wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 06:44 pm BST

PDB ID	:	1TYP
Title	:	SUBSTRATE INTERACTIONS BETWEEN TRYPANOTHIONE REDUCTASE AND N1-GLUTATHIONYLSPERMIDINE DISULPHIDE AT 0.28-NM RESOLUTION
Authors	:	Bailey, S.; Hunter, W.N.
Deposited on	:	1992-06-29
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 (i) symbol.

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

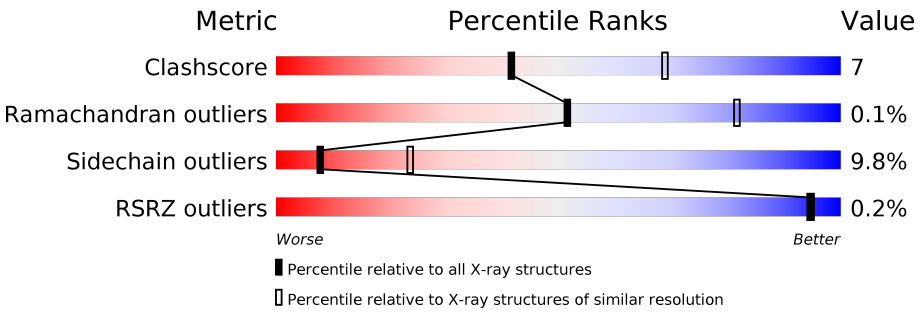
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	487	75% 21% •
1	B	487	74% 22% • •

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
2	FAD	A	493	X	-	-	-
2	FAD	B	493	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	A	494	X	-	-	-
3	NAP	B	494	X	-	-	-
5	SPD	A	496	-	-	X	-
5	SPD	A	498	-	-	-	X
5	SPD	B	498	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8136 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.

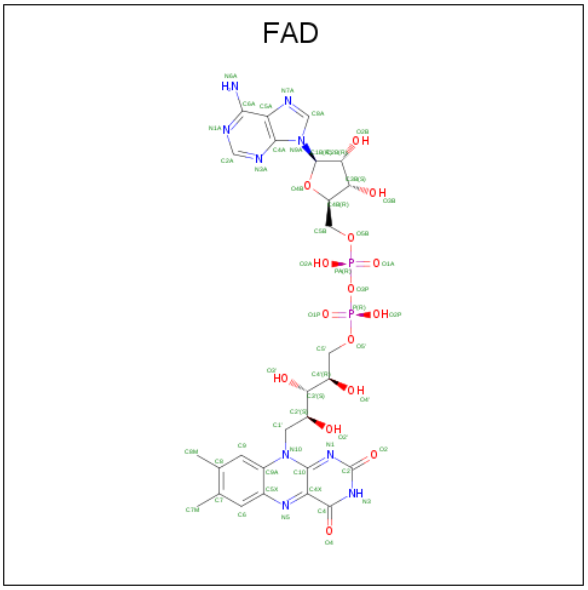
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3713	2336	645	711	21	0	0	0
1	B	486	3705	2331	644	710	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	TRP	PHE	CONFLICT	UNP P39040
B	126	TRP	PHE	CONFLICT	UNP P39040

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

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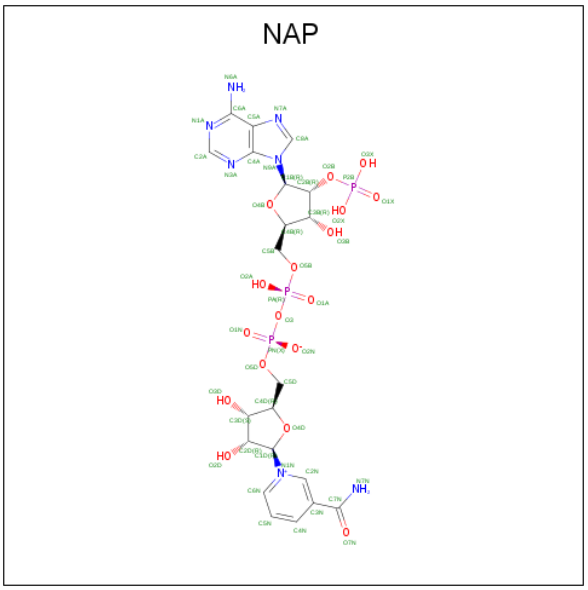
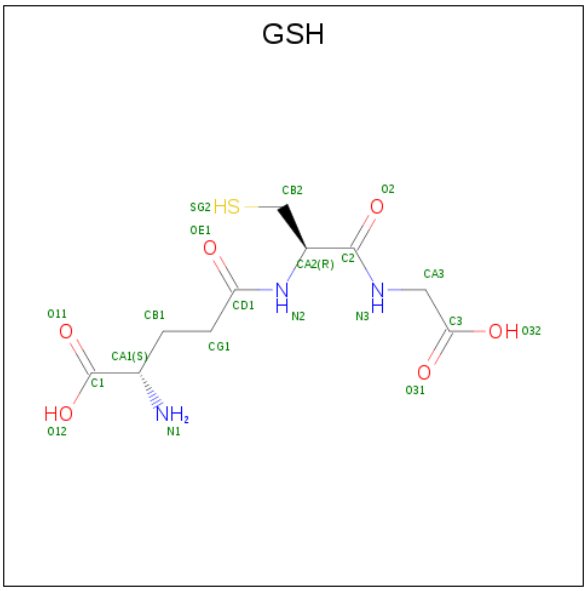
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	53	27	9	15	2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



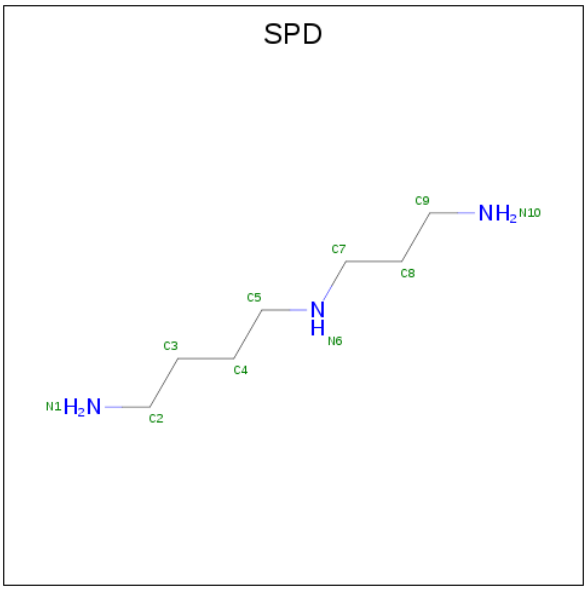
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0

- Molecule 4 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			19	10	3	5	1		
4	A	1	Total	C	N	O	S	0	0
			19	10	3	5	1		
4	B	1	Total	C	N	O	S	0	0
			19	10	3	5	1		
4	B	1	Total	C	N	O	S	0	0
			19	10	3	5	1		

- Molecule 5 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	A	1	10	7	3	0	0
			Total	C	N		
5	A	1	10	7	3	0	0
			Total	C	N		
5	B	1	10	7	3	0	0
			Total	C	N		
5	B	1	10	7	3	0	0

- Molecule 6 is water.

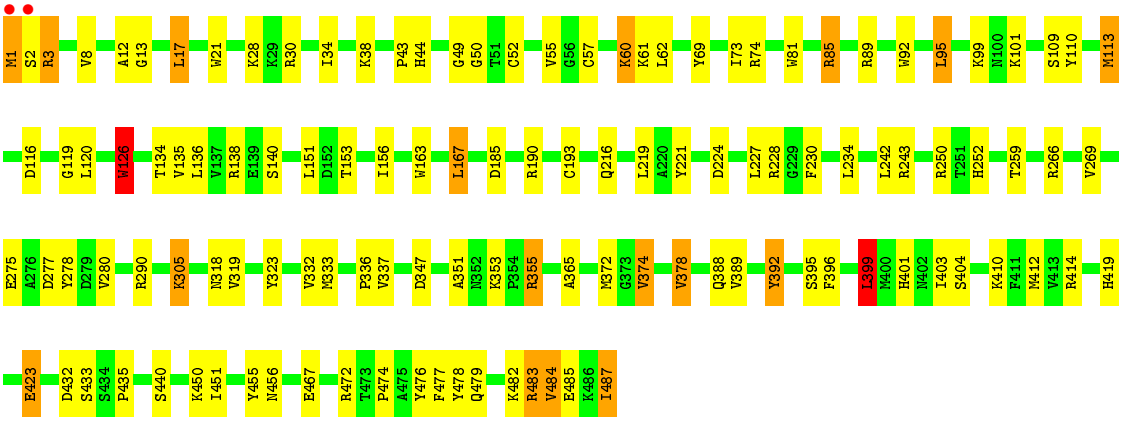
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	196	196	196	0	0
			Total	O		
6	B	204	204	204	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

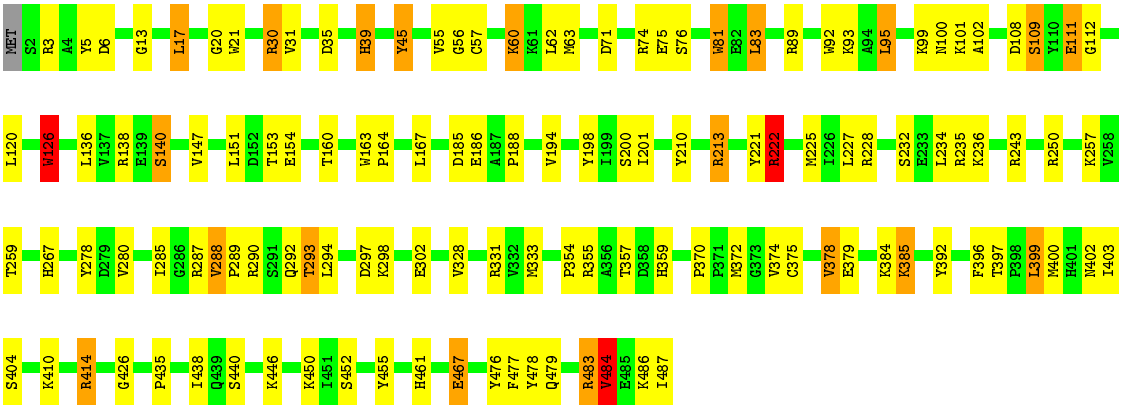
- Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A:



- Molecule 1: TRYPANOTHIONE REDUCTASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	128.80Å 128.80Å 92.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 31.47 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 91.3 (31.47-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.148 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 70.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8136	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, NAP, SPD, 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	0.87	0/3787	1.66	55/5131 (1.1%)
1	B	0.88	1/3779 (0.0%)	1.65	73/5121 (1.4%)
All	All	0.87	1/7566 (0.0%)	1.66	128/10252 (1.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	VAL	CA-CB	5.38	1.66	1.54

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	MET	CA-CB-CG	16.40	141.19	113.30
1	A	113	MET	CB-CG-SD	16.40	161.60	112.40
1	B	30	ARG	NE-CZ-NH1	15.20	127.90	120.30
1	A	414	ARG	NE-CZ-NH1	13.68	127.14	120.30
1	B	126	TRP	CD1-CG-CD2	12.31	116.15	106.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	45	TYR	Sidechain

5.2 Too-close contacts (i)

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	3713	0	3658	59	0
1	B	3705	0	3646	51	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
3	A	48	0	24	3	0
3	B	48	0	24	10	0
4	A	38	0	27	0	0
4	B	38	0	28	0	0
5	A	20	0	34	8	0
5	B	20	0	35	1	0
6	A	196	0	0	6	0
6	B	204	0	0	7	0
All	All	8136	0	7538	107	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 7.

The worst 5 of 107 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:A:113:MET:HG3	5:A:496:SPD:N10	1.32	1.41
1:A:113:MET:CG	5:A:496:SPD:N10	2.27	0.98
1:A:113:MET:CG	5:A:496:SPD:H102	1.79	0.94
1:A:113:MET:HG3	5:A:496:SPD:H101	1.41	0.86
1:B:198:TYR:HE1	3:B:494:NAP:H3D	1.47	0.79

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	485/487 (100%)	464 (96%)	20 (4%)	1 (0%)	47	78
1	B	484/487 (99%)	461 (95%)	23 (5%)	0	100	100
All	All	969/974 (100%)	925 (96%)	43 (4%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG

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	390/390 (100%)	352 (90%)	38 (10%)	8	24
1	B	389/390 (100%)	351 (90%)	38 (10%)	8	24
All	All	779/780 (100%)	703 (90%)	76 (10%)	8	24

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	483	ARG
1	B	83	LEU
1	B	450	LYS
1	A	484	VAL
1	B	17	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	B	39	HIS
1	B	130	GLN
1	B	479	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	SPD	A	498	4	9,9,9	0.93	0	8,8,8	1.04	0
5	SPD	B	498	4	9,9,9	1.69	2 (22%)	8,8,8	2.51	3 (37%)
4	GSH	B	495	5,4	14,18,19	0.70	0	16,22,24	1.94	5 (31%)
4	GSH	A	495	5,4	14,18,19	0.41	0	16,22,24	1.84	4 (25%)
4	GSH	B	497	5,4	14,18,19	1.24	1 (7%)	16,22,24	4.78	9 (56%)
5	SPD	B	496	4	9,9,9	0.36	0	8,8,8	1.35	1 (12%)
3	NAP	A	494	-	45,52,52	1.41	6 (13%)	56,80,80	2.38	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAP	B	494	-	45,52,52	1.69	6 (13%)	56,80,80	2.15	12 (21%)
2	FAD	B	493	-	51,58,58	1.40	7 (13%)	60,89,89	2.81	14 (23%)
5	SPD	A	496	4	9,9,9	0.33	0	8,8,8	2.55	3 (37%)
4	GSH	A	497	5,4	14,18,19	0.97	0	16,22,24	4.34	7 (43%)
2	FAD	A	493	-	51,58,58	1.33	5 (9%)	60,89,89	2.69	11 (18%)

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	SPD	A	498	4	-	0/7/7/7	-
5	SPD	B	498	4	-	4/7/7/7	-
4	GSH	B	495	5,4	-	1/18/23/24	-
4	GSH	A	495	5,4	-	2/18/23/24	-
4	GSH	B	497	5,4	-	5/18/23/24	-
5	SPD	B	496	4	-	1/7/7/7	-
3	NAP	A	494	-	3/3/12/12	10/31/67/67	0/5/5/5
3	NAP	B	494	-	3/3/12/12	10/31/67/67	0/5/5/5
2	FAD	B	493	-	1/1/9/9	4/30/50/50	0/6/6/6
5	SPD	A	496	4	-	1/7/7/7	-
4	GSH	A	497	5,4	-	5/18/23/24	-
2	FAD	A	493	-	1/1/9/9	4/30/50/50	0/6/6/6

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	494	NAP	O4D-C1D	5.50	1.48	1.41
2	A	493	FAD	C4-C4X	4.49	1.49	1.41
3	B	494	NAP	C2N-N1N	4.45	1.40	1.35
3	B	494	NAP	C2D-C3D	-4.18	1.41	1.53
3	B	494	NAP	C2D-C1D	4.11	1.60	1.53

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	493	FAD	C4-N3-C2	13.17	126.26	115.14
4	B	497	GSH	CA2-CB2-SG2	-13.07	99.50	114.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	497	GSH	CA2-CB2-SG2	-12.80	99.81	114.19
2	B	493	FAD	C4-N3-C2	11.89	125.18	115.14
2	B	493	FAD	C3B-C2B-C1B	-10.49	85.19	100.98

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	494	NAP	C3D
3	A	494	NAP	C4D
3	A	494	NAP	C1D
3	B	494	NAP	C3D
3	B	494	NAP	C4D

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	495	GSH	N1-CA1-CB1-CG1
4	A	495	GSH	C1-CA1-CB1-CG1
4	B	497	GSH	N2-CA2-CB2-SG2
4	B	497	GSH	C2-CA2-CB2-SG2
3	A	494	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

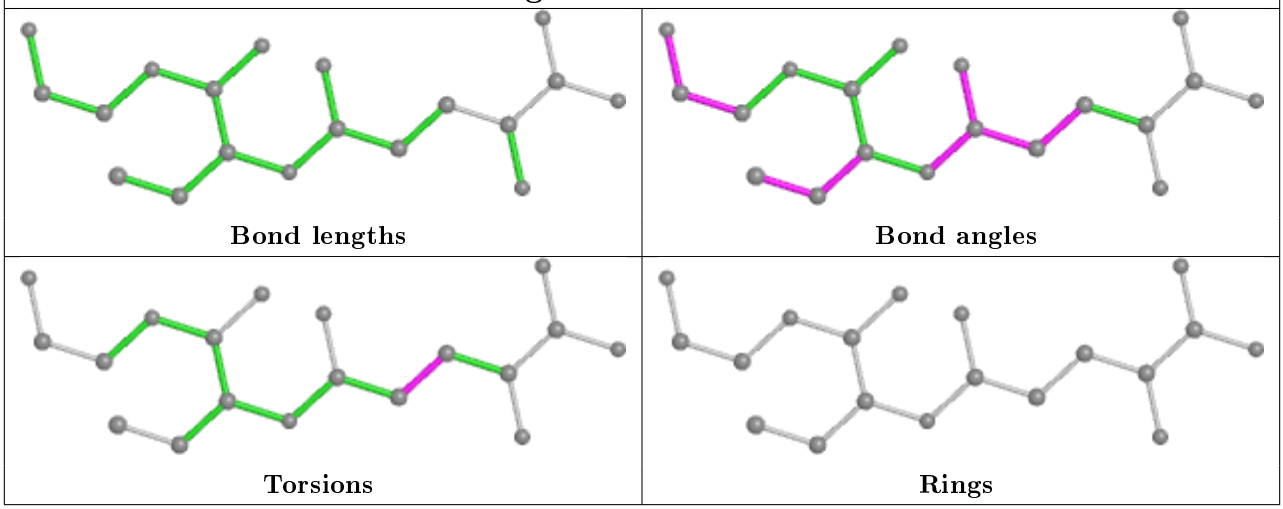
7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	498	SPD	1	0
5	B	498	SPD	1	0
3	A	494	NAP	3	0
3	B	494	NAP	10	0
2	B	493	FAD	2	0
5	A	496	SPD	7	0
2	A	493	FAD	2	0

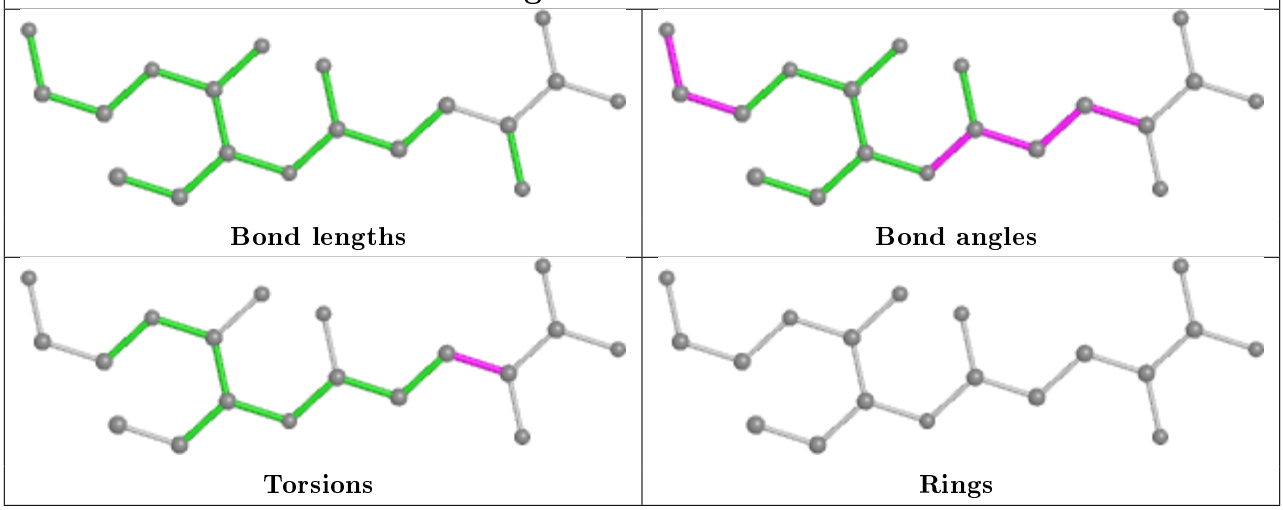
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

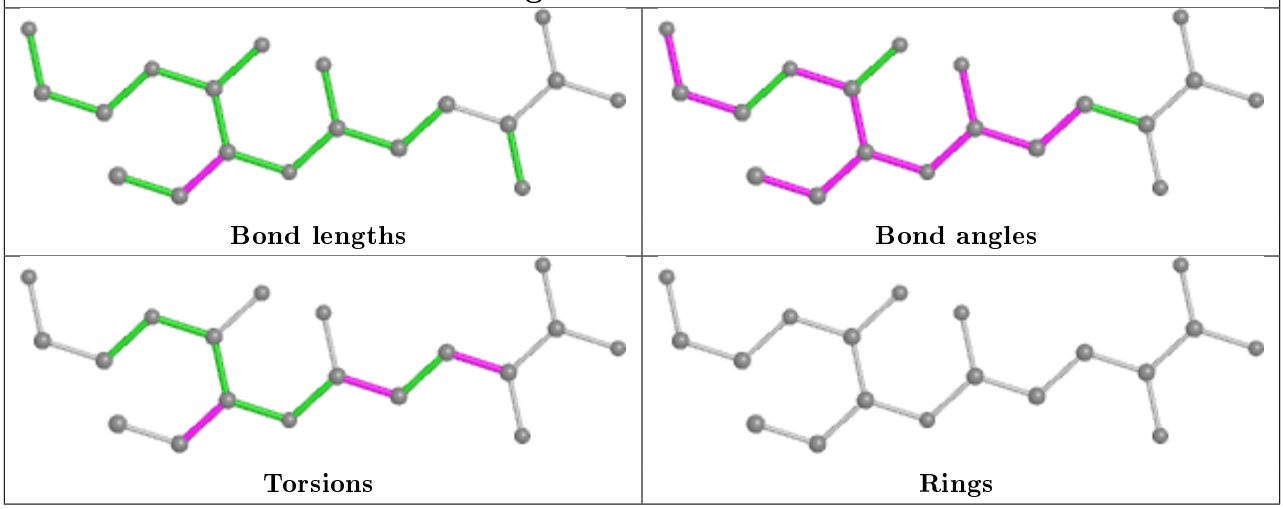
Ligand GSH B 495



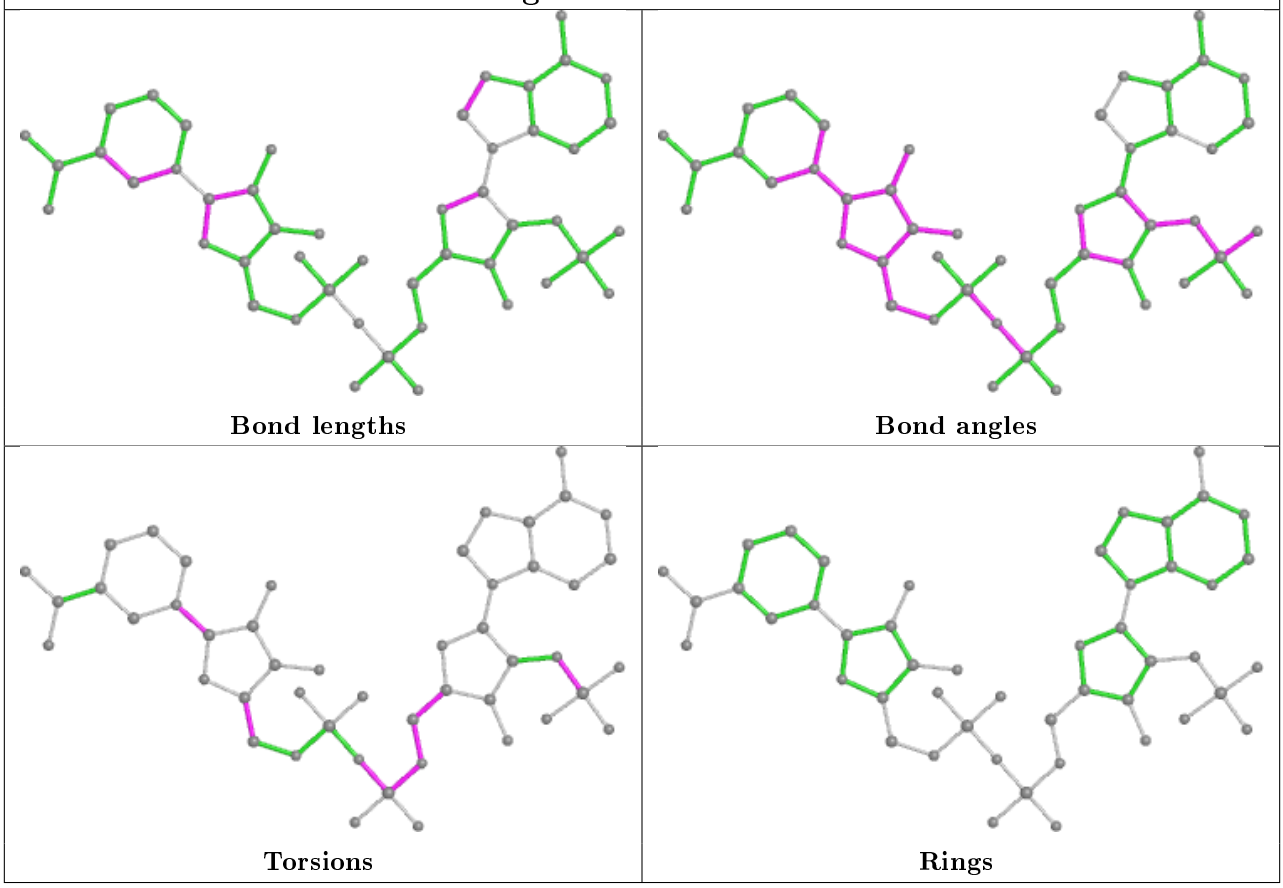
Ligand GSH A 495



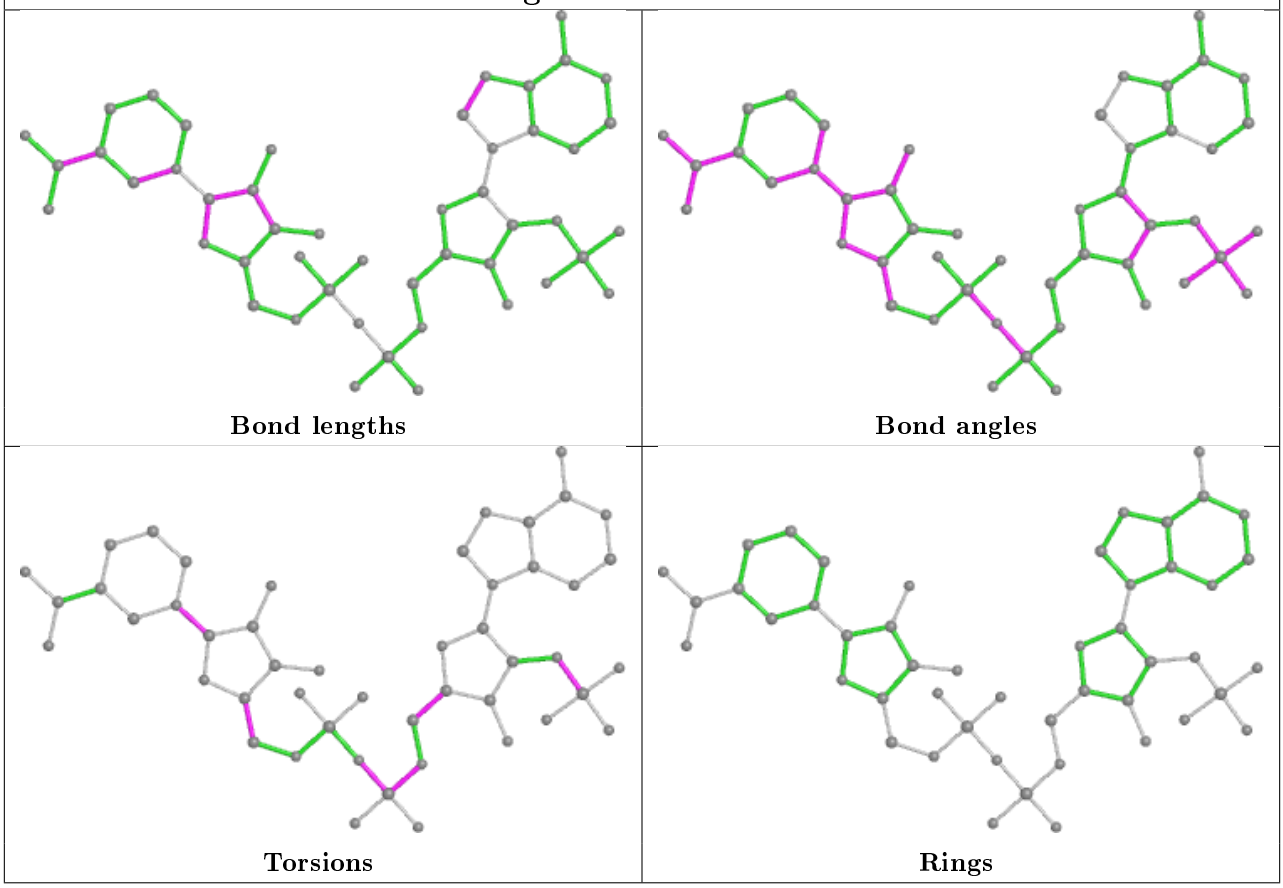
Ligand GSH B 497



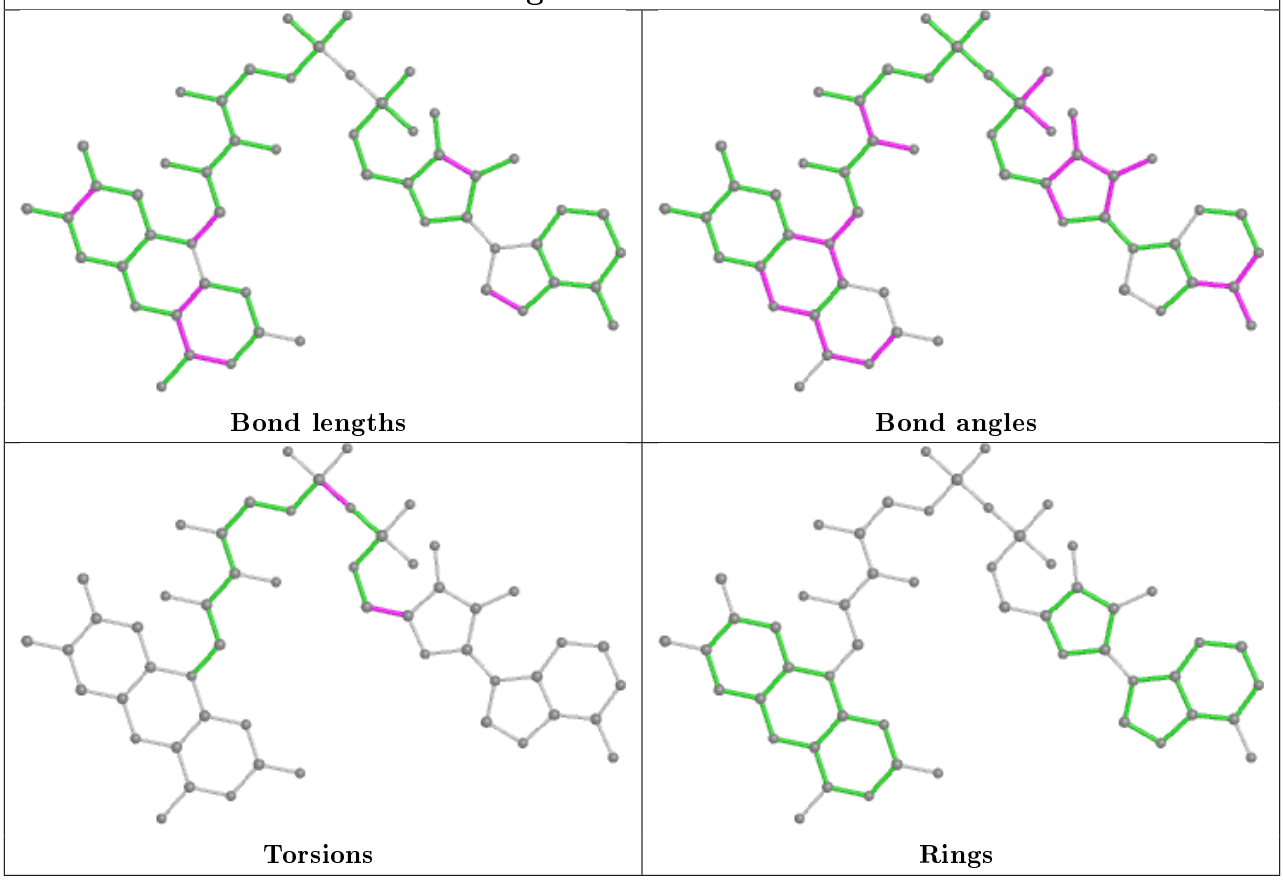
Ligand NAP A 494



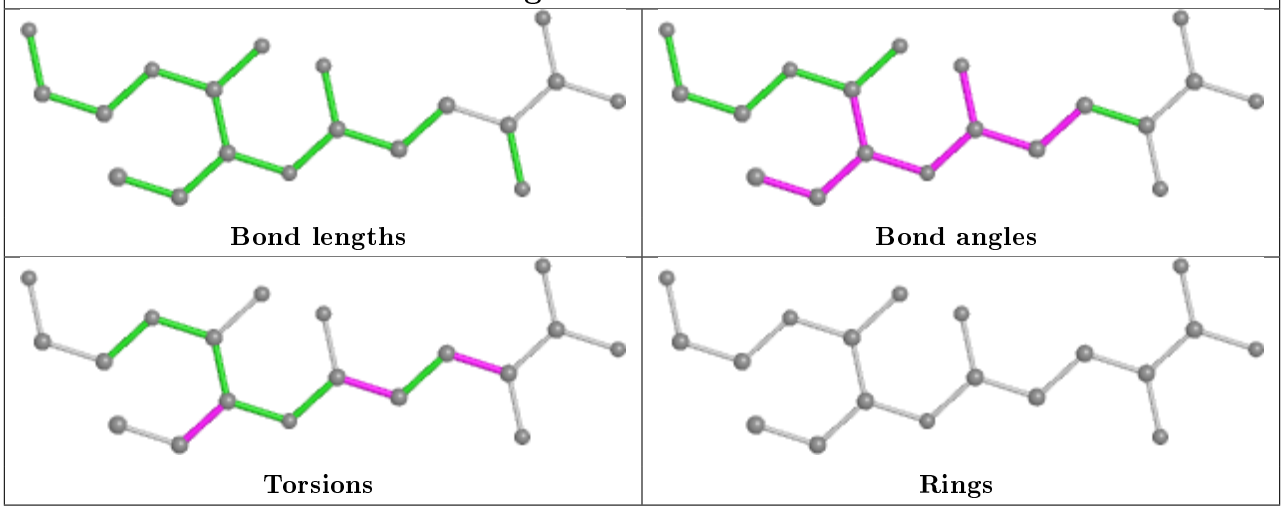
Ligand NAP B 494



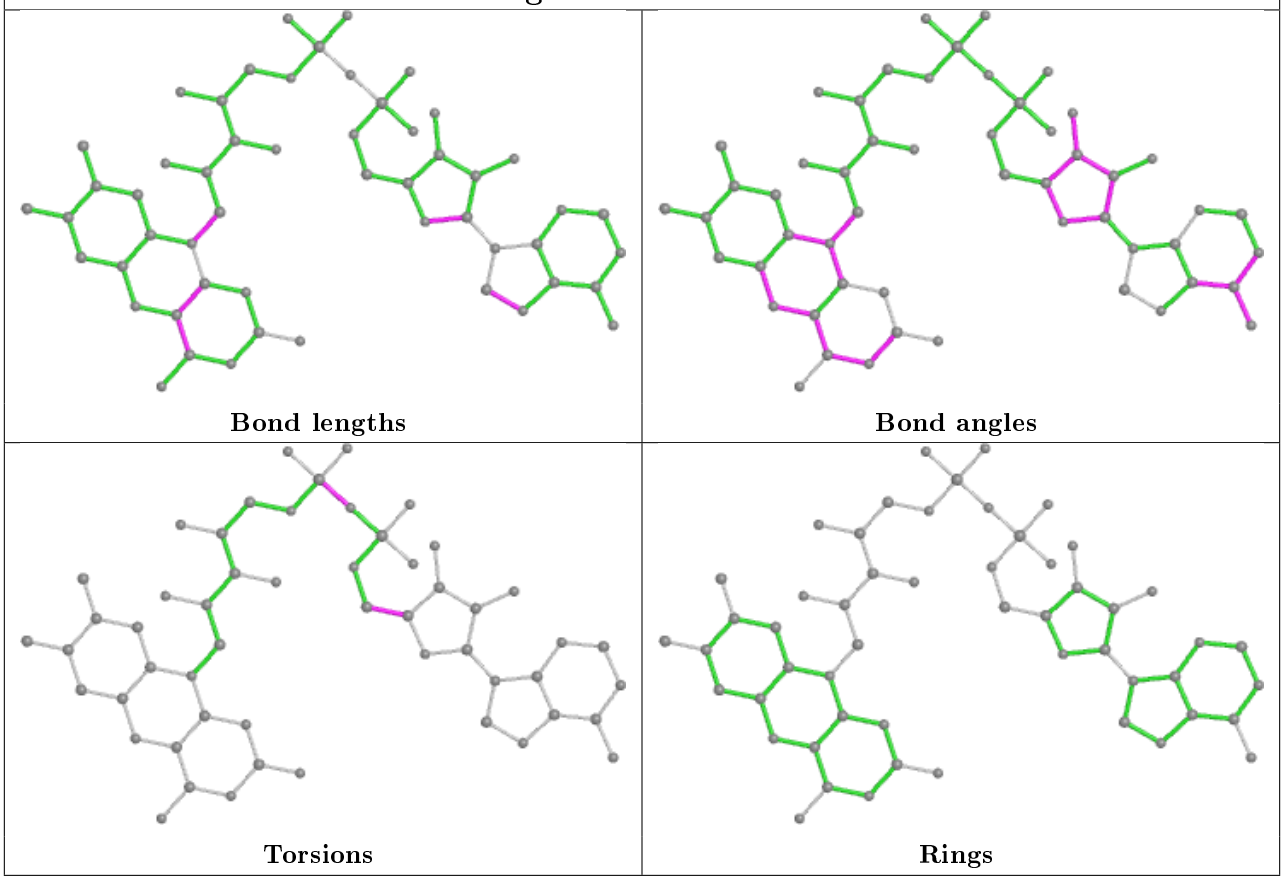
Ligand FAD B 493



Ligand GSH A 497



Ligand FAD A 493



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	487/487 (100%)	-0.95	2 (0%) 92 91	3, 10, 30, 70	0
1	B	486/487 (99%)	-0.89	0 100 100	3, 9, 29, 48	0
All	All	973/974 (99%)	-0.92	2 (0%) 95 94	3, 10, 30, 70	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.0
1	A	2	SER	2.9

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	SPD	A	498	10/10	0.72	0.69	53,56,59,60	0
5	SPD	B	498	10/10	0.79	0.63	64,66,73,73	0

Continued on next page...

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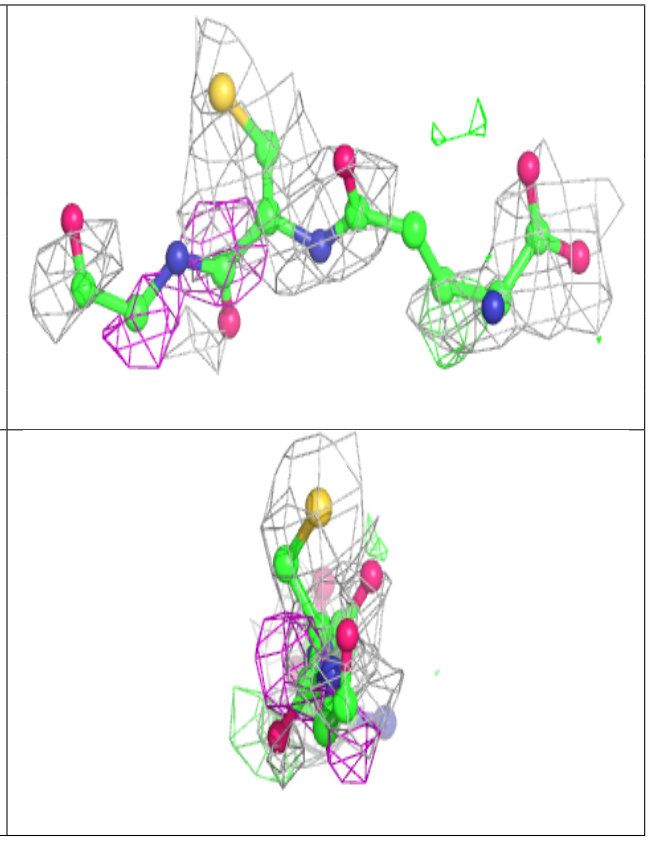
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GSH	B	497	19/20	0.79	0.33	48,63,66,66	0
5	SPD	A	496	10/10	0.89	0.25	25,40,62,65	0
4	GSH	A	497	19/20	0.89	0.26	30,50,54,59	0
4	GSH	B	495	19/20	0.91	0.18	29,35,38,39	0
5	SPD	B	496	10/10	0.92	0.30	27,43,53,54	0
4	GSH	A	495	19/20	0.93	0.17	23,26,38,40	0
3	NAP	B	494	48/48	0.93	0.18	22,49,61,66	0
3	NAP	A	494	48/48	0.94	0.17	28,50,71,73	0
2	FAD	B	493	53/53	0.99	0.14	3,4,11,13	0
2	FAD	A	493	53/53	0.99	0.11	3,4,7,10	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.

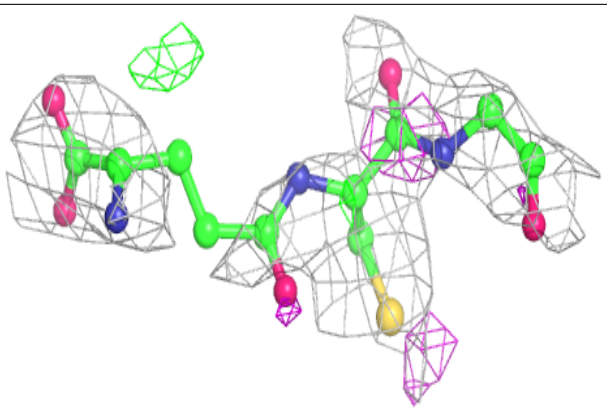
Electron density around GSH B 497:

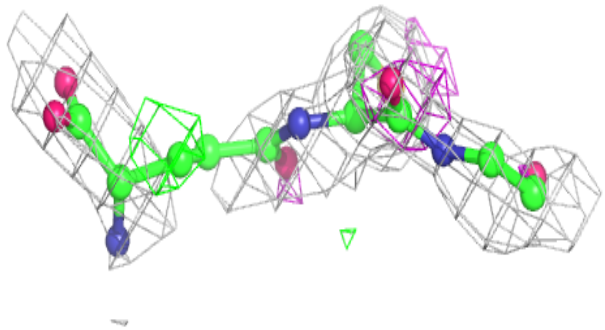
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

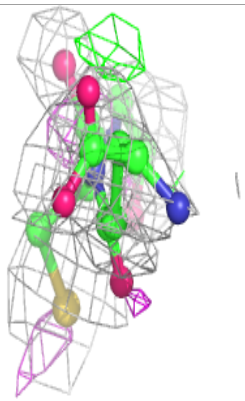


Electron density around GSH A 497:

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

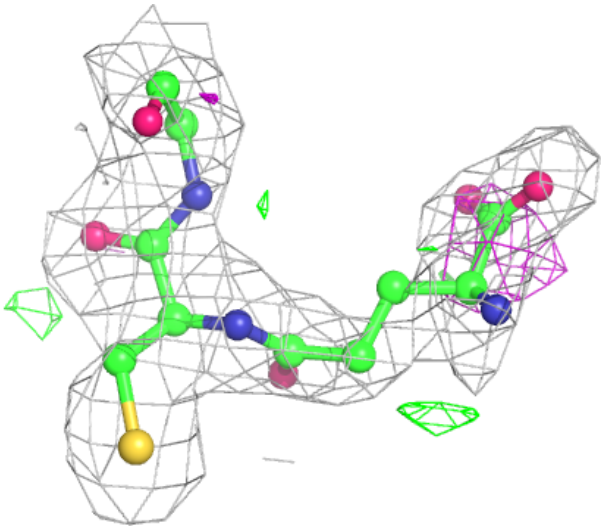


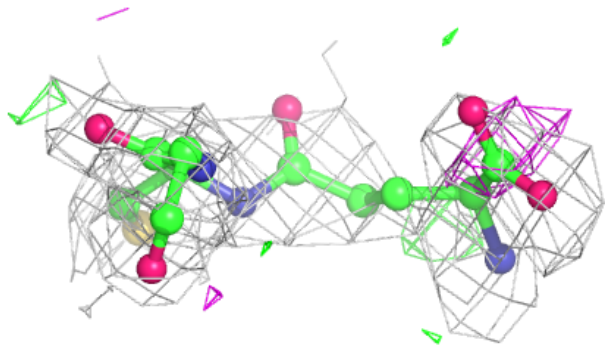


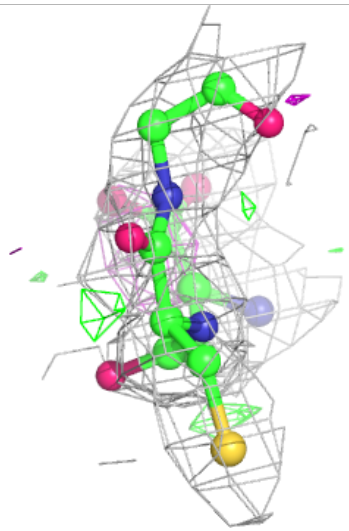


Electron density around GSH B 495:

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

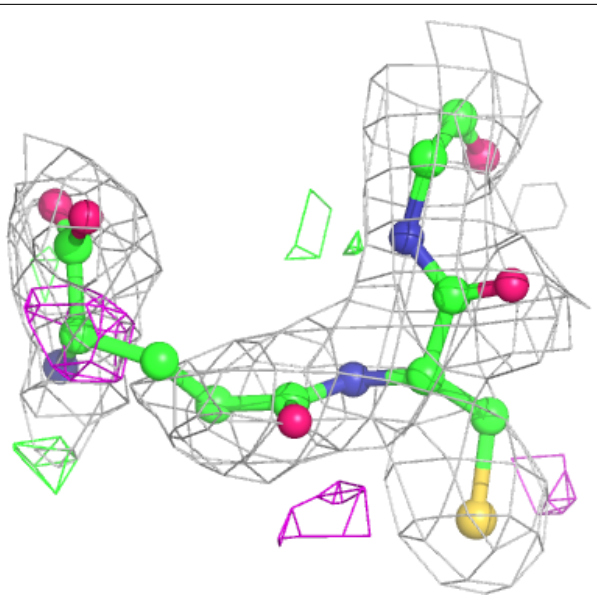


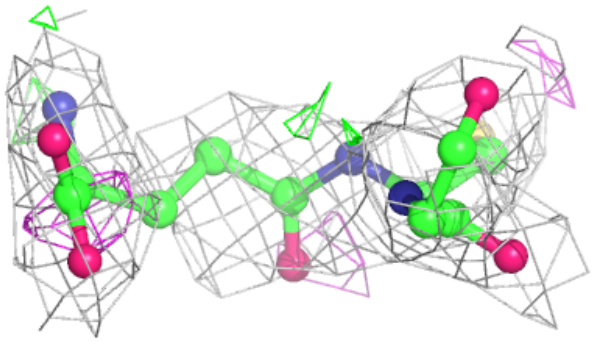


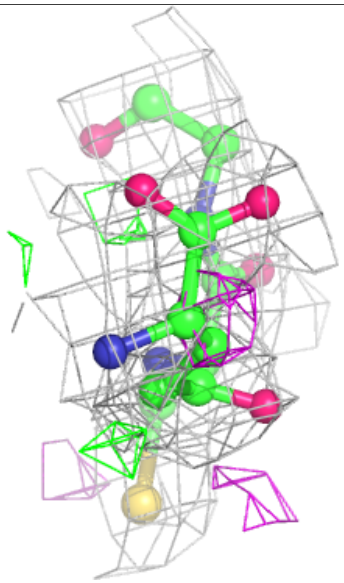


Electron density around GSH A 495:

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

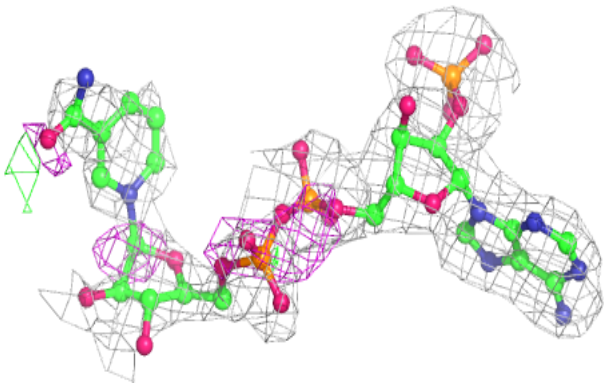


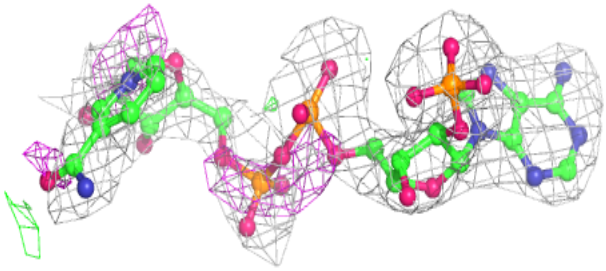


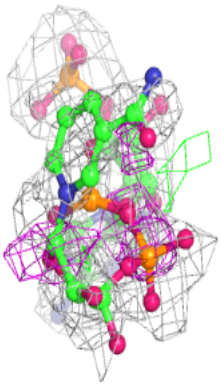


Electron density around NAP B 494:

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

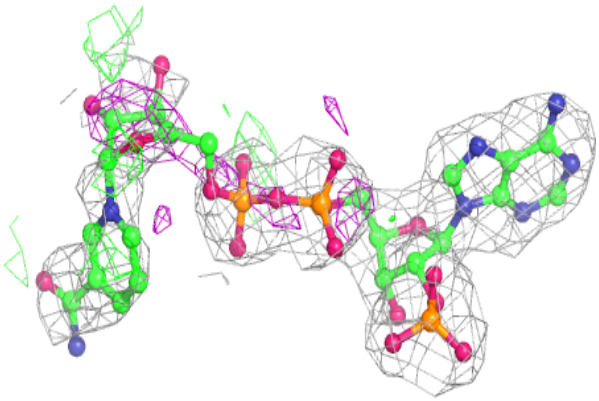


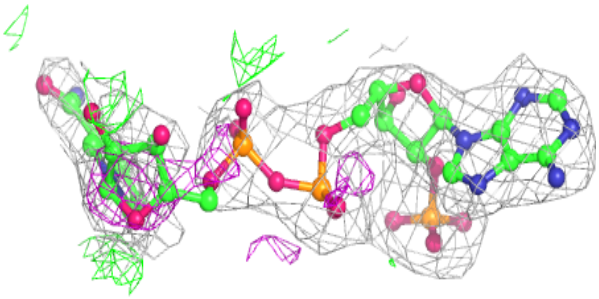




Electron density around NAP A 494:

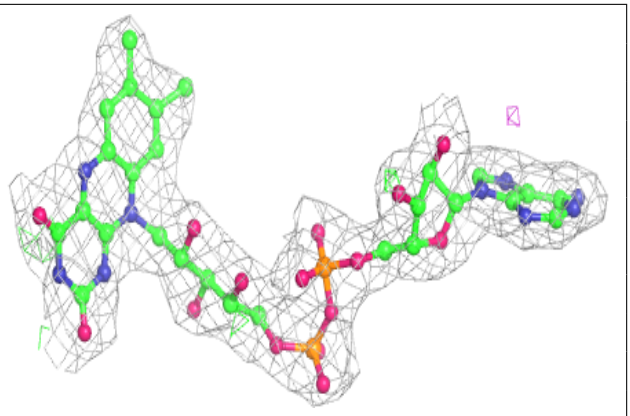
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

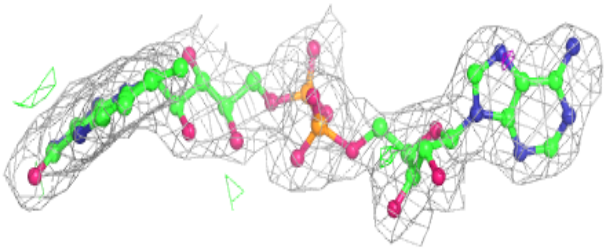


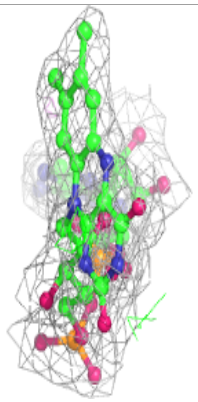


Electron density around FAD B 493:

$2mF_o$-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 493:

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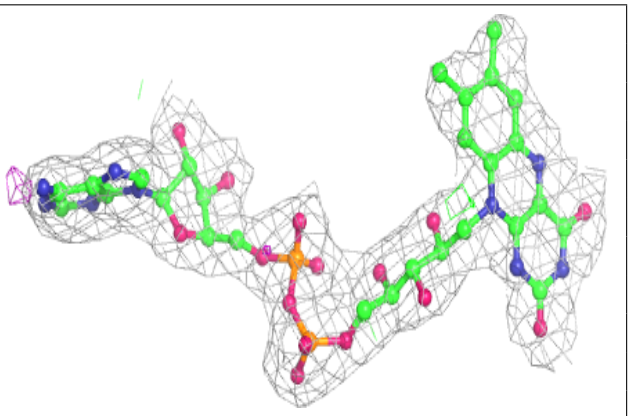
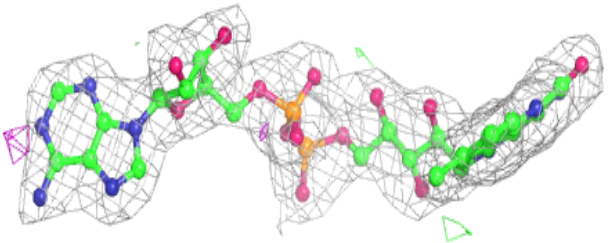
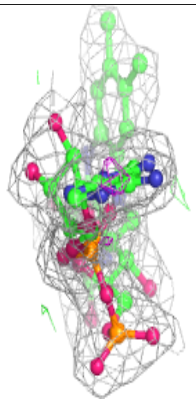
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.