



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:25 PM UTC

PDB ID : 1TYP / pdb\_00001typ  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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)  
Xtrriage (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

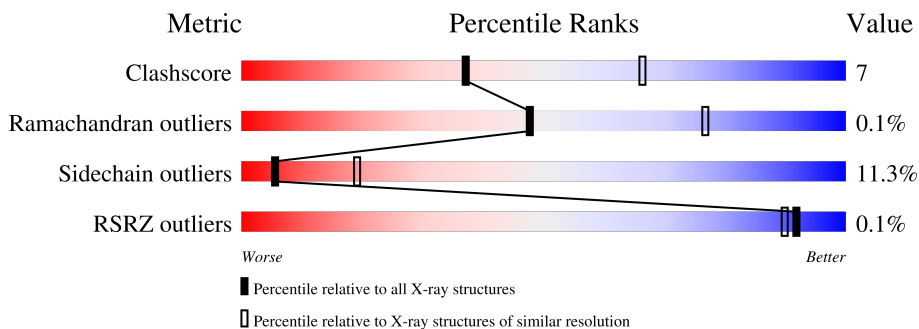
# 1 Overall quality at a glance

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))
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	487	
1	B	487	

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	-	-	-
3	NAP	A	494	X	-	-	-
3	NAP	B	494	X	-	-	-
5	SPD	A	496	-	-	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.

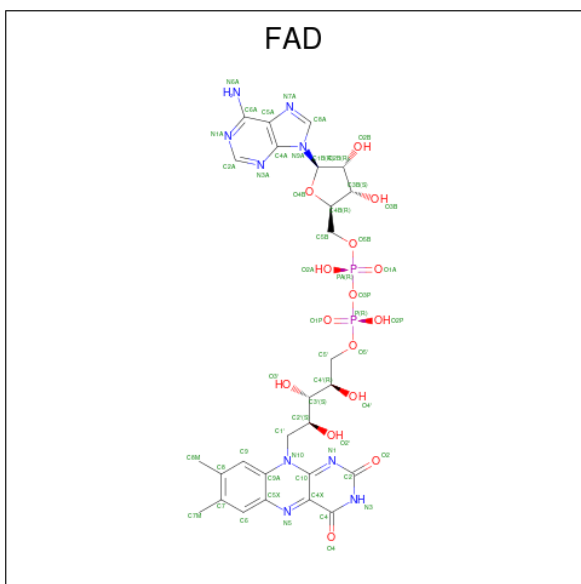
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

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 (CCD ID: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



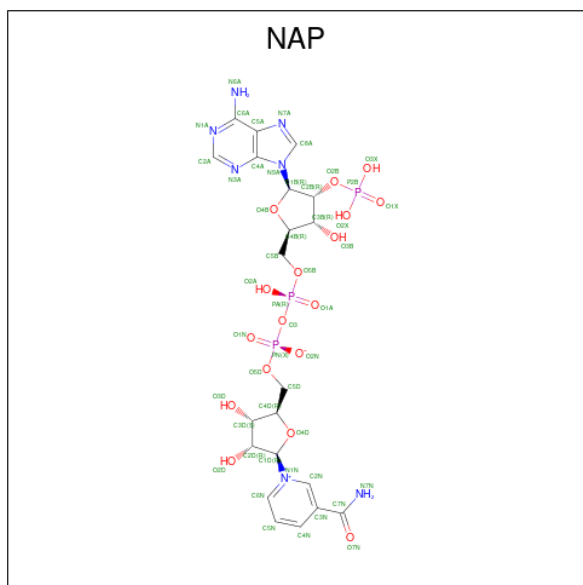
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0

*Continued on next page...*

Continued from previous page...

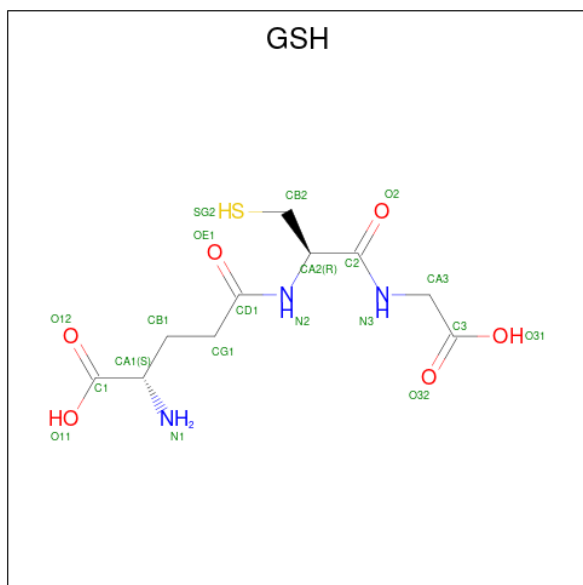
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	B	1	53	27	9	15	2	0	0

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



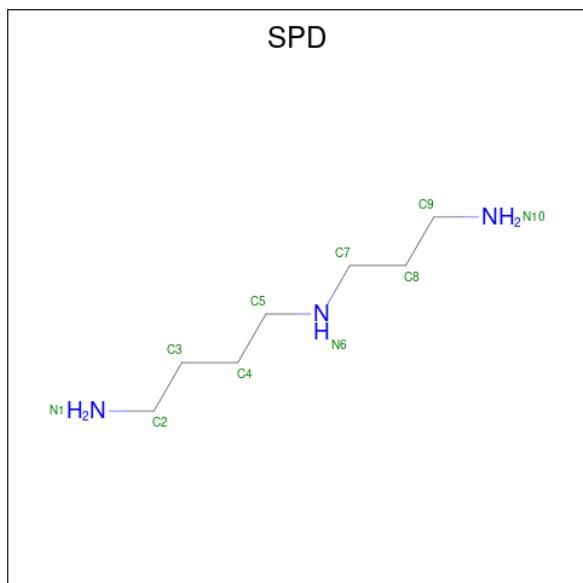
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	48	21	7	17	3	0	0
3	B	1	48	21	7	17	3	0	0

- Molecule 4 is GLUTATHIONE (CCD ID: GSH) (formula:  $C_{10}H_{17}N_3O_6S$ ).



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

- Molecule 5 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ).



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



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.80Å 128.80Å 92.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 88.6 (8.00-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.81Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.148 , (Not available) 0.160 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtrriage
Anisotropy	0.001	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, NAP, GSH, 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	1.12	17/3787 (0.4%)	1.89	94/5131 (1.8%)
1	B	1.14	17/3779 (0.4%)	1.88	93/5121 (1.8%)
All	All	1.13	34/7566 (0.4%)	1.88	187/10252 (1.8%)

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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	VAL	CA-CB	9.50	1.66	1.54
1	B	194	VAL	CA-CB	8.40	1.64	1.54
1	B	27	HIS	CD2-NE2	-7.74	1.29	1.37
1	B	428	HIS	CD2-NE2	-7.72	1.29	1.37
1	A	194	VAL	CA-CB	7.68	1.63	1.54
1	B	44	HIS	CD2-NE2	-7.55	1.29	1.37
1	A	166	HIS	CD2-NE2	-6.95	1.30	1.37
1	B	166	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	133	HIS	CD2-NE2	-6.63	1.30	1.37
1	B	133	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	359	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	123	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	39	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	428	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	401	HIS	CD2-NE2	-6.15	1.31	1.37
1	B	252	HIS	CD2-NE2	-6.12	1.31	1.37

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	252	HIS	CD2-NE2	-6.03	1.31	1.37
1	B	40	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	73	ILE	CA-CB	5.82	1.61	1.54
1	A	39	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	419	HIS	CG-ND1	-5.76	1.31	1.38
1	A	44	HIS	CD2-NE2	-5.71	1.31	1.37
1	B	401	HIS	CD2-NE2	-5.68	1.31	1.37
1	B	267	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	123	HIS	CD2-NE2	-5.59	1.31	1.37
1	A	267	HIS	CD2-NE2	-5.59	1.31	1.37
1	A	40	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	419	HIS	CD2-NE2	-5.45	1.31	1.37
1	B	461	HIS	CD2-NE2	-5.42	1.31	1.37
1	A	461	HIS	CD2-NE2	-5.19	1.32	1.37
1	B	419	HIS	CD2-NE2	-5.19	1.32	1.37
1	A	42	PRO	CA-CB	-5.10	1.49	1.53
1	B	90	PRO	CA-CB	-5.05	1.47	1.53

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	MET	CB-CG-SD	16.30	161.60	112.70
1	A	113	MET	CA-CB-CG	13.54	141.19	114.10
1	B	288	VAL	N-CA-CB	-9.57	97.81	111.21
1	A	166	HIS	CB-CG-CD2	-9.44	118.93	131.20
1	B	39	HIS	CA-CB-CG	-9.21	104.59	113.80
1	A	173	ASP	CA-CB-CG	9.14	121.74	112.60
1	A	213	ARG	N-CA-C	8.81	121.68	111.11
1	B	428	HIS	CB-CG-CD2	-8.79	119.78	131.20
1	A	295	GLN	OE1-CD-NE2	-8.78	113.82	122.60
1	B	484	VAL	N-CA-C	8.59	127.21	109.34
1	A	1	MET	CA-C-O	-8.56	106.25	120.80
1	B	44	HIS	CB-CG-CD2	-8.53	120.11	131.20
1	B	231	ASP	CA-CB-CG	8.52	121.12	112.60
1	B	312	ASP	CA-CB-CG	8.52	121.12	112.60
1	B	401	HIS	CA-CB-CG	-8.26	105.54	113.80
1	A	401	HIS	CA-CB-CG	-8.24	105.56	113.80
1	A	374	VAL	N-CA-CB	-8.19	98.02	111.45
1	A	320	ASP	N-CA-C	8.09	122.25	112.38
1	B	369	ILE	N-CA-C	-8.04	100.19	108.15
1	B	54	ASN	OD1-CG-ND2	-8.02	114.58	122.60

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	GLN	CG-CD-NE2	7.75	128.02	116.40
1	B	461	HIS	CB-CG-CD2	-7.71	121.18	131.20
1	B	109	SER	CA-CB-OG	-7.70	95.70	111.10
1	A	319	VAL	N-CA-C	-7.58	96.81	107.80
1	B	378	VAL	N-CA-CB	-7.48	98.89	110.86
1	A	428	HIS	CB-CG-CD2	-7.47	121.49	131.20
1	B	378	VAL	CB-CA-C	7.43	121.46	110.98
1	A	397	THR	N-CA-C	-7.43	98.91	109.24
1	B	111	GLU	CB-CA-C	-7.39	96.95	110.63
1	A	142	ASP	CA-CB-CG	7.37	119.97	112.60
1	B	232	SER	N-CA-C	7.36	119.94	111.11
1	A	27	HIS	CA-CB-CG	-7.33	106.47	113.80
1	A	107	ASN	CA-CB-CG	7.33	119.93	112.60
1	B	374	VAL	N-CA-CB	-7.31	100.15	112.44
1	B	111	GLU	N-CA-CB	7.31	121.48	110.22
1	B	166	HIS	CB-CG-CD2	-7.30	121.71	131.20
1	A	166	HIS	CB-CG-ND1	7.27	133.61	122.70
1	A	3	ARG	N-CA-C	-7.21	95.45	110.80
1	A	312	ASP	CA-CB-CG	7.15	119.75	112.60
1	B	167	LEU	O-C-N	-7.15	114.87	123.16
1	A	461	HIS	CB-CG-CD2	-7.14	121.92	131.20
1	A	71	ASP	CA-CB-CG	7.11	119.71	112.60
1	A	91	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	A	359	HIS	CB-CG-CD2	-7.03	122.07	131.20
1	B	461	HIS	CA-CB-CG	7.00	120.80	113.80
1	B	237	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	A	349	VAL	N-CA-C	6.95	118.58	111.00
1	B	394	SER	N-CA-C	-6.92	98.50	109.23
1	A	352	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	B	402	ASN	CA-CB-CG	6.88	119.48	112.60
1	B	461	HIS	CB-CG-ND1	6.75	132.83	122.70
1	B	39	HIS	CA-C-O	-6.75	113.53	121.16
1	A	109	SER	CA-CB-OG	-6.67	97.77	111.10
1	A	401	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	B	267	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	B	126	TRP	CD2-CE2-CZ2	-6.54	115.86	122.40
1	B	379	GLU	CA-C-O	-6.53	113.58	120.63
1	A	68	ASN	CA-CB-CG	-6.48	106.12	112.60
1	B	133	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	B	269	VAL	N-CA-C	-6.47	98.30	107.75
1	B	484	VAL	N-CA-CB	-6.45	100.59	111.23
1	B	295	GLN	OE1-CD-NE2	-6.42	116.18	122.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	TRP	CH2-CZ2-CE2	6.42	125.84	117.50
1	A	461	HIS	CA-CB-CG	6.41	120.21	113.80
1	B	30	ARG	NE-CZ-NH1	6.40	127.90	121.50
1	B	44	HIS	CB-CG-ND1	6.39	132.29	122.70
1	A	222	ARG	N-CA-C	6.39	120.34	112.54
1	A	461	HIS	CB-CG-ND1	6.39	132.28	122.70
1	A	295	GLN	CG-CD-NE2	6.37	125.95	116.40
1	A	130	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	A	411	PHE	N-CA-C	-6.34	100.23	110.32
1	A	377	TYR	CA-C-N	6.31	129.97	120.75
1	A	377	TYR	C-N-CA	6.31	129.97	120.75
1	A	44	HIS	CA-CB-CG	-6.30	107.50	113.80
1	B	302	GLU	CA-CB-CG	6.27	126.65	114.10
1	B	126	TRP	CG-CD1-NE1	-6.19	102.15	110.20
1	B	126	TRP	CD1-CG-CD2	6.16	116.15	106.30
1	B	166	HIS	CA-CB-CG	-6.13	107.67	113.80
1	B	40	HIS	CB-CG-CD2	-6.11	123.25	131.20
1	A	2	SER	CA-C-N	6.09	133.17	121.54
1	A	2	SER	C-N-CA	6.09	133.17	121.54
1	B	107	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	352	ASN	CA-C-O	6.07	129.19	120.51
1	B	163	TRP	CG-CD2-CE3	6.07	139.97	133.90
1	B	126	TRP	CB-CG-CD1	-6.04	117.84	126.90
1	B	104	SER	CA-CB-OG	-6.03	99.04	111.10
1	A	428	HIS	CB-CG-ND1	6.02	131.74	122.70
1	A	486	LYS	CA-C-N	6.02	132.53	121.70
1	A	486	LYS	C-N-CA	6.02	132.53	121.70
1	B	456	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	A	89	ARG	CB-CA-C	-5.96	102.23	110.16
1	B	378	VAL	N-CA-C	-5.94	99.86	108.71
1	B	377	TYR	N-CA-C	5.91	118.83	110.50
1	A	359	HIS	CB-CG-ND1	5.90	131.54	122.70
1	A	267	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	B	71	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	83	LEU	CA-CB-CG	5.88	136.87	116.30
1	B	320	ASP	N-CA-C	5.84	119.51	112.38
1	B	352	ASN	CA-CB-CG	-5.84	106.76	112.60
1	A	116	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	236	LYS	N-CA-CB	-5.83	101.61	110.07
1	A	252	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	B	25	SER	N-CA-C	5.83	117.44	111.14
1	A	85	ARG	CG-CD-NE	-5.82	99.19	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	GLY	N-CA-C	-5.81	107.78	114.69
1	A	42	PRO	N-CA-C	-5.80	104.90	110.47
1	A	421	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	378	VAL	CB-CA-C	5.75	119.22	111.28
1	A	232	SER	N-CA-C	5.72	118.25	111.33
1	A	273	GLY	N-CA-C	-5.72	107.77	115.21
1	B	288	VAL	CB-CA-C	5.72	121.76	111.36
1	B	73	ILE	N-CA-C	-5.71	105.16	110.53
1	A	167	LEU	N-CA-C	-5.71	102.84	110.55
1	B	250	ARG	CB-CG-CD	-5.71	98.17	111.30
1	A	9	VAL	CA-C-O	-5.70	114.38	120.59
1	A	471	MET	CA-C-O	5.69	127.19	120.70
1	B	222	ARG	CA-CB-CG	5.67	125.44	114.10
1	A	318	ASN	CB-CG-ND2	5.67	124.90	116.40
1	B	37	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	B	110	TYR	CA-C-O	-5.65	113.12	119.79
1	A	456	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	254	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	414	ARG	NE-CZ-NH1	5.64	127.14	121.50
1	A	285	ILE	N-CA-C	5.64	117.63	111.77
1	A	305	LYS	CB-CG-CD	5.64	124.27	111.30
1	A	388	GLN	CA-CB-CG	-5.58	102.93	114.10
1	B	68	ASN	N-CA-C	5.57	118.07	111.33
1	B	126	TRP	CA-CB-CG	-5.57	103.02	113.60
1	A	402	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	A	484	VAL	N-CA-CB	-5.55	102.07	111.23
1	B	404	SER	N-CA-C	5.53	118.24	111.82
1	B	428	HIS	CB-CG-ND1	5.53	130.99	122.70
1	A	138	ARG	NE-CZ-NH2	-5.53	114.23	119.20
1	B	116	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	40	HIS	CA-C-O	-5.52	115.80	121.87
1	A	378	VAL	N-CA-CB	-5.49	99.74	110.45
1	B	160	THR	N-CA-C	5.49	119.84	113.20
1	B	44	HIS	CA-CB-CG	-5.49	108.31	113.80
1	B	203	PHE	CA-CB-CG	-5.49	108.31	113.80
1	B	477	PHE	O-C-N	5.48	129.40	123.10
1	A	116	ASP	CA-C-N	-5.47	115.73	122.84
1	A	116	ASP	C-N-CA	-5.47	115.73	122.84
1	A	92	TRP	CE2-CD2-CG	-5.46	100.64	107.20
1	A	412	MET	CB-CG-SD	-5.45	96.34	112.70
1	B	397	THR	N-CA-C	-5.45	102.79	109.65
1	A	21	TRP	CD2-CE2-CZ2	-5.42	116.98	122.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	357	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	477	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	84	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	38	LYS	N-CA-CB	-5.37	102.63	110.47
1	B	236	LYS	CA-CB-CG	5.37	124.83	114.10
1	B	457	THR	O-C-N	-5.34	116.70	123.01
1	B	163	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	A	133	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	B	186	GLU	CA-CB-CG	5.31	124.72	114.10
1	A	24	ALA	N-CA-C	5.29	116.85	111.14
1	A	386	TYR	O-C-N	-5.28	117.14	123.27
1	A	104	SER	CA-CB-OG	-5.28	100.54	111.10
1	B	267	HIS	CB-CG-ND1	5.26	130.59	122.70
1	B	107	ASN	CB-CG-ND2	5.26	124.28	116.40
1	A	203	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	257	LYS	CG-CD-CE	5.23	123.33	111.30
1	A	41	GLY	CA-C-N	5.23	123.48	119.66
1	A	41	GLY	C-N-CA	5.23	123.48	119.66
1	B	100	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	B	120	LEU	CA-C-O	-5.22	114.58	120.43
1	A	95	LEU	N-CA-C	-5.22	105.28	110.97
1	B	163	TRP	CB-CG-CD1	-5.21	119.08	126.90
1	A	335	THR	CA-CB-OG1	-5.18	101.83	109.60
1	B	237	GLN	CA-CB-CG	-5.18	103.75	114.10
1	A	163	TRP	CE2-CD2-CG	-5.17	100.99	107.20
1	A	460	VAL	N-CA-C	-5.17	100.93	108.17
1	B	167	LEU	N-CA-C	-5.12	101.36	109.96
1	B	384	LYS	CB-CG-CD	-5.12	99.53	111.30
1	B	431	GLY	O-C-N	-5.11	119.09	123.43
1	A	270	PHE	CA-CB-CG	-5.11	108.69	113.80
1	B	216	GLN	CA-CB-CG	5.10	124.30	114.10
1	B	197	GLY	CA-C-O	-5.08	117.20	122.28
1	B	163	TRP	CG-CD1-NE1	-5.06	103.62	110.20
1	A	172	ASP	N-CA-C	5.05	117.52	111.71
1	A	380	GLU	CA-CB-CG	5.05	124.20	114.10
1	B	467	GLU	CB-CG-CD	5.03	121.16	112.60
1	A	218	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	179	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	B	218	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	288	VAL	N-CA-CB	-5.02	104.18	111.21

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	61	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	9	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	109	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 (109) 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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.66
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
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: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:8:VAL:HG11	1:A:135:VAL:HG21	1.93	0.51
1:A:403:ILE:HD12	1:B:62:LEU:HD22	1.91	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:285:ILE:C	3:B:494:NAP:H52A	2.35	0.50
1:A:203:PHE:CB	1:A:282:MET:HE1	2.42	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:353:LYS:HB3	1:A:353:LYS:HE2	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:375:CYS:O	1:B:426:GLY:HA2	2.16	0.44
1:B:397:THR:OG1	1:B:410:LYS:HD2	2.17	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:393:GLU:CD	1:A:414:ARG:HH11	2.27	0.43
1:A:224:ASP:HA	1:A:252:HIS:CE1	2.54	0.43
1:B:5:TYR:O	1:B:153:THR:HA	2.19	0.43
1:B:222:ARG:HD2	3:B:494:NAP:N3A	2.34	0.43
1:B:259:THR:OG1	1:B:267:HIS:HB3	2.19	0.43
2:B:493:FAD:H9	2:B:493:FAD:H1'1	1.77	0.43
1:A:17:LEU:HD12	1:A:17:LEU:HA	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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:138:ARG:HH22	1:B:295:GLN:CD	2.28	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%)	43	72
1	B	484/487 (99%)	461 (95%)	23 (5%)	0	100	100
All	All	969/974 (100%)	925 (96%)	43 (4%)	1 (0%)	48	77

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%)	348 (89%)	42 (11%)	6	21
1	B	389/390 (100%)	343 (88%)	46 (12%)	5	17
All	All	779/780 (100%)	691 (89%)	88 (11%)	5	19

All (88) 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	38	LYS
1	A	55	VAL
1	A	57	CYS
1	A	60	LYS
1	A	95	LEU
1	A	101	LYS
1	A	116	ASP
1	A	120	LEU
1	A	136	LEU
1	A	147	VAL
1	A	167	LEU
1	A	194	VAL
1	A	216	GLN
1	A	219	LEU
1	A	242	LEU
1	A	259	THR
1	A	260	LYS
1	A	305	LYS
1	A	328	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	335	THR
1	A	341	GLU
1	A	355	ARG
1	A	374	VAL
1	A	378	VAL
1	A	380	GLU
1	A	385	LYS
1	A	395	SER
1	A	399	LEU
1	A	410	LYS
1	A	413	VAL
1	A	423	GLU
1	A	440	SER
1	A	451	ILE
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	38	LYS
1	B	57	CYS
1	B	60	LYS
1	B	68	ASN
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	136	LEU
1	B	140	SER
1	B	147	VAL
1	B	151	LEU
1	B	162	SER
1	B	194	VAL
1	B	200	SER
1	B	213	ARG
1	B	222	ARG
1	B	225	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	232	SER
1	B	242	LEU
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	305	LYS
1	B	331	ARG
1	B	354	PRO
1	B	355	ARG
1	B	370	PRO
1	B	374	VAL
1	B	378	VAL
1	B	385	LYS
1	B	399	LEU
1	B	440	SER
1	B	452	SER
1	B	473	THR
1	B	484	VAL
1	B	486	LYS
1	B	487	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	252	HIS
1	A	479	GLN
1	B	39	HIS
1	B	130	GLN
1	B	402	ASN
1	B	479	GLN

### 5.3.3 RNA ⓘ

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](#)

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
4	GSH	B	497	5,4	17,18,19	1.53	3 (17%)	19,22,24	4.43	10 (52%)
5	SPD	A	498	4	9,9,9	0.94	0	8,8,8	1.07	0
5	SPD	A	496	4	9,9,9	0.32	0	8,8,8	2.64	3 (37%)
2	FAD	B	493	-	58,58,58	1.48	8 (13%)	85,89,89	2.04	16 (18%)
5	SPD	B	498	4	9,9,9	1.71	2 (22%)	8,8,8	2.51	3 (37%)
4	GSH	B	495	5,4	17,18,19	1.18	1 (5%)	19,22,24	1.77	4 (21%)
4	GSH	A	495	5,4	17,18,19	1.01	1 (5%)	19,22,24	1.75	4 (21%)
5	SPD	B	496	4	9,9,9	0.35	0	8,8,8	1.36	1 (12%)
3	NAP	A	494	-	50,52,52	1.23	5 (10%)	71,80,80	1.92	16 (22%)
2	FAD	A	493	-	58,58,58	1.17	3 (5%)	85,89,89	1.57	10 (11%)
4	GSH	A	497	5,4	17,18,19	1.50	3 (17%)	19,22,24	4.10	10 (52%)
3	NAP	B	494	-	50,52,52	1.86	7 (14%)	71,80,80	2.55	14 (19%)

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
4	GSH	B	497	5,4	-	10/23/23/24	-
5	SPD	A	498	4	-	0/7/7/7	-
5	SPD	A	496	4	-	1/7/7/7	-
2	FAD	B	493	-	1/1/9/9	3/34/50/50	0/6/6/6
5	SPD	B	498	4	-	4/7/7/7	-
4	GSH	B	495	5,4	-	2/23/23/24	-
4	GSH	A	495	5,4	-	3/23/23/24	-
5	SPD	B	496	4	-	1/7/7/7	-
3	NAP	A	494	-	3/3/12/12	10/35/67/67	0/5/5/5
2	FAD	A	493	-	1/1/9/9	5/34/50/50	0/6/6/6
4	GSH	A	497	5,4	-	8/23/23/24	-
3	NAP	B	494	-	3/3/12/12	8/35/67/67	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	494	NAP	O4D-C1D	5.99	1.48	1.40
3	B	494	NAP	PA-O3	5.21	1.65	1.59
2	B	493	FAD	C9-C8	-5.01	1.32	1.39
3	B	494	NAP	C2N-N1N	4.91	1.40	1.35
3	B	494	NAP	PN-O3	4.76	1.64	1.59
2	B	493	FAD	C6-C7	-4.63	1.33	1.39
3	B	494	NAP	C2D-C3D	-4.23	1.41	1.53
3	A	494	NAP	O4D-C1D	3.93	1.46	1.40
2	A	493	FAD	C6-C7	-3.93	1.34	1.39
3	A	494	NAP	C2N-C3N	-3.79	1.33	1.39
5	B	498	SPD	C8-C7	3.76	1.66	1.51
4	B	495	GSH	O31-C3	-3.62	1.23	1.42
4	A	497	GSH	O31-C3	-3.56	1.24	1.42
2	B	493	FAD	C5X-N5	-3.53	1.32	1.39
2	A	493	FAD	C5X-N5	-3.50	1.33	1.39
4	A	495	GSH	O31-C3	-3.45	1.24	1.42
2	A	493	FAD	C9-C8	-3.36	1.35	1.39
4	B	497	GSH	CB2-CA2	-3.22	1.49	1.53
4	B	497	GSH	O31-C3	-3.17	1.25	1.42
4	A	497	GSH	CB1-CA1	2.85	1.59	1.53
2	B	493	FAD	C1'-C2'	-2.83	1.48	1.52
2	B	493	FAD	C9A-N10	-2.82	1.36	1.41
3	B	494	NAP	C3N-C7N	2.72	1.54	1.50
3	A	494	NAP	C2N-N1N	2.62	1.37	1.35
2	B	493	FAD	PA-O3P	-2.59	1.56	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	498	SPD	C8-C9	2.55	1.63	1.51
4	A	497	GSH	O11-C1	-2.30	1.23	1.30
4	B	497	GSH	CB1-CA1	2.24	1.58	1.53
2	B	493	FAD	C8-C7	2.22	1.46	1.40
3	A	494	NAP	C4N-C3N	-2.11	1.36	1.39
2	B	493	FAD	C2B-C3B	-2.05	1.47	1.53
3	A	494	NAP	C2B-C1B	-2.04	1.48	1.53
3	B	494	NAP	C5N-C4N	-2.01	1.35	1.38

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	494	NAP	O2A-PA-O3	14.85	147.42	107.27
4	B	497	GSH	CA2-CB2-SG2	-13.00	99.50	114.16
4	A	497	GSH	CA2-CB2-SG2	-12.73	99.81	114.16
2	B	493	FAD	C3B-C2B-C1B	-8.60	85.19	101.46
4	B	497	GSH	CG1-CD1-N2	8.14	130.21	115.86
3	A	494	NAP	C4D-O4D-C1D	-7.19	103.34	109.92
2	A	493	FAD	C3B-C2B-C1B	-7.09	88.06	101.46
4	A	497	GSH	CG1-CD1-N2	6.86	127.95	115.86
3	B	494	NAP	C6N-N1N-C2N	-6.73	116.16	121.88
5	A	496	SPD	C8-C9-N10	6.53	157.57	112.60
4	B	497	GSH	CB1-CG1-CD1	6.26	127.02	113.06
2	B	493	FAD	O4B-C4B-C3B	-5.83	93.58	105.15
3	A	494	NAP	O4D-C4D-C5D	5.38	126.58	109.33
2	B	493	FAD	O3P-PA-O1A	5.32	126.71	110.70
3	A	494	NAP	C6N-N1N-C2N	-5.21	117.45	121.88
2	B	493	FAD	O4B-C1B-N9A	5.18	118.03	108.09
3	B	494	NAP	O3-PA-O1A	-5.17	95.14	110.70
4	A	497	GSH	C2-CA2-N2	5.10	124.91	111.11
2	B	493	FAD	O2A-PA-O3P	-5.10	93.49	107.27
2	B	493	FAD	C2B-C3B-C4B	4.97	112.21	102.61
3	B	494	NAP	O4D-C4D-C5D	4.84	124.83	109.33
4	B	497	GSH	OE1-CD1-CG1	-4.81	113.30	122.02
4	B	495	GSH	CA2-CB2-SG2	4.61	119.35	114.16
4	A	497	GSH	OE1-CD1-CG1	-4.58	113.72	122.02
3	B	494	NAP	O7N-C7N-C3N	4.55	125.16	119.60
4	B	497	GSH	CB2-CA2-N2	-4.55	104.80	111.28
5	B	498	SPD	C4-C5-N6	-4.37	100.33	112.07
3	A	494	NAP	O4D-C4D-C3D	4.27	113.62	105.15
3	A	494	NAP	C2D-C3D-C4D	-4.13	94.64	102.61
4	A	495	GSH	CG1-CB1-CA1	4.04	123.14	113.86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	498	SPD	C7-N6-C5	4.01	132.37	113.40
3	B	494	NAP	P2B-O2B-C2B	-3.87	113.10	123.43
4	A	497	GSH	CB2-CA2-N2	-3.86	105.78	111.28
4	B	497	GSH	OE1-CD1-N2	-3.83	116.47	122.95
2	B	493	FAD	O3B-C3B-C4B	3.78	121.93	111.08
2	A	493	FAD	O4B-C4B-C3B	-3.68	97.86	105.15
4	A	495	GSH	CB1-CG1-CD1	-3.62	104.98	113.06
2	A	493	FAD	O3B-C3B-C4B	3.57	121.33	111.08
3	A	494	NAP	O4B-C4B-C3B	-3.51	98.19	105.15
3	A	494	NAP	O2N-PN-O3	3.43	116.54	107.27
2	A	493	FAD	O3P-PA-O1A	3.36	120.82	110.70
5	B	498	SPD	C8-C7-N6	-3.35	103.07	112.07
3	B	494	NAP	C2N-N1N-C1D	3.31	126.44	119.13
2	A	493	FAD	C10-N1-C2	3.24	123.86	116.85
4	B	495	GSH	CG1-CD1-N2	3.17	121.45	115.86
5	B	496	SPD	C4-C5-N6	-3.16	103.58	112.07
4	B	497	GSH	C2-CA2-N2	3.16	119.66	111.11
2	B	493	FAD	C2'-C1'-N10	3.01	124.44	110.20
3	B	494	NAP	O3-PN-O1N	2.93	119.51	110.70
2	B	493	FAD	O3'-C3'-C4'	-2.90	102.33	108.93
3	B	494	NAP	O7N-C7N-N7N	-2.87	118.47	122.62
3	B	494	NAP	C2B-C1B-N9A	-2.86	109.05	113.75
2	B	493	FAD	O3P-P-O1P	-2.82	102.21	110.70
3	A	494	NAP	O3D-C3D-C4D	2.79	119.11	111.08
2	B	493	FAD	C2B-C1B-N9A	2.78	120.21	113.30
4	A	497	GSH	CB1-CG1-CD1	2.78	119.25	113.06
2	A	493	FAD	C2B-C1B-N9A	2.76	120.16	113.30
4	A	497	GSH	OE1-CD1-N2	-2.74	118.32	122.95
4	A	497	GSH	CA3-N3-C2	2.72	127.43	122.55
4	A	497	GSH	CB1-CA1-C1	2.69	117.56	110.45
3	A	494	NAP	O4B-C1B-N9A	2.68	113.23	108.09
2	B	493	FAD	O2B-C2B-C3B	-2.60	103.48	111.82
4	A	495	GSH	CG1-CD1-N2	2.52	120.30	115.86
4	B	495	GSH	OE1-CD1-CG1	-2.52	117.46	122.02
2	B	493	FAD	C10-N1-C2	2.48	122.21	116.85
5	A	496	SPD	C4-C5-N6	-2.47	105.43	112.07
2	B	493	FAD	C4X-C10-N10	2.46	120.01	116.48
2	A	493	FAD	O3P-P-O1P	-2.46	103.31	110.70
4	A	497	GSH	O31-C3-CA3	2.44	120.45	111.50
3	B	494	NAP	C3N-C7N-N7N	-2.39	114.79	117.74
4	B	497	GSH	CA2-C2-N3	2.35	121.58	116.54
5	A	496	SPD	C7-C8-C9	-2.34	105.82	114.17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	497	GSH	C3-CA3-N3	2.29	117.00	111.60
2	A	493	FAD	O4B-C1B-C2B	-2.28	101.73	106.62
3	A	494	NAP	O5D-C5D-C4D	-2.28	101.23	108.99
3	A	494	NAP	C2N-N1N-C1D	2.26	124.11	119.13
3	B	494	NAP	O2B-P2B-O1X	-2.24	101.35	109.33
3	A	494	NAP	C2B-C1B-N9A	-2.24	110.07	113.75
4	B	495	GSH	CB1-CG1-CD1	-2.21	108.14	113.06
3	A	494	NAP	O2B-P2B-O1X	-2.20	101.50	109.33
3	A	494	NAP	O3-PA-O1A	2.18	117.27	110.70
3	A	494	NAP	O2B-C2B-C1B	-2.14	102.54	110.05
3	B	494	NAP	O3X-P2B-O2X	2.13	115.80	107.80
2	B	493	FAD	O2A-PA-O1A	2.12	122.31	112.44
4	A	495	GSH	O31-C3-CA3	2.12	119.28	111.50
3	B	494	NAP	C3B-C2B-C1B	2.11	106.84	102.81
2	B	493	FAD	C8M-C8-C9	-2.11	115.86	119.57
2	A	493	FAD	C1'-C2'-C3'	2.11	115.37	109.66
4	B	497	GSH	O31-C3-CA3	2.11	119.24	111.50
2	A	493	FAD	C4X-C10-N1	-2.06	119.55	124.59
3	A	494	NAP	O3D-C3D-C2D	-2.00	105.40	111.82

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	493	FAD	C3B
2	B	493	FAD	C3B
3	A	494	NAP	C1D
3	A	494	NAP	C4D
3	A	494	NAP	C3D
3	B	494	NAP	C4D
3	B	494	NAP	C1D
3	B	494	NAP	C3D

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	493	FAD	PA-O3P-P-O5'
3	A	494	NAP	C5B-O5B-PA-O1A
3	A	494	NAP	C5B-O5B-PA-O3
3	A	494	NAP	PN-O3-PA-O5B
3	A	494	NAP	C2D-C1D-N1N-C6N
3	B	494	NAP	C5B-O5B-PA-O2A
3	B	494	NAP	C2D-C1D-N1N-C2N

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	494	NAP	C2D-C1D-N1N-C6N
4	A	495	GSH	N1-CA1-CB1-CG1
4	A	495	GSH	C1-CA1-CB1-CG1
4	A	497	GSH	N2-CA2-CB2-SG2
4	A	497	GSH	C2-CA2-CB2-SG2
4	B	497	GSH	N2-CA2-CB2-SG2
4	B	497	GSH	C2-CA2-CB2-SG2
5	B	498	SPD	C3-C4-C5-N6
4	B	497	GSH	O11-C1-CA1-N1
4	A	495	GSH	O31-C3-CA3-N3
4	B	497	GSH	O31-C3-CA3-N3
4	B	497	GSH	N2-CD1-CG1-CB1
4	B	497	GSH	OE1-CD1-CG1-CB1
4	A	497	GSH	O11-C1-CA1-N1
4	A	497	GSH	O31-C3-CA3-N3
4	B	495	GSH	O31-C3-CA3-N3
4	A	497	GSH	N2-CD1-CG1-CB1
4	A	497	GSH	OE1-CD1-CG1-CB1
5	B	498	SPD	C8-C7-N6-C5
5	B	498	SPD	N6-C7-C8-C9
2	A	493	FAD	C3B-C4B-C5B-O5B
3	B	494	NAP	O4B-C4B-C5B-O5B
3	B	494	NAP	C3B-C4B-C5B-O5B
2	B	493	FAD	PA-O3P-P-O1P
5	A	496	SPD	N1-C2-C3-C4
5	B	498	SPD	C2-C3-C4-C5
4	A	497	GSH	O12-C1-CA1-N1
4	B	497	GSH	O12-C1-CA1-N1
2	B	493	FAD	PA-O3P-P-O5'
3	A	494	NAP	C3D-C4D-C5D-O5D
4	A	497	GSH	C1-CA1-CB1-CG1
3	A	494	NAP	O4D-C4D-C5D-O5D
3	B	494	NAP	PN-O3-PA-O2A
4	B	495	GSH	CA1-CB1-CG1-CD1
3	B	494	NAP	O4D-C4D-C5D-O5D
3	B	494	NAP	C5B-O5B-PA-O1A
2	A	493	FAD	O4B-C4B-C5B-O5B
5	B	496	SPD	N1-C2-C3-C4
3	A	494	NAP	C2B-O2B-P2B-O2X
2	A	493	FAD	PA-O3P-P-O2P
3	A	494	NAP	PN-O3-PA-O2A
4	B	497	GSH	O11-C1-CA1-CB1

*Continued on next page...*

*Continued from previous page...*

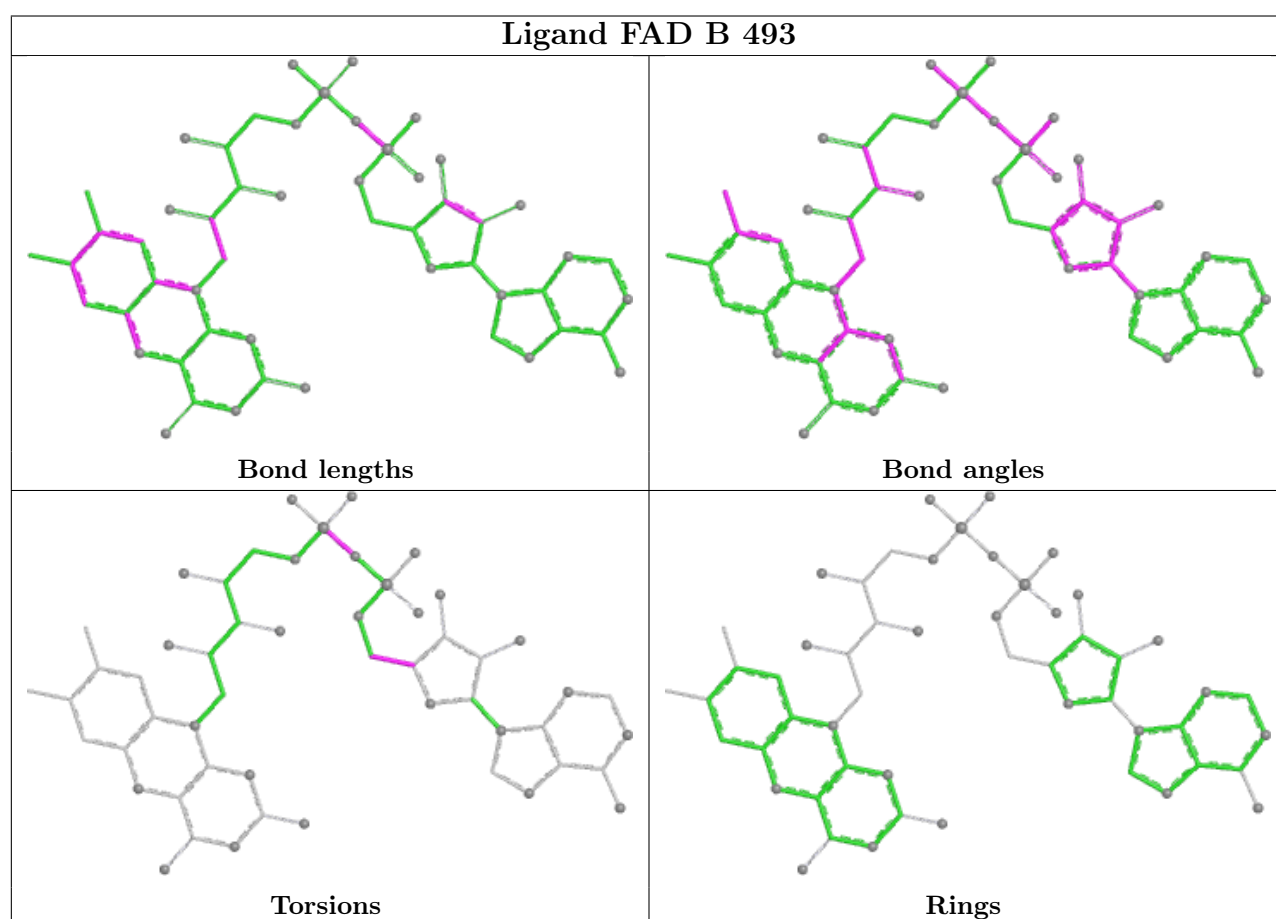
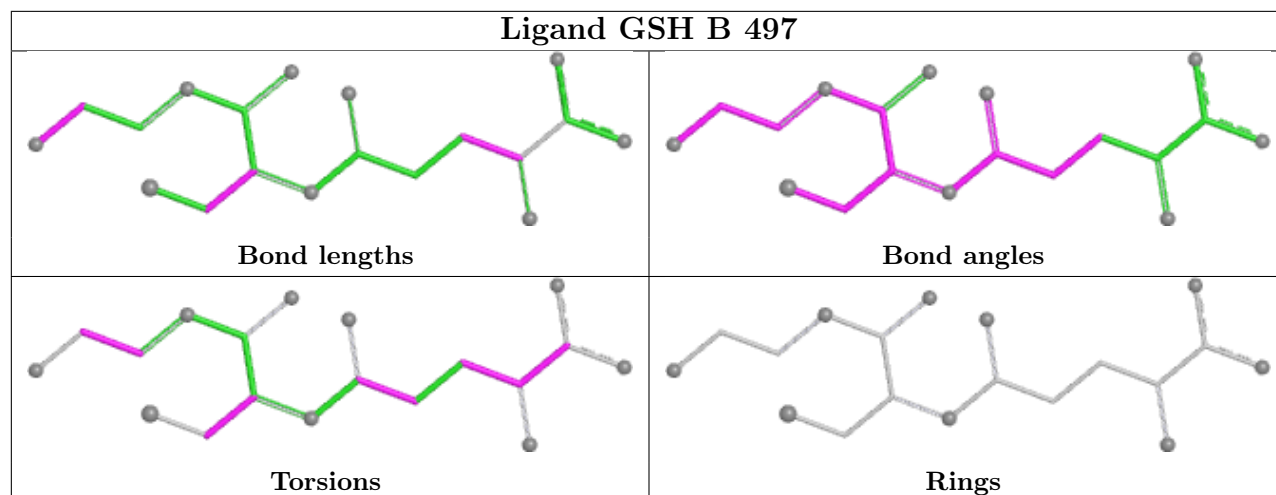
Mol	Chain	Res	Type	Atoms
2	B	493	FAD	C3B-C4B-C5B-O5B
3	A	494	NAP	C4B-C5B-O5B-PA
4	B	497	GSH	O12-C1-CA1-CB1
4	B	497	GSH	N1-CA1-CB1-CG1
2	A	493	FAD	PA-O3P-P-O1P
3	A	494	NAP	O4B-C4B-C5B-O5B

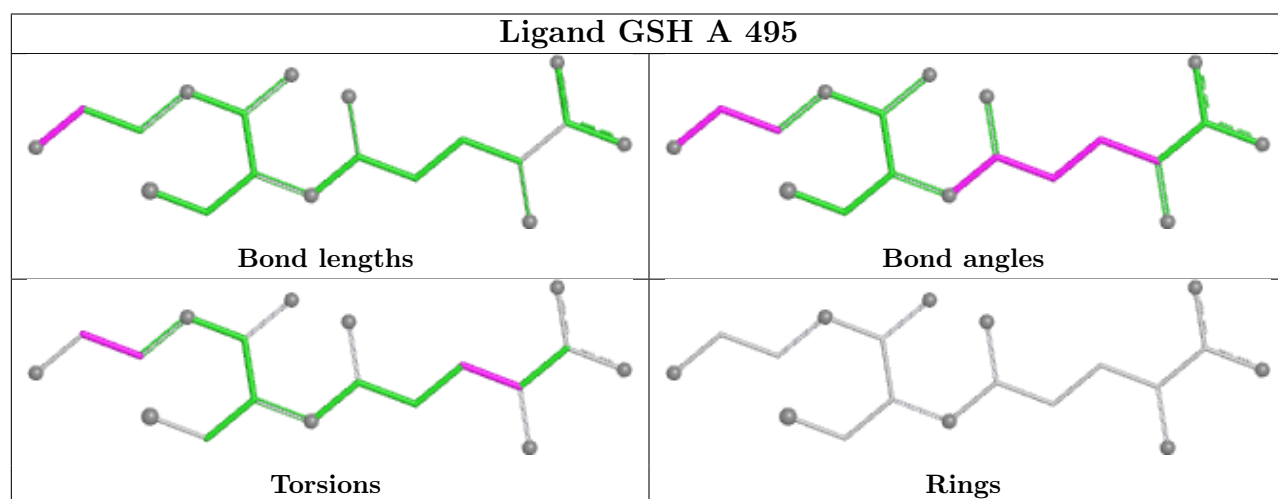
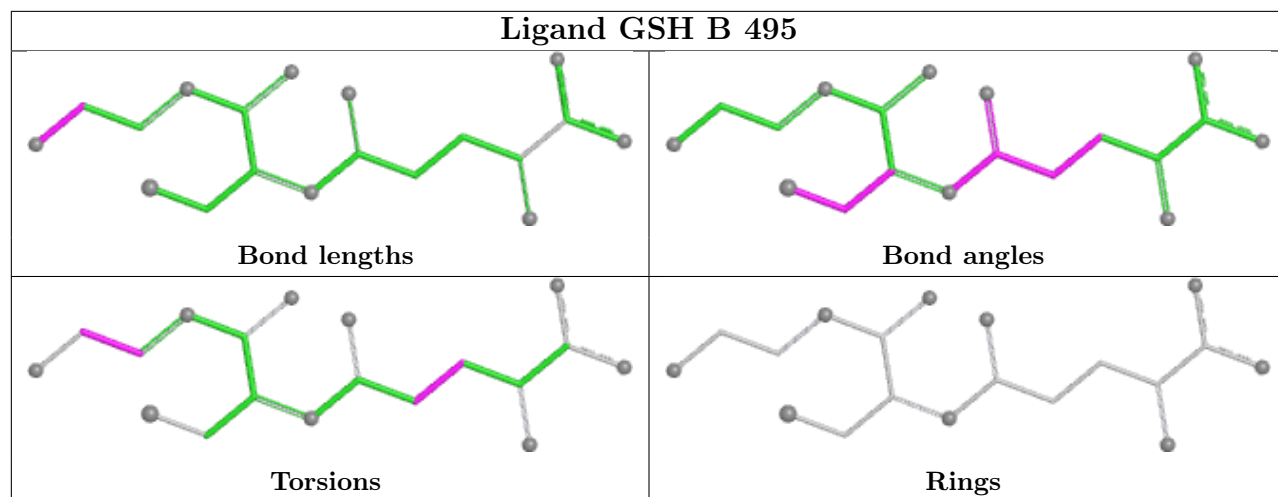
There are no ring outliers.

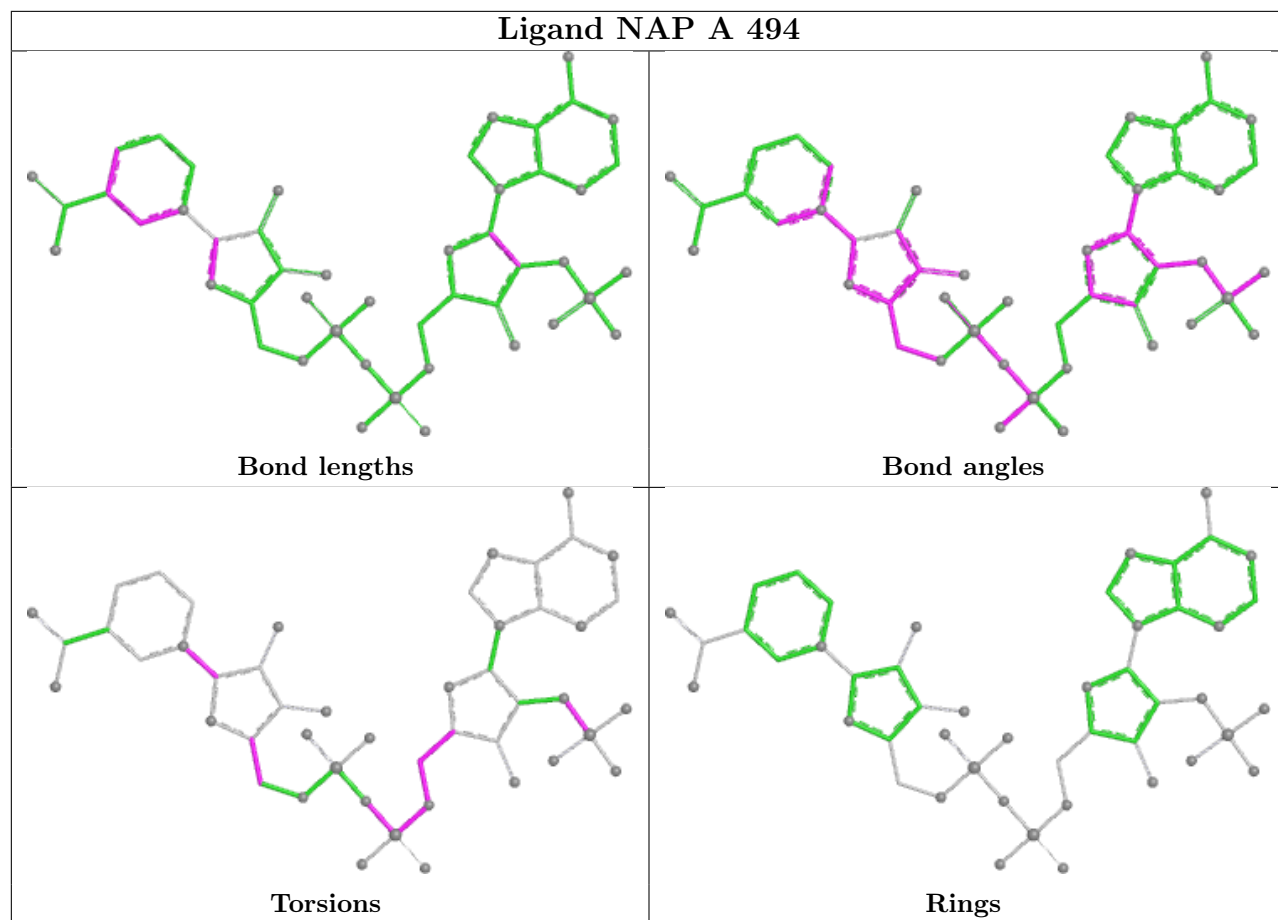
7 monomers are involved in 25 short contacts:

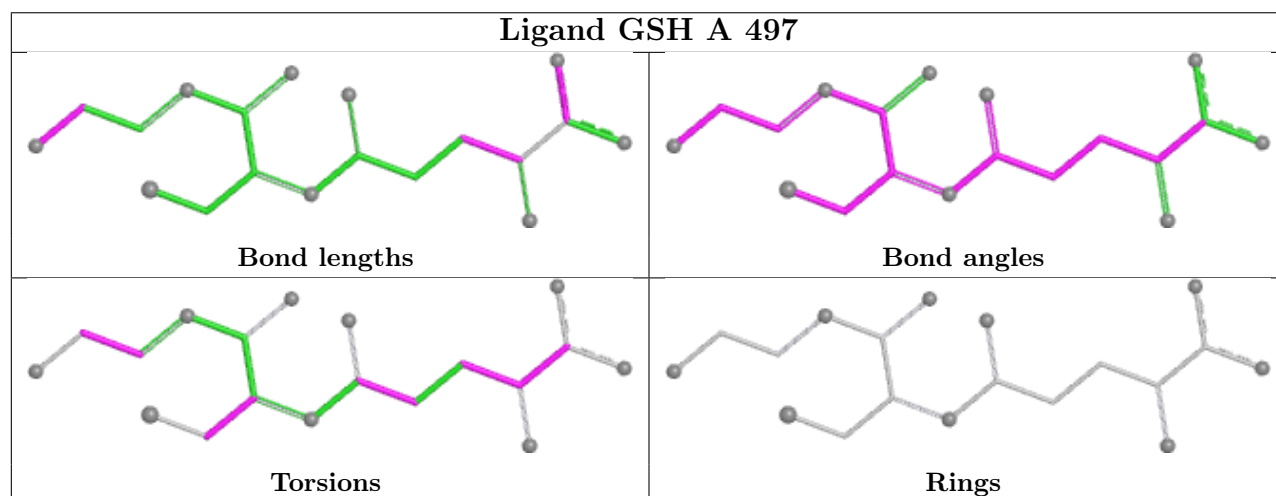
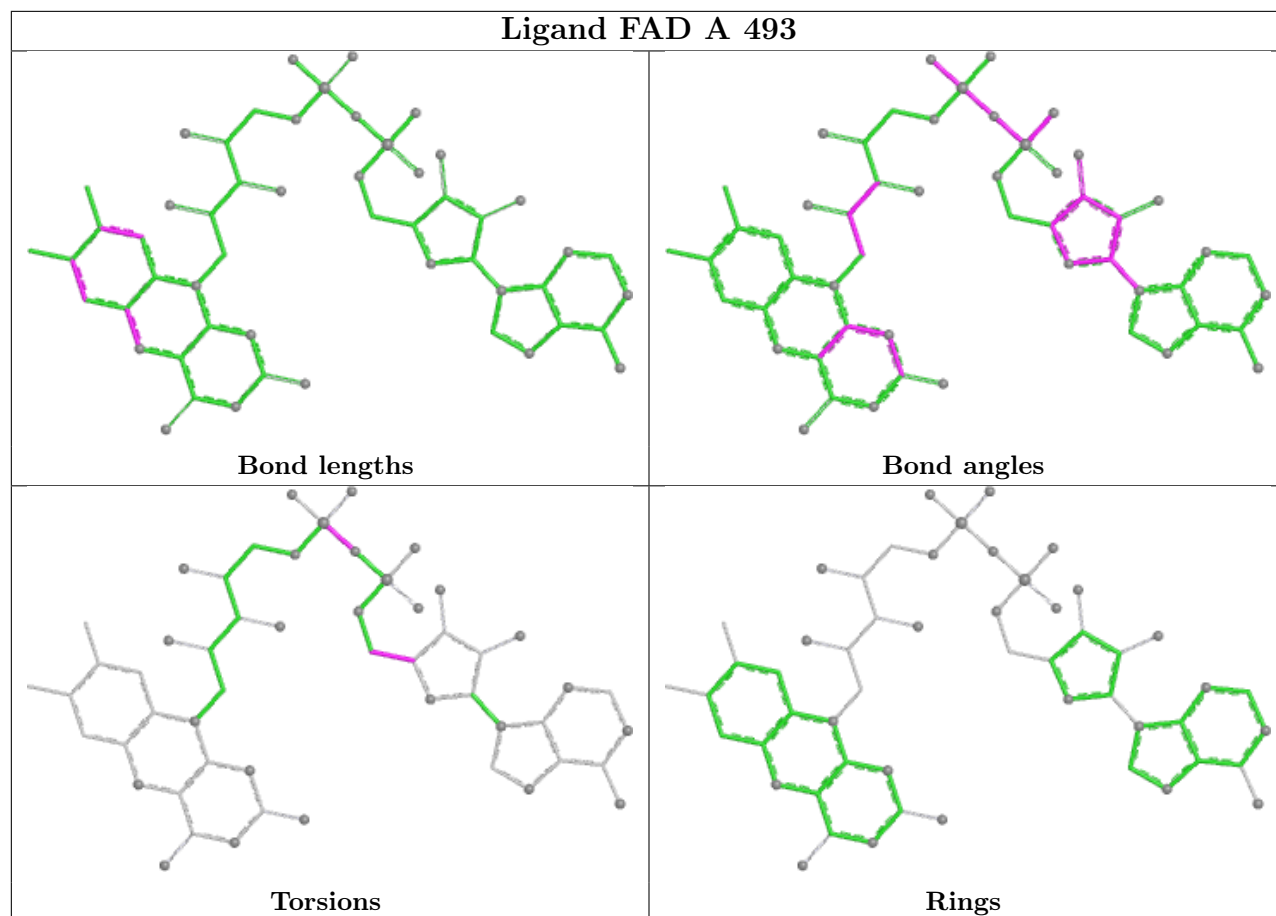
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	498	SPD	1	0
5	A	496	SPD	7	0
2	B	493	FAD	2	0
5	B	498	SPD	1	0
3	A	494	NAP	3	0
2	A	493	FAD	2	0
3	B	494	NAP	9	0

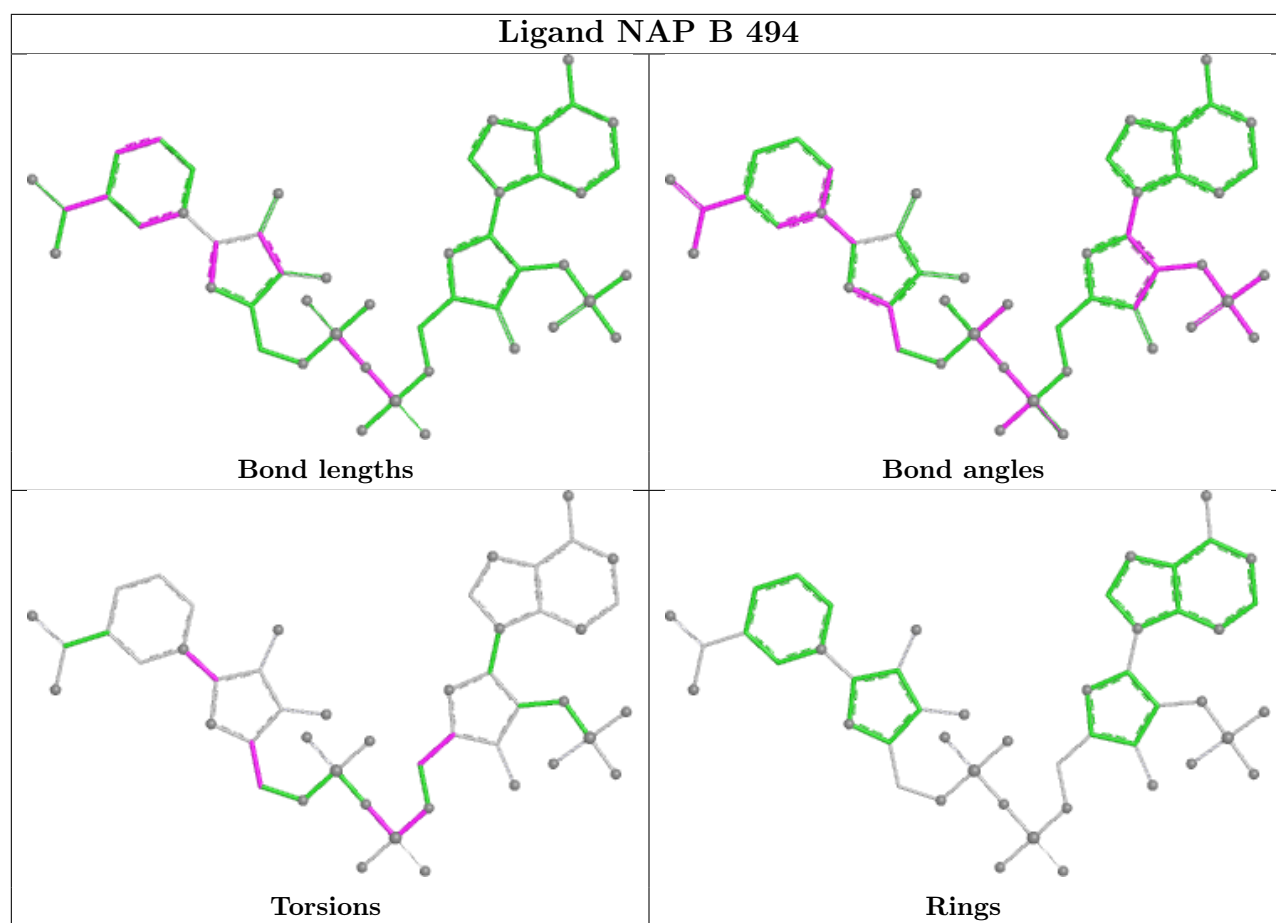
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	487/487 (100%)	-1.04	1 (0%) 91   88	3, 10, 30, 70	0
1	B	486/487 (99%)	-1.04	0 100   100	3, 9, 29, 48	0
All	All	973/974 (99%)	-1.04	1 (0%) 92   90	3, 10, 30, 70	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

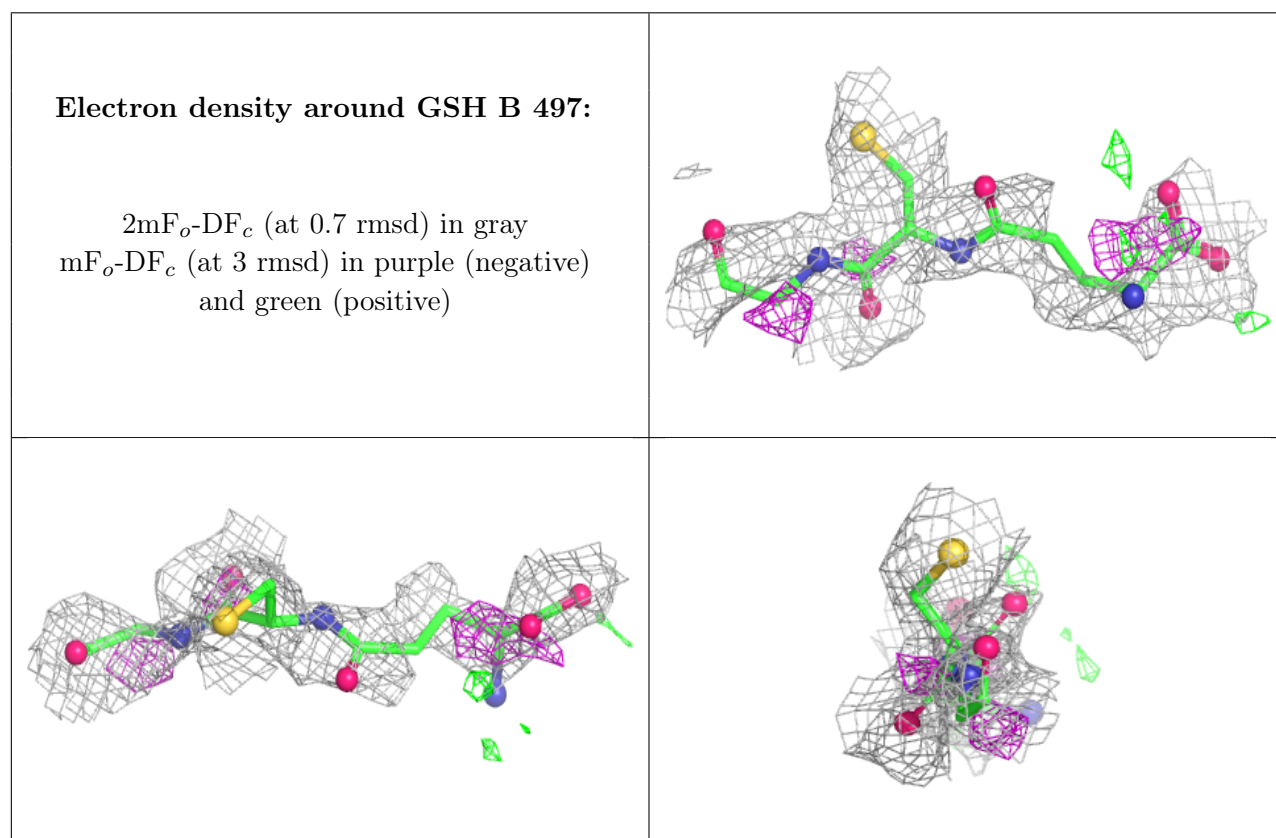
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SPD	A	498	10/10	0.56	0.17	53,56,59,60	0
5	SPD	B	498	10/10	0.81	0.14	64,66,73,73	0
4	GSH	B	497	19/20	0.82	0.16	48,63,66,66	0
5	SPD	B	496	10/10	0.87	0.14	27,43,53,54	0

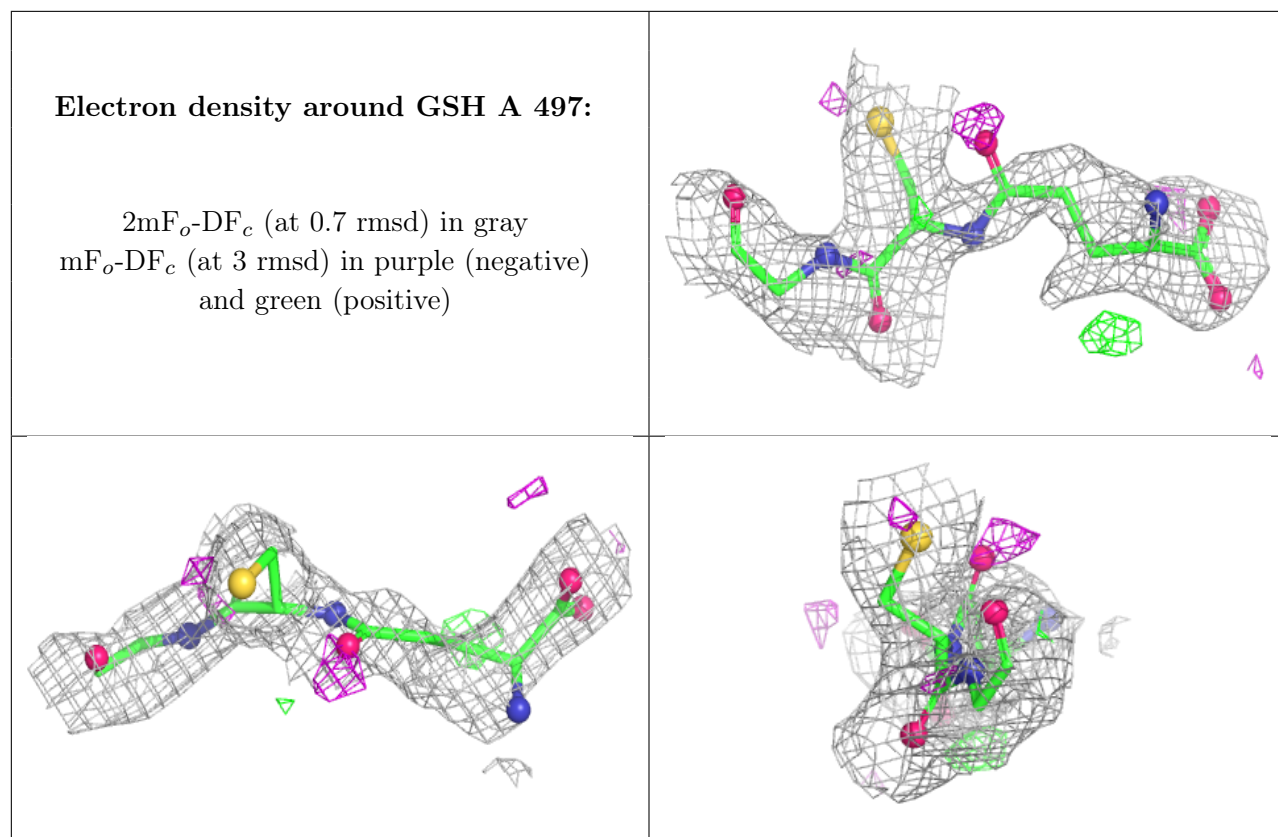
*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GSH	A	497	19/20	0.88	0.14	30,50,54,59	0
4	GSH	B	495	19/20	0.89	0.10	29,35,38,39	0
3	NAP	B	494	48/48	0.90	0.11	22,49,61,66	0
5	SPD	A	496	10/10	0.91	0.13	25,40,62,65	0
4	GSH	A	495	19/20	0.93	0.09	23,26,38,40	0
3	NAP	A	494	48/48	0.93	0.09	28,50,71,73	0
2	FAD	B	493	53/53	0.98	0.04	3,4,11,13	0
2	FAD	A	493	53/53	0.99	0.04	3,4,7,10	0

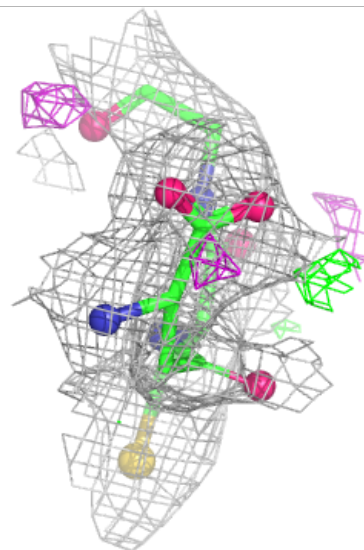
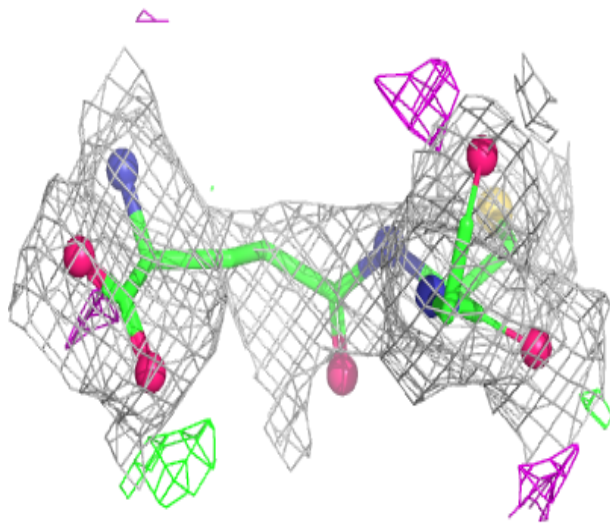
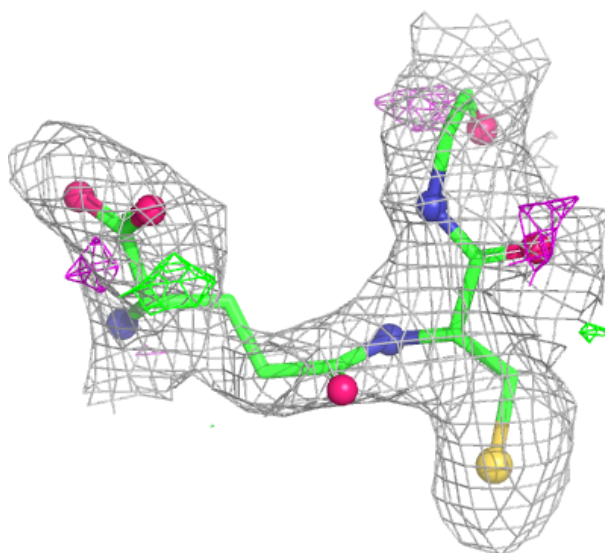
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

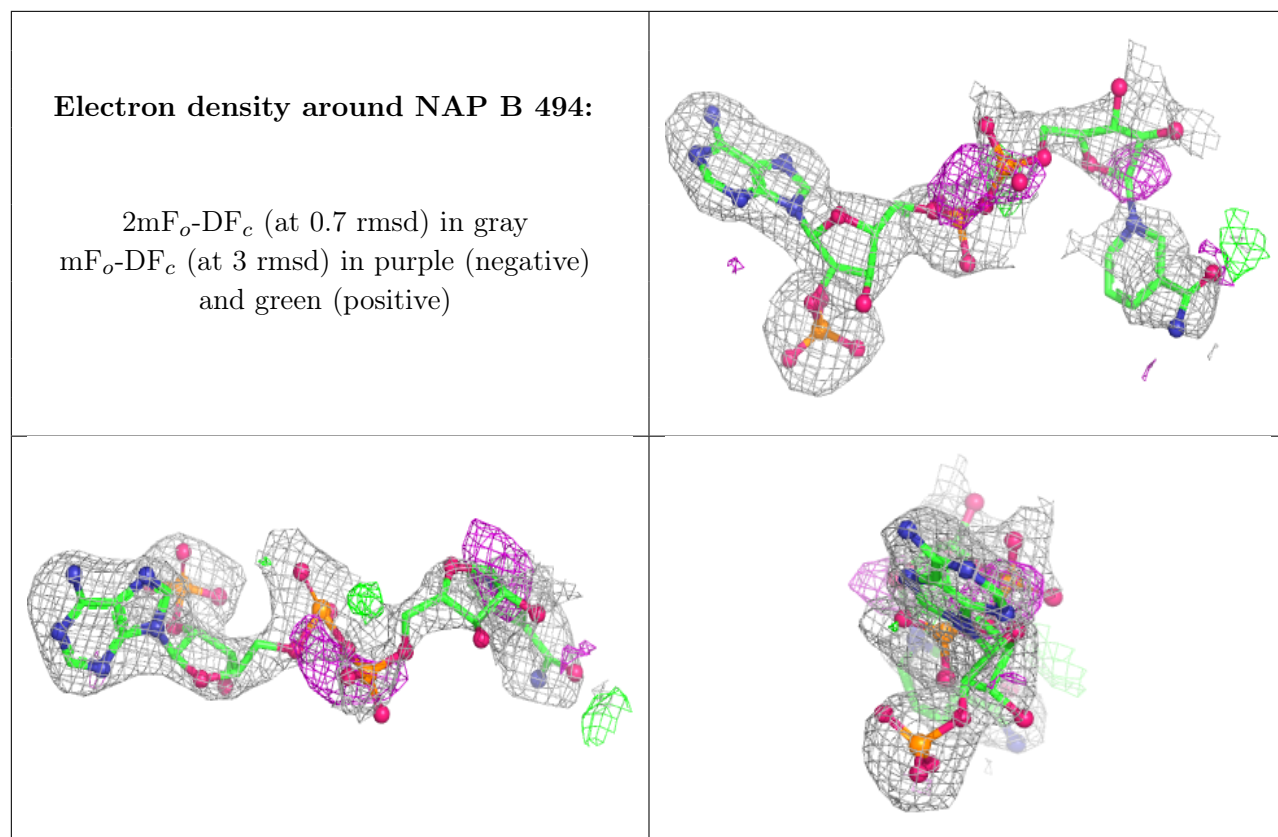


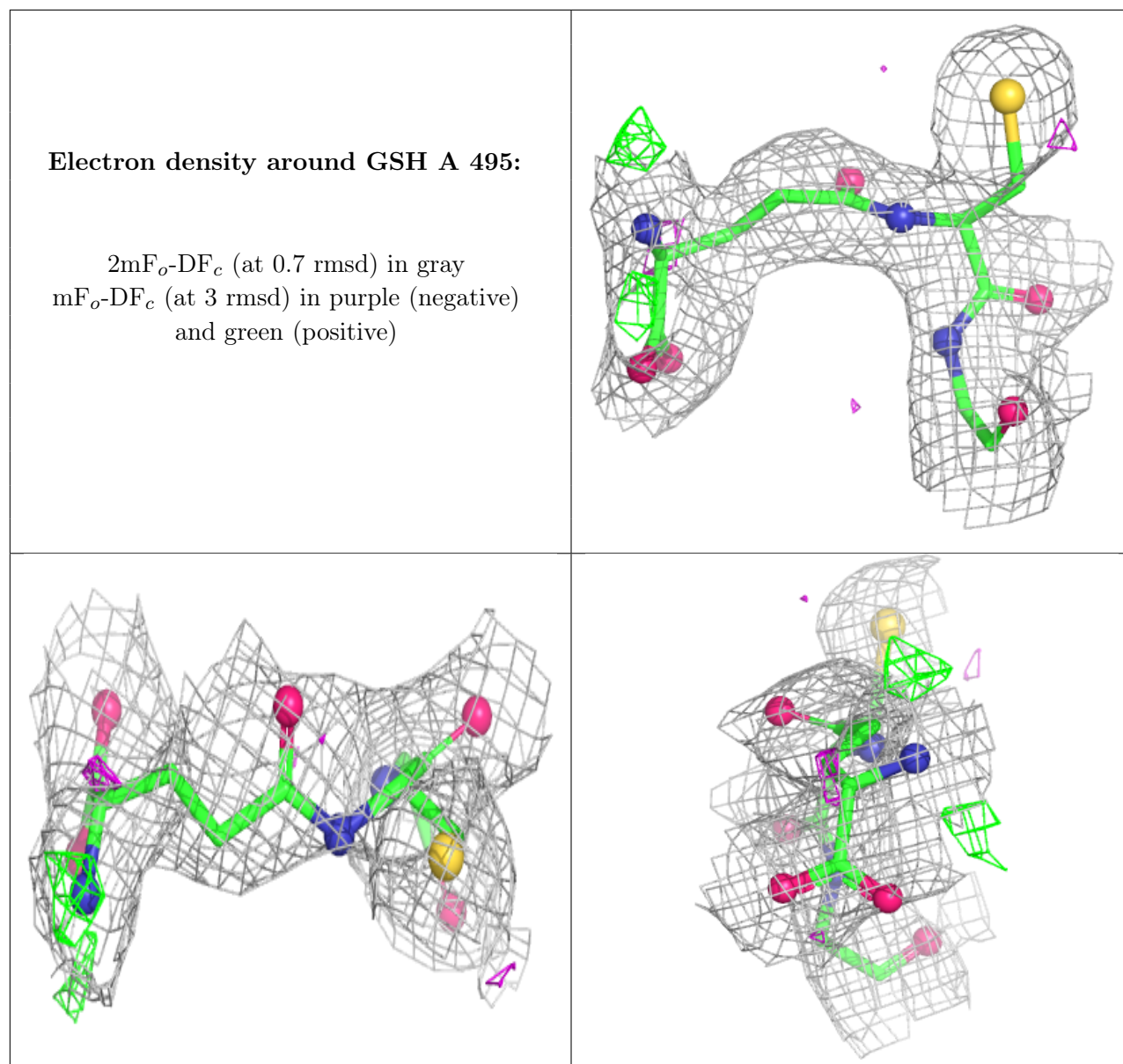


**Electron density around GSH B 495:**

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

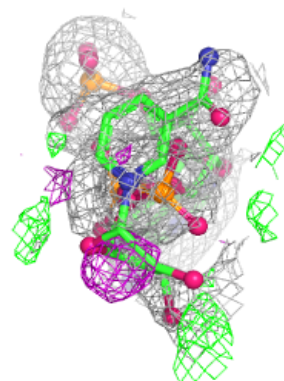
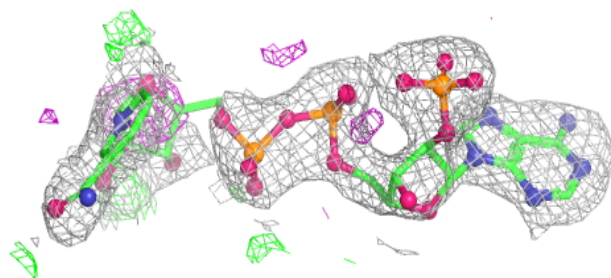
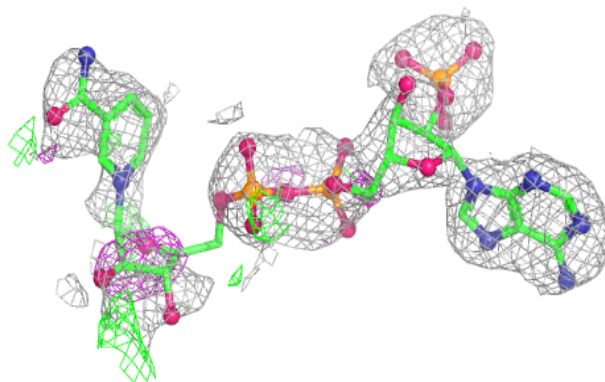




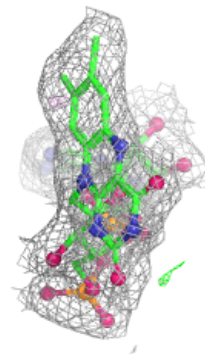
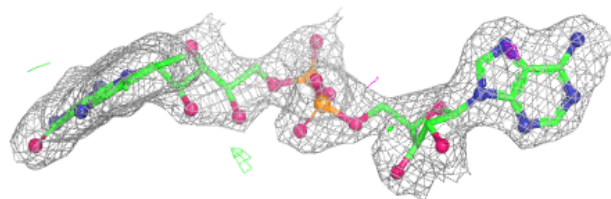
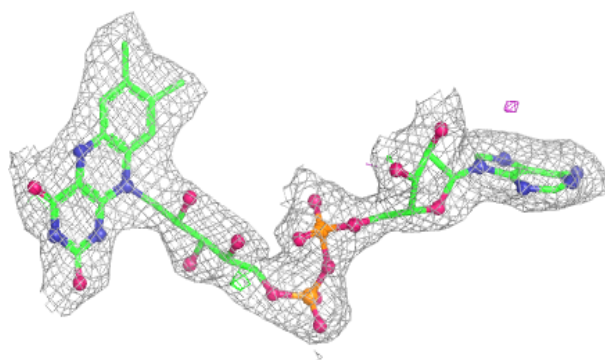


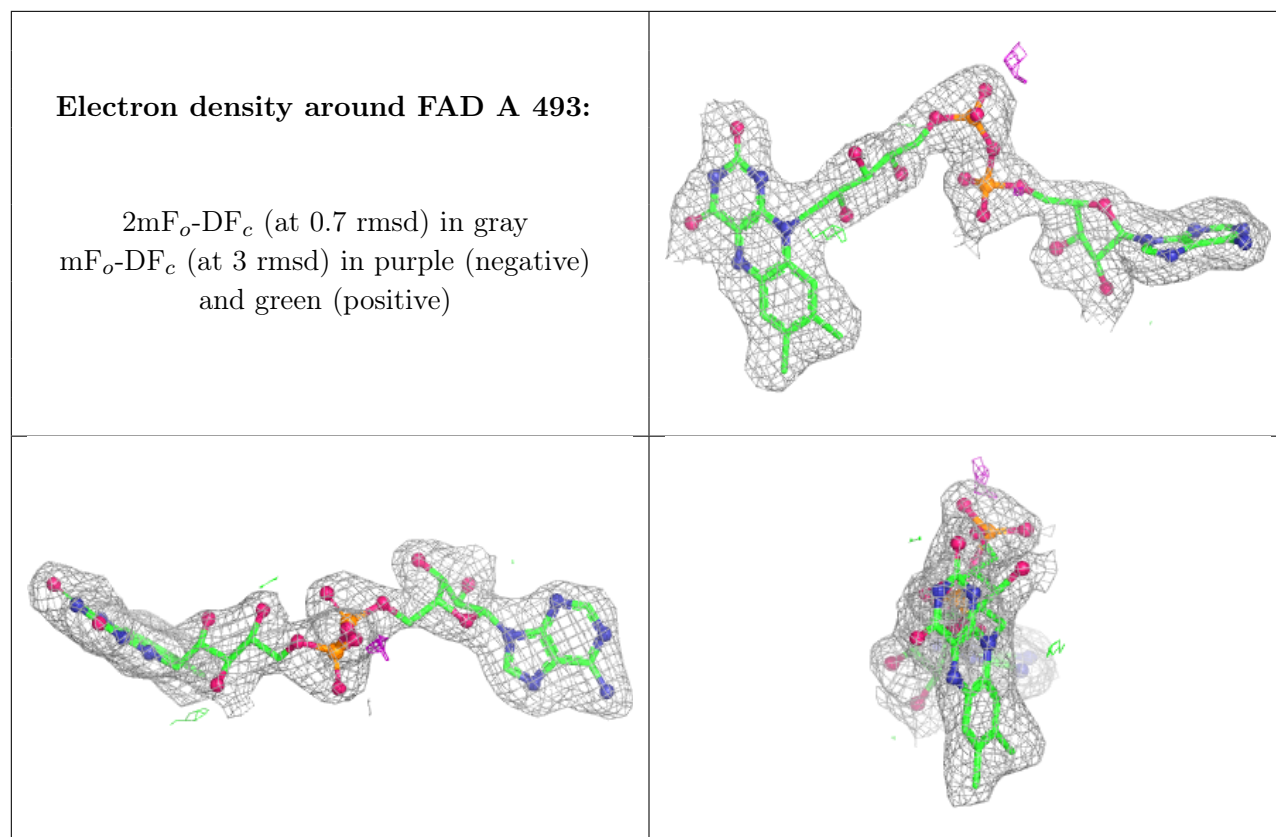
**Electron density around NAP A 494:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.