



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:44 pm BST

PDB ID : 1TYP
Title : SUBSTRATE INTERACTIONS BETWEEN TRYPTOPHAN 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

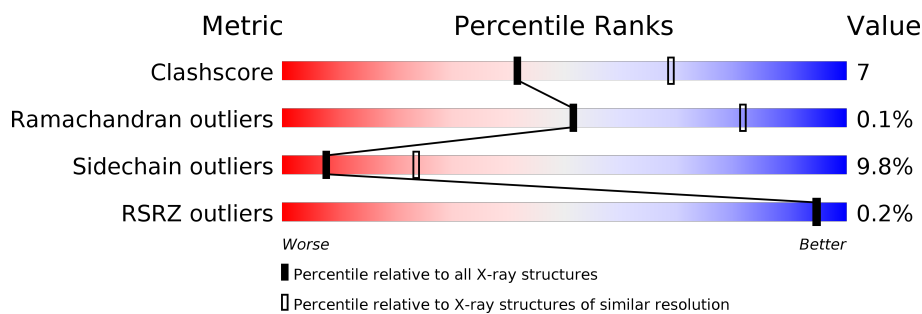
1 Overall quality at a glance

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 $\leq 5\%$. 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	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.

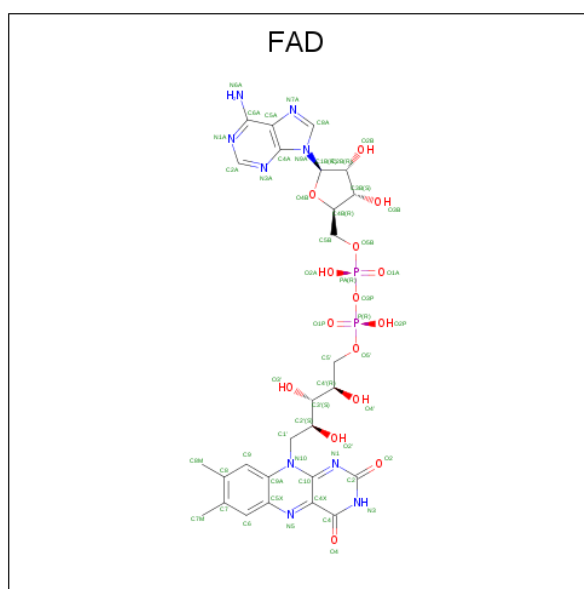
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	Total 3713	C 2336	N 645	O 711	S 21	0	0	0
1	B	486	Total 3705	C 2331	N 644	O 710	S 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: $C_{27}H_{33}N_9O_{15}P_2$).



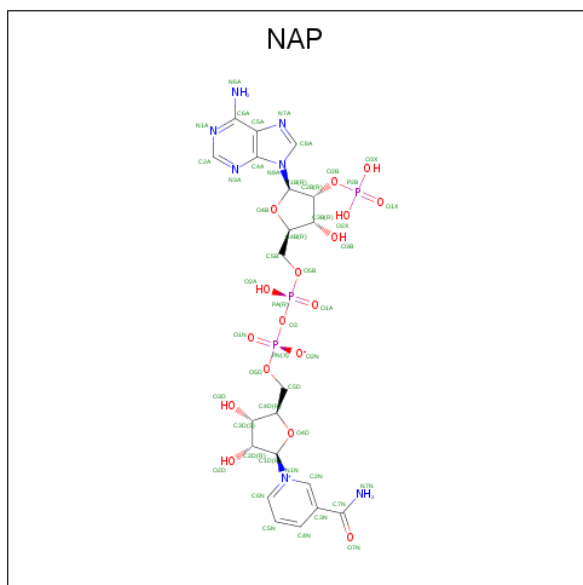
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0

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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
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
5	A	1	Total C N 10 7 3	0	0
5	A	1	Total C N 10 7 3	0	0
5	B	1	Total C N 10 7 3	0	0
5	B	1	Total C N 10 7 3	0	0

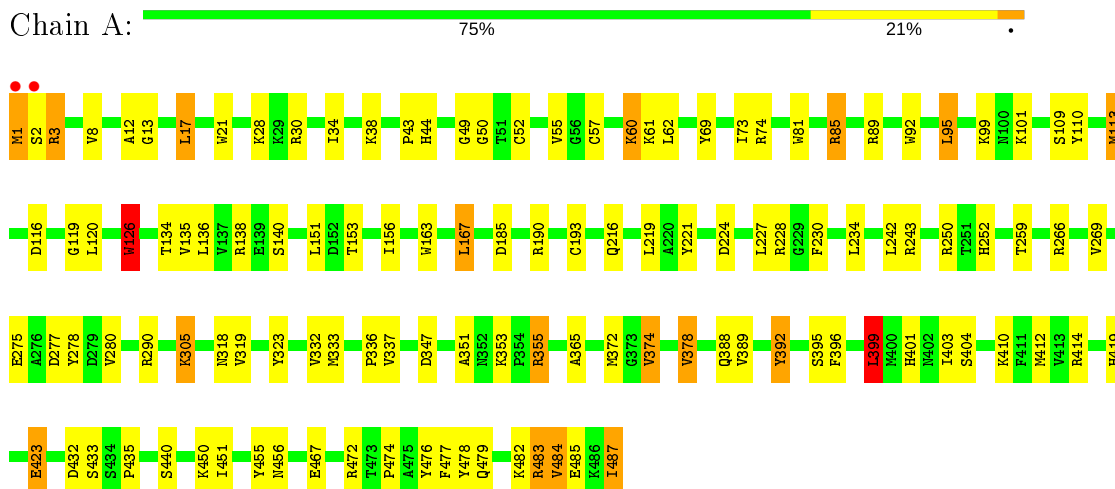
- Molecule 6 is water.

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

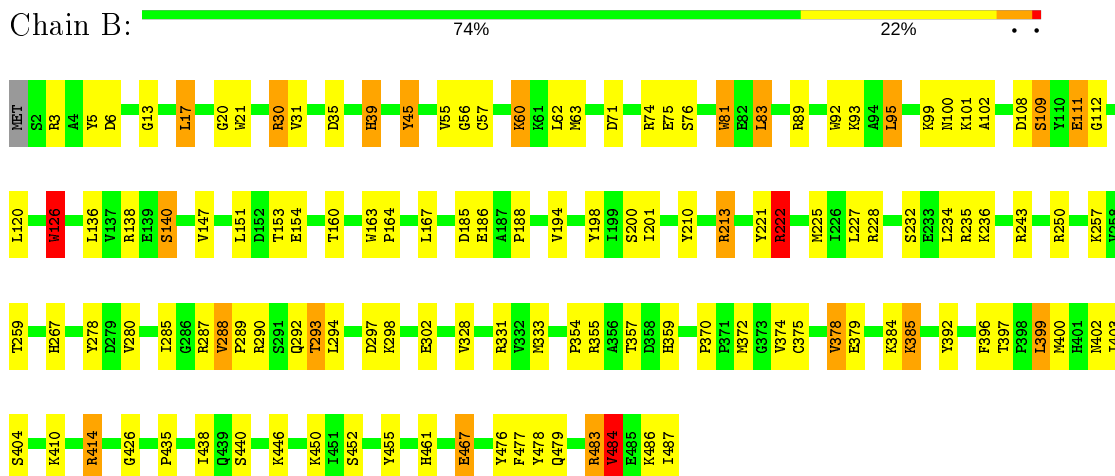
3 Residue-property plots

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: TRYPANOTHIONE REDUCTASE



- Molecule 1: TRYPANOTHIONE REDUCTASE



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.81Å)	Xtrriage
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	Xtrriage
Anisotropy	0.001	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtrriage
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

Xtrriage'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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality 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

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	138	ARG	NE-CZ-NH2	-12.15	114.23	120.30
1	B	483	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	A	414	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	B	83	LEU	CA-CB-CG	9.38	136.87	115.30
1	B	414	ARG	NE-CZ-NH1	9.38	124.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	B	163	TRP	CD1-CG-CD2	9.07	113.56	106.30
1	B	138	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	290	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	B	74	ARG	NE-CZ-NH2	-8.91	115.85	120.30
1	B	92	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	B	138	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	A	92	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	B	74	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	B	126	TRP	CH2-CZ2-CE2	8.44	125.84	117.40
1	A	92	TRP	CE2-CD2-CG	-8.32	100.64	107.30
1	A	163	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	B	163	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	A	81	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	B	126	TRP	CG-CD1-NE1	-7.95	102.15	110.10
1	A	163	TRP	CE2-CD2-CG	-7.88	100.99	107.30
1	B	81	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	A	74	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	472	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	472	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	89	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	B	213	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	92	TRP	CE2-CD2-CG	-7.59	101.22	107.30
1	A	21	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	B	250	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	A	74	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	126	TRP	CE2-CD2-CG	-7.44	101.34	107.30
1	B	243	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	81	TRP	CE2-CD2-CG	-7.42	101.37	107.30
1	B	476	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	B	21	TRP	CD1-CG-CD2	7.34	112.18	106.30
1	A	323	TYR	CB-CG-CD2	-7.34	116.60	121.00
1	B	483	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	222	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	A	69	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	21	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	B	126	TRP	CB-CG-CD1	-7.04	117.84	127.00
1	A	228	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	B	222	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	81	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	A	126	TRP	CD1-CG-CD2	6.75	111.70	106.30
1	B	163	TRP	CG-CD2-CE3	6.74	139.97	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	GLU	CB-CA-C	-6.72	96.95	110.40
1	B	392	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	A	1	MET	CA-C-O	-6.60	106.25	120.10
1	B	30	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	235	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	3	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	163	TRP	CG-CD1-NE1	-6.48	103.62	110.10
1	B	478	TYR	CB-CG-CD2	-6.44	117.13	121.00
1	B	21	TRP	CE2-CD2-CG	-6.27	102.28	107.30
1	B	414	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	243	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	288	VAL	N-CA-CB	-6.22	97.81	111.50
1	A	374	VAL	N-CA-CB	-6.13	98.02	111.50
1	A	250	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	163	TRP	CB-CG-CD1	-6.09	119.08	127.00
1	A	392	TYR	CB-CG-CD2	-6.08	117.36	121.00
1	B	111	GLU	N-CA-CB	6.04	121.48	110.60
1	A	138	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	B	167	LEU	CA-C-N	6.02	128.25	116.20
1	B	302	GLU	CA-CB-CG	6.02	126.65	113.40
1	A	85	ARG	CG-CD-NE	-6.01	99.19	111.80
1	B	484	VAL	N-CA-C	6.00	127.21	111.00
1	B	71	ASP	CB-CG-OD1	5.98	123.69	118.30
1	A	278	TYR	CB-CG-CD1	-5.91	117.45	121.00
1	A	221	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	A	476	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	89	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	290	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	3	ARG	N-CA-C	-5.76	95.45	111.00
1	A	113	MET	CG-SD-CE	-5.75	91.00	100.20
1	B	109	SER	CA-CB-OG	-5.74	95.70	111.20
1	B	378	VAL	N-CA-CB	-5.73	98.89	111.50
1	B	278	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	A	355	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	126	TRP	CA-CB-CG	-5.62	103.02	113.70
1	B	92	TRP	CB-CG-CD1	-5.56	119.77	127.00
1	A	392	TYR	CB-CG-CD1	5.56	124.33	121.00
1	B	222	ARG	CA-CB-CG	5.47	125.44	113.40
1	B	250	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	288	VAL	CB-CA-C	5.45	121.76	111.40
1	A	95	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	399	LEU	CA-CB-CG	5.42	127.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	A	280	VAL	CG1-CB-CG2	-5.37	102.30	110.90
1	B	92	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	B	126	TRP	CD2-CE2-CZ2	-5.37	115.86	122.30
1	B	213	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	412	MET	CB-CG-SD	-5.35	96.34	112.40
1	B	126	TRP	CG-CD2-CE3	5.35	138.71	133.90
1	A	378	VAL	N-CA-CB	-5.34	99.74	111.50
1	B	39	HIS	CA-CB-CG	-5.30	104.59	113.60
1	B	378	VAL	CB-CA-C	5.30	121.46	111.40
1	A	193	CYS	CA-CB-SG	-5.29	104.48	114.00
1	A	219	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	483	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	235	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	92	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	A	92	TRP	CB-CG-CD1	-5.27	120.15	127.00
1	B	331	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	319	VAL	N-CA-C	-5.26	96.81	111.00
1	B	228	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	163	TRP	CG-CD1-NE1	-5.25	104.86	110.10
1	B	95	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	236	LYS	CA-CB-CG	5.20	124.83	113.40
1	A	1	MET	CA-C-N	5.20	128.63	117.20
1	B	210	TYR	CB-CG-CD1	-5.19	117.89	121.00
1	B	250	ARG	CB-CG-CD	-5.17	98.17	111.60
1	B	374	VAL	N-CA-CB	-5.16	100.15	111.50
1	B	186	GLU	CA-CB-CG	5.15	124.72	113.40
1	B	328	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	A	167	LEU	CA-CB-CG	5.13	127.11	115.30
1	B	136	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	81	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	69	TYR	CD1-CG-CD2	5.07	123.47	117.90
1	A	266	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	63	MET	CG-SD-CE	5.02	108.23	100.20

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.

All (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
1:A:113:MET:HG3	5:A:496:SPD:H102	0.92	0.75
1:A:396:PHE:CE1	1:A:467:GLU:HG3	2.21	0.74
1:B:467:GLU:HG3	6:B:587:HOH:O	1.87	0.74
1:B:112:GLY:HA3	5:B:498:SPD:H71	1.72	0.70
1:A:388:GLN:HG2	1:A:487:ILE:HD11	1.75	0.68
1:B:198:TYR:CE1	3:B:494:NAP:H3D	2.28	0.68
1:A:234:LEU:HD23	1:A:372:MET:HE3	1.77	0.67
1:B:13:GLY:O	1:B:17:LEU:HB2	1.96	0.65
1:A:333:MET:HB2	3:A:494:NAP:H2D	1.79	0.64
1:B:477:PHE:HB2	1:B:484:VAL:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ARG:HG2	3:B:494:NAP:H51N	1.83	0.60
1:A:62:LEU:HD13	1:B:403:ILE:HD11	1.83	0.59
1:A:389:VAL:HB	1:A:478:TYR:HB2	1.86	0.58
1:B:126:TRP:CE3	1:B:140:SER:HA	2.40	0.57
1:A:109:SER:HB3	5:A:498:SPD:H31	1.86	0.56
1:A:269:VAL:HG13	1:A:275:GLU:HG2	1.85	0.56
1:A:305:LYS:H	1:A:305:LYS:CD	2.19	0.56
1:B:76:SER:HB2	1:B:81:TRP:HB2	1.88	0.55
1:A:399:LEU:HD11	1:B:102:ALA:HB1	1.89	0.55
1:B:333:MET:HB2	3:B:494:NAP:H2D	1.88	0.54
1:A:126:TRP:CE3	1:A:140:SER:HA	2.42	0.54
1:A:365:ALA:HB1	1:A:435:PRO:HB3	1.90	0.54
1:B:287:ARG:CG	3:B:494:NAP:H51N	2.37	0.54
1:B:479:GLN:HE21	1:B:487:ILE:HG13	1.72	0.54
1:B:93:LYS:HE2	1:B:185:ASP:O	2.08	0.54
1:A:230:PHE:HZ	3:A:494:NAP:H71N	1.56	0.53
1:A:365:ALA:CB	1:A:435:PRO:HB3	2.39	0.52
1:A:12:ALA:O	1:A:17:LEU:HD22	2.09	0.52
1:A:126:TRP:HD1	6:A:625:HOH:O	1.92	0.52
1:B:188:PRO:HD2	6:B:562:HOH:O	2.08	0.51
1:B:221:TYR:HE1	3:B:494:NAP:HO3A	1.57	0.51
1:A:305:LYS:H	1:A:305:LYS:HD2	1.76	0.51
1:A:318:ASN:HB3	6:A:598:HOH:O	2.11	0.51
1:B:399:LEU:O	1:B:402:ASN:HB3	2.11	0.51
1:A:403:ILE:HD12	1:B:62:LEU:HD22	1.91	0.51
1:A:8:VAL:HG11	1:A:135:VAL:HG21	1.93	0.51
1:A:388:GLN:HB3	1:A:419:HIS:HB3	1.93	0.50
1:A:50:GLY:HA2	2:A:493:FAD:O3B	2.11	0.50
1:B:333:MET:CB	3:B:494:NAP:H2D	2.42	0.50
1:A:396:PHE:HE1	1:A:467:GLU:HG3	1.76	0.49
1:B:357:THR:HB	1:B:359:HIS:CE1	2.48	0.49
1:A:234:LEU:HD23	1:A:372:MET:CE	2.42	0.49
1:A:190:ARG:NH1	1:A:277:ASP:O	2.46	0.49
1:A:332:VAL:HB	1:A:337:VAL:HG11	1.95	0.49
6:A:550:HOH:O	1:B:400:MET:HB3	2.11	0.48
1:B:201:ILE:HD12	1:B:227:LEU:HD13	1.96	0.48
1:A:477:PHE:HB2	1:A:484:VAL:HG12	1.96	0.48
1:B:384:LYS:HD2	1:B:385:LYS:NZ	2.28	0.48
1:B:160:THR:HG21	1:B:294:LEU:HD21	1.96	0.47
1:A:13:GLY:O	1:A:17:LEU:HB2	2.14	0.47
1:B:396:PHE:CE1	1:B:467:GLU:HG2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:HE2	1:B:100:ASN:OD1	2.15	0.47
1:A:73:ILE:O	1:A:85:ARG:NH1	2.49	0.46
1:A:227:LEU:HG	1:A:230:PHE:CD1	2.50	0.46
1:A:401:HIS:HA	1:A:404:SER:OG	2.15	0.46
1:A:134:THR:HA	1:A:151:LEU:O	2.15	0.46
1:A:347:ASP:HA	1:A:351:ALA:HB3	1.97	0.46
1:A:60:LYS:HD3	1:A:61:LYS:N	2.30	0.46
1:B:285:ILE:C	3:B:494:NAP:H52A	2.35	0.46
1:A:353:LYS:HE2	1:A:353:LYS:HB3	1.68	0.45
1:A:49:GLY:HA2	6:A:635:HOH:O	2.17	0.45
1:A:392:TYR:CZ	1:A:474:PRO:HG3	2.52	0.45
1:A:62:LEU:HD13	1:B:403:ILE:CD1	2.46	0.45
1:A:336:PRO:HG3	6:B:633:HOH:O	2.17	0.45
1:B:75:GLU:HB3	1:B:404:SER:HB2	1.99	0.45
1:B:461:HIS:HB2	6:B:633:HOH:O	2.17	0.44
1:B:397:THR:OG1	1:B:410:LYS:HD2	2.17	0.44
1:B:375:CYS:O	1:B:426:GLY:HA2	2.16	0.44
1:B:484:VAL:HG13	1:B:486:LYS:O	2.18	0.44
3:B:494:NAP:PA	6:B:655:HOH:O	2.74	0.44
1:A:110:TYR:O	1:A:113:MET:HB3	2.18	0.44
1:A:456:ASN:O	1:B:446:LYS:HE3	2.17	0.44
1:B:288:VAL:HA	1:B:289:PRO:HD3	1.95	0.44
1:A:119:GLY:HA3	6:A:556:HOH:O	2.17	0.44
1:A:224:ASP:HA	1:A:252:HIS:CE1	2.54	0.43
1:B:259:THR:OG1	1:B:267:HIS:HB3	2.19	0.43
1:B:222:ARG:HD2	3:B:494:NAP:N3A	2.34	0.43
1:B:5:TYR:O	1:B:153:THR:HA	2.19	0.43
2:B:493:FAD:H9	2:B:493:FAD:H1'1	1.77	0.43
1:A:17:LEU:HA	1:A:17:LEU:HD12	1.82	0.42
1:B:435:PRO:O	1:B:438:ILE:HG22	2.19	0.42
1:A:432:ASP:O	1:A:433:SER:HB2	2.19	0.42
1:B:35:ASP:OD2	2:B:493:FAD:H3B	2.19	0.42
1:B:234:LEU:HD23	1:B:372:MET:HE3	2.00	0.42
1:A:333:MET:CB	3:A:494:NAP:H2D	2.46	0.42
1:B:56:GLY:O	1:B:60:LYS:HB3	2.20	0.42
1:B:45:TYR:HB3	1:B:55:VAL:HG11	2.00	0.42
1:B:379:GLU:OE1	1:B:414:ARG:NH2	2.53	0.42
1:A:113:MET:SD	5:A:496:SPD:N10	2.91	0.42
1:B:39:HIS:HE1	1:B:108:ASP:OD1	2.03	0.42
1:A:34:ILE:HD11	1:A:151:LEU:HD12	2.03	0.41
1:A:52:CYS:HB3	6:A:633:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ASP:O	1:B:154:GLU:HB3	2.19	0.41
1:B:293:THR:HB	6:B:646:HOH:O	2.19	0.41
1:A:34:ILE:HG22	2:A:493:FAD:H2A	2.02	0.41
1:B:20:GLY:HA2	1:B:31:VAL:HG11	2.02	0.41
1:A:113:MET:HB2	5:A:496:SPD:H101	1.86	0.41
1:A:43:PRO:HG2	1:A:44:HIS:CE1	2.56	0.40
1:A:423:GLU:HA	1:A:450:LYS:HA	2.03	0.40
1:B:126:TRP:HD1	6:B:550:HOH:O	2.04	0.40
1:B:164:PRO:HD3	1:B:287:ARG:NH1	2.36	0.40
1:A:153:THR:HG21	1:A:156:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	17	LEU
1	A	28	LYS
1	A	30	ARG
1	A	38	LYS
1	A	55	VAL
1	A	57	CYS
1	A	60	LYS
1	A	95	LEU
1	A	99	LYS
1	A	101	LYS
1	A	116	ASP
1	A	120	LEU
1	A	126	TRP
1	A	136	LEU
1	A	167	LEU
1	A	185	ASP
1	A	216	GLN
1	A	242	LEU
1	A	259	THR
1	A	305	LYS
1	A	355	ARG
1	A	374	VAL
1	A	378	VAL
1	A	395	SER
1	A	399	LEU
1	A	410	LYS
1	A	423	GLU
1	A	440	SER
1	A	451	ILE
1	A	455	TYR
1	A	479	GLN

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Mol	Chain	Res	Type
1	A	482	LYS
1	A	483	ARG
1	A	484	VAL
1	A	485	GLU
1	A	487	ILE
1	B	17	LEU
1	B	30	ARG
1	B	57	CYS
1	B	60	LYS
1	B	83	LEU
1	B	95	LEU
1	B	101	LYS
1	B	109	SER
1	B	111	GLU
1	B	120	LEU
1	B	126	TRP
1	B	140	SER
1	B	151	LEU
1	B	194	VAL
1	B	200	SER
1	B	213	ARG
1	B	222	ARG
1	B	225	MET
1	B	232	SER
1	B	257	LYS
1	B	280	VAL
1	B	292	GLN
1	B	293	THR
1	B	297	ASP
1	B	298	LYS
1	B	354	PRO
1	B	355	ARG
1	B	370	PRO
1	B	378	VAL
1	B	385	LYS
1	B	399	LEU
1	B	440	SER
1	B	450	LYS
1	B	452	SER
1	B	455	TYR
1	B	467	GLU
1	B	483	ARG

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Mol	Chain	Res	Type
1	B	484	VAL

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

All (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
2	A	493	FAD	C1'-N10	4.06	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	493	FAD	C4X-C10	3.99	1.42	1.38
3	A	494	NAP	C2N-C3N	-3.87	1.33	1.39
3	A	494	NAP	C2D-C1D	3.81	1.59	1.53
2	B	493	FAD	C4-C4X	3.73	1.47	1.41
5	B	498	SPD	C8-C7	3.70	1.66	1.51
3	A	494	NAP	O4D-C1D	3.56	1.46	1.41
2	A	493	FAD	C4X-C10	3.41	1.42	1.38
4	B	497	GSH	CB2-CA2	-3.17	1.49	1.53
2	B	493	FAD	C1'-N10	2.95	1.51	1.48
3	B	494	NAP	C3N-C7N	2.71	1.54	1.50
2	A	493	FAD	C8A-N7A	-2.61	1.30	1.34
2	B	493	FAD	C4-N3	2.53	1.37	1.33
5	B	498	SPD	C8-C9	2.53	1.63	1.51
3	A	494	NAP	C8A-N7A	-2.46	1.30	1.34
3	B	494	NAP	C8A-N7A	-2.42	1.30	1.34
3	A	494	NAP	C2N-N1N	2.38	1.37	1.35
2	A	493	FAD	O4B-C1B	2.18	1.44	1.41
2	B	493	FAD	C8-C7	2.15	1.46	1.40
2	B	493	FAD	C8A-N7A	-2.14	1.30	1.34
3	A	494	NAP	O4B-C1B	2.07	1.44	1.41
2	B	493	FAD	C2B-C3B	-2.02	1.47	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
3	A	494	NAP	O4D-C1D-C2D	-8.88	93.95	106.93
2	A	493	FAD	C3B-C2B-C1B	-8.58	88.06	100.98
4	B	497	GSH	CG1-CD1-N2	8.29	130.21	115.83
3	B	494	NAP	O4D-C1D-C2D	-7.58	95.85	106.93
2	B	493	FAD	C4X-C4-N3	-7.13	113.68	123.43
4	A	497	GSH	CG1-CD1-N2	6.99	127.95	115.83
3	B	494	NAP	C6N-N1N-C2N	-6.38	116.16	121.97
2	A	493	FAD	C4X-C4-N3	-6.32	114.78	123.43
4	B	497	GSH	CB1-CG1-CD1	6.26	127.02	113.04
5	A	496	SPD	C8-C9-N10	6.26	157.57	112.78
3	A	494	NAP	O2D-C2D-C1D	5.86	132.50	110.85
2	B	493	FAD	O4B-C4B-C3B	-5.83	93.58	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	494	NAP	O4D-C4D-C5D	5.23	126.58	109.37
4	A	497	GSH	C2-CA2-N2	5.05	124.91	111.16
3	A	494	NAP	C6N-N1N-C2N	-4.96	117.45	121.97
2	B	493	FAD	C2B-C3B-C4B	4.92	112.21	102.64
3	A	494	NAP	C3D-C2D-C1D	4.79	108.19	100.98
4	B	497	GSH	OE1-CD1-CG1	-4.77	113.30	122.02
3	B	494	NAP	O4D-C4D-C5D	4.70	124.83	109.37
3	B	494	NAP	O7N-C7N-C3N	4.62	125.16	119.63
4	B	495	GSH	CA2-CB2-SG2	4.59	119.35	114.19
4	B	497	GSH	CB2-CA2-N2	-4.55	104.80	111.28
4	A	497	GSH	OE1-CD1-CG1	-4.54	113.72	122.02
5	B	498	SPD	C4-C5-N6	-4.38	100.33	112.14
3	A	494	NAP	O4D-C4D-C3D	4.30	113.62	105.11
3	B	494	NAP	O2D-C2D-C1D	4.23	126.48	110.85
2	A	493	FAD	C4X-N5-C5X	4.21	120.98	116.77
3	A	494	NAP	C2D-C3D-C4D	-4.12	94.64	102.64
2	A	493	FAD	C1'-N10-C9A	4.08	121.50	118.29
5	B	498	SPD	C7-N6-C5	4.01	132.37	113.45
4	A	495	GSH	CG1-CB1-CA1	3.99	123.14	113.84
4	A	497	GSH	CB2-CA2-N2	-3.86	105.78	111.28
4	B	497	GSH	OE1-CD1-N2	-3.84	116.47	122.95
2	B	493	FAD	O3B-C3B-C4B	3.76	121.93	111.05
2	A	493	FAD	O4B-C4B-C3B	-3.67	97.86	105.11
4	A	495	GSH	CB1-CG1-CD1	-3.61	104.98	113.04
2	A	493	FAD	O3B-C3B-C4B	3.55	121.33	111.05
2	A	493	FAD	O4B-C1B-C2B	-3.55	101.73	106.93
3	A	494	NAP	O4B-C4B-C3B	-3.50	98.19	105.11
3	A	494	NAP	PN-O3-PA	3.49	144.80	132.83
5	B	498	SPD	C8-C7-N6	-3.36	103.07	112.14
2	B	493	FAD	C1'-N10-C10	3.35	121.41	118.41
2	B	493	FAD	C5A-C6A-N6A	3.32	125.40	120.35
3	B	494	NAP	C2N-N1N-C1D	3.28	126.44	119.14
4	B	495	GSH	CG1-CD1-N2	3.24	121.45	115.83
5	B	496	SPD	C4-C5-N6	-3.17	103.58	112.14
4	B	497	GSH	C2-CA2-N2	3.12	119.66	111.16
3	B	494	NAP	PN-O3-PA	3.07	143.38	132.83
2	B	493	FAD	C4X-N5-C5X	2.92	119.69	116.77
3	B	494	NAP	O7N-C7N-N7N	-2.89	118.47	122.58
3	A	494	NAP	O3D-C3D-C4D	2.79	119.11	111.05
4	A	497	GSH	CB1-CG1-CD1	2.78	119.25	113.04
4	A	497	GSH	OE1-CD1-N2	-2.75	118.32	122.95
2	B	493	FAD	O3'-C3'-C4'	-2.68	102.33	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	495	GSH	CG1-CD1-N2	2.58	120.30	115.83
2	B	493	FAD	O2B-C2B-C3B	-2.58	103.48	111.82
4	B	497	GSH	CA2-C2-N3	2.50	121.58	116.54
4	B	495	GSH	OE1-CD1-CG1	-2.49	117.46	122.02
5	A	496	SPD	C4-C5-N6	-2.49	105.43	112.14
3	B	494	NAP	C3N-C7N-N7N	-2.46	114.79	117.75
2	B	493	FAD	C9A-N10-C10	-2.40	118.77	121.91
4	B	495	GSH	O31-C3-CA3	-2.36	118.59	125.42
5	A	496	SPD	C7-C8-C9	-2.31	105.82	114.28
3	A	494	NAP	O5D-C5D-C4D	-2.26	101.23	108.99
3	A	494	NAP	C2N-N1N-C1D	2.23	124.11	119.14
4	B	495	GSH	CB1-CG1-CD1	-2.19	108.14	113.04
4	B	497	GSH	O31-C3-CA3	-2.14	119.24	125.42
3	B	494	NAP	O3X-P2B-O2X	2.14	115.80	107.64
2	B	493	FAD	C5A-C6A-N1A	-2.13	115.52	120.35
4	A	495	GSH	O31-C3-CA3	-2.12	119.28	125.42
3	B	494	NAP	C3B-C2B-C1B	2.10	106.84	102.89
3	A	494	NAP	O2B-C2B-C1B	-2.10	102.54	110.10
2	A	493	FAD	C5A-C6A-N1A	-2.10	115.60	120.35
3	B	494	NAP	O2B-P2B-O1X	-2.08	101.35	109.39
2	A	493	FAD	C9A-N10-C10	-2.08	119.19	121.91
3	A	494	NAP	O2B-P2B-O1X	-2.04	101.50	109.39
2	B	493	FAD	O2A-PA-O1A	2.04	122.31	112.24
2	A	493	FAD	C5A-C6A-N6A	2.01	123.41	120.35

All (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
3	B	494	NAP	C1D
2	B	493	FAD	C3B
2	A	493	FAD	C3B

All (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

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Mol	Chain	Res	Type	Atoms
4	B	497	GSH	N2-CA2-CB2-SG2
4	B	497	GSH	C2-CA2-CB2-SG2
3	A	494	NAP	C5B-O5B-PA-O1A
3	A	494	NAP	PN-O3-PA-O5B
3	A	494	NAP	C2B-O2B-P2B-O2X
3	A	494	NAP	C2D-C1D-N1N-C6N
3	B	494	NAP	C5B-O5B-PA-O2A
3	B	494	NAP	C2D-C1D-N1N-C2N
3	B	494	NAP	C2D-C1D-N1N-C6N
4	A	497	GSH	C1-CA1-CB1-CG1
4	A	497	GSH	N2-CA2-CB2-SG2
4	A	497	GSH	C2-CA2-CB2-SG2
2	A	493	FAD	PA-O3P-P-O5'
5	B	498	SPD	C3-C4-C5-N6
3	B	494	NAP	O4B-C4B-C5B-O5B
2	A	493	FAD	C3B-C4B-C5B-O5B
5	B	498	SPD	C8-C7-N6-C5
4	B	497	GSH	N2-CD1-CG1-CB1
4	B	497	GSH	OE1-CD1-CG1-CB1
3	B	494	NAP	C3B-C4B-C5B-O5B
5	B	498	SPD	N6-C7-C8-C9
4	A	497	GSH	N2-CD1-CG1-CB1
4	A	497	GSH	OE1-CD1-CG1-CB1
3	A	494	NAP	C3D-C4D-C5D-O5D
5	B	498	SPD	C2-C3-C4-C5
2	B	493	FAD	PA-O3P-P-O1P
2	A	493	FAD	O4B-C4B-C5B-O5B
5	A	496	SPD	N1-C2-C3-C4
2	B	493	FAD	PA-O3P-P-O5'
3	A	494	NAP	O4D-C4D-C5D-O5D
3	B	494	NAP	O4D-C4D-C5D-O5D
3	B	494	NAP	PN-O3-PA-O2A
3	B	494	NAP	C5B-O5B-PA-O1A
4	B	495	GSH	CA1-CB1-CG1-CD1
5	B	496	SPD	N1-C2-C3-C4
3	A	494	NAP	O4B-C4B-C5B-O5B
2	B	493	FAD	C3B-C4B-C5B-O5B
3	A	494	NAP	C5B-O5B-PA-O3
3	B	494	NAP	C5B-O5B-PA-O3
3	B	494	NAP	C2B-O2B-P2B-O2X
3	A	494	NAP	PN-O3-PA-O2A
2	A	493	FAD	PA-O3P-P-O2P

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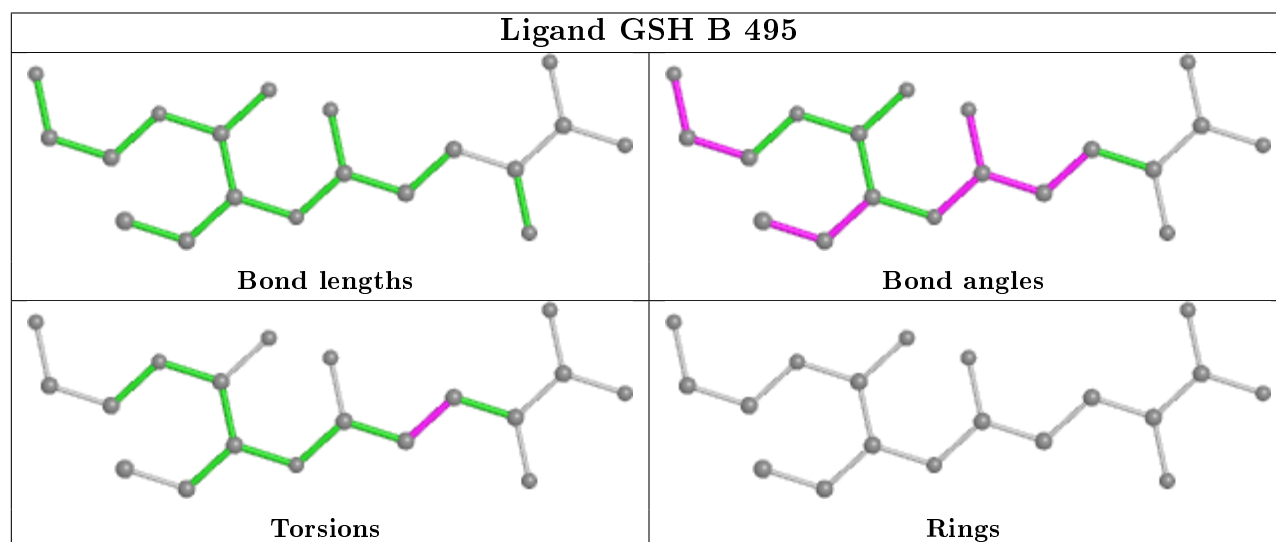
Mol	Chain	Res	Type	Atoms
3	A	494	NAP	C4B-C5B-O5B-PA
2	B	493	FAD	O4B-C4B-C5B-O5B
4	B	497	GSH	N1-CA1-CB1-CG1

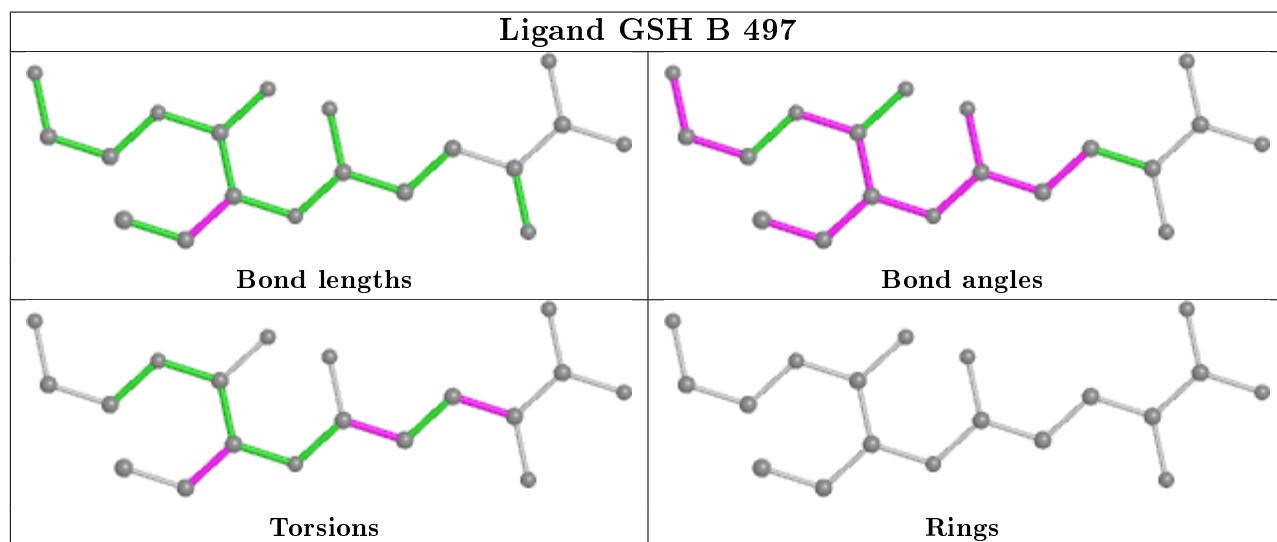
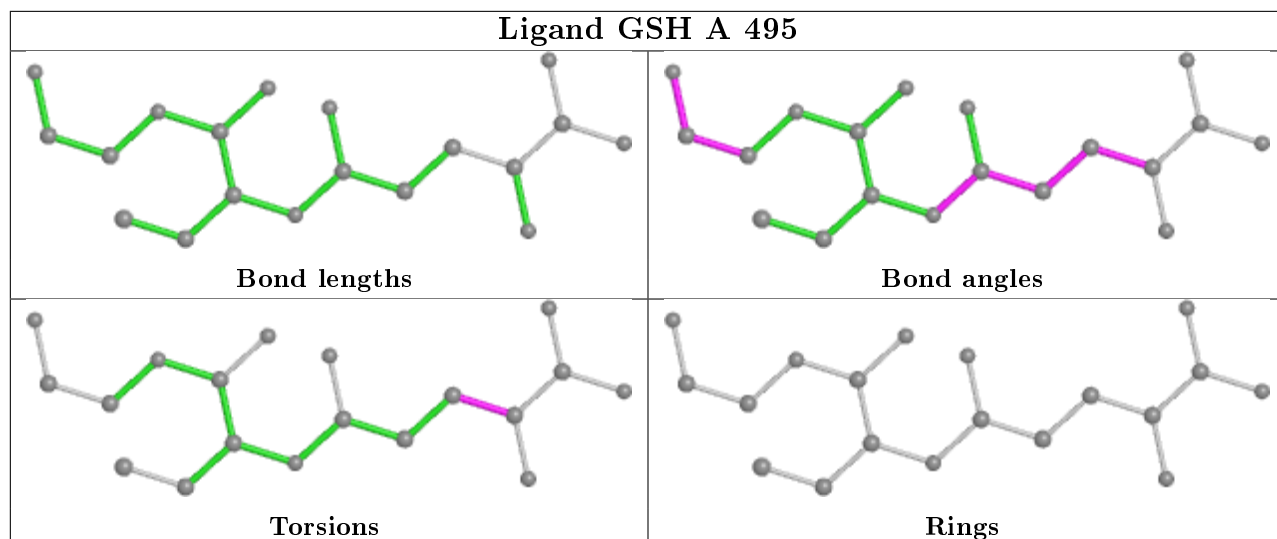
There are no ring outliers.

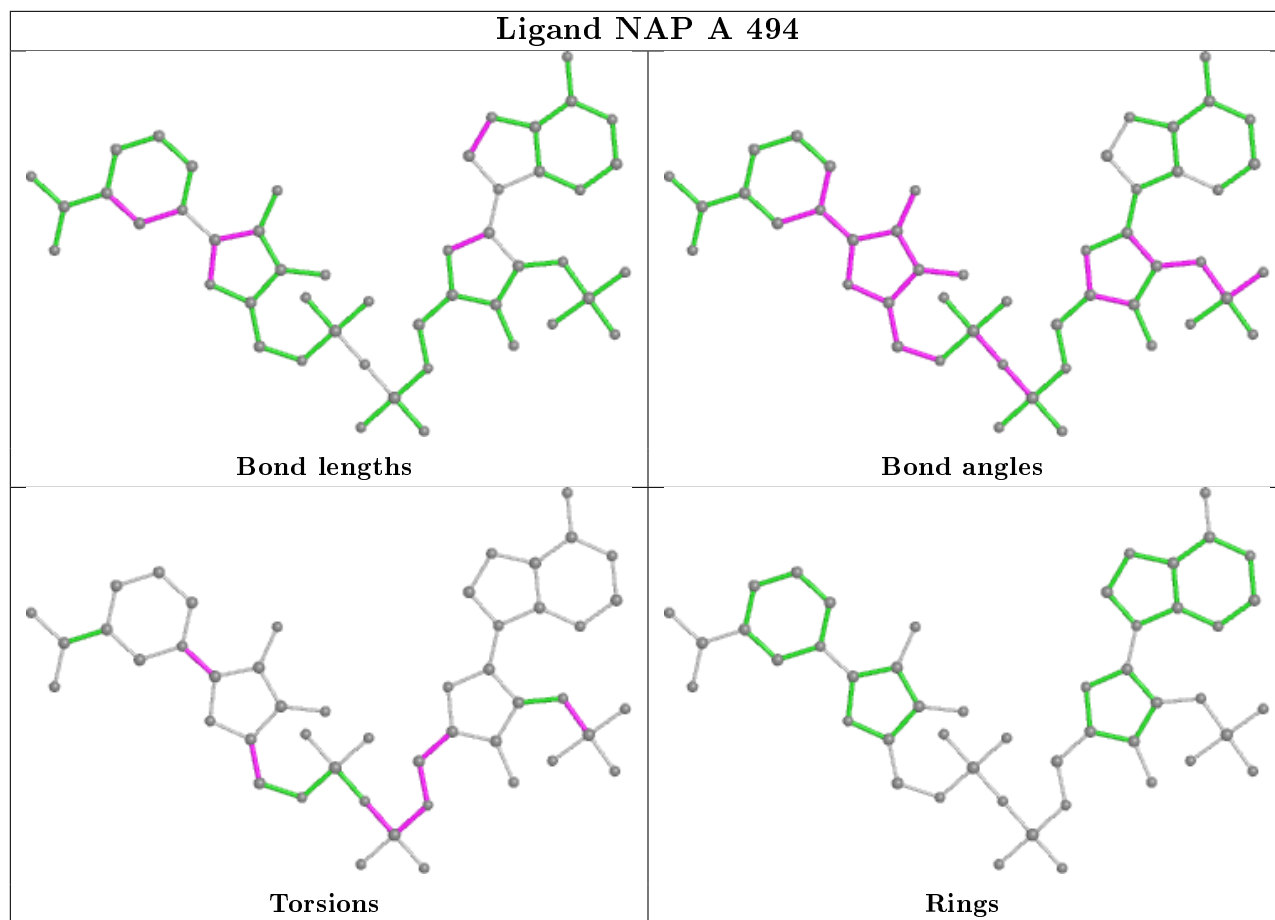
7 monomers are involved in 26 short contacts:

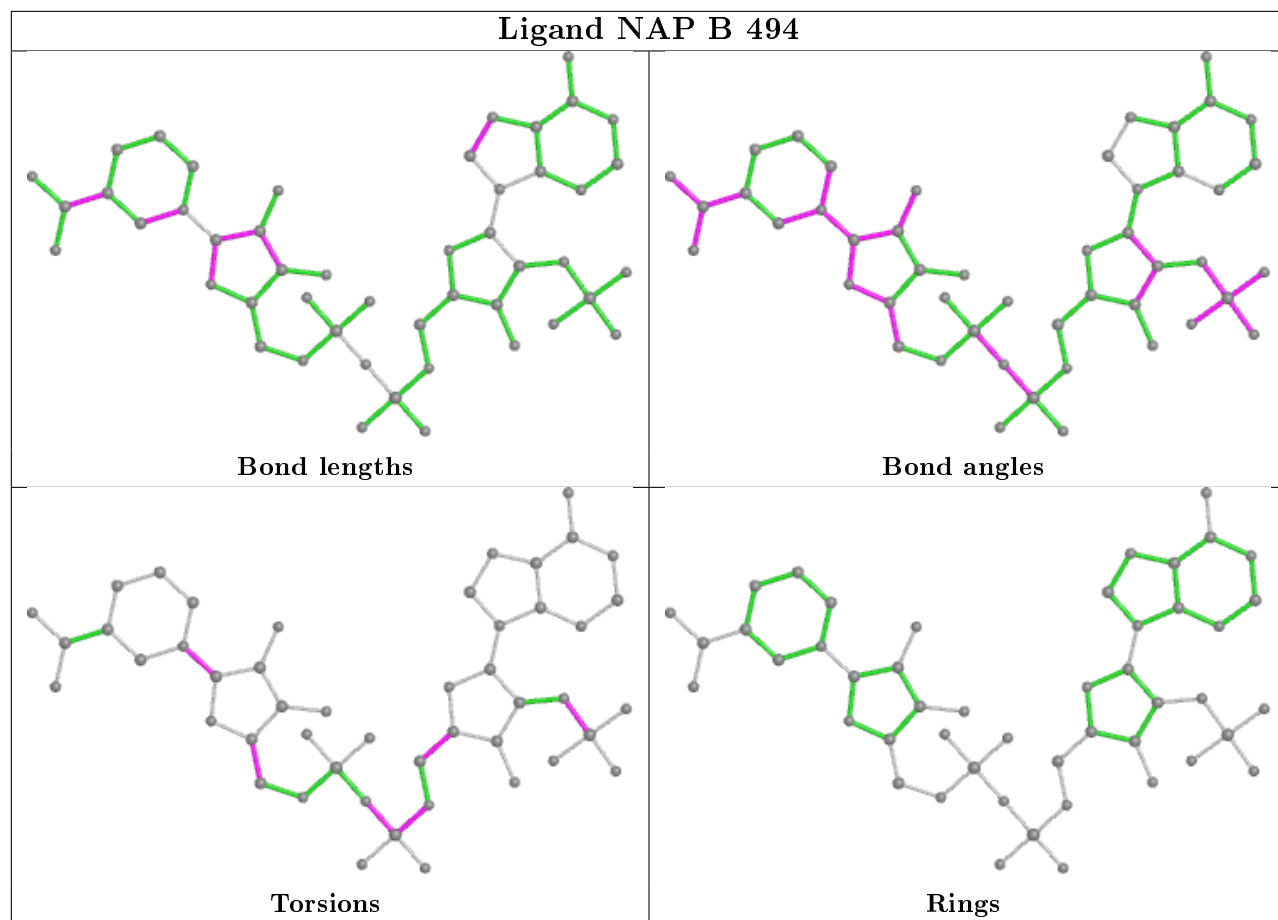
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	498	SPD	1	0
5	B	498	SPD	1	0
3	A	494	NAP	3	0
3	B	494	NAP	10	0
2	B	493	FAD	2	0
5	A	496	SPD	7	0
2	A	493	FAD	2	0

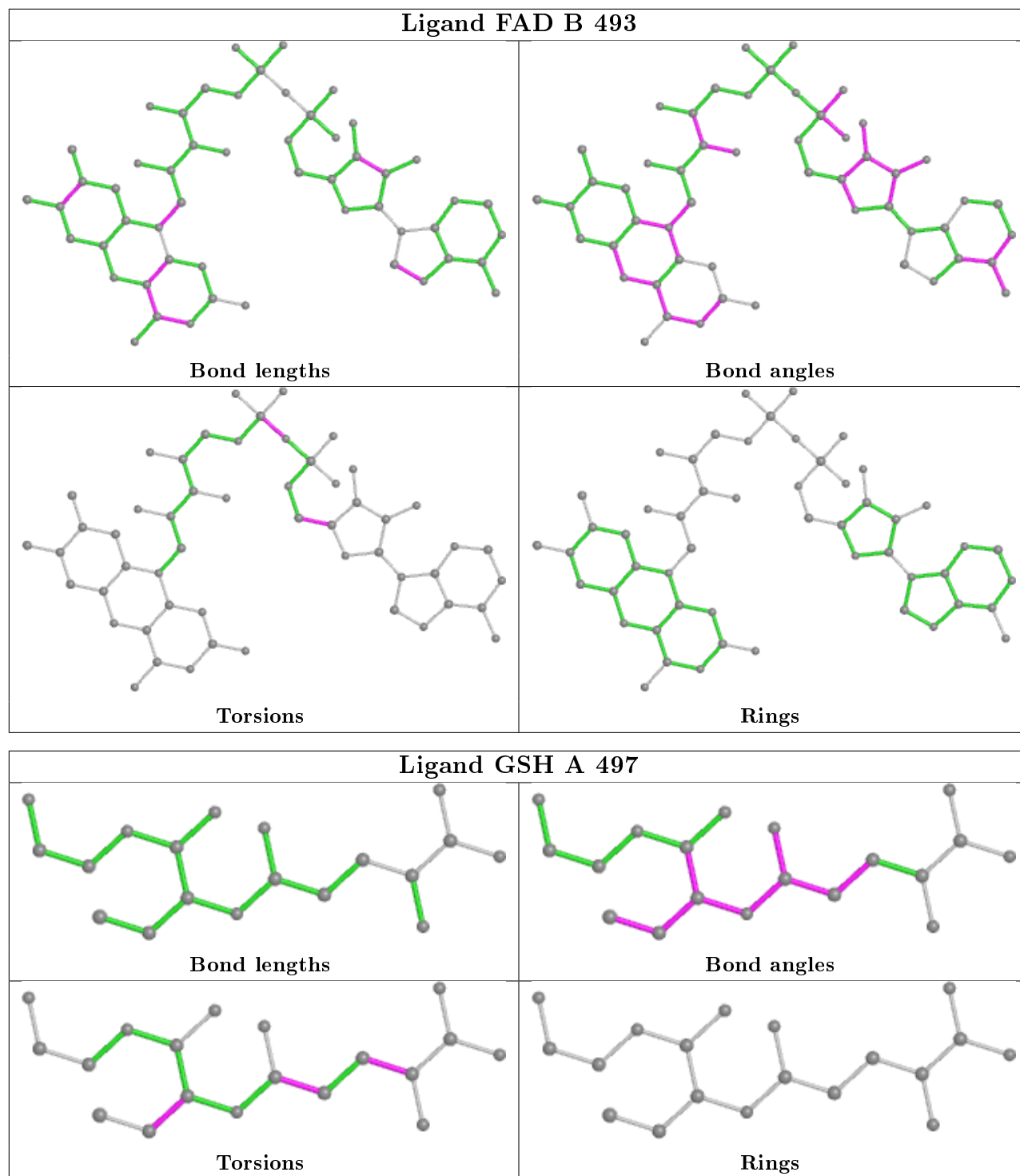
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

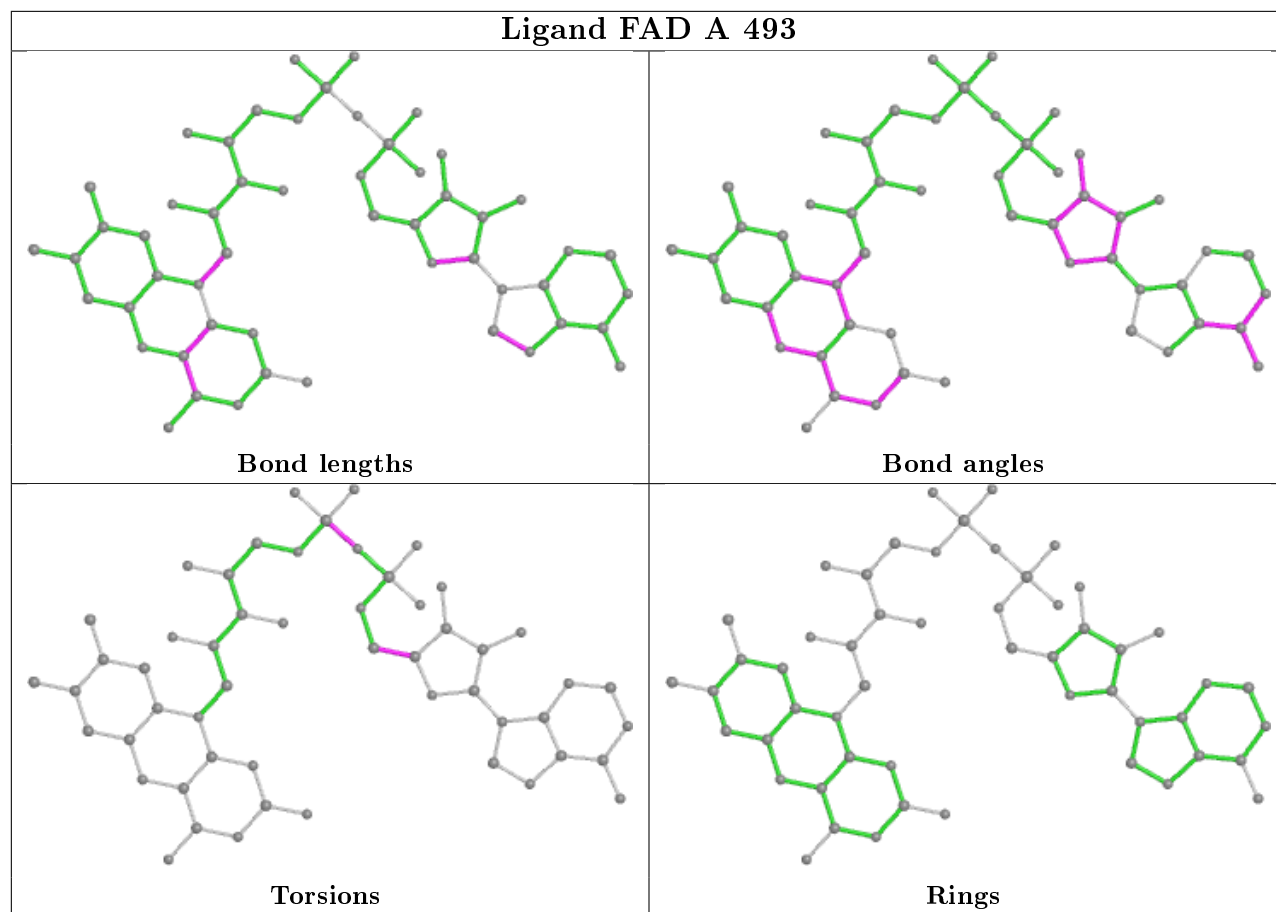












5.7 Other polymers [i](#)

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	487/487 (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.

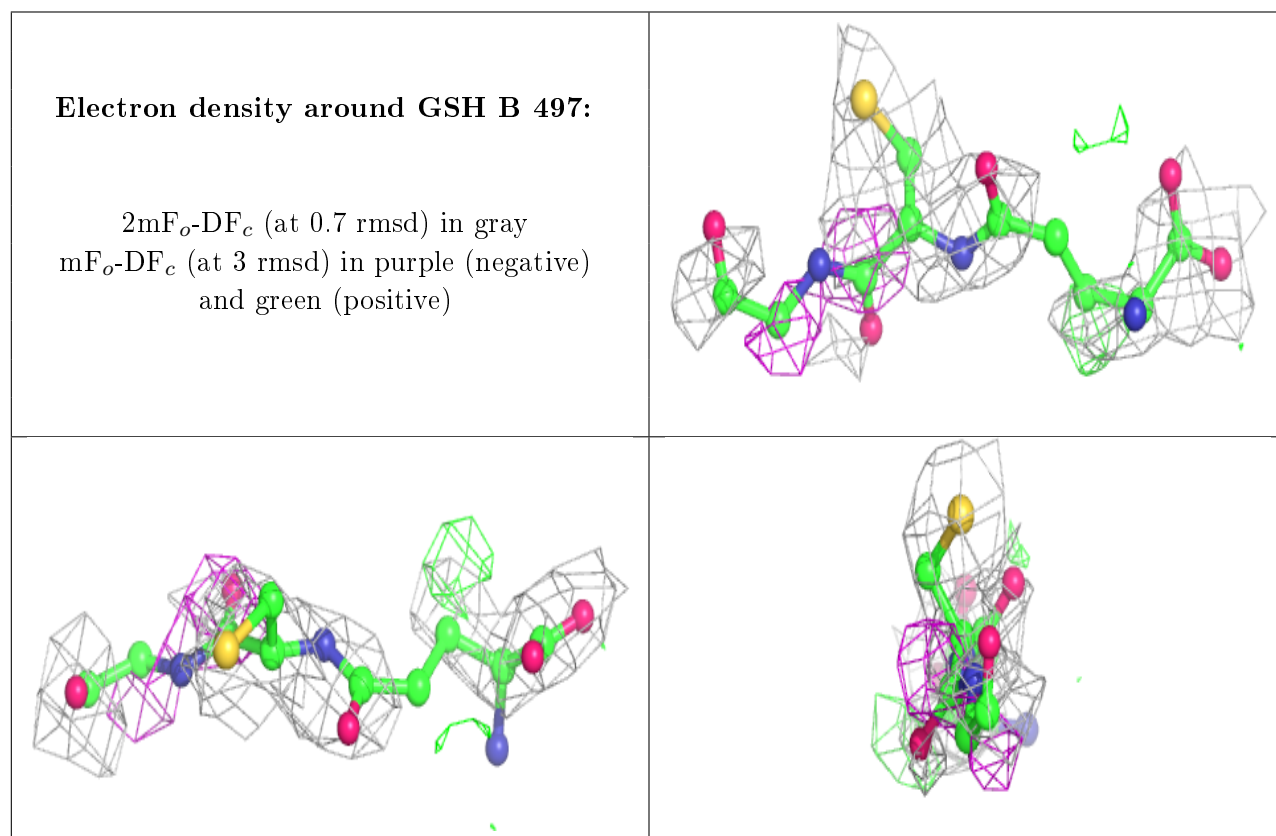
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SPD	A	498	10/10	0.72	0.69	53,56,59,60	0
5	SPD	B	498	10/10	0.79	0.63	64,66,73,73	0

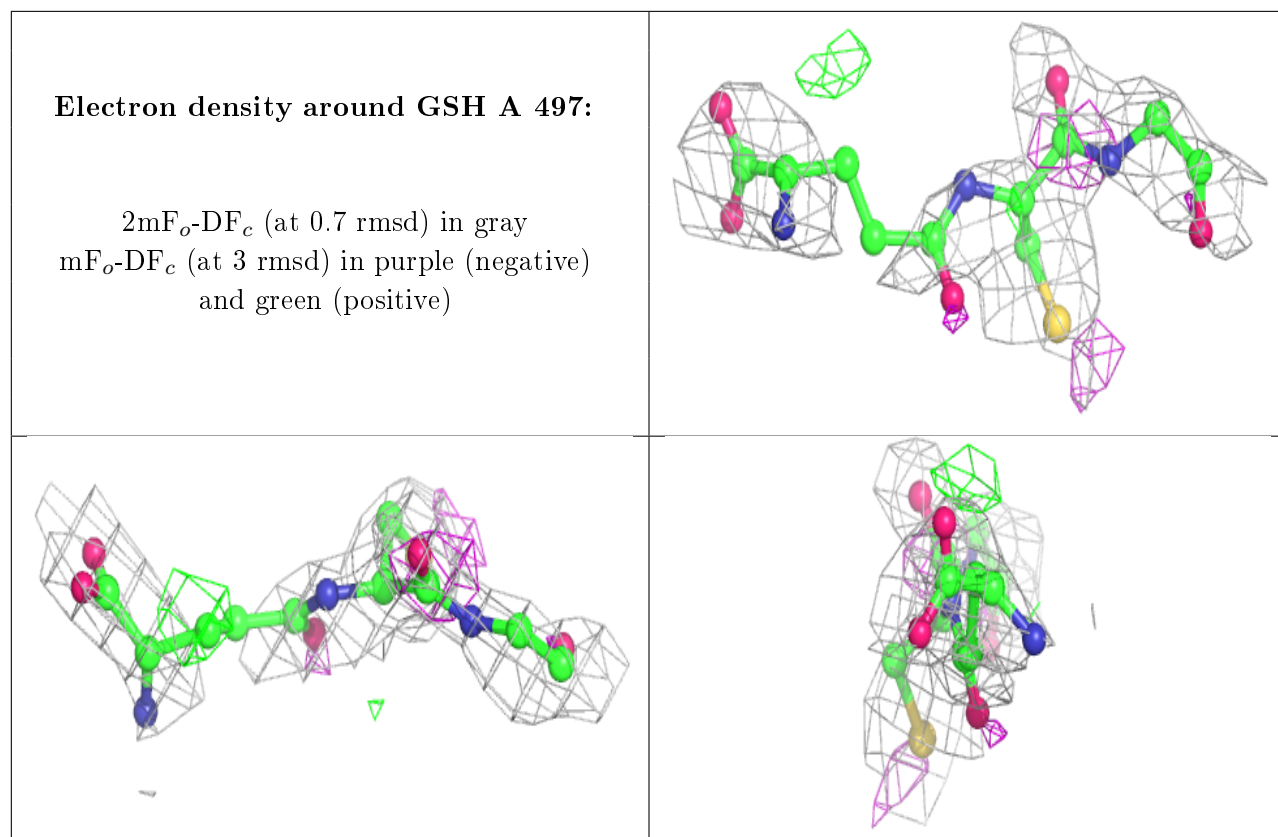
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GSH	B	497	19/20	0.79	0.33	48,63,66,66	0
5	SPD	A	496	10/10	0.89	0.25	25,40,62,65	0
4	GSH	A	497	19/20	0.89	0.26	30,50,54,59	0
4	GSH	B	495	19/20	0.91	0.18	29,35,38,39	0
5	SPD	B	496	10/10	0.92	0.30	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

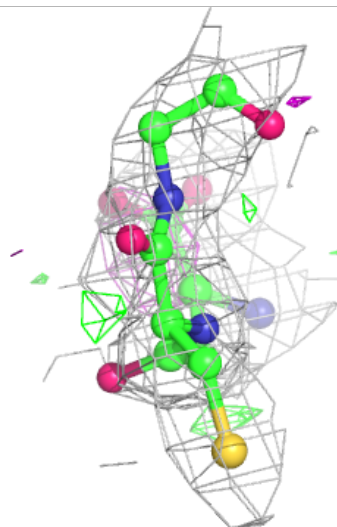
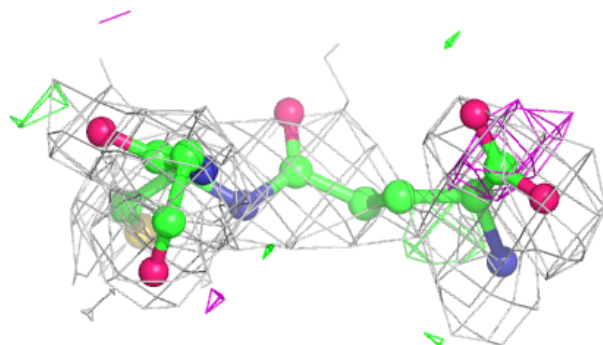
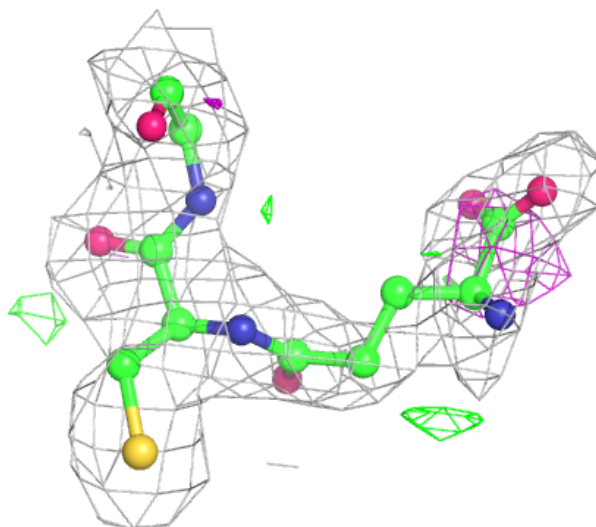
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





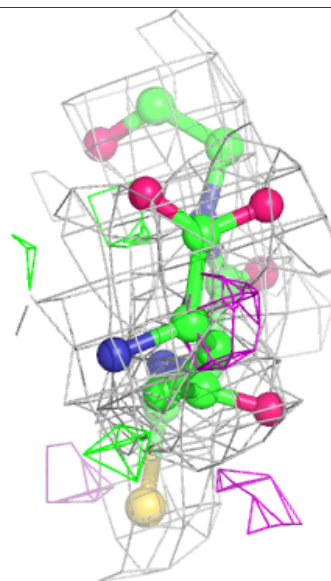
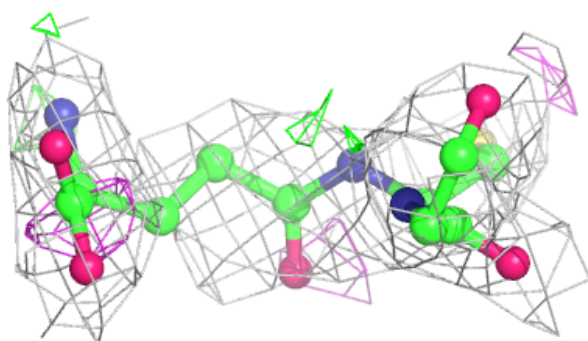
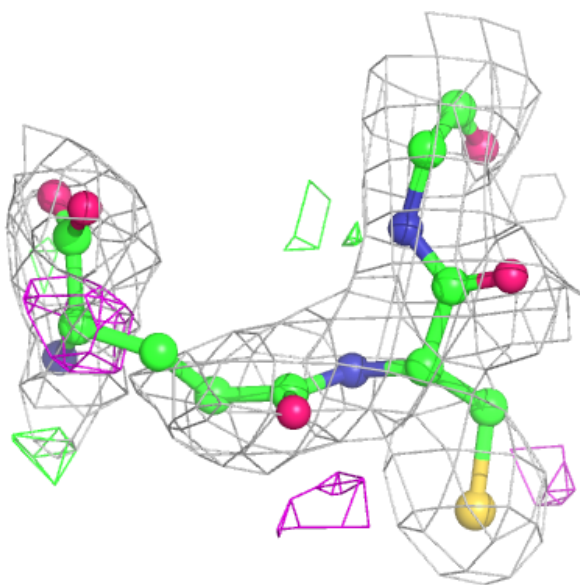
Electron density around GSH B 495:

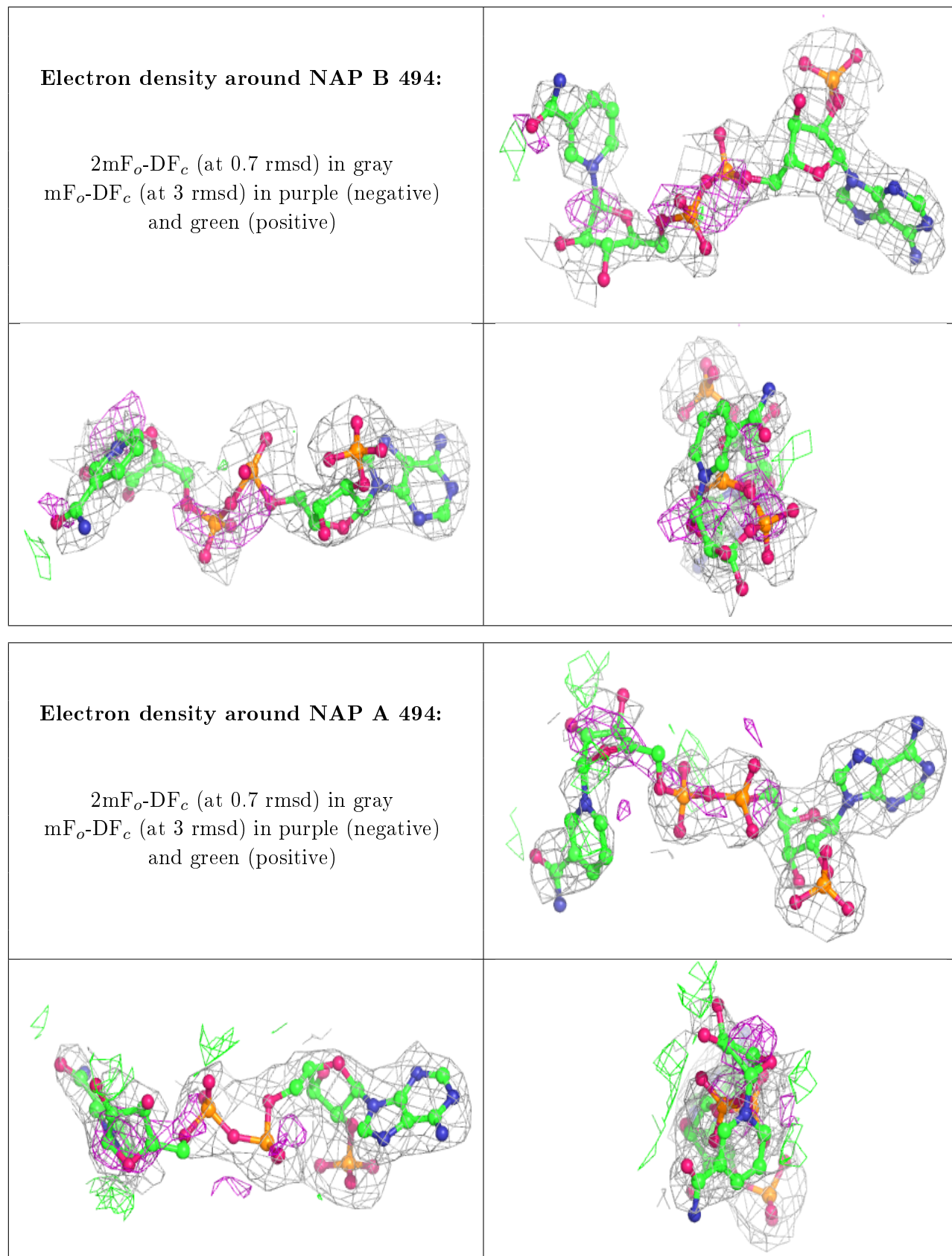
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GSH A 495:

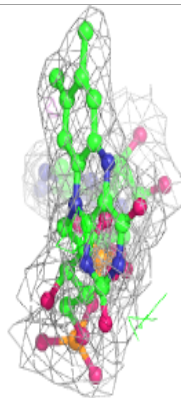
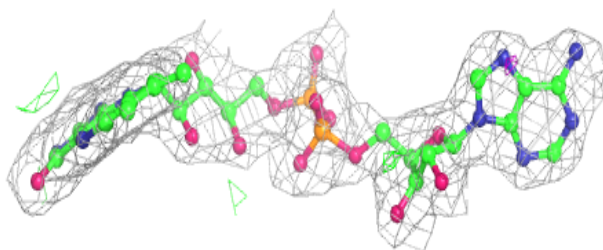
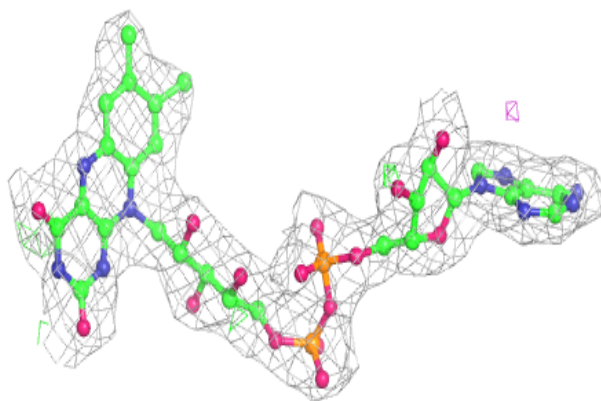
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



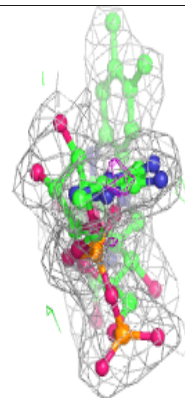
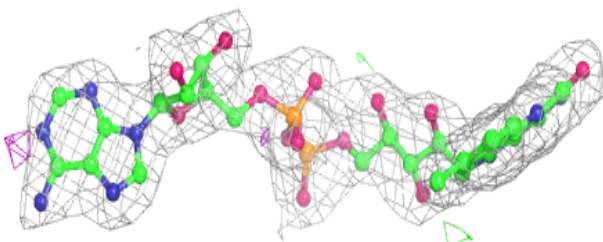
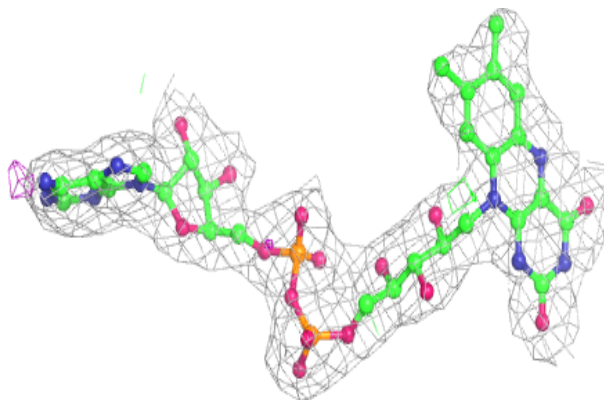


Electron density around FAD B 493:

$2mF_o-DF_c$ (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:**

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



6.5 Other polymers

There are no such residues in this entry.