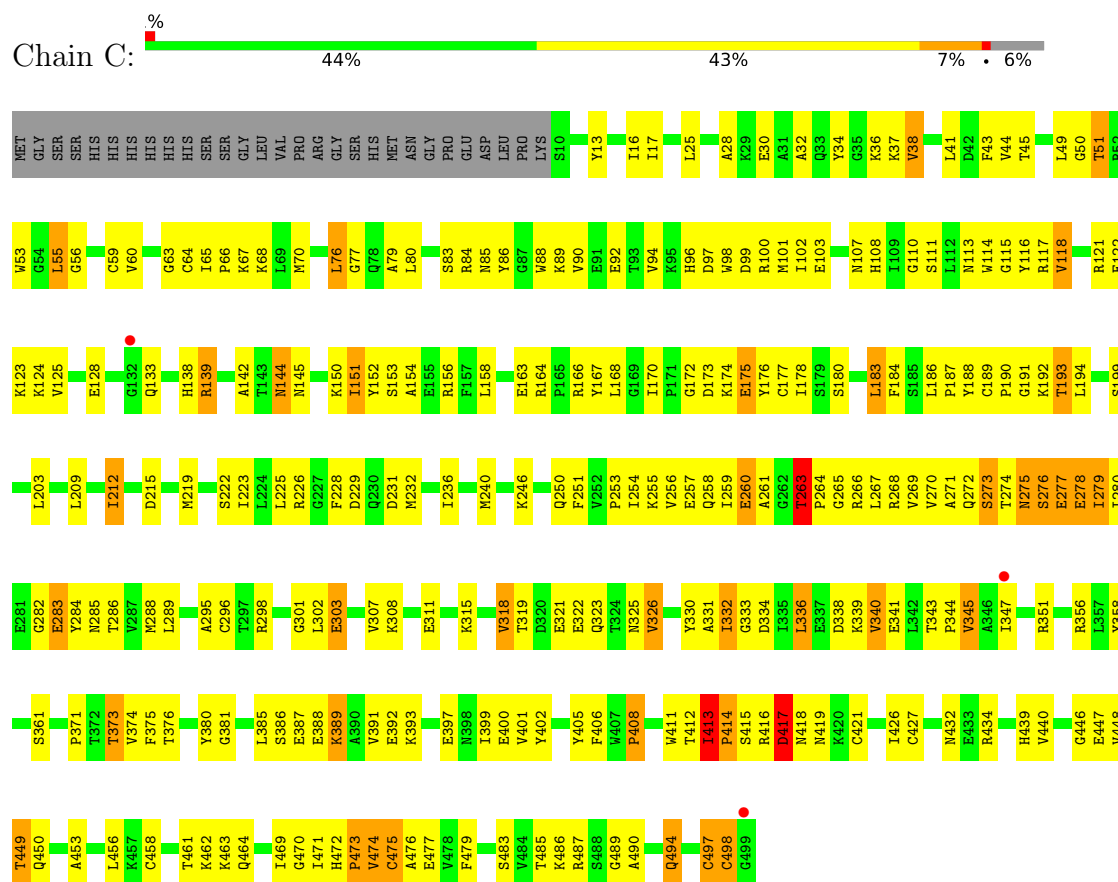


• Molecule 1: THIOREDOXIN REDUCTASE 1

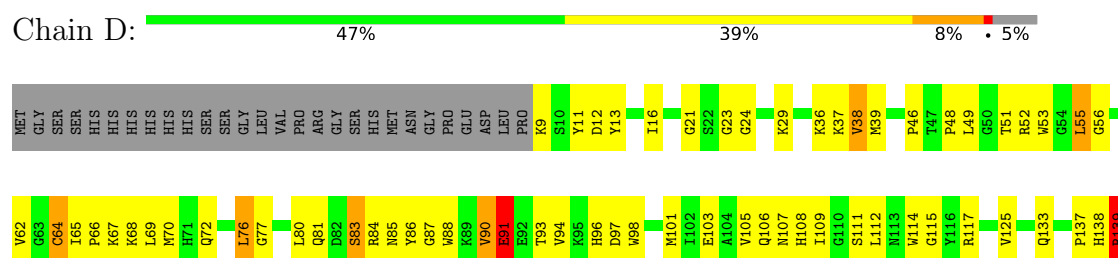


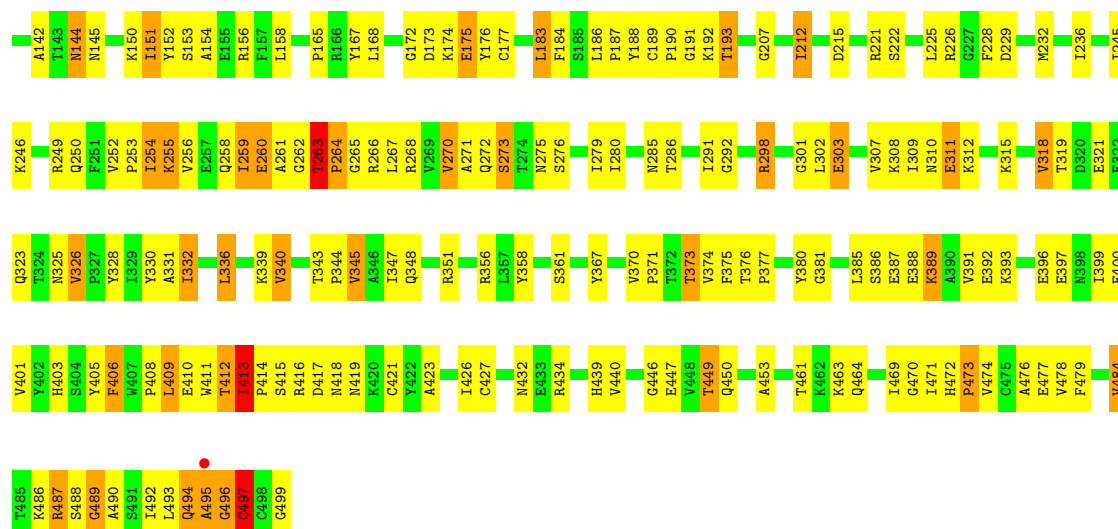


• Molecule 1: THIOREDOXIN REDUCTASE 1

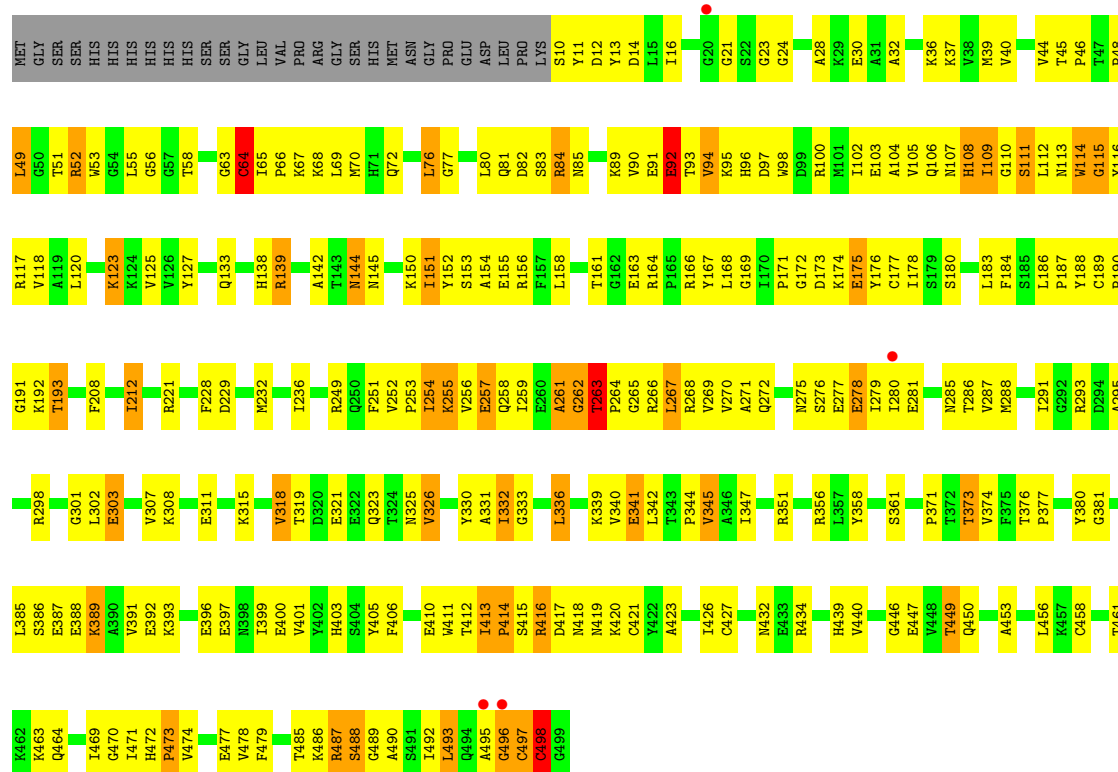
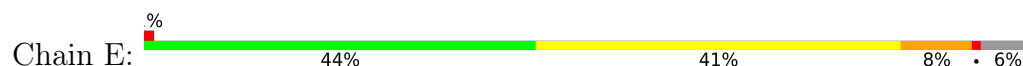


• Molecule 1: THIOREDOXIN REDUCTASE 1





• Molecule 1: THIOREDOXIN REDUCTASE 1



• Molecule 1: THIOREDOXIN REDUCTASE 1



A453	V374	Y284	L203	Y116	T47
L456	T376	W288	E204	R117	P48
K457	P377		C205	V118	L49
C458		I291	A206	A119	R52
G459	Y380	G292	F208	L120	
L460	G381	R293	L209		G57
T461		D294		V125	T58
K462	L385	A295	I212	Q133	C59
K463	S386				V60
Q464	E387	R298	D215	H138	M61
	E388			R139	V62
	K389	G301	I223	I140	G63
I469	A390	L302	R226	K141	C64
G470	V391	E303	G227	A142	I65
I471	E392	V307	F228	T143	P66
H472	K393	K308	D229	N144	K67
P473			Q230	N145	K68
V474	E397	E311	D231	K150	L69
C475	N398		W232	I151	M70
A476	I399	V318	K235	Y152	H71
E477	E400	T319		S153	Q72
V478	V401	D320	M240	A154	L75
F479	Y402	E321		E155	L76
	H403	E322	I245	R156	G77
S483	S404	Q323	K246	F157	Q78
V484	Y405	T324		L158	A79
T485	F406	N325	F251	T161	L80
K486	W407	V326	V252	G162	Q81
R487	P408	Y330	P253	E163	D82
S488	L409	A331	I254	R164	S83
G489	E410	I332	K255		R84
A490	W411	G333	V256	Y167	N85
S491	T412	D334	E257	W88	Y86
I492	I413	I335	Q258	L168	G87
L493	P414	S415	I259	G172	X88
Q494	R416	E337	E260	D173	K89
ALA	D417	D338	A261	G174	V90
GLY	W418	K339	G262	E175	E91
CYS	N419	V340	T263	G176	E92
CYS	K420	E341	G265	C177	T93
GLY	C421	L342	R266	I178	V94
		T343	L267		K95
		P344	R268	D182	H96
		V345	V269	D181	D97
		A346	V270	L183	W98
		E433	A271	F184	
		R434	Q272	S185	M101
			S273	L186	I102
					E103
					A104

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	144.63Å 90.64Å 166.60Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.8 (15.00-2.80) 98.8 (15.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.287 (Not available) , 0.271	Depositor DCC
R_{free} test set	4885 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23294	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: FAD, MPD, NAP

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	0.54	1/3830 (0.0%)	1.01	11/5187 (0.2%)
1	B	0.55	1/3834 (0.0%)	0.99	11/5191 (0.2%)
1	C	0.53	1/3850 (0.0%)	1.00	12/5211 (0.2%)
1	D	0.55	1/3859 (0.0%)	1.08	19/5222 (0.4%)
1	E	0.47	0/3850	0.99	18/5211 (0.3%)
1	F	0.48	1/3825 (0.0%)	0.99	13/5179 (0.3%)
All	All	0.52	5/23048 (0.0%)	1.01	84/31201 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	413	ILE	CA-CB	7.69	1.59	1.53
1	F	493	LEU	C-N	-5.57	1.25	1.33
1	B	494	GLN	C-N	-5.56	1.25	1.33
1	A	495	ALA	C-N	-5.45	1.25	1.33
1	C	497	CYS	CA-C	5.10	1.59	1.52

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	THR	CA-C-N	-15.27	101.44	120.23
1	D	263	THR	C-N-CA	-15.27	101.44	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH2	13.00	130.90	119.20
1	D	139	ARG	NE-CZ-NH1	-11.64	109.86	121.50
1	A	263	THR	CA-C-N	-11.59	105.72	120.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	13	TYR	Sidechain

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	3756	0	3764	261	0
1	B	3760	0	3772	272	0
1	C	3776	0	3780	288	0
1	D	3785	0	3793	272	0
1	E	3776	0	3778	344	0
1	F	3751	0	3764	298	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	5	0
2	E	53	0	31	4	0
2	F	53	0	31	10	0
3	A	48	0	24	1	0
3	B	48	0	24	6	0
3	C	48	0	24	1	0
3	D	48	0	25	4	0
3	E	48	0	25	2	0
3	F	48	0	25	1	0
4	A	8	0	14	2	0
4	B	16	0	28	5	0
4	D	8	0	14	3	0
4	F	8	0	14	5	0
5	A	9	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	9	0	0	3	0
5	C	7	0	0	1	0
5	D	8	0	0	3	0
5	E	4	0	0	2	0
5	F	7	0	0	2	0
All	All	23294	0	23054	1590	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 34.

The worst 5 of 1590 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:F:46:PRO:HG3	1:F:52:ARG:HE	1.15	1.10
1:E:80:LEU:HD23	1:F:80:LEU:HD23	1.34	1.10
1:B:199:SER:HB3	3:B:601:NAP:H52A	1.37	1.05
1:D:418:ASN:HD21	1:D:495:ALA:HB2	1.19	1.05
1:A:199:SER:HB3	3:A:601:NAP:H52A	1.39	1.04

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	485/519 (93%)	426 (88%)	51 (10%)	8 (2%)	7	27
1	B	485/519 (93%)	419 (86%)	60 (12%)	6 (1%)	10	34
1	C	430/519 (83%)	373 (87%)	47 (11%)	10 (2%)	5	18
1	D	489/519 (94%)	424 (87%)	51 (10%)	14 (3%)	3	13
1	E	488/519 (94%)	421 (86%)	54 (11%)	13 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	484/519 (93%)	417 (86%)	55 (11%)	12 (2%)	4	16
All	All	2861/3114 (92%)	2480 (87%)	318 (11%)	63 (2%)	5	19

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	GLY
1	B	263	THR
1	C	263	THR
1	C	276	SER
1	C	278	GLU

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	399/426 (94%)	365 (92%)	34 (8%)	10	31
1	B	400/426 (94%)	366 (92%)	34 (8%)	10	31
1	C	401/426 (94%)	363 (90%)	38 (10%)	8	26
1	D	402/426 (94%)	368 (92%)	34 (8%)	10	31
1	E	401/426 (94%)	367 (92%)	34 (8%)	10	31
1	F	399/426 (94%)	366 (92%)	33 (8%)	10	32
All	All	2402/2556 (94%)	2195 (91%)	207 (9%)	10	31

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	133	GLN
1	E	64	CYS
1	F	345	VAL
1	D	175	GLU
1	D	332	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	138	HIS
1	E	106	GLN
1	F	428	ASN
1	D	258	GLN
1	D	428	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	NAP	A	601	-	50,52,52	1.78	8 (16%)	71,80,80	2.74	12 (16%)
4	MPD	F	700	-	7,7,7	0.41	0	9,10,10	0.42	0
4	MPD	A	701	-	7,7,7	0.33	0	9,10,10	0.41	0
2	FAD	F	600	-	58,58,58	1.50	7 (12%)	85,89,89	1.94	8 (9%)
2	FAD	C	600	-	58,58,58	1.86	10 (17%)	85,89,89	1.81	9 (10%)
3	NAP	C	601	-	50,52,52	1.68	7 (14%)	71,80,80	2.69	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	B	701	-	7,7,7	0.37	0	9,10,10	0.33	0
3	NAP	D	601	-	50,52,52	1.79	11 (22%)	71,80,80	1.13	4 (5%)
3	NAP	B	601	-	50,52,52	1.70	7 (14%)	71,80,80	2.49	11 (15%)
4	MPD	B	700	-	7,7,7	0.35	0	9,10,10	0.41	0
4	MPD	D	700	-	7,7,7	0.36	0	9,10,10	0.25	0
2	FAD	E	600	-	58,58,58	1.61	8 (13%)	85,89,89	1.76	7 (8%)
3	NAP	E	601	-	50,52,52	1.47	7 (14%)	71,80,80	1.12	7 (9%)
2	FAD	D	600	-	58,58,58	1.92	12 (20%)	85,89,89	1.80	9 (10%)
3	NAP	F	601	-	50,52,52	1.49	8 (16%)	71,80,80	1.27	6 (8%)
2	FAD	B	600	-	58,58,58	1.70	10 (17%)	85,89,89	1.79	8 (9%)
2	FAD	A	600	-	58,58,58	1.70	9 (15%)	85,89,89	1.83	7 (8%)

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	NAP	A	601	-	1/1/12/12	6/35/67/67	0/5/5/5
4	MPD	F	700	-	-	1/5/5/5	-
4	MPD	A	701	-	-	0/5/5/5	-
2	FAD	F	600	-	-	5/34/50/50	0/6/6/6
2	FAD	C	600	-	-	8/34/50/50	0/6/6/6
3	NAP	C	601	-	1/1/12/12	14/35/67/67	0/5/5/5
4	MPD	B	701	-	-	0/5/5/5	-
3	NAP	D	601	-	-	12/35/67/67	0/5/5/5
3	NAP	B	601	-	1/1/12/12	6/35/67/67	0/5/5/5
4	MPD	B	700	-	-	1/5/5/5	-
4	MPD	D	700	-	-	1/5/5/5	-
2	FAD	E	600	-	-	5/34/50/50	0/6/6/6
3	NAP	E	601	-	-	10/35/67/67	0/5/5/5
2	FAD	D	600	-	-	8/34/50/50	0/6/6/6
3	NAP	F	601	-	-	15/35/67/67	0/5/5/5
2	FAD	B	600	-	-	9/34/50/50	0/6/6/6
2	FAD	A	600	-	-	9/34/50/50	0/6/6/6

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	P-O3P	6.36	1.66	1.59
3	A	601	NAP	O4B-C4B	6.00	1.58	1.45
2	D	600	FAD	C4X-N5	5.99	1.43	1.30
2	C	600	FAD	P-O3P	5.90	1.65	1.59
2	C	600	FAD	C4X-N5	5.50	1.42	1.30

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAP	C5B-C4B-C3B	15.76	171.93	115.21
3	B	601	NAP	C5B-C4B-C3B	15.08	169.49	115.21
3	C	601	NAP	C5B-C4B-C3B	14.93	168.96	115.21
2	F	600	FAD	O2A-PA-O3P	-11.78	75.42	107.27
2	D	600	FAD	O2A-PA-O3P	-11.39	76.49	107.27

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	NAP	C4B
3	B	601	NAP	C4B
3	C	601	NAP	C4B

5 of 110 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	O4B-C4B-C5B-O5B
2	C	600	FAD	C5B-O5B-PA-O2A
2	C	600	FAD	C4B-C5B-O5B-PA

There are no ring outliers.

16 monomers are involved in 52 short contacts:

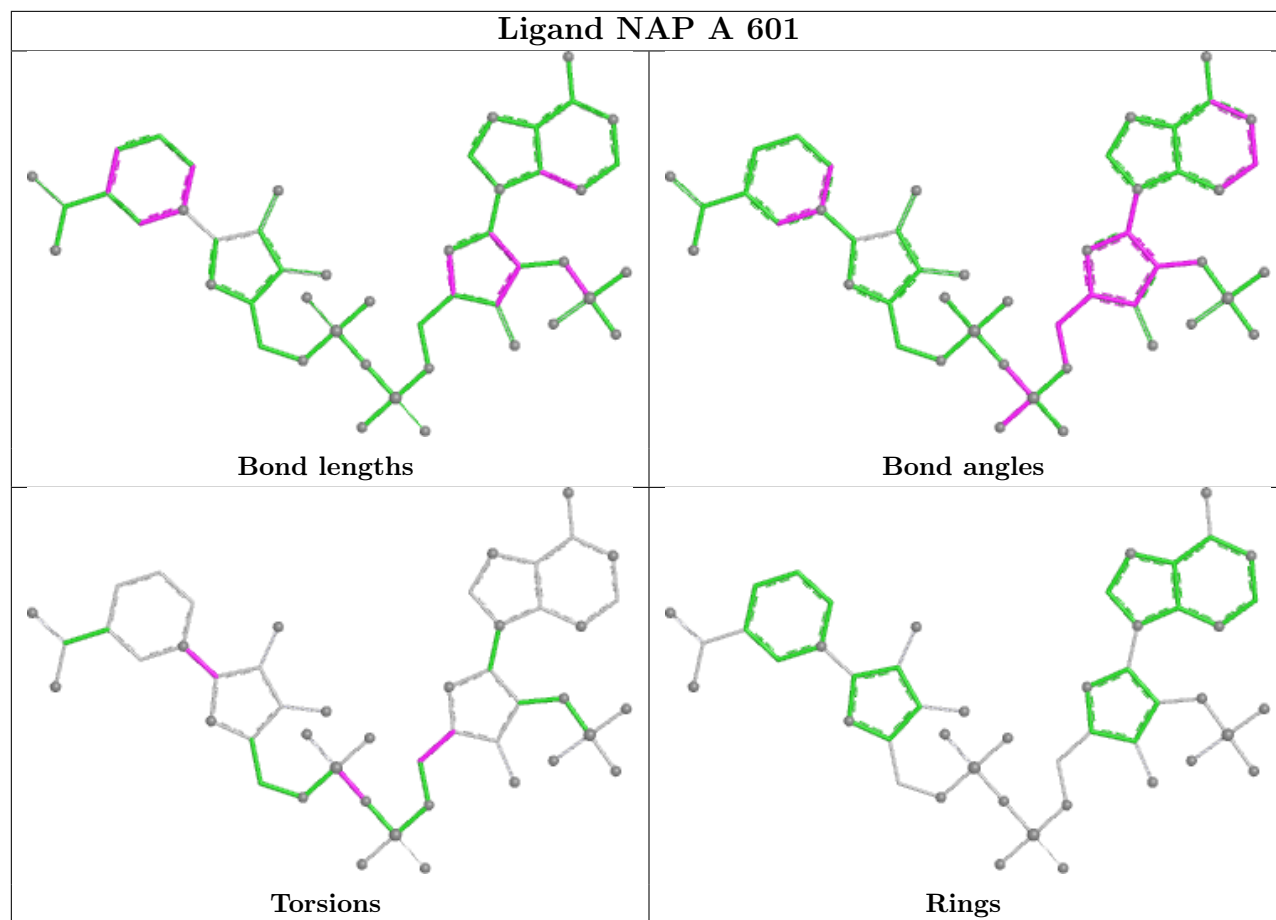
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAP	1	0
4	F	700	MPD	5	0
4	A	701	MPD	2	0
2	F	600	FAD	10	0
3	C	601	NAP	1	0
4	B	701	MPD	3	0
3	D	601	NAP	4	0

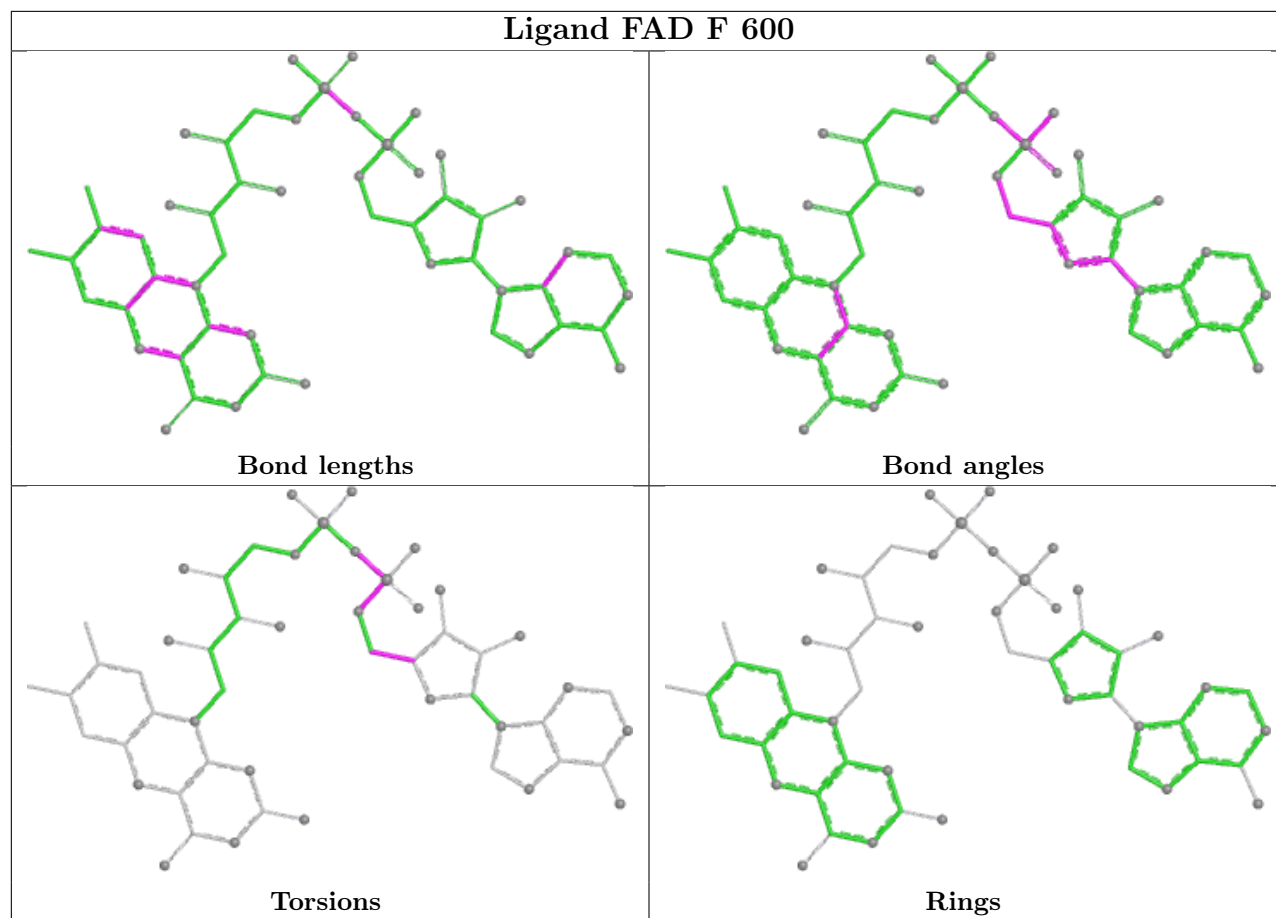
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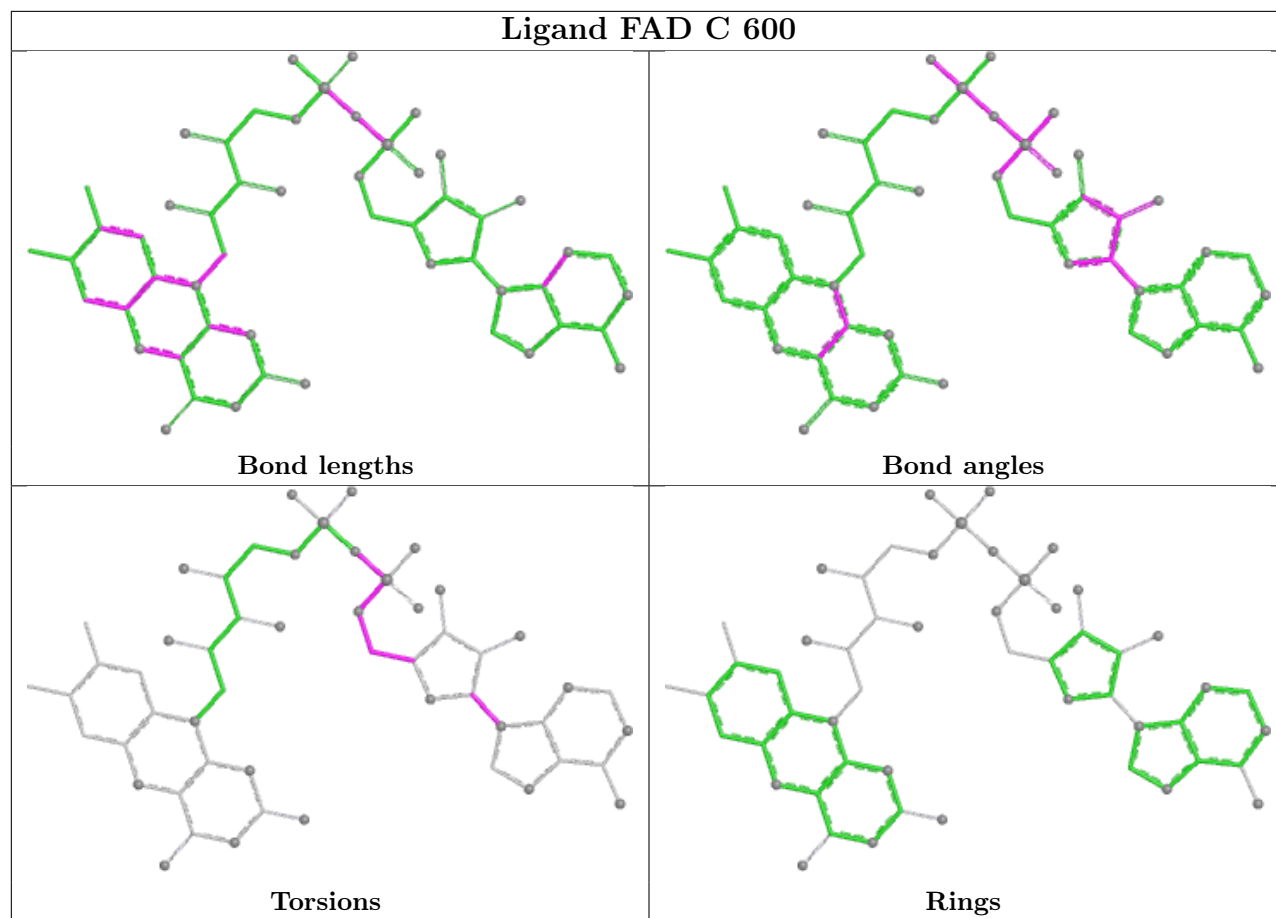
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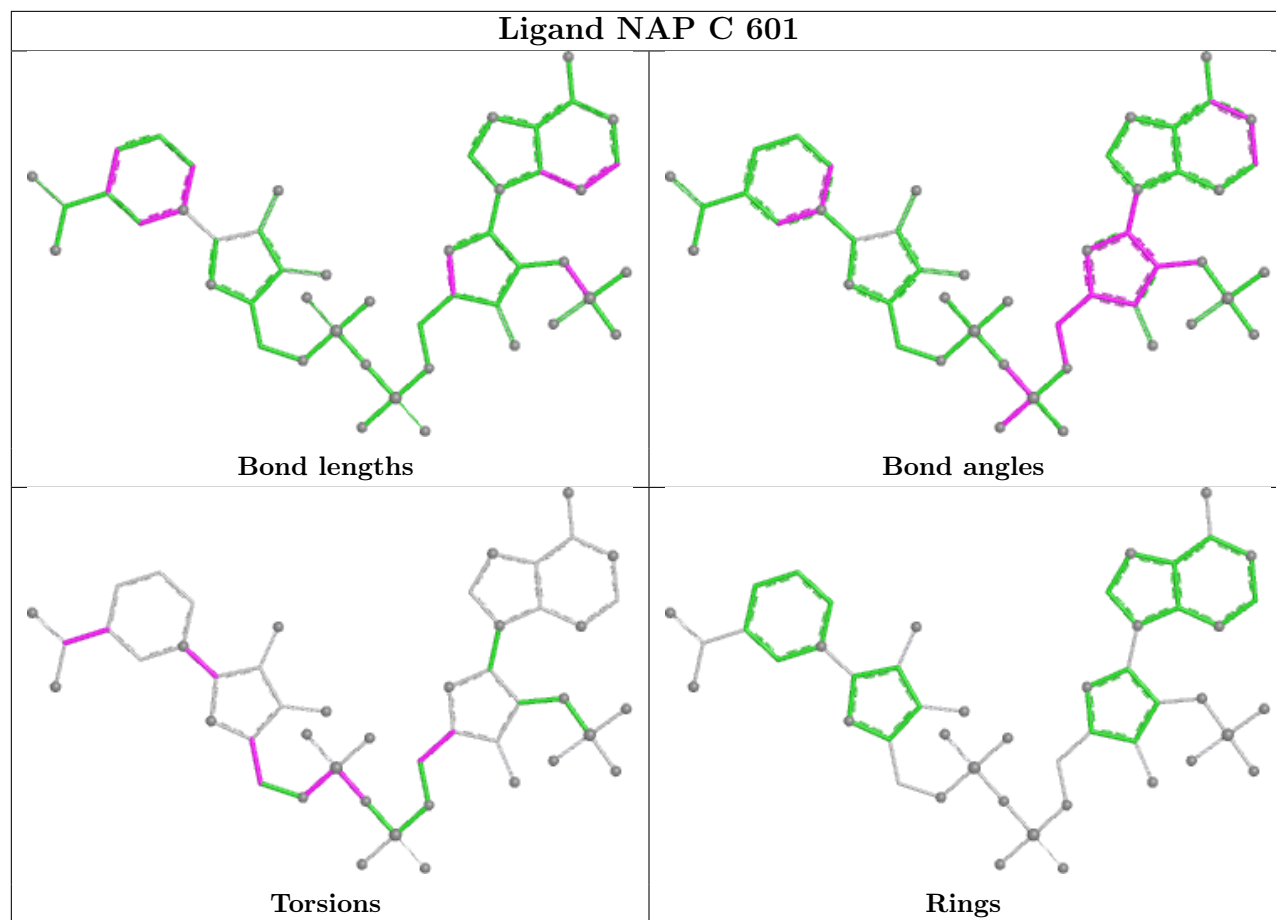
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAP	6	0
4	B	700	MPD	2	0
4	D	700	MPD	3	0
2	E	600	FAD	4	0
3	E	601	NAP	2	0
2	D	600	FAD	5	0
3	F	601	NAP	1	0
2	B	600	FAD	1	0
2	A	600	FAD	2	0

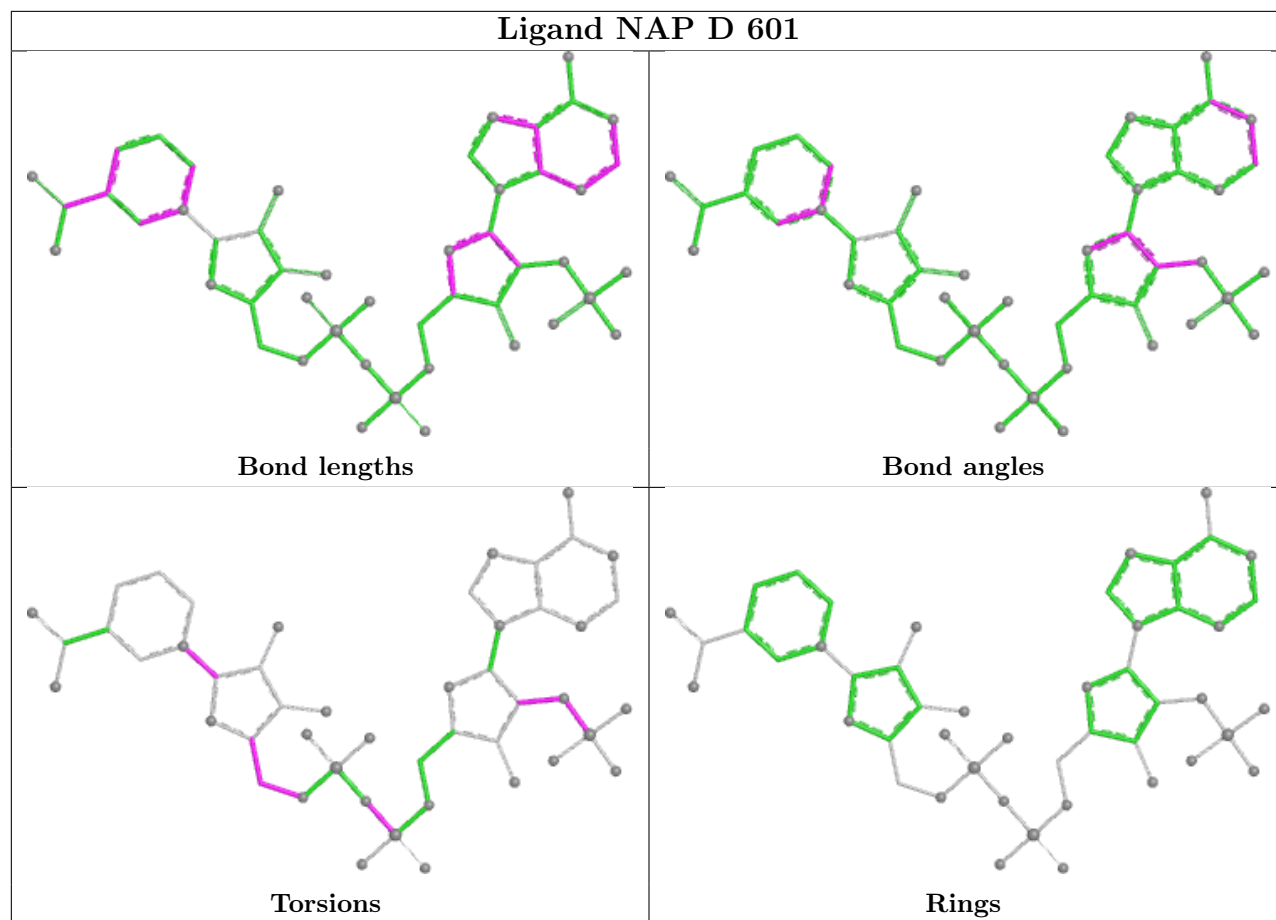
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

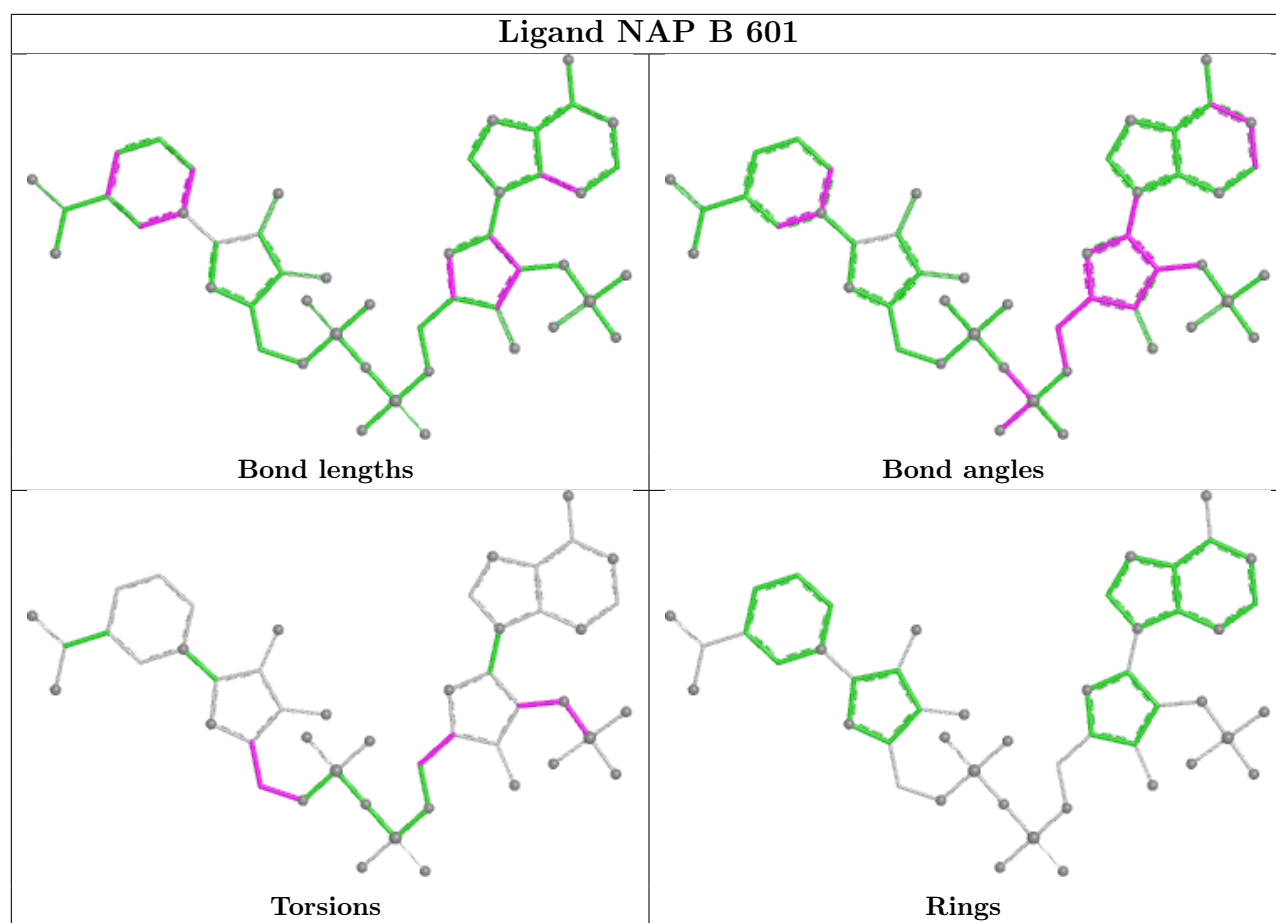


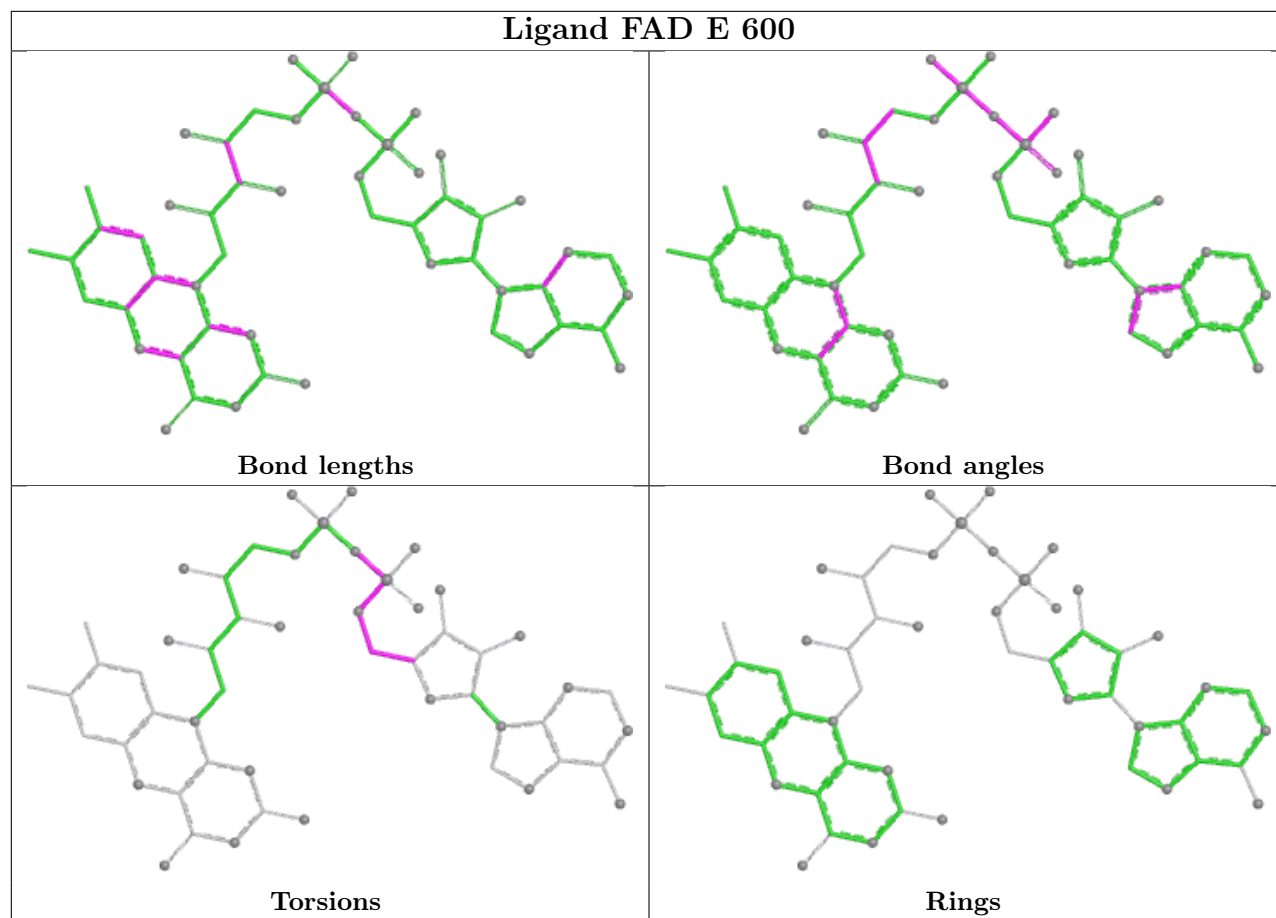


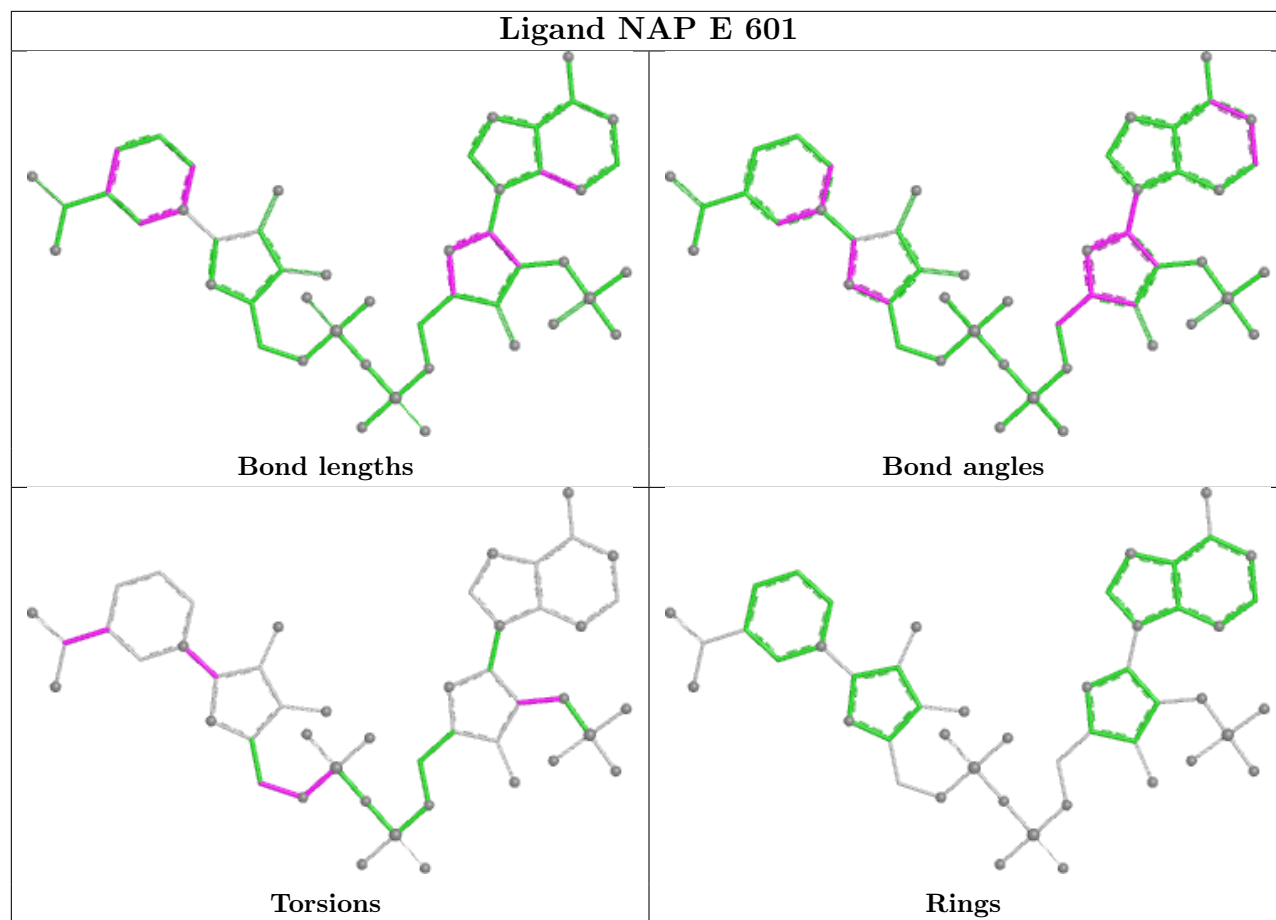


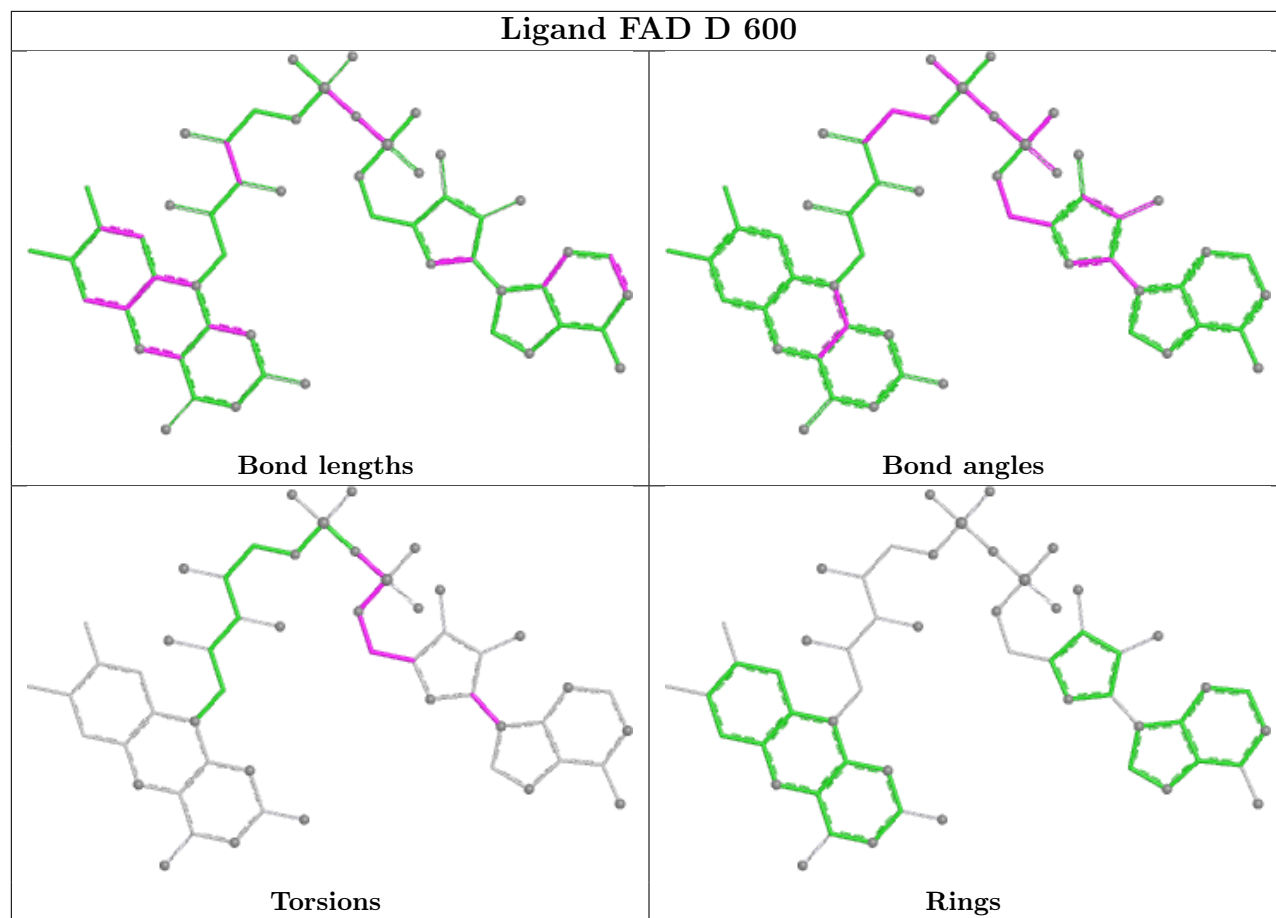


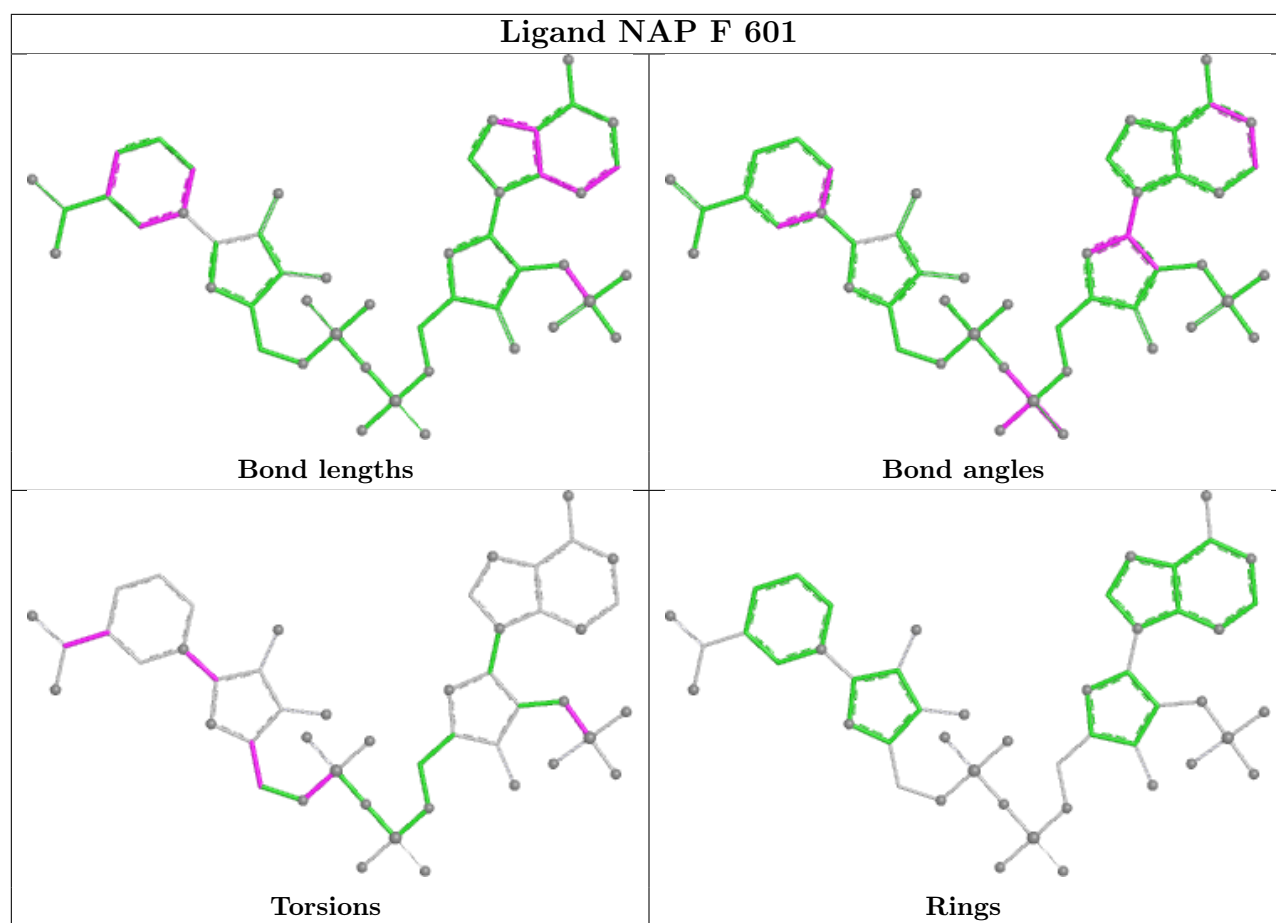


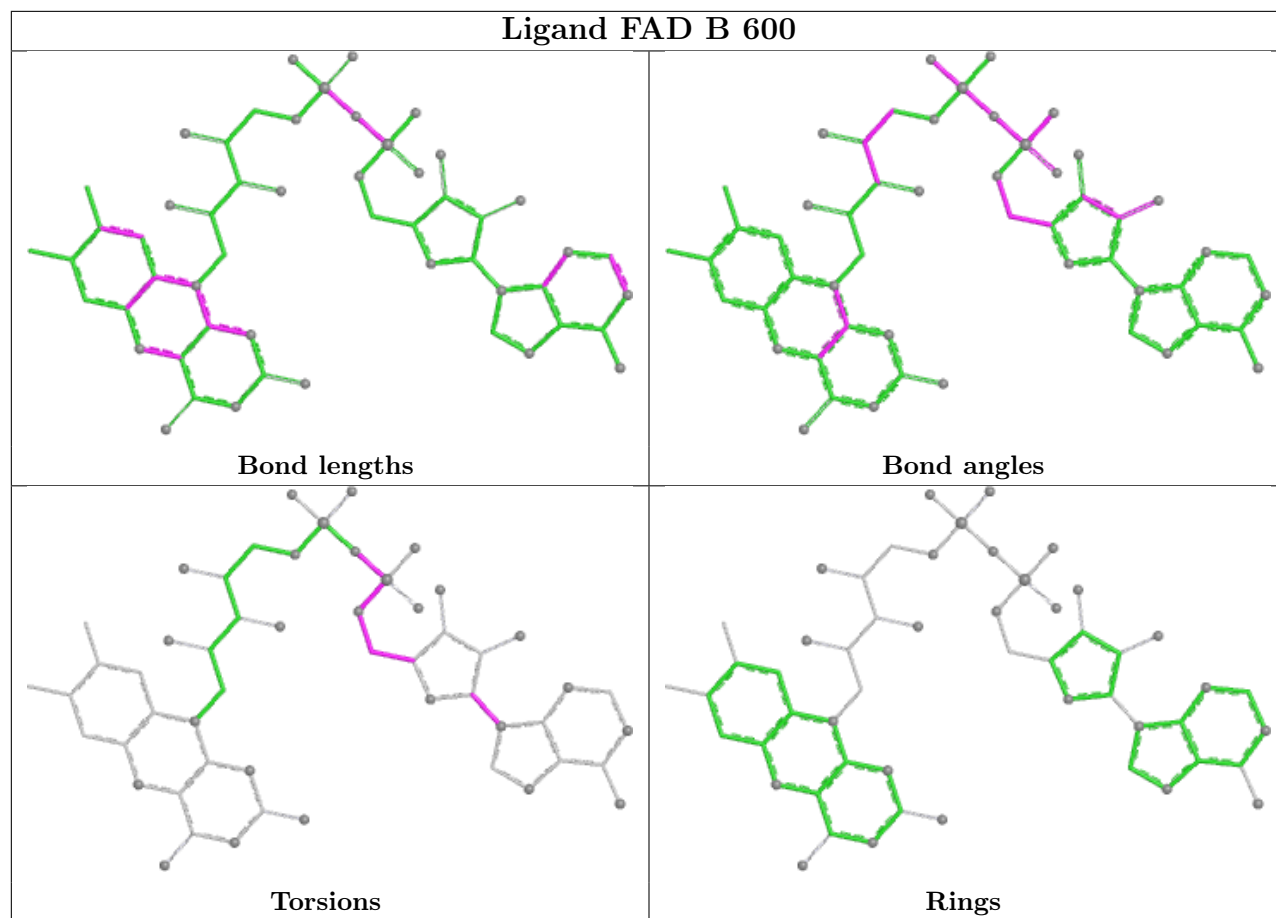


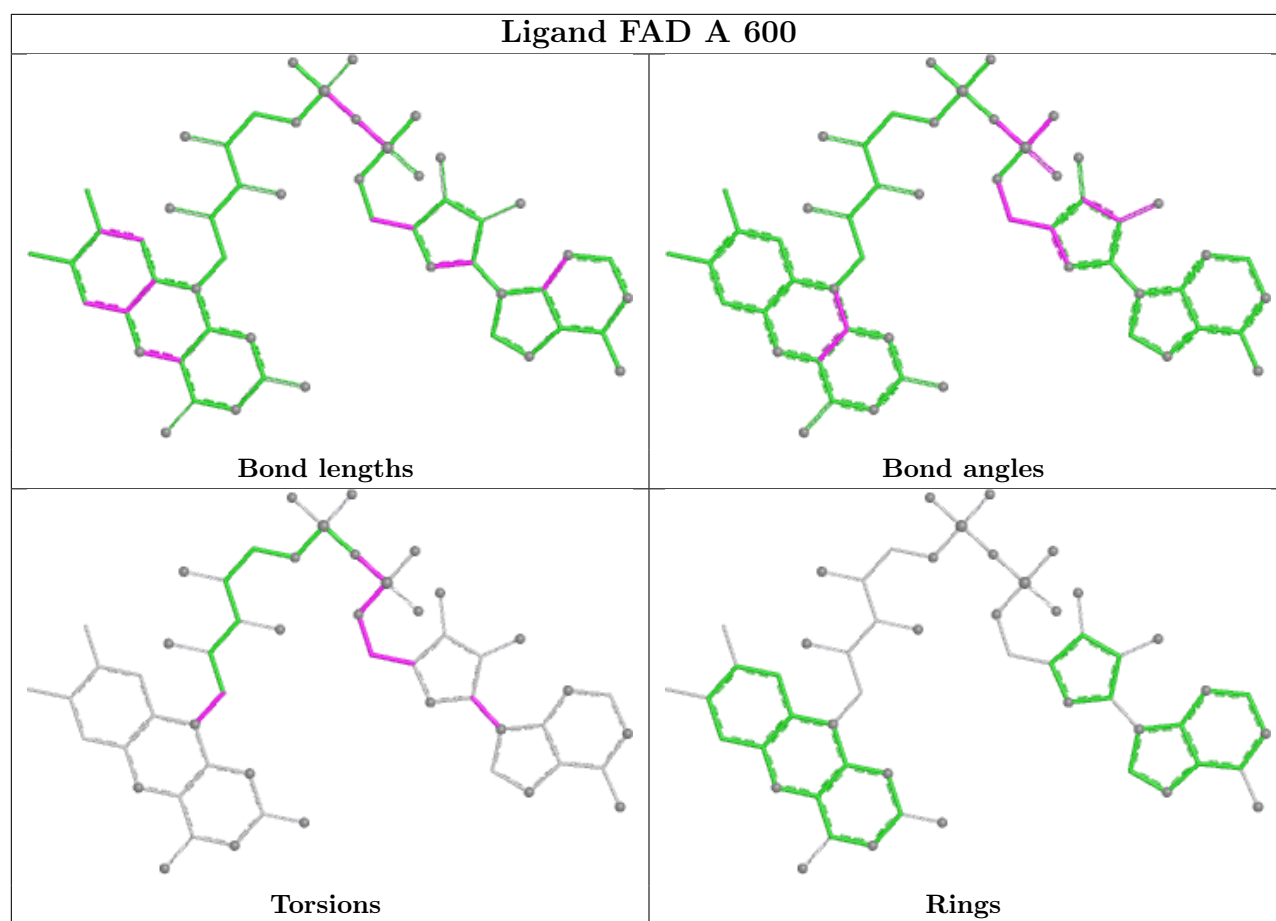












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/519 (93%)	-0.10	0 100 100	25, 51, 70, 83	0
1	B	487/519 (93%)	-0.13	1 (0%) 91 88	26, 51, 69, 93	0
1	C	490/519 (94%)	0.01	3 (0%) 85 80	31, 55, 75, 102	0
1	D	491/519 (94%)	-0.08	1 (0%) 91 88	26, 52, 73, 107	0
1	E	490/519 (94%)	0.06	4 (0%) 82 75	32, 59, 82, 105	0
1	F	486/519 (93%)	-0.01	1 (0%) 91 88	29, 57, 77, 91	0
All	All	2931/3114 (94%)	-0.04	10 (0%) 90 86	25, 54, 75, 107	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	495	ALA	2.7
1	E	20	GLY	2.6
1	C	132	GLY	2.5
1	E	496	GLY	2.2
1	C	347	ILE	2.2

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 ⓘ

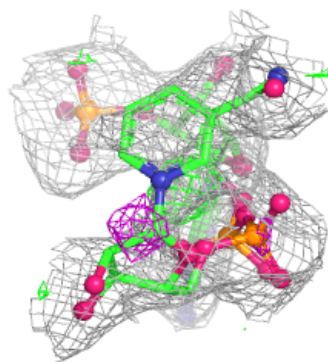
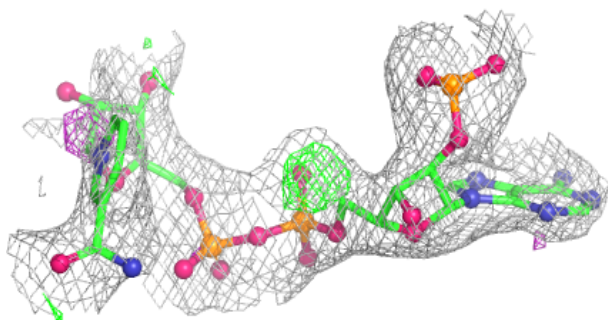
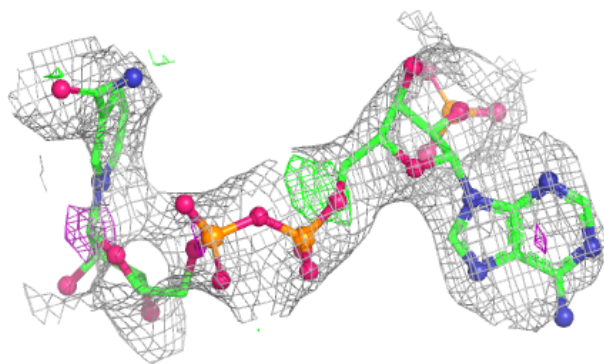
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MPD	A	701	8/8	0.71	0.20	76,78,79,79	0
3	NAP	F	601	48/48	0.74	0.15	83,108,119,120	0
3	NAP	E	601	48/48	0.77	0.14	73,104,121,121	0
4	MPD	B	701	8/8	0.77	0.15	58,60,61,62	0
3	NAP	C	601	48/48	0.83	0.12	80,95,101,102	0
3	NAP	D	601	48/48	0.85	0.12	26,68,87,87	0
3	NAP	A	601	48/48	0.86	0.12	68,86,102,104	0
3	NAP	B	601	48/48	0.86	0.13	63,86,104,105	0
4	MPD	B	700	8/8	0.91	0.12	34,38,39,44	0
2	FAD	E	600	53/53	0.91	0.12	54,59,83,84	0
4	MPD	D	700	8/8	0.91	0.11	39,41,43,43	0
2	FAD	D	600	53/53	0.92	0.10	25,49,70,70	0
2	FAD	F	600	53/53	0.92	0.12	52,60,62,64	0
2	FAD	B	600	53/53	0.94	0.09	35,45,50,52	0
2	FAD	C	600	53/53	0.95	0.08	20,40,61,62	0
2	FAD	A	600	53/53	0.95	0.08	25,35,44,47	0
4	MPD	F	700	8/8	0.95	0.08	34,35,37,37	0

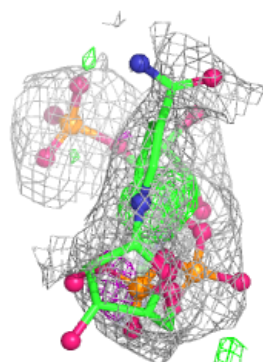
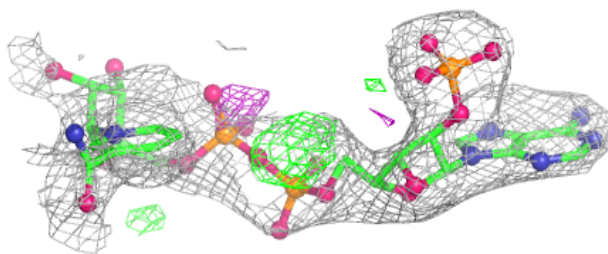
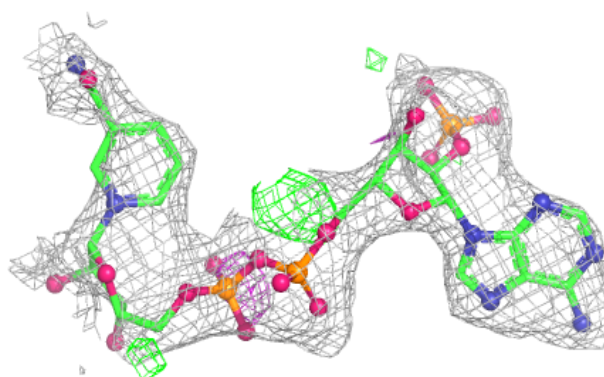
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP 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)

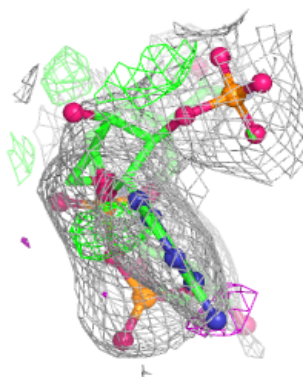
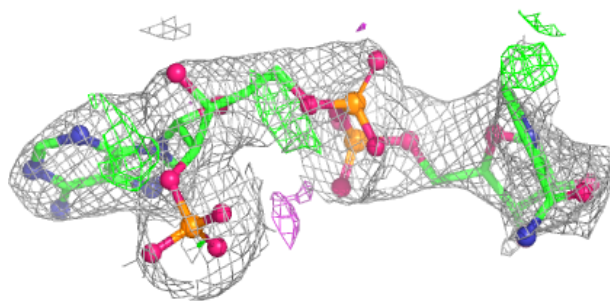
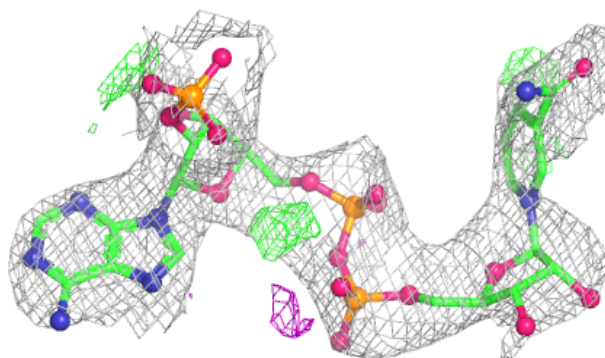
**Electron density around NAP E 601:**

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and green (positive)

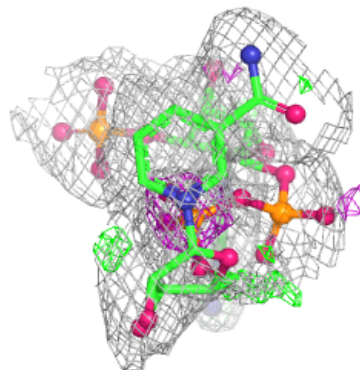
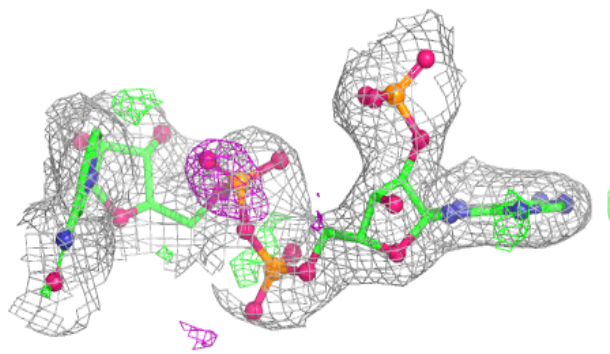
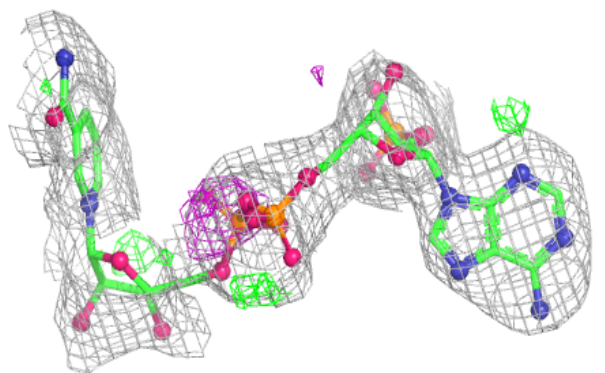


Electron density around NAP C 601:

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and green (positive)

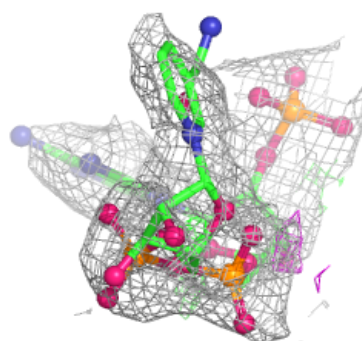
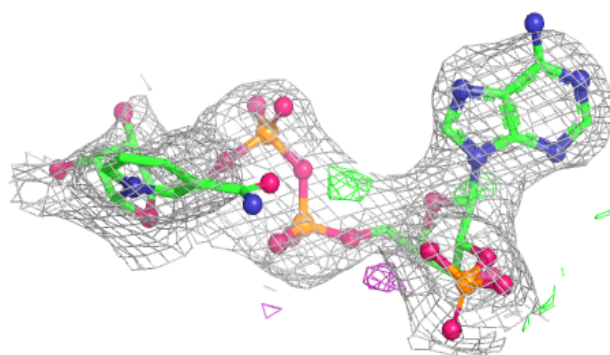
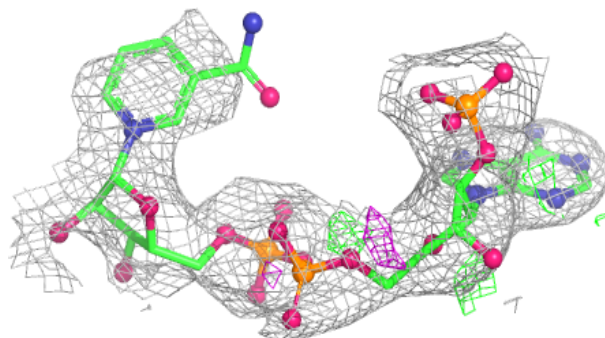
**Electron density around NAP D 601:**

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and green (positive)

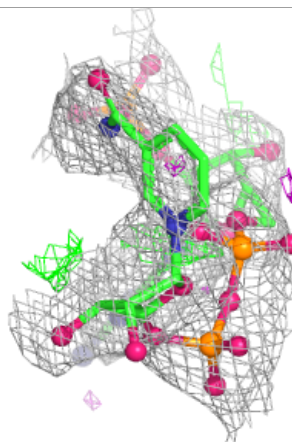
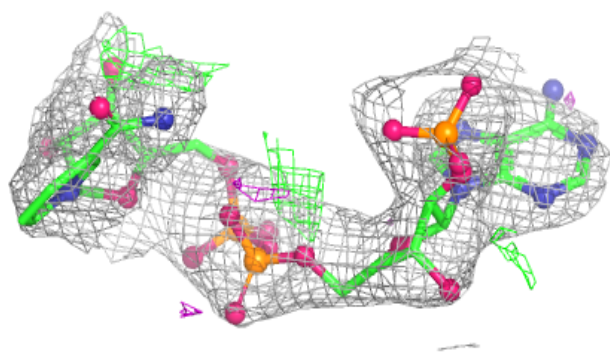
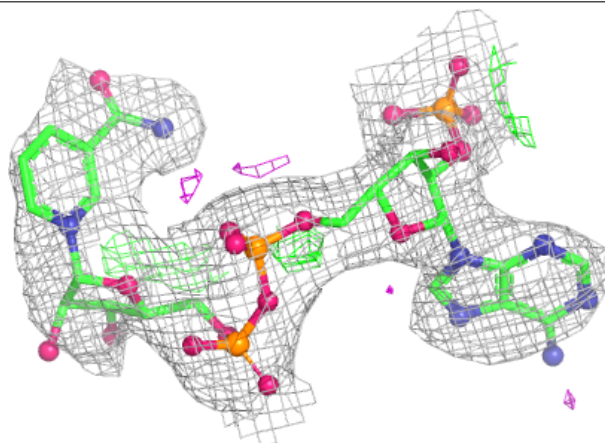


Electron density around NAP A 601:

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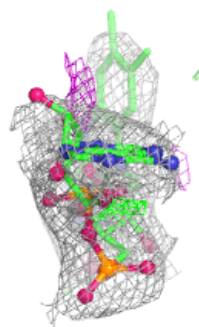
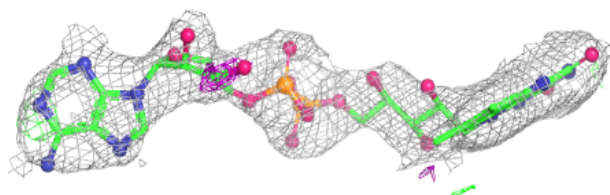
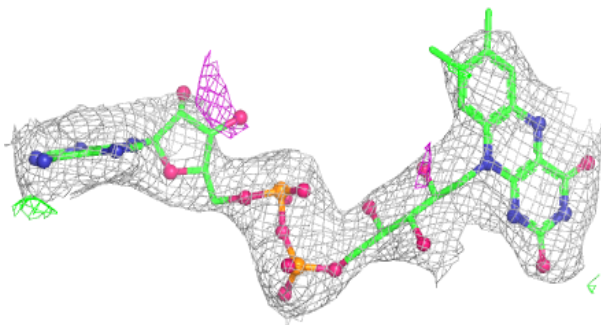
**Electron density around NAP B 601:**

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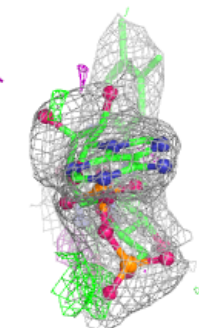
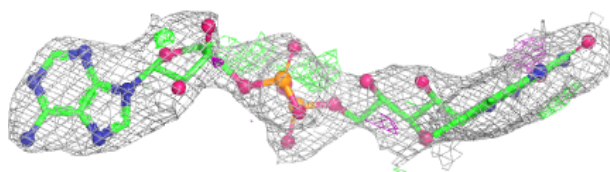
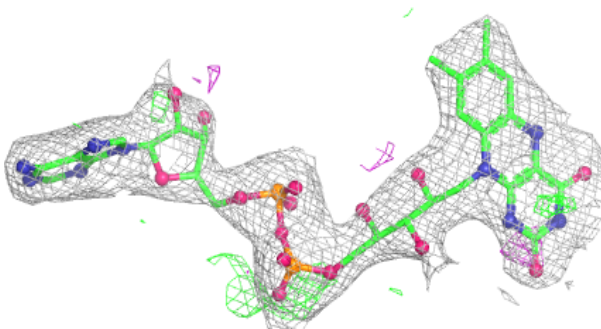


Electron density around FAD E 600:

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and green (positive)

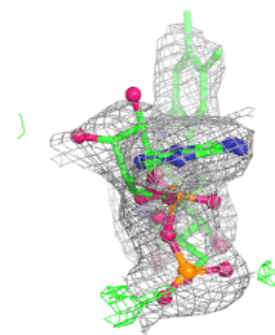
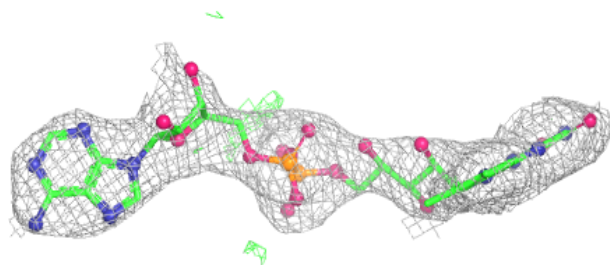
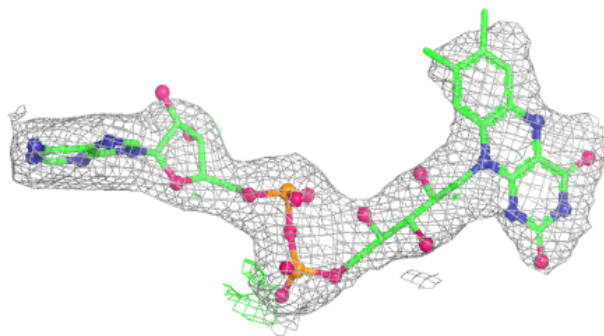
**Electron density around FAD D 600:**

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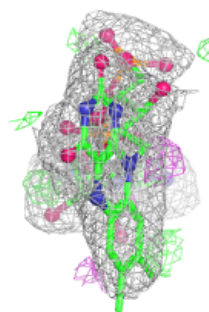
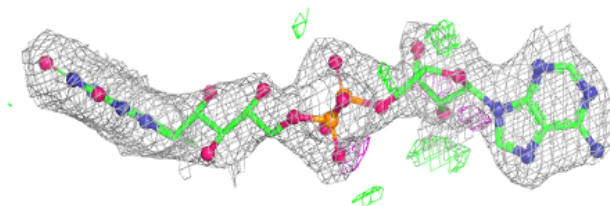
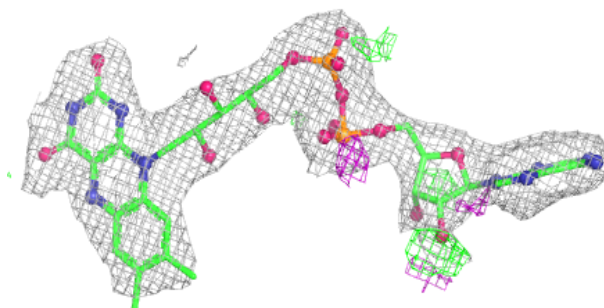


Electron density around FAD F 600:

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and green (positive)

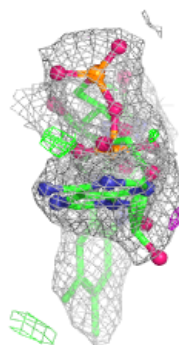
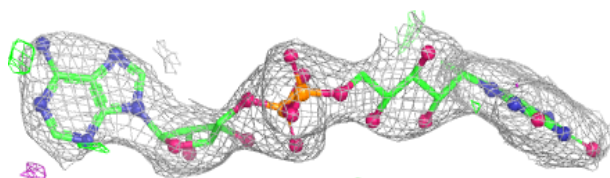
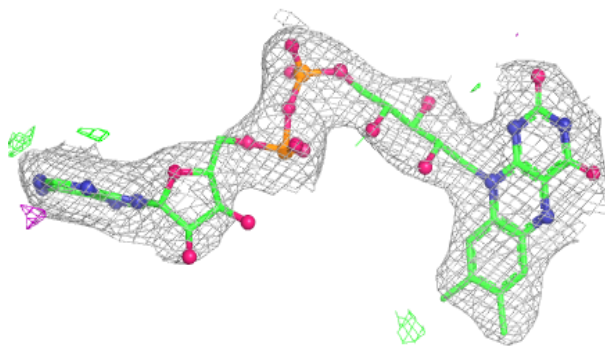
**Electron density around FAD B 600:**

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

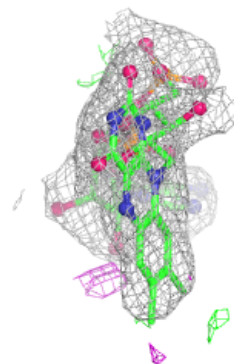
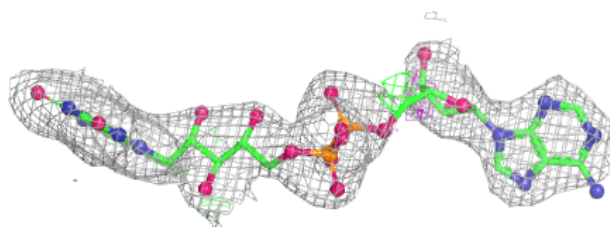
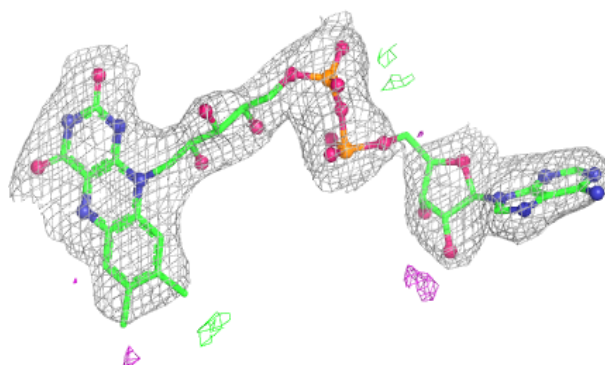


Electron density around FAD C 600:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.