



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:57 AM UTC

PDB ID : 2ZZB / pdb\_00002zzb  
Title : Crystal structure of human thioredoxin reductase I and terpyridine platinum(II)  
Authors : Lo, Y.C.; Ko, T.P.; Wang, A.H.J.  
Deposited on : 2009-02-09  
Resolution : 3.20 Å (reported)

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

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

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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>.

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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

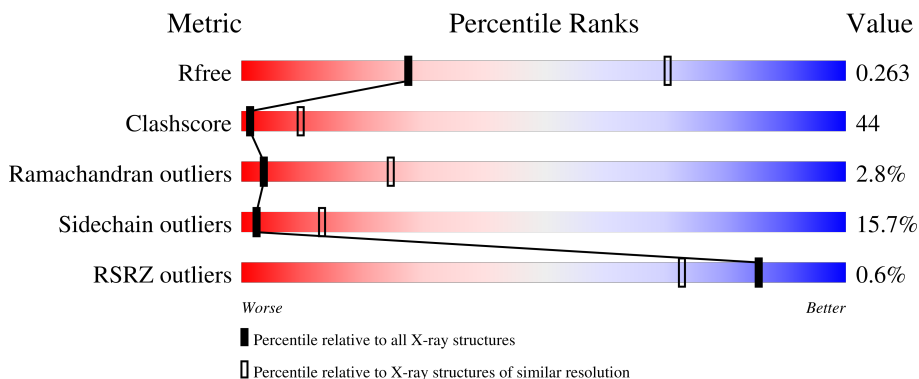
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	513	
1	B	513	
1	C	513	
1	D	513	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15394 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thioredoxin reductase 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3776	2397	645	713	21	0	0	0
1	B	485	3750	2385	640	706	19	0	0	0
1	C	493	3800	2414	649	716	21	0	0	0
1	D	484	3741	2379	638	705	19	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

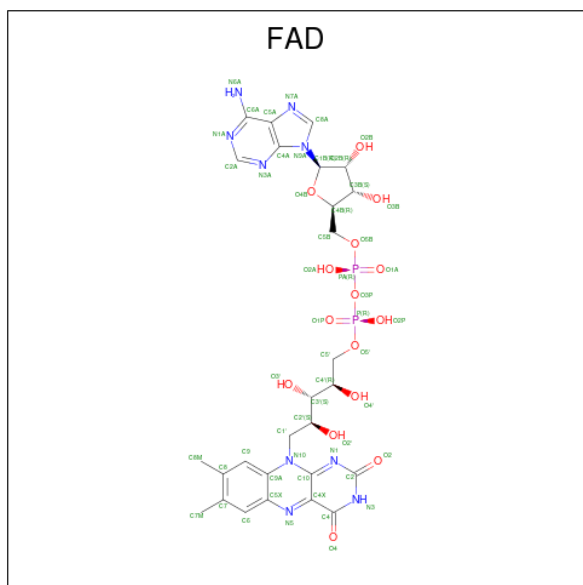
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q16881
A	-12	ALA	-	expression tag	UNP Q16881
A	-11	HIS	-	expression tag	UNP Q16881
A	-10	HIS	-	expression tag	UNP Q16881
A	-9	HIS	-	expression tag	UNP Q16881
A	-8	HIS	-	expression tag	UNP Q16881
A	-7	HIS	-	expression tag	UNP Q16881
A	-6	HIS	-	expression tag	UNP Q16881
A	-5	VAL	-	expression tag	UNP Q16881
A	-4	ASP	-	expression tag	UNP Q16881
A	-3	ASP	-	expression tag	UNP Q16881
A	-2	ASP	-	expression tag	UNP Q16881
A	-1	ASP	-	expression tag	UNP Q16881
A	498	CYS	U	SEE REMARK 999	UNP Q16881
B	-13	MET	-	expression tag	UNP Q16881
B	-12	ALA	-	expression tag	UNP Q16881
B	-11	HIS	-	expression tag	UNP Q16881
B	-10	HIS	-	expression tag	UNP Q16881
B	-9	HIS	-	expression tag	UNP Q16881
B	-8	HIS	-	expression tag	UNP Q16881
B	-7	HIS	-	expression tag	UNP Q16881

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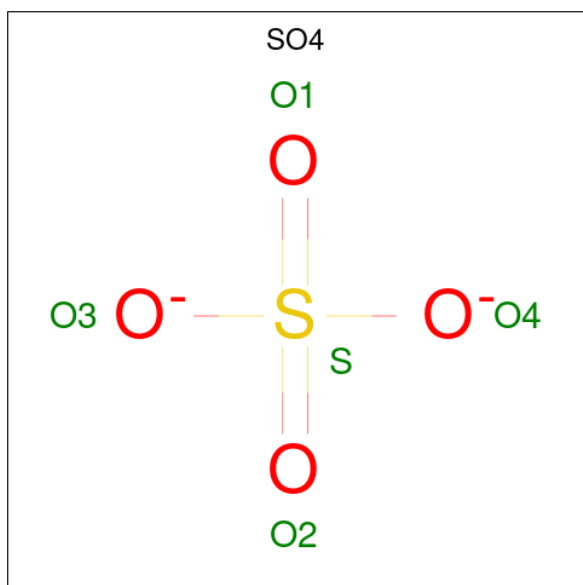
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q16881
B	-5	VAL	-	expression tag	UNP Q16881
B	-4	ASP	-	expression tag	UNP Q16881
B	-3	ASP	-	expression tag	UNP Q16881
B	-2	ASP	-	expression tag	UNP Q16881
B	-1	ASP	-	expression tag	UNP Q16881
B	498	CYS	U	SEE REMARK 999	UNP Q16881
C	-13	MET	-	expression tag	UNP Q16881
C	-12	ALA	-	expression tag	UNP Q16881
C	-11	HIS	-	expression tag	UNP Q16881
C	-10	HIS	-	expression tag	UNP Q16881
C	-9	HIS	-	expression tag	UNP Q16881
C	-8	HIS	-	expression tag	UNP Q16881
C	-7	HIS	-	expression tag	UNP Q16881
C	-6	HIS	-	expression tag	UNP Q16881
C	-5	VAL	-	expression tag	UNP Q16881
C	-4	ASP	-	expression tag	UNP Q16881
C	-3	ASP	-	expression tag	UNP Q16881
C	-2	ASP	-	expression tag	UNP Q16881
C	-1	ASP	-	expression tag	UNP Q16881
C	498	CYS	U	SEE REMARK 999	UNP Q16881
D	-13	MET	-	expression tag	UNP Q16881
D	-12	ALA	-	expression tag	UNP Q16881
D	-11	HIS	-	expression tag	UNP Q16881
D	-10	HIS	-	expression tag	UNP Q16881
D	-9	HIS	-	expression tag	UNP Q16881
D	-8	HIS	-	expression tag	UNP Q16881
D	-7	HIS	-	expression tag	UNP Q16881
D	-6	HIS	-	expression tag	UNP Q16881
D	-5	VAL	-	expression tag	UNP Q16881
D	-4	ASP	-	expression tag	UNP Q16881
D	-3	ASP	-	expression tag	UNP Q16881
D	-2	ASP	-	expression tag	UNP Q16881
D	-1	ASP	-	expression tag	UNP Q16881
D	498	CYS	U	SEE REMARK 999	UNP Q16881

- 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>).



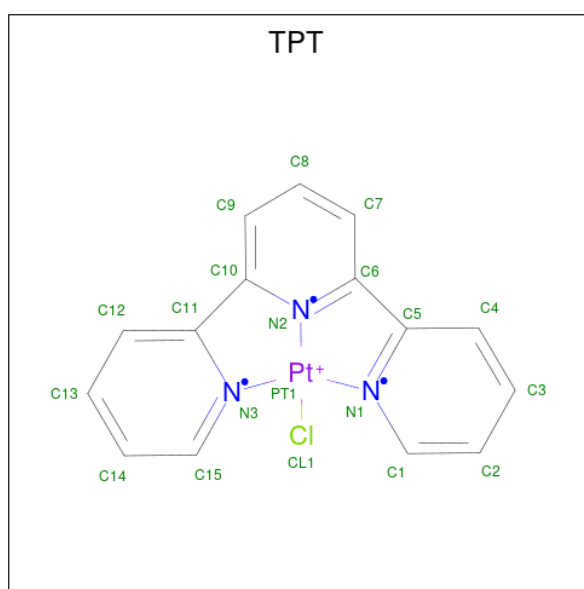
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
2	A	1	Total	53	27	9	15	2	0	0
2	B	1	Total	53	27	9	15	2	0	0
2	C	1	Total	53	27	9	15	2	0	0
2	D	1	Total	53	27	9	15	2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is 2,2':6',2''-TERPYRIDINE PLATINUM(II) Chloride (CCD ID: TPT) (formula:  $C_{15}H_{11}ClN_3Pt$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N Pt 19 15 3 1	0	0
4	D	1	Total C N Pt 19 15 3 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total O 19 19	0	0
5	B	17	Total O 17 17	0	0
5	C	13	Total O 13 13	0	0

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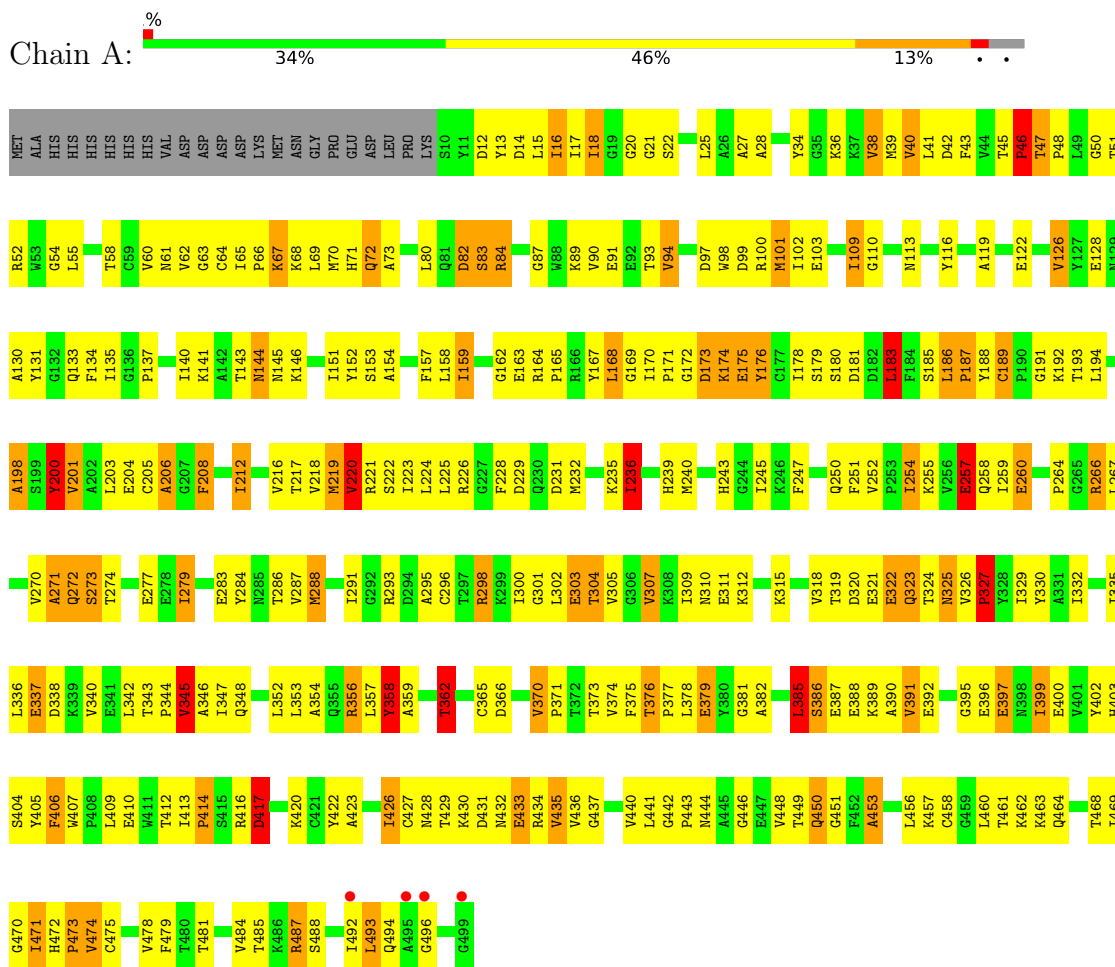
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	D	8	Total	O	0	0
			8	8		

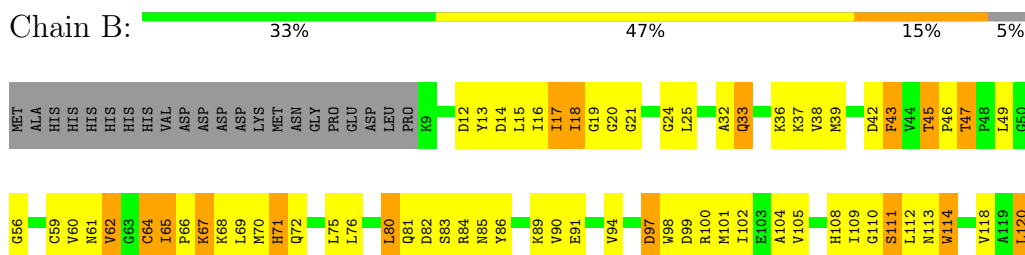
### 3 Residue-property plots

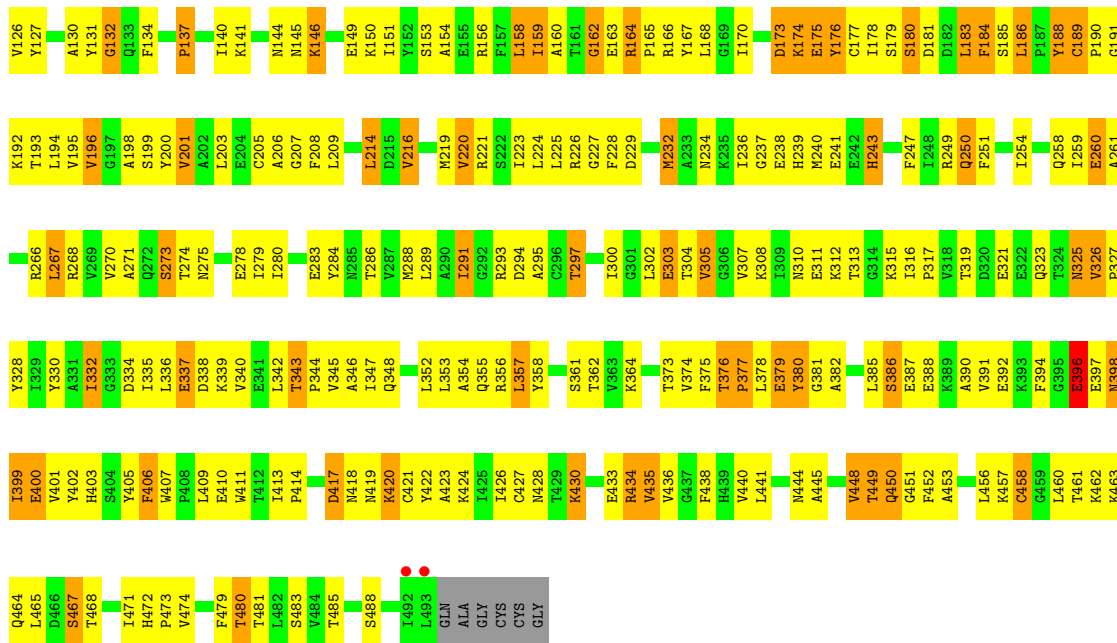
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Thioredoxin reductase 1, cytoplasmic

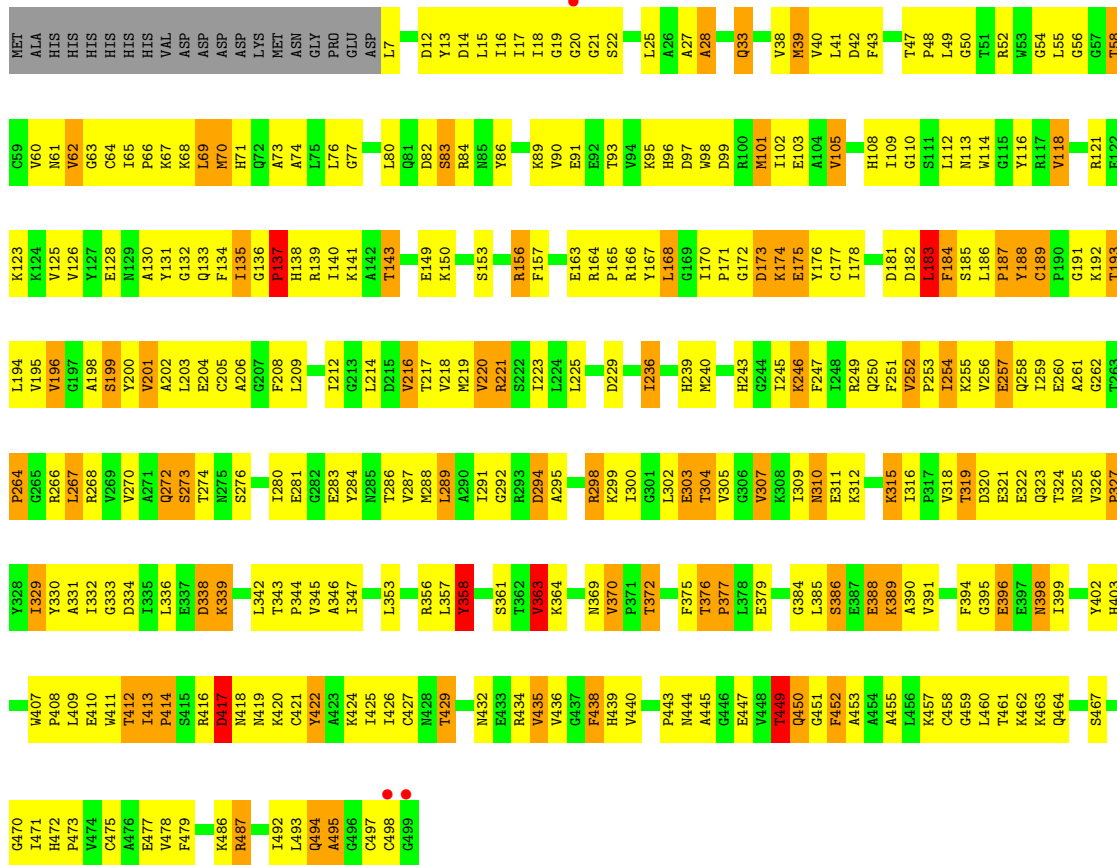


- Molecule 1: Thioredoxin reductase 1, cytoplasmic





● Molecule 1: Thioredoxin reductase 1, cytoplasmic



● Molecule 1: Thioredoxin reductase 1, cytoplasmic



MET	ALA	HIS	HIS	HIS	HIS	HIS	HIS	VAL	ASP	ASP	ASP	ASP	LYS	MET	ASN	GLY	PRO	GLU	ASP	LEU	PRO	PRO	LYS	S10	Y11	D12	Y13	D14	L15	I16	I17	I18	G19	G20	G21	S22	G23	G24	L25	A26	A27	A28	K29	A32	K36	K37	V38	M39	V40	L41	D42	F43	F46	T47	P48	L49	G50		
T51	R52	W53	G54	L55	G56	G57	F58	I59	C59	V60	N61	V62	G63	C64	A65	P66	K67	K68	L69	H70	H71	Q72	L76	G77	Q78	A79	L80	Q81	I84	R84	R85	R86	E91	E92	T93	Y94	R100	M101	Q106	N107	H108	I109	G110	S111	L112	N113	W114	R117	V118	K123	K124	V125	L126	Y127					
E128	N129	A130	Y131	G132	Q133	F134	I135	G136	P137	H138	R139	I140	K141	A142	T143	E204	N144	N145	K146	G147	K148	E149	K150	I151	Y152	S153	A154	E155	L156	F157	R158	I159	A160	T161	G162	E163	R164	P165	R166	Y167	G169	I170	P171	G172	D173	K174	E175	Y176	C177	I178	S179	S180	D181	D182	L183	F184	S185	L186	P187
Y188	C189	P190	G191	K192	T193	L194	V195	V196	G197	A198	L267	S199	V200	V201	A202	L203	E204	C205	A206	G207	F208	L209	I212	G213	L214	D215	V216	T217	V218	V219	V220	R221	S222	L223	E224	L225	F228	D229	Q230	D231	M232	A233	M234	K235	E238	H239	M240	L245	R117	L248	R249	Q250	F251	V252	P253	I254			
K255	V256	E257	Q258	L259	E260	A261	P264	G265	R266	L267	R268	V269	A270	A271	Q272	S273	T274	E277	E278	L279	I280	E283	Y284	M285	V286	V287	M288	D294	A295	C296	T297	R298	K299	I300	E303	T304	V305	G306	V307	K308	I309	N310	E323	H323	L316	F317	V318	T319	D320	E321	E322	Q323	T324	N325	V326				
P327	Y328	I329	Y330	A331	I332	G333	D334	I335	L336	V340	F341	L342	T343	P344	I347	Q348	L352	L353	A354	R355	Q356	L357	Y358	K364	Y367	E368	N369	V370	V374	F375	T376	P377	L378	G384	L385	S386	E387	A390	F394	G395	E396	E397	N398	V401	Y402	H403	S404	Y405	F406										
W407	P408	L409	E410	W411	T412	I413	D417	N418	N419	K420	C421	Y422	A423	K424	C427	N428	T429	K430	R434	F438	H439	V440	L441	G442	P443	N444	E447	V448	T449	Q450	G451	F452	A453	A454	A455	L456	K457	C458	G459	L460	T461	K462	K463	Q464	L465	D466	L469	G470	L471	H472	P473	V474	C475						
A476	E477	V478	F479	T480	T481	L482	S483	K486	R487	S488	G489	I492	L493	GLN	ALA	GLY	CYS	CYS	GLY	E447	V448	T449	Q450	G451	F452	A453	A454	A455	L456	K457	C458	G459	L460	T461	K462	K463	Q464	L465	D466	L469	G470	L471	H472	P473	V474	C475													

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.95Å 135.16Å 346.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.21	Depositor EDS
% Data completeness (in resolution range)	95.3 (30.00-3.20) 95.3 (30.00-3.21)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 3.18Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.242 , 0.305 0.210 , 0.263	Depositor DCC
$R_{free}$ test set	2246 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.2	Xtrriage
Anisotropy	0.286	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15394	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: TPT, SO4, 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	1.14	7/3850 (0.2%)	1.37	40/5211 (0.8%)
1	B	1.20	11/3824 (0.3%)	1.36	34/5177 (0.7%)
1	C	1.04	3/3875 (0.1%)	1.33	33/5245 (0.6%)
1	D	1.11	8/3815 (0.2%)	1.33	32/5166 (0.6%)
All	All	1.12	29/15364 (0.2%)	1.35	139/20799 (0.7%)

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	A	0	4
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	10

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	ILE	CA-CB	10.43	1.67	1.54
1	B	60	VAL	CA-CB	-7.51	1.45	1.54
1	D	300	ILE	CA-CB	7.34	1.62	1.54
1	A	189	CYS	CB-SG	7.08	2.04	1.81
1	D	196	VAL	CA-CB	-6.15	1.46	1.54

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	VAL	N-CA-C	9.25	121.06	108.11
1	C	452	PHE	N-CA-C	-9.09	102.58	114.31
1	B	183	LEU	N-CA-C	8.82	120.59	110.97
1	C	413	ILE	CB-CA-C	-8.67	102.64	114.00
1	C	453	ALA	N-CA-C	-8.54	101.91	111.14

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	TYR	Sidechain
1	A	176	TYR	Sidechain
1	A	200	TYR	Sidechain
1	A	406	PHE	Sidechain
1	B	43	PHE	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	3776	0	3779	352	0
1	B	3750	0	3763	340	0
1	C	3800	0	3809	372	2
1	D	3741	0	3750	355	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
2	C	53	0	31	3	0
2	D	53	0	31	4	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	19	0	11	0	0
4	D	19	0	11	3	0
5	A	19	0	0	0	0
5	B	17	0	0	0	0
5	C	13	0	0	1	0
5	D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15394	0	15247	1352	2

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 44.

The worst 5 of 1352 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:189:CYS:CB	1:A:189:CYS:SG	2.04	1.42
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.11	1.16
1:C:163:GLU:HG2	1:C:295:ALA:HA	1.29	1.14
1:C:498:CYS:HB3	4:D:501:TPT:H15	1.27	1.12
1:A:163:GLU:HG2	1:A:295:ALA:HA	1.33	1.11

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:CYS:O	1:C:497:CYS:O[3_554]	1.59	0.61
1:C:498:CYS:SG	1:C:498:CYS:SG[3_554]	1.70	0.50

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	488/513 (95%)	418 (86%)	57 (12%)	13 (3%)	4	25
1	B	483/513 (94%)	409 (85%)	64 (13%)	10 (2%)	5	31
1	C	491/513 (96%)	404 (82%)	67 (14%)	20 (4%)	2	17
1	D	482/513 (94%)	407 (84%)	63 (13%)	12 (2%)	4	27
All	All	1944/2052 (95%)	1638 (84%)	251 (13%)	55 (3%)	4	25

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	A	174	LYS
1	A	379	GLU
1	B	184	PHE
1	C	173	ASP

### 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	401/422 (95%)	332 (83%)	69 (17%)	2 10
1	B	399/422 (94%)	340 (85%)	59 (15%)	3 15
1	C	404/422 (96%)	339 (84%)	65 (16%)	2 13
1	D	398/422 (94%)	340 (85%)	58 (15%)	3 16
All	All	1602/1688 (95%)	1351 (84%)	251 (16%)	2 13

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	396	GLU
1	D	254	ILE
1	C	101	MET
1	D	216	VAL
1	D	340	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	428	ASN
1	D	234	ASN
1	C	129	ASN
1	D	133	GLN
1	D	323	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	TPT	B	501	-	19,23,24	0.92	0	15,35,38	1.98	4 (26%)
2	FAD	A	500	-	58,58,58	1.39	8 (13%)	85,89,89	1.58	17 (20%)
4	TPT	D	501	-	19,23,24	0.94	0	15,35,38	1.95	4 (26%)
2	FAD	B	500	-	58,58,58	1.58	8 (13%)	85,89,89	1.61	15 (17%)
3	SO4	D	502	-	4,4,4	0.38	0	6,6,6	0.34	0
3	SO4	B	502	-	4,4,4	0.41	0	6,6,6	0.20	0
3	SO4	C	502	-	4,4,4	0.42	0	6,6,6	0.14	0
2	FAD	C	500	-	58,58,58	1.75	8 (13%)	85,89,89	1.64	17 (20%)
3	SO4	A	502	-	4,4,4	0.45	0	6,6,6	0.26	0
2	FAD	D	500	-	58,58,58	1.74	9 (15%)	85,89,89	1.57	16 (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
4	TPT	B	501	-	-	-	0/5/5/5
2	FAD	A	500	-	-	2/34/50/50	0/6/6/6
4	TPT	D	501	-	-	-	0/5/5/5
2	FAD	B	500	-	-	2/34/50/50	0/6/6/6
2	FAD	C	500	-	-	2/34/50/50	0/6/6/6
2	FAD	D	500	-	-	3/34/50/50	0/6/6/6

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	FAD	P-O3P	7.54	1.67	1.59
2	C	500	FAD	P-O3P	7.45	1.67	1.59
2	B	500	FAD	P-O3P	6.19	1.66	1.59
2	C	500	FAD	PA-O3P	5.44	1.65	1.59
2	A	500	FAD	PA-O3P	4.55	1.64	1.59

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FAD	N3A-C2A-N1A	-5.31	120.54	128.58
2	A	500	FAD	N3A-C2A-N1A	-5.23	120.67	128.58
2	B	500	FAD	N3A-C2A-N1A	-5.01	121.00	128.58
2	D	500	FAD	N3A-C2A-N1A	-4.82	121.29	128.58
2	C	500	FAD	C5A-C4A-N3A	-4.75	120.17	126.72

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	FAD	O4B-C4B-C5B-O5B
2	A	500	FAD	C3B-C4B-C5B-O5B
2	B	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	C3B-C4B-C5B-O5B
2	C	500	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 14 short contacts:

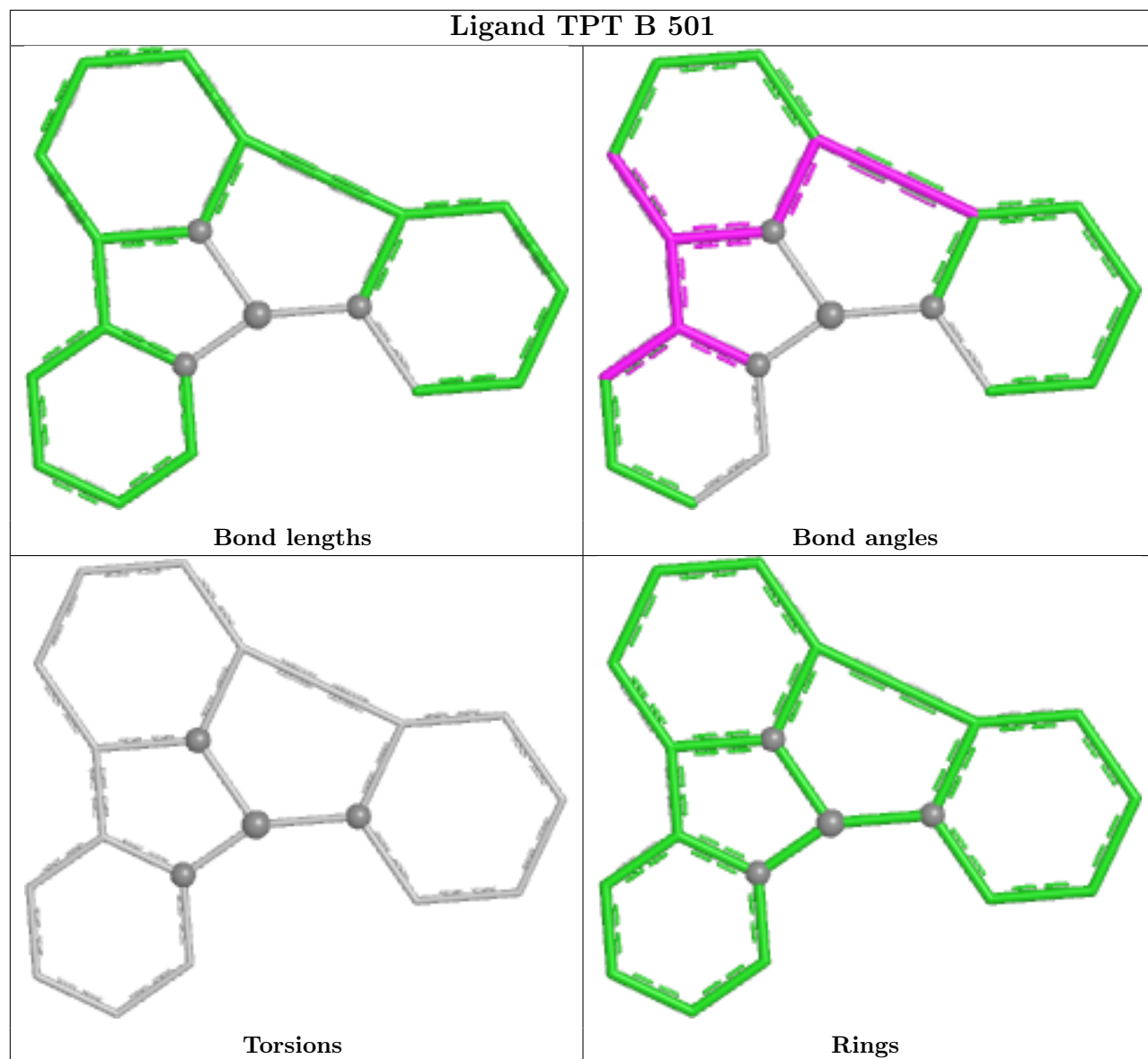
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FAD	1	0
4	D	501	TPT	3	0

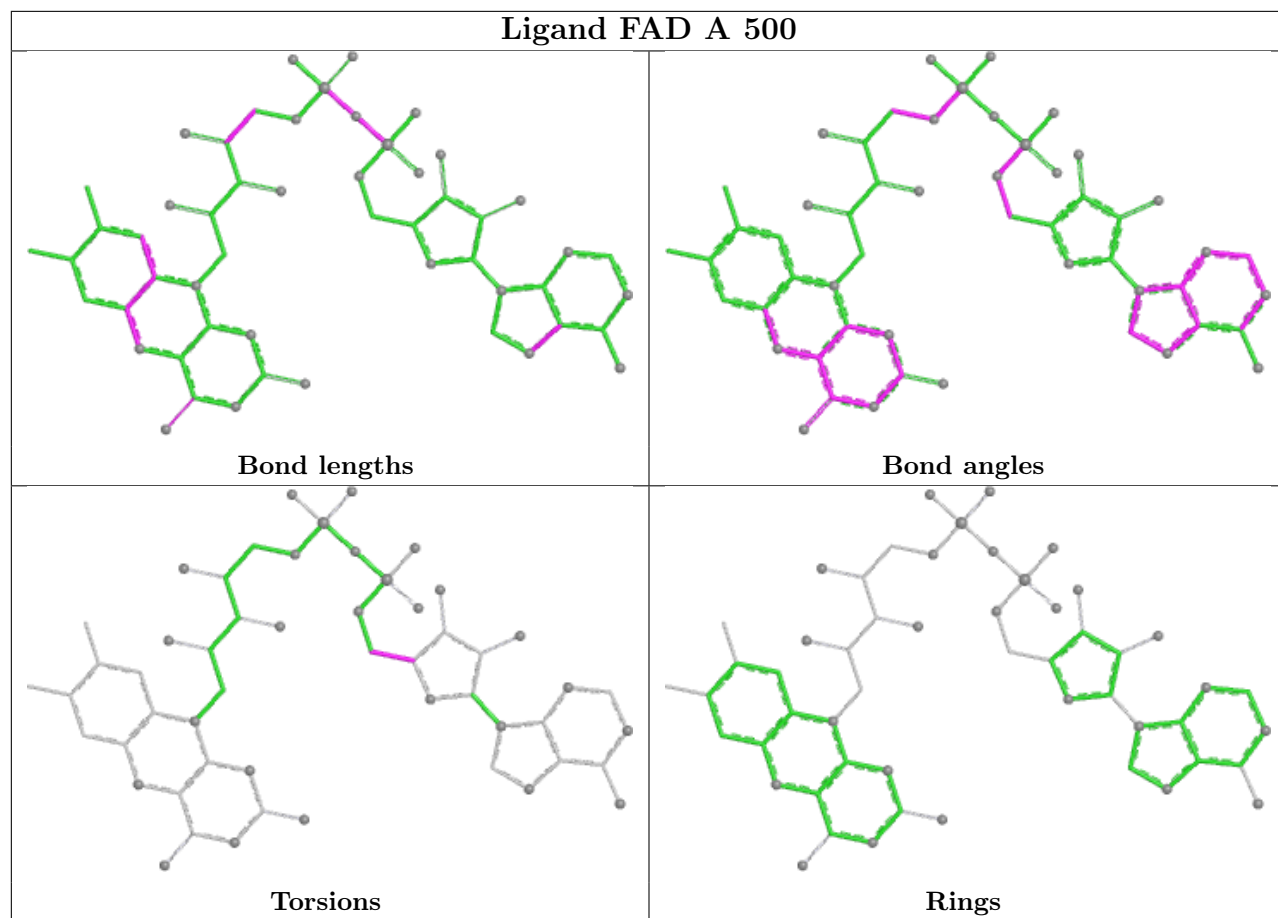
*Continued on next page...*

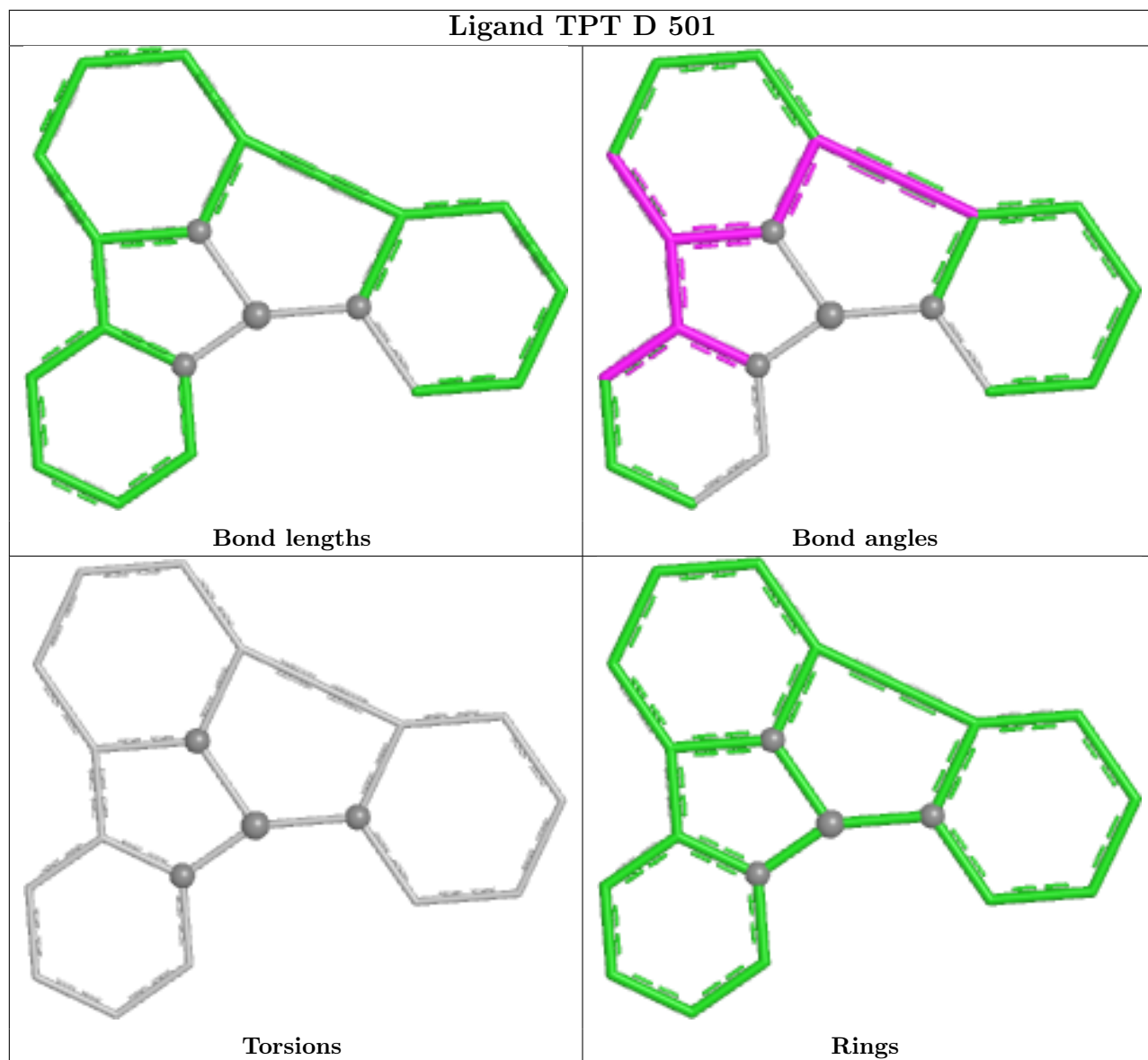
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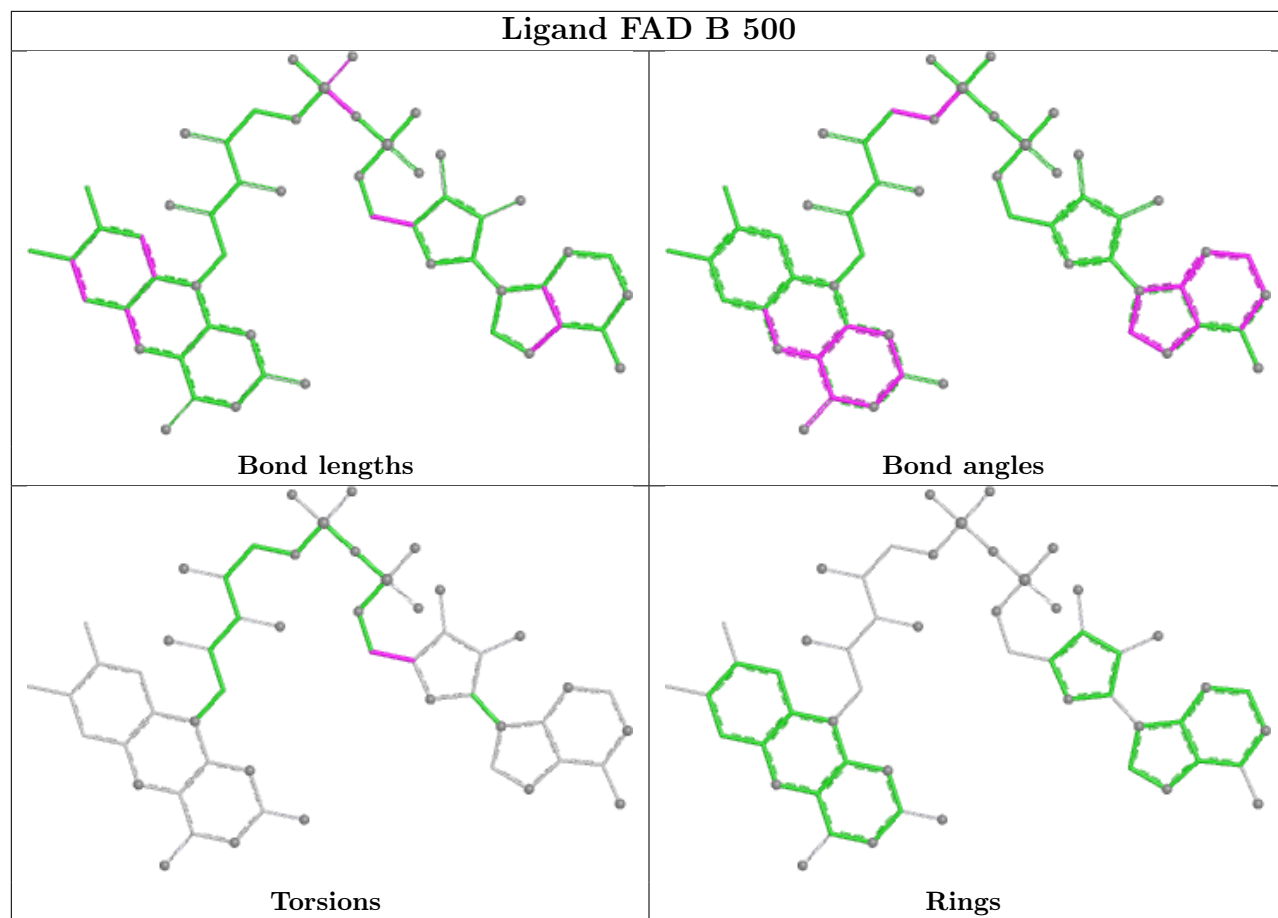
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	FAD	2	0
2	C	500	FAD	3	0
3	A	502	SO4	1	0
2	D	500	FAD	4	0

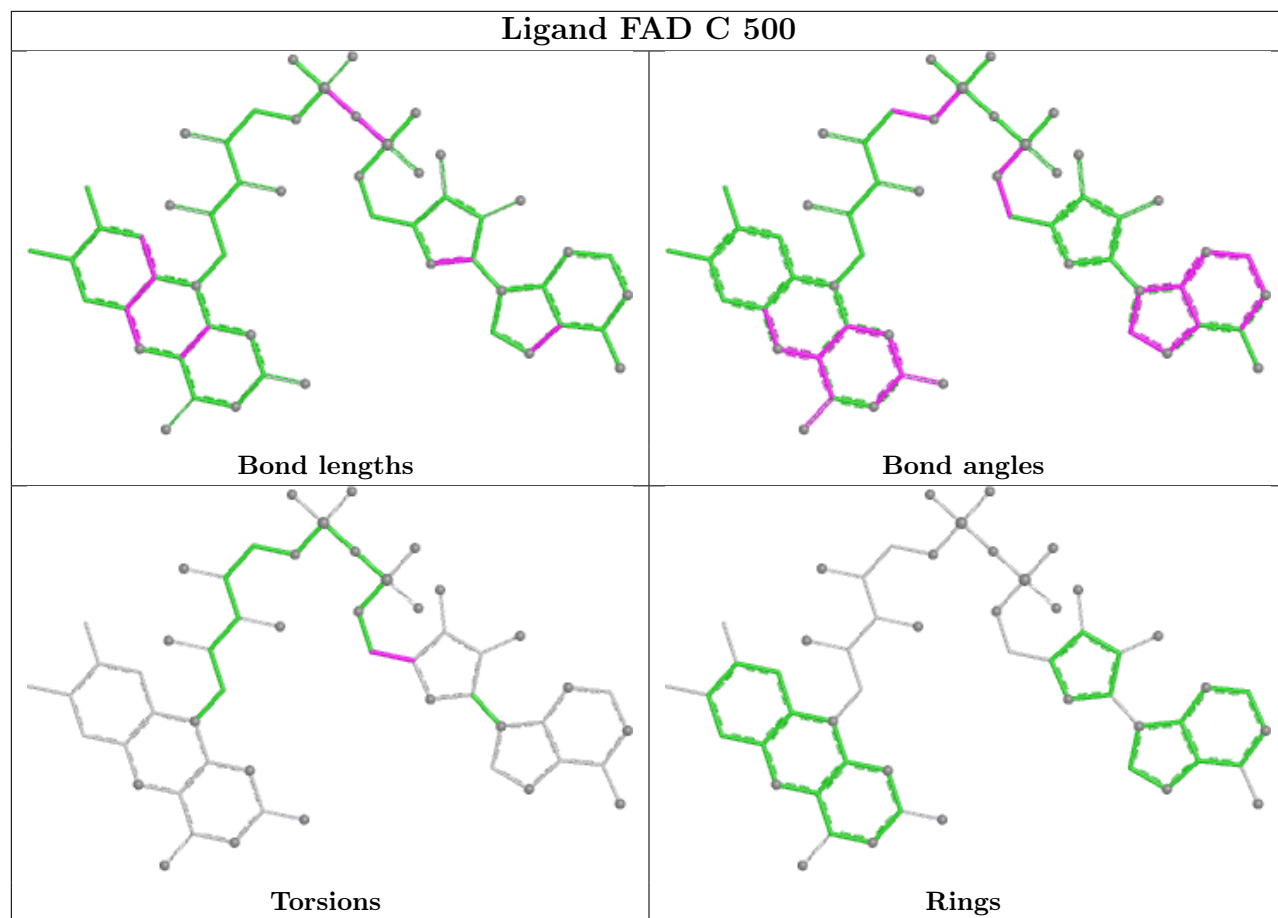
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

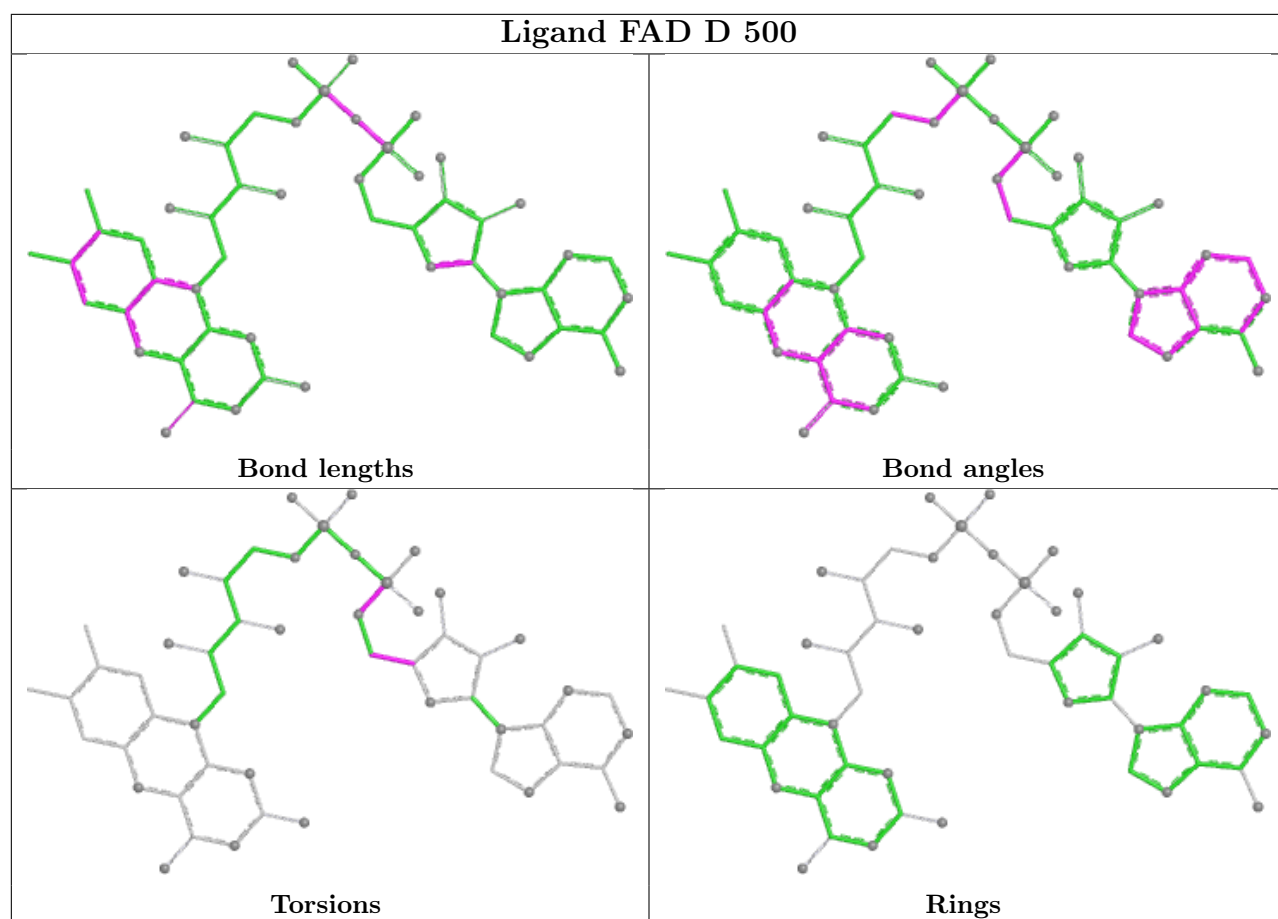












## 5.7 Other polymers [i](#)

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	490/513 (95%)	-0.45	4 (0%) 82 67	15, 50, 81, 128	0
1	B	485/513 (94%)	-0.49	2 (0%) 88 79	18, 45, 76, 107	0
1	C	493/513 (96%)	-0.28	3 (0%) 85 73	21, 58, 85, 137	0
1	D	484/513 (94%)	-0.36	3 (0%) 85 73	23, 53, 83, 104	0
All	All	1952/2052 (95%)	-0.39	12 (0%) 85 73	15, 51, 83, 137	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	499	GLY	5.7
1	B	493	LEU	3.8
1	D	493	LEU	3.4
1	C	498	CYS	2.6
1	C	20	GLY	2.5

### 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](#)

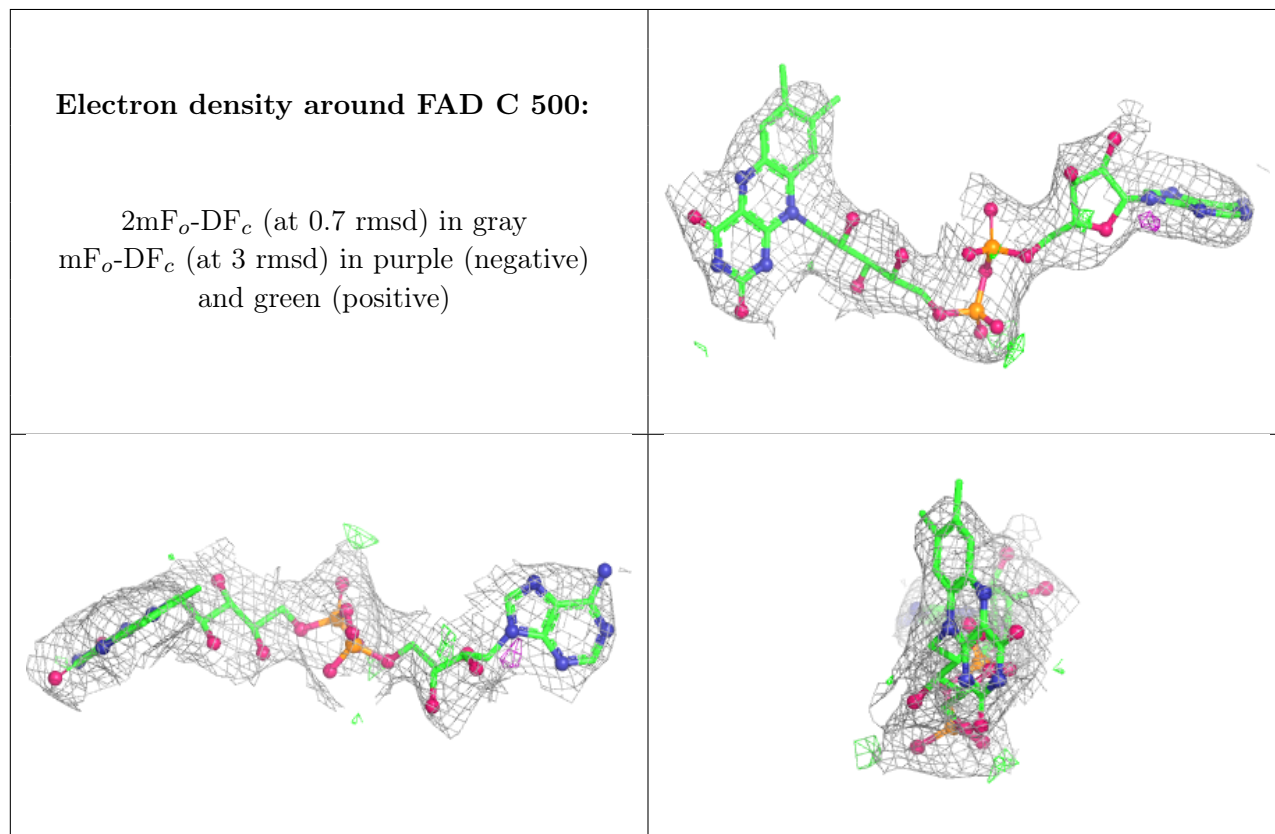
There are no oligosaccharides in this entry.

### 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.

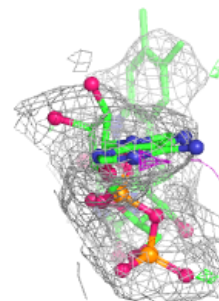
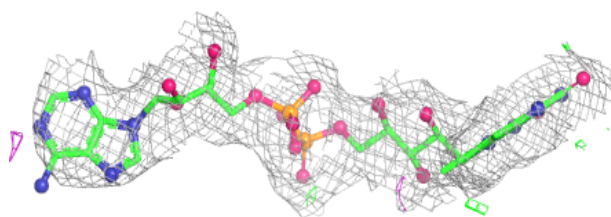
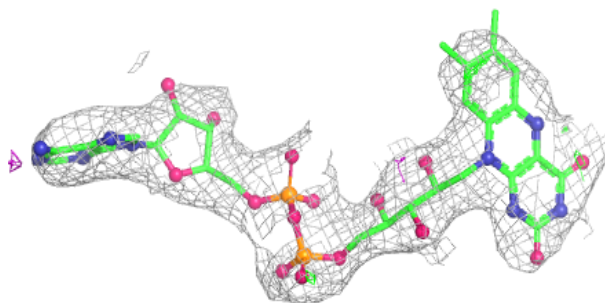
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	502	5/5	0.84	0.10	71,73,74,75	0
3	SO4	B	502	5/5	0.86	0.07	81,81,82,82	0
3	SO4	A	502	5/5	0.89	0.07	72,73,75,75	0
3	SO4	C	502	5/5	0.90	0.07	83,83,83,83	0
2	FAD	C	500	53/53	0.93	0.10	43,58,61,62	0
2	FAD	A	500	53/53	0.94	0.09	42,56,69,70	0
4	TPT	B	501	19/20	0.94	0.19	29,36,38,39	19
4	TPT	D	501	19/20	0.94	0.19	42,46,48,48	19
2	FAD	D	500	53/53	0.95	0.08	33,41,57,58	0
2	FAD	B	500	53/53	0.96	0.07	24,32,44,45	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.

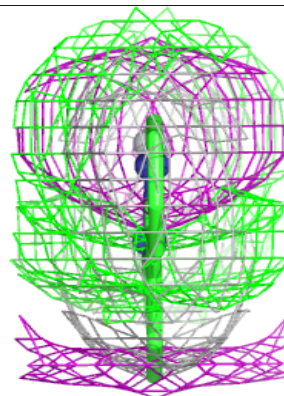
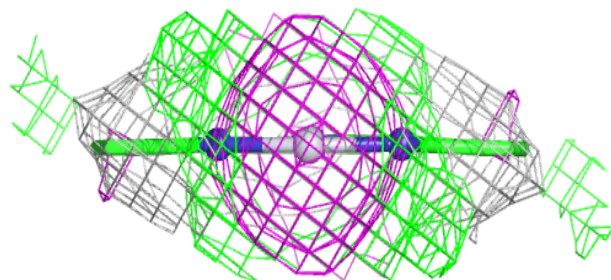
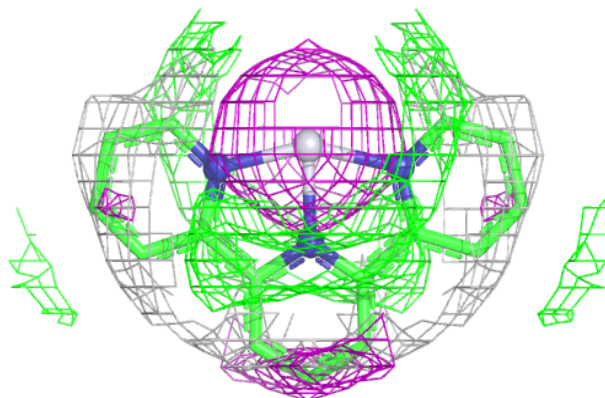


**Electron density around FAD A 500:**

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

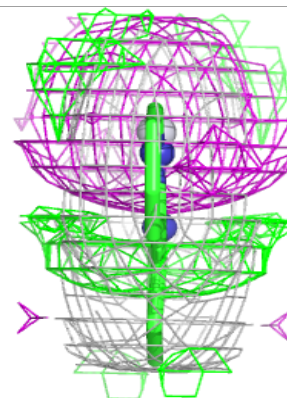
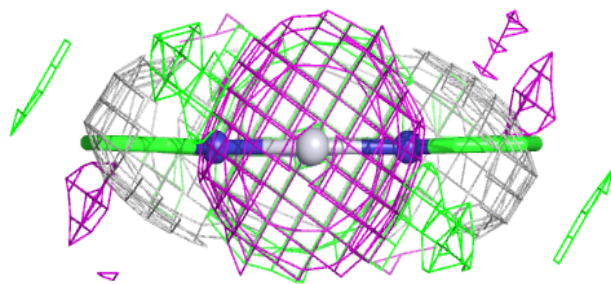
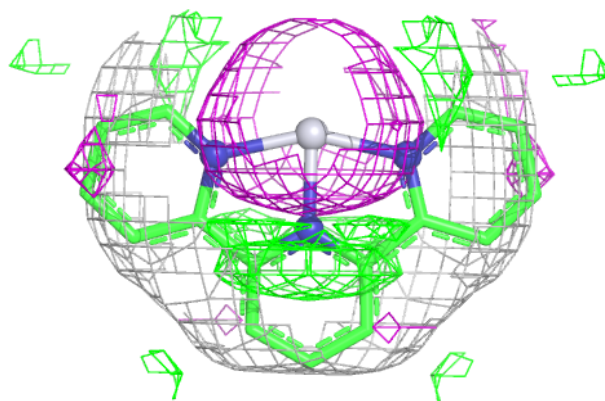
**Electron density around TPT B 501:**

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

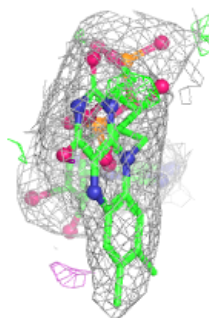
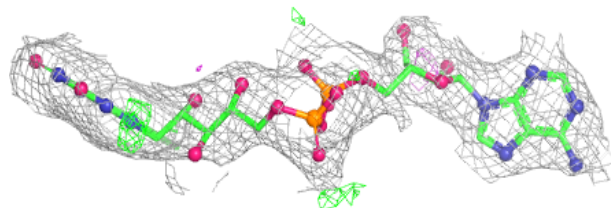
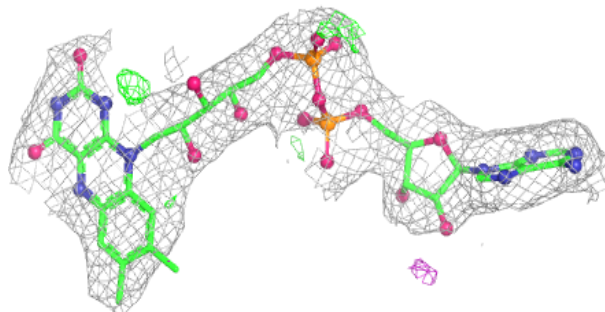


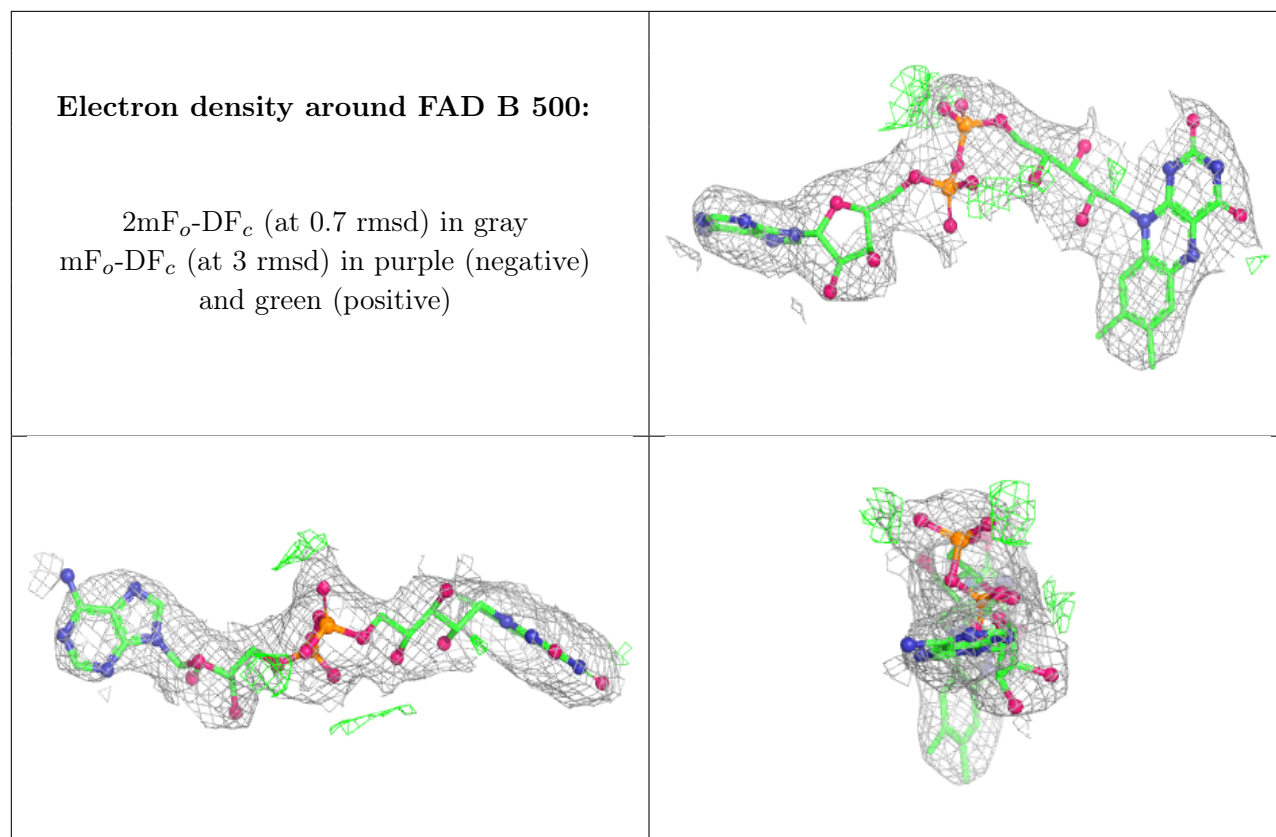
**Electron density around TPT D 501:**

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

**Electron density around FAD D 500:**

$2mF_o-DF_c$  (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.