



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:43 pm BST

PDB ID : 4NEV
Title : Crystal structure of Trypanothione Reductase from Trypanosoma brucei in complex with inhibitor EP127 (5-{5-[1-(PYRROLIDIN-1-YL)CYCLOHEXYL]-1,3-THIAZOL-2-YL}-1H-INDOLE)
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Deposited on : 2013-10-30
Resolution : 2.50 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

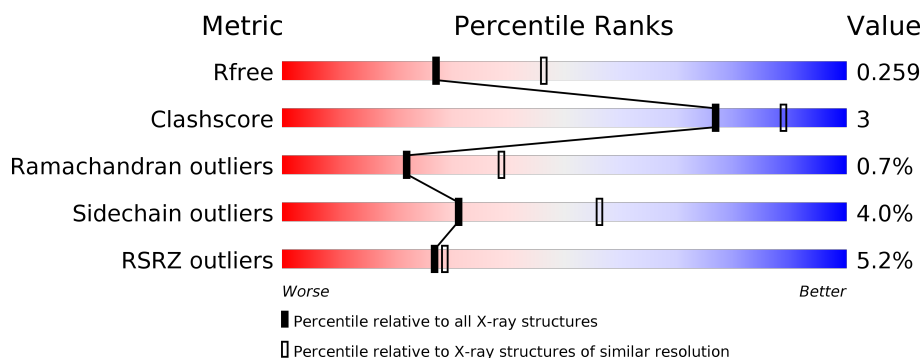
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	495	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	495	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>•</div> </div> </div>

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7667 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.

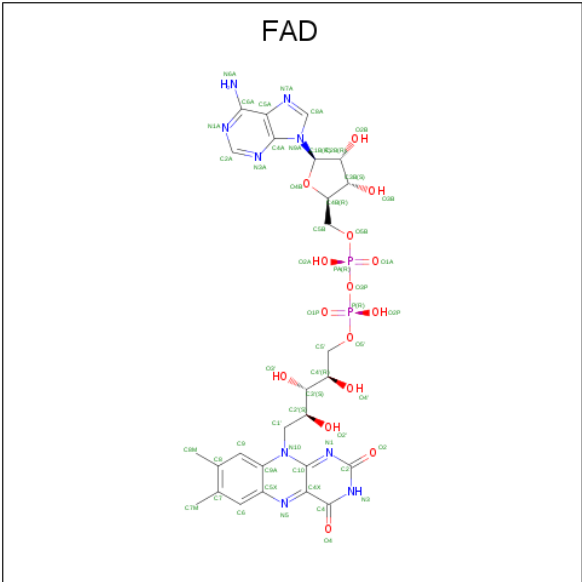
- Molecule 1 is a protein called Trypanothione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3683	2344	625	695	19			
1	B	485	Total	C	N	O	S	0	0	0
			3685	2345	626	695	19			

There are 6 discrepancies between the modelled and reference sequences:

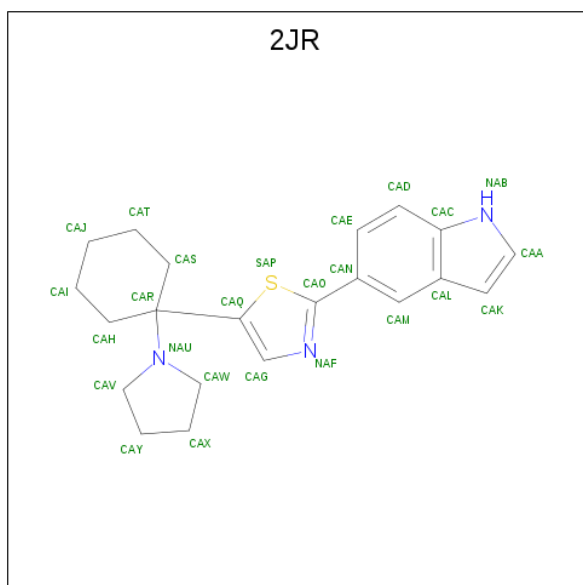
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q389T8
A	-1	SER	-	EXPRESSION TAG	UNP Q389T8
A	0	HIS	-	EXPRESSION TAG	UNP Q389T8
B	-2	GLY	-	EXPRESSION TAG	UNP Q389T8
B	-1	SER	-	EXPRESSION TAG	UNP Q389T8
B	0	HIS	-	EXPRESSION TAG	UNP Q389T8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 3 is 5-{5-[1-(pyrrolidin-1-yl)cyclohexyl]-1,3-thiazol-2-yl}-1H-indole (three-letter code: 2JR) (formula: C₂₁H₂₅N₃S).



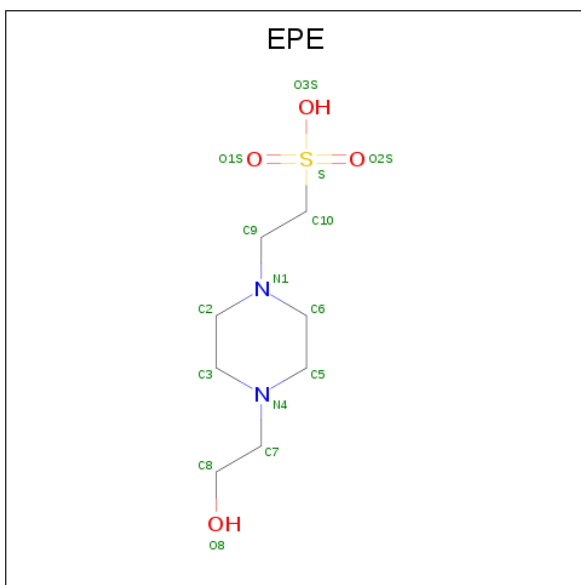
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			25	21	3	1		
3	B	1	Total	C	N	S	0	0
			25	21	3	1		
3	B	1	Total	C	N	S	0	0
			25	21	3	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

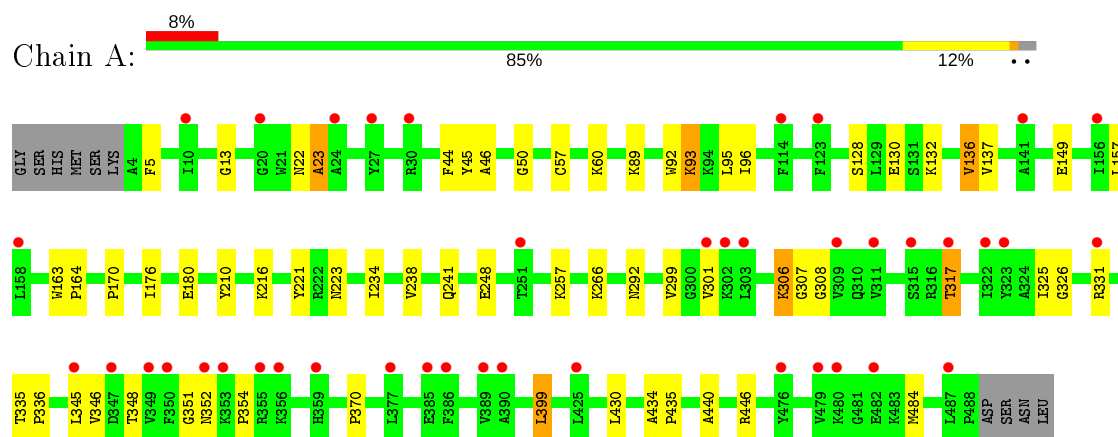
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	28	Total O 28 28	0	0
6	B	35	Total O 35 35	0	0

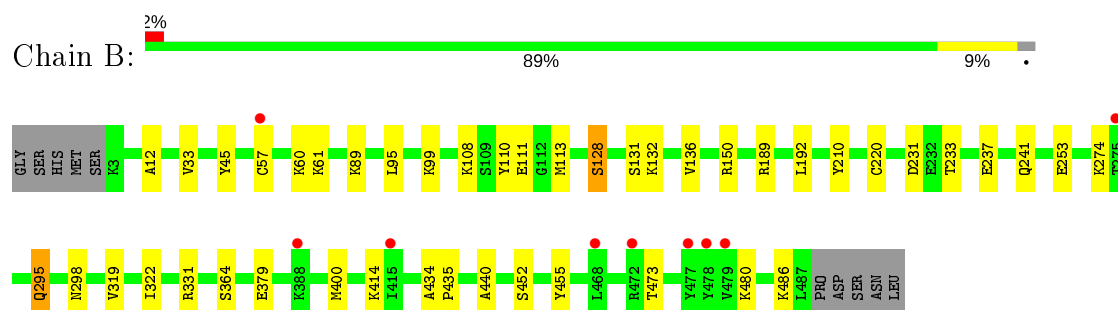
3 Residue-property plots [i](#)

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

• Molecule 1: Trypanothione reductase



• Molecule 1: Trypanothione reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.20 Å 117.20 Å 224.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.00 – 2.50 66.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.00-2.50) 99.9 (66.68-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.234 , 0.258 0.230 , 0.259	Depositor DCC
R_{free} test set	2779 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7667	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 2JR, FAD, SO4

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	0.25	0/3761	0.43	0/5104
1	B	0.25	0/3762	0.42	0/5103
All	All	0.25	0/7523	0.42	0/10207

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3683	0	3690	27	0
1	B	3685	0	3696	18	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	25	0	25	0	0
3	B	50	0	50	2	0
4	A	15	0	0	0	0
4	B	25	0	0	1	0
5	B	15	0	18	0	0
6	A	28	0	0	0	0
6	B	35	0	0	1	0
All	All	7667	0	7541	46	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 3.

All (46) 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:348:THR:HG22	1:A:354:PRO:HA	1.69	0.74
1:A:130:GLU:HB2	1:A:136:VAL:HG22	1.69	0.73
1:A:22:ASN:O	1:A:346:VAL:HG11	1.93	0.68
1:B:192:LEU:HD11	1:B:220:CYS:SG	2.34	0.67
1:B:253:GLU:OE2	1:B:274:LYS:HE2	1.98	0.63
1:A:370:PRO:HG2	1:A:430:LEU:HD11	1.84	0.58
1:A:306:LYS:O	1:A:308:GLY:N	2.34	0.56
1:B:128:SER:HB2	6:B:608:HOH:O	2.07	0.53
1:A:299:VAL:O	1:A:299:VAL:HG12	2.09	0.52
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.44	0.52
1:B:452:SER:HA	1:B:455:TYR:CZ	2.46	0.51
1:A:301:VAL:HG13	1:A:317:THR:HG21	1.92	0.51
1:A:93:LYS:HD2	1:A:93:LYS:H	1.77	0.49
1:A:176:ILE:HB	1:A:180:GLU:HB2	1.94	0.49
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.94	0.48
3:B:509:2JR:H19	3:B:509:2JR:H10	1.37	0.47
1:A:170:PRO:HG2	1:A:257:LYS:HB3	1.97	0.46
1:A:241:GLN:OE1	1:A:370:PRO:HG3	2.16	0.46
1:B:237:GLU:O	1:B:241:GLN:HG3	2.15	0.46
1:B:189:ARG:NH2	4:B:504:SO4:O2	2.49	0.45
1:B:319:VAL:HG11	1:B:322:ILE:HD12	1.98	0.45
1:A:13:GLY:HA2	1:A:50:GLY:CA	2.46	0.45
1:A:137:VAL:HB	1:A:149:GLU:HB2	1.99	0.44
1:B:136:VAL:HG12	1:B:150:ARG:HG2	1.99	0.44
1:B:95:LEU:HD22	1:B:210:TYR:CZ	2.53	0.44
1:A:345:LEU:O	1:A:348:THR:OG1	2.34	0.44
1:A:163:TRP:CG	1:A:164:PRO:HD2	2.53	0.44
1:A:234:ILE:O	1:A:238:VAL:HG12	2.18	0.44
1:A:22:ASN:O	1:A:23:ALA:HB2	2.18	0.44
1:A:95:LEU:HD22	1:A:210:TYR:CZ	2.53	0.44
1:A:157:LEU:HD11	1:A:325:ILE:HG12	2.00	0.43
1:B:295:GLN:HG2	1:B:298:ASN:ND2	2.34	0.43
1:A:434:ALA:HB3	1:A:435:PRO:HD3	2.00	0.43
1:A:266:LYS:HD2	1:A:266:LYS:N	2.34	0.43
1:B:110:TYR:O	1:B:113:MET:HB3	2.18	0.42
1:B:12:ALA:HB2	1:B:33:VAL:HG12	2.02	0.42
1:B:108:LYS:O	1:B:111:GLU:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TRP:CZ2	1:A:96:ILE:HD11	2.55	0.41
1:B:379:GLU:OE1	1:B:414:LYS:NZ	2.53	0.41
3:B:502:2JR:H20	3:B:502:2JR:H9	1.98	0.41
1:A:326:GLY:HA3	2:A:501:FAD:O2P	2.20	0.41
1:A:335:THR:HB	1:A:336:PRO:HD3	2.03	0.40
1:B:253:GLU:OE2	1:B:274:LYS:CE	2.67	0.40
1:A:44:PHE:O	1:A:46:ALA:N	2.54	0.40
1:B:231:ASP:OD2	1:B:233:THR:OG1	2.29	0.40
1:B:434:ALA:HB3	1:B:435:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	483/495 (98%)	451 (93%)	26 (5%)	6 (1%)	13	24
1	B	483/495 (98%)	465 (96%)	17 (4%)	1 (0%)	47	68
All	All	966/990 (98%)	916 (95%)	43 (4%)	7 (1%)	22	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	LEU
1	A	5	PHE
1	A	23	ALA
1	A	45	TYR
1	B	45	TYR
1	A	307	GLY
1	A	351	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/407 (98%)	381 (96%)	17 (4%)	29	53
1	B	398/407 (98%)	383 (96%)	15 (4%)	33	58
All	All	796/814 (98%)	764 (96%)	32 (4%)	31	56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	CYS
1	A	60	LYS
1	A	89	LYS
1	A	93	LYS
1	A	128	SER
1	A	132	LYS
1	A	136	VAL
1	A	216	LYS
1	A	248	GLU
1	A	292	ASN
1	A	306	LYS
1	A	317	THR
1	A	331	ARG
1	A	352	ASN
1	A	399	LEU
1	A	446	ARG
1	A	484	MET
1	B	57	CYS
1	B	60	LYS
1	B	61	LYS
1	B	89	LYS
1	B	99	LYS
1	B	128	SER
1	B	131	SER
1	B	132	LYS
1	B	295	GLN
1	B	331	ARG

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Mol	Chain	Res	Type
1	B	364	SER
1	B	400	MET
1	B	473	THR
1	B	480	LYS
1	B	486	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	B	456	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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	SO4	B	503	-	4,4,4	0.36	0	6,6,6	0.05	0
4	SO4	B	504	-	4,4,4	0.34	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	504	-	4,4,4	0.34	0	6,6,6	0.06	0
3	2JR	A	502	-	24,29,29	2.46	4 (16%)	23,42,42	1.54	5 (21%)
3	2JR	B	509	-	24,29,29	2.26	5 (20%)	23,42,42	1.91	5 (21%)
5	EPE	B	508	-	15,15,15	1.86	1 (6%)	18,20,20	2.83	9 (50%)
4	SO4	B	505	-	4,4,4	0.35	0	6,6,6	0.06	0
4	SO4	A	505	-	4,4,4	0.32	0	6,6,6	0.08	0
2	FAD	A	501	-	51,58,58	1.88	6 (11%)	60,89,89	2.03	11 (18%)
2	FAD	B	501	-	51,58,58	1.87	6 (11%)	60,89,89	2.03	11 (18%)
4	SO4	B	506	-	4,4,4	0.33	0	6,6,6	0.05	0
3	2JR	B	502	-	24,29,29	2.59	7 (29%)	23,42,42	2.04	7 (30%)
4	SO4	B	507	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	A	503	-	4,4,4	0.33	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2JR	A	502	-	-	1/10/33/33	0/5/5/5
3	2JR	B	509	-	-	6/10/33/33	0/5/5/5
5	EPE	B	508	-	-	7/9/19/19	0/1/1/1
2	FAD	A	501	-	-	5/30/50/50	0/6/6/6
2	FAD	B	501	-	-	3/30/50/50	0/6/6/6
3	2JR	B	502	-	-	0/10/33/33	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C4X-C10	9.52	1.48	1.38
2	A	501	FAD	C4X-C10	9.41	1.48	1.38
3	A	502	2JR	CAO-SAP	-7.98	1.62	1.73
3	B	502	2JR	CAO-SAP	-7.06	1.63	1.73
5	B	508	EPE	C10-S	-6.86	1.67	1.77
3	B	509	2JR	CAQ-SAP	-5.68	1.63	1.74
3	B	502	2JR	CAQ-SAP	-5.48	1.63	1.74
3	B	509	2JR	CAO-SAP	-5.32	1.66	1.73
3	A	502	2JR	CAQ-SAP	-4.98	1.64	1.74
3	B	509	2JR	CAD-CAC	-4.74	1.33	1.41
3	B	502	2JR	CAD-CAC	-4.68	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	2JR	CAS-CAR	4.64	1.58	1.54
3	A	502	2JR	CAD-CAC	-4.54	1.34	1.41
2	A	501	FAD	C4-C4X	4.53	1.49	1.41
2	B	501	FAD	C4-C4X	4.45	1.49	1.41
2	A	501	FAD	C9A-C5X	3.75	1.50	1.42
3	A	502	2JR	CAM-CAL	-3.59	1.33	1.42
2	B	501	FAD	C9A-C5X	3.56	1.49	1.42
3	B	509	2JR	CAM-CAL	-3.54	1.34	1.42
3	B	502	2JR	CAM-CAL	-3.45	1.34	1.42
2	B	501	FAD	C8-C7	3.26	1.49	1.40
2	A	501	FAD	C8-C7	3.23	1.49	1.40
3	B	509	2JR	CAH-CAR	-2.73	1.51	1.54
2	A	501	FAD	C9A-N10	2.55	1.42	1.38
2	A	501	FAD	C5A-C4A	2.46	1.47	1.40
2	B	501	FAD	C9A-N10	2.34	1.41	1.38
3	B	502	2JR	CAH-CAR	2.28	1.56	1.54
2	B	501	FAD	C5A-C4A	2.22	1.46	1.40
3	B	502	2JR	CAH-CAI	-2.03	1.47	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C4-N3-C2	8.17	122.04	115.14
2	B	501	FAD	C4-N3-C2	8.16	122.03	115.14
2	B	501	FAD	C4-C4X-C10	-6.20	115.85	119.95
2	A	501	FAD	C4-C4X-C10	-6.01	115.97	119.95
2	B	501	FAD	C1'-N10-C9A	5.46	122.59	118.29
2	A	501	FAD	C1'-N10-C9A	5.35	122.51	118.29
5	B	508	EPE	C5-N4-C3	5.25	120.65	108.83
3	B	502	2JR	CAY-CAV-NAU	-5.06	96.61	103.95
3	B	509	2JR	CAI-CAH-CAR	-5.02	104.66	113.15
5	B	508	EPE	C6-N1-C2	4.94	119.95	108.83
2	A	501	FAD	C4X-N5-C5X	4.57	121.34	116.77
3	B	509	2JR	CAW-NAU-CAV	-4.26	97.95	106.37
2	B	501	FAD	C4X-N5-C5X	4.25	121.02	116.77
5	B	508	EPE	C7-N4-C3	4.24	122.09	111.23
2	A	501	FAD	C4-C4X-N5	4.19	123.39	118.60
5	B	508	EPE	O3S-S-C10	4.07	112.35	105.77
2	B	501	FAD	C4-C4X-N5	4.06	123.24	118.60
5	B	508	EPE	C9-N1-C6	3.95	121.33	111.23
2	B	501	FAD	N3A-C2A-N1A	-3.80	122.73	128.68
3	B	509	2JR	CAY-CAV-NAU	-3.78	98.46	103.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	N3A-C2A-N1A	-3.74	122.84	128.68
3	A	502	2JR	CAG-CAQ-SAP	-3.47	108.55	112.00
2	B	501	FAD	C4X-C4-N3	-3.32	118.89	123.43
3	B	502	2JR	CAS-CAR-CAH	3.31	113.84	108.44
3	B	502	2JR	CAG-CAQ-SAP	-3.29	108.73	112.00
2	A	501	FAD	C4X-C4-N3	-3.25	118.98	123.43
5	B	508	EPE	C2-C3-N4	-2.98	104.53	110.64
5	B	508	EPE	C3-C2-N1	-2.97	104.54	110.64
3	A	502	2JR	CAS-CAT-CAJ	-2.96	106.79	111.37
3	B	502	2JR	CAT-CAS-CAR	2.95	118.14	113.15
5	B	508	EPE	C9-N1-C2	2.93	118.72	111.23
3	A	502	2JR	CAY-CAV-NAU	2.87	108.11	103.95
2	A	501	FAD	C4A-C5A-N7A	-2.80	106.48	109.40
2	B	501	FAD	C4A-C5A-N7A	-2.71	106.58	109.40
3	B	502	2JR	CAH-CAI-CAJ	-2.67	107.24	111.37
3	B	502	2JR	CAW-NAU-CAV	-2.65	101.15	106.37
2	B	501	FAD	P-O3P-PA	-2.59	123.95	132.83
2	A	501	FAD	P-O3P-PA	-2.43	124.50	132.83
5	B	508	EPE	C7-N4-C5	2.36	117.26	111.23
3	A	502	2JR	CAW-NAU-CAV	-2.29	101.85	106.37
3	B	509	2JR	CAH-CAI-CAJ	-2.27	107.86	111.37
2	A	501	FAD	C9A-N10-C10	-2.26	118.94	121.91
2	B	501	FAD	C9A-N10-C10	-2.21	119.01	121.91
3	B	502	2JR	CAX-CAW-NAU	-2.20	100.76	103.95
3	A	502	2JR	CAK-CAL-CAC	2.13	108.02	106.20
2	A	501	FAD	C2A-N1A-C6A	2.11	122.36	118.75
3	B	509	2JR	CAX-CAY-CAV	-2.10	99.26	105.19
2	B	501	FAD	C1B-N9A-C4A	-2.03	123.07	126.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	2JR	CAQ-CAR-NAU-CAW
3	B	509	2JR	CAH-CAR-NAU-CAW
3	B	509	2JR	CAS-CAR-NAU-CAV
3	B	509	2JR	CAS-CAR-NAU-CAW
3	B	509	2JR	CAQ-CAR-NAU-CAV
3	B	509	2JR	CAQ-CAR-NAU-CAW
5	B	508	EPE	C8-C7-N4-C3
5	B	508	EPE	C9-C10-S-O1S
5	B	508	EPE	C9-C10-S-O2S

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Mol	Chain	Res	Type	Atoms
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C3B-C4B-C5B-O5B
5	B	508	EPE	N4-C7-C8-O8
5	B	508	EPE	C9-C10-S-O3S
2	A	501	FAD	P-O3P-PA-O1A
5	B	508	EPE	S-C10-C9-N1
5	B	508	EPE	C10-C9-N1-C2
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
3	B	509	2JR	CAH-CAR-NAU-CAV
2	A	501	FAD	P-O3P-PA-O2A
2	B	501	FAD	P-O3P-PA-O2A
2	B	501	FAD	O4B-C4B-C5B-O5B

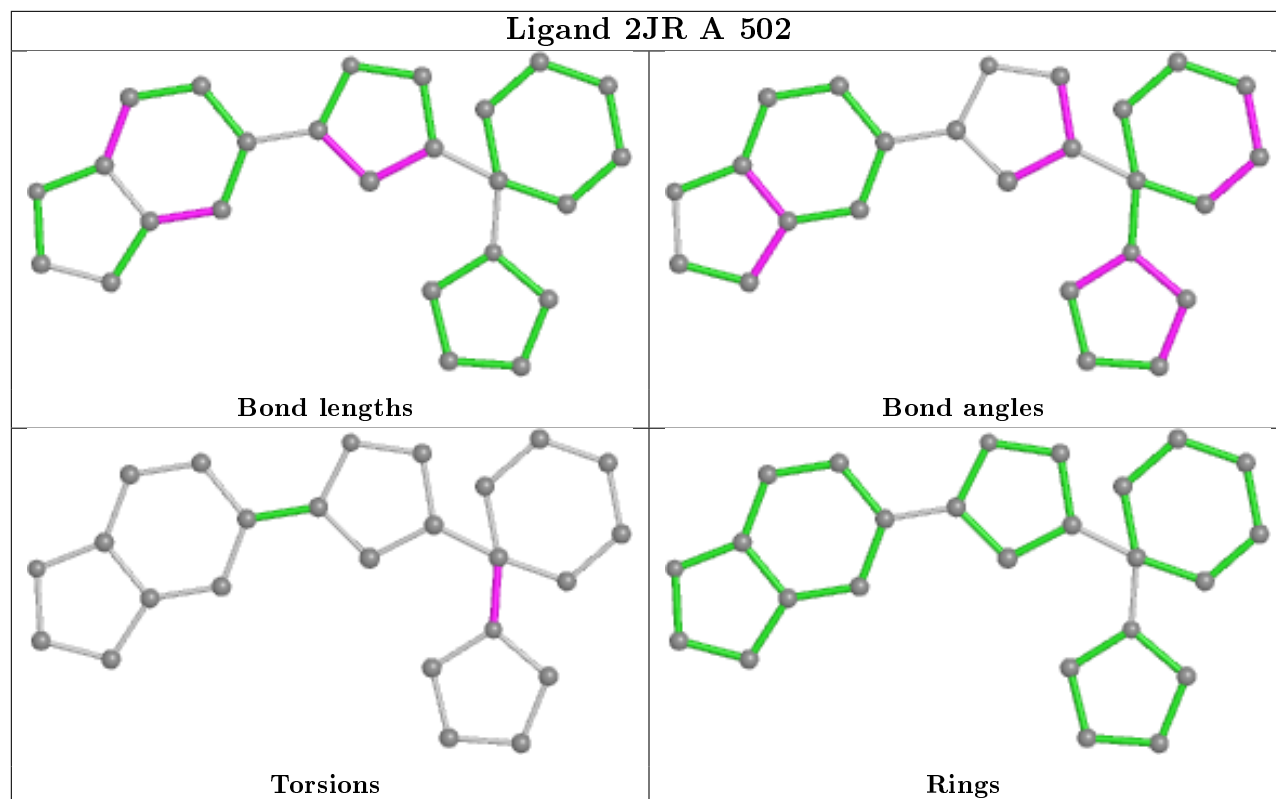
There are no ring outliers.

4 monomers are involved in 4 short contacts:

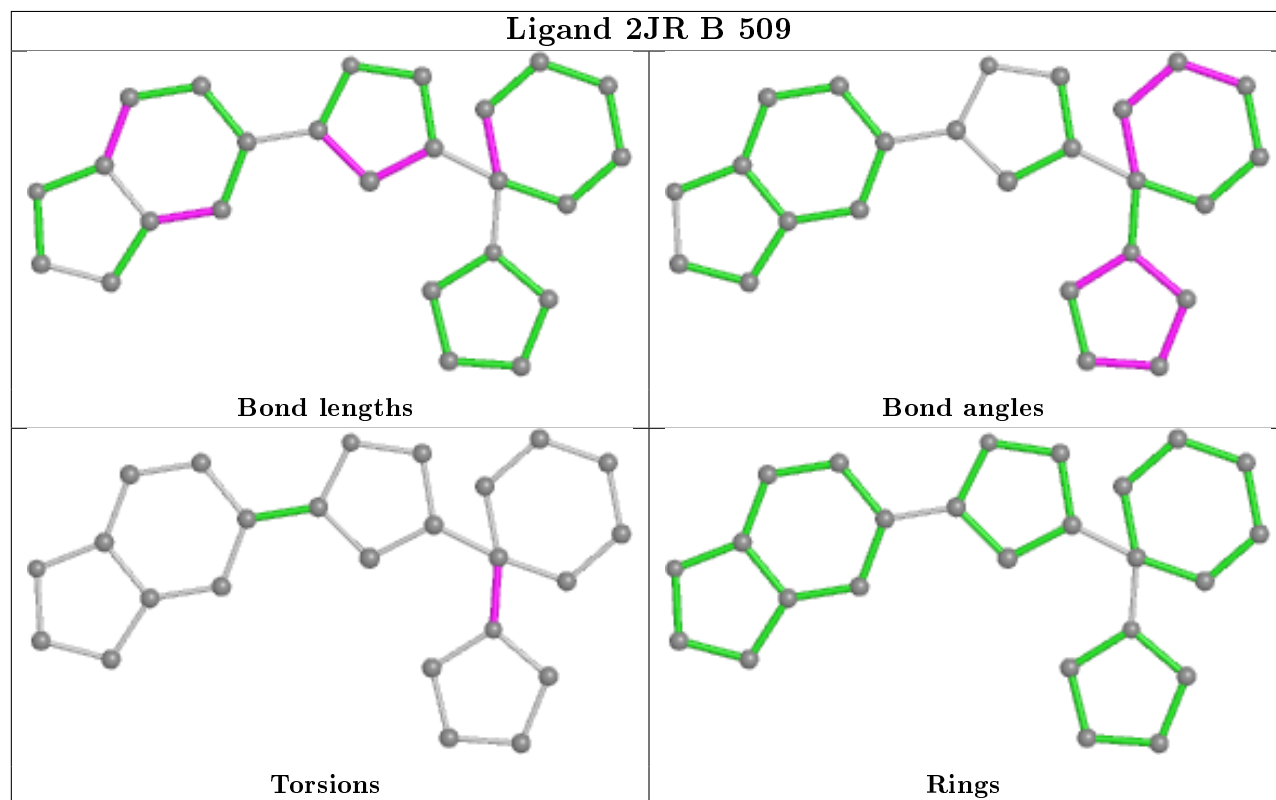
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	SO4	1	0
3	B	509	2JR	1	0
2	A	501	FAD	1	0
3	B	502	2JR	1	0

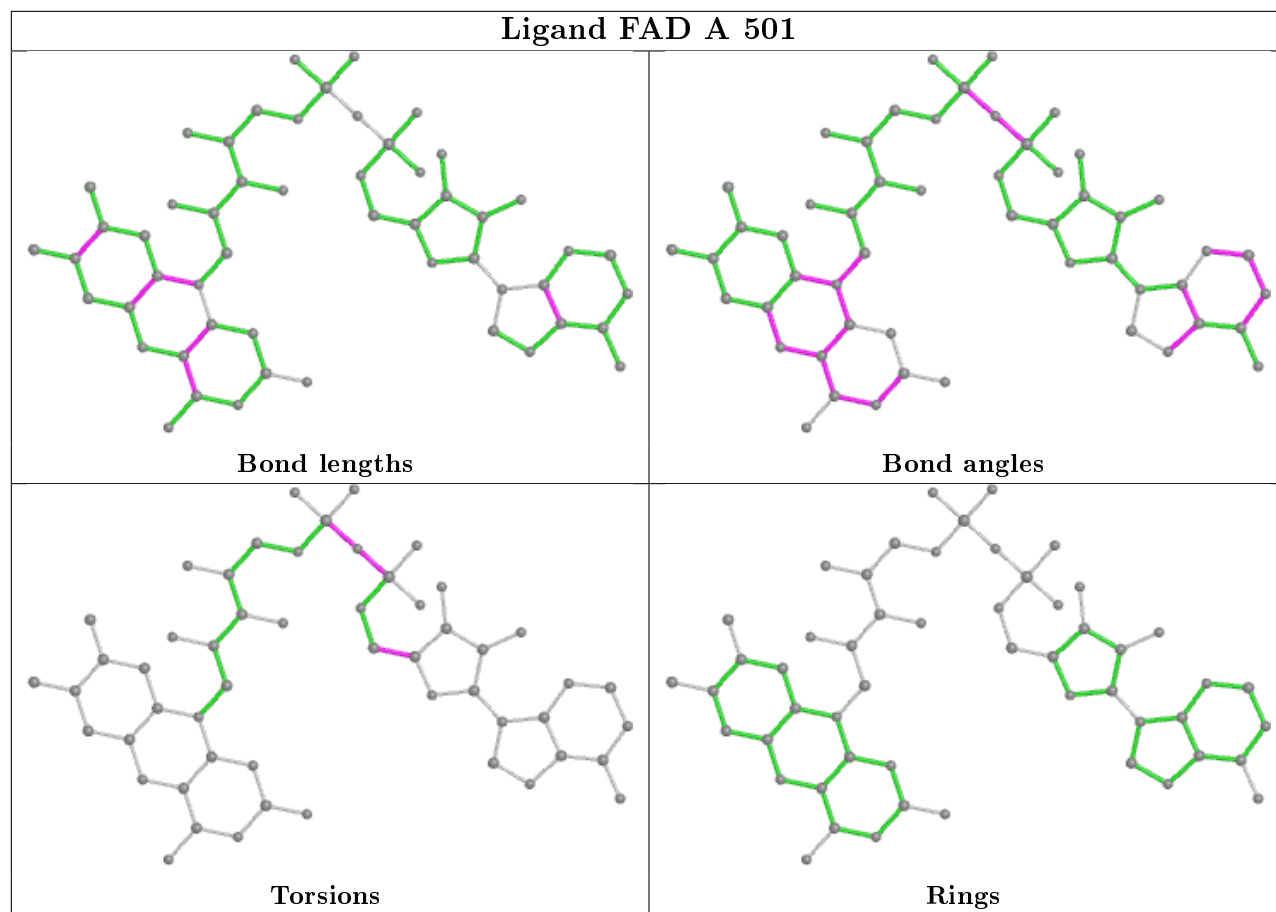
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 2JR A 502

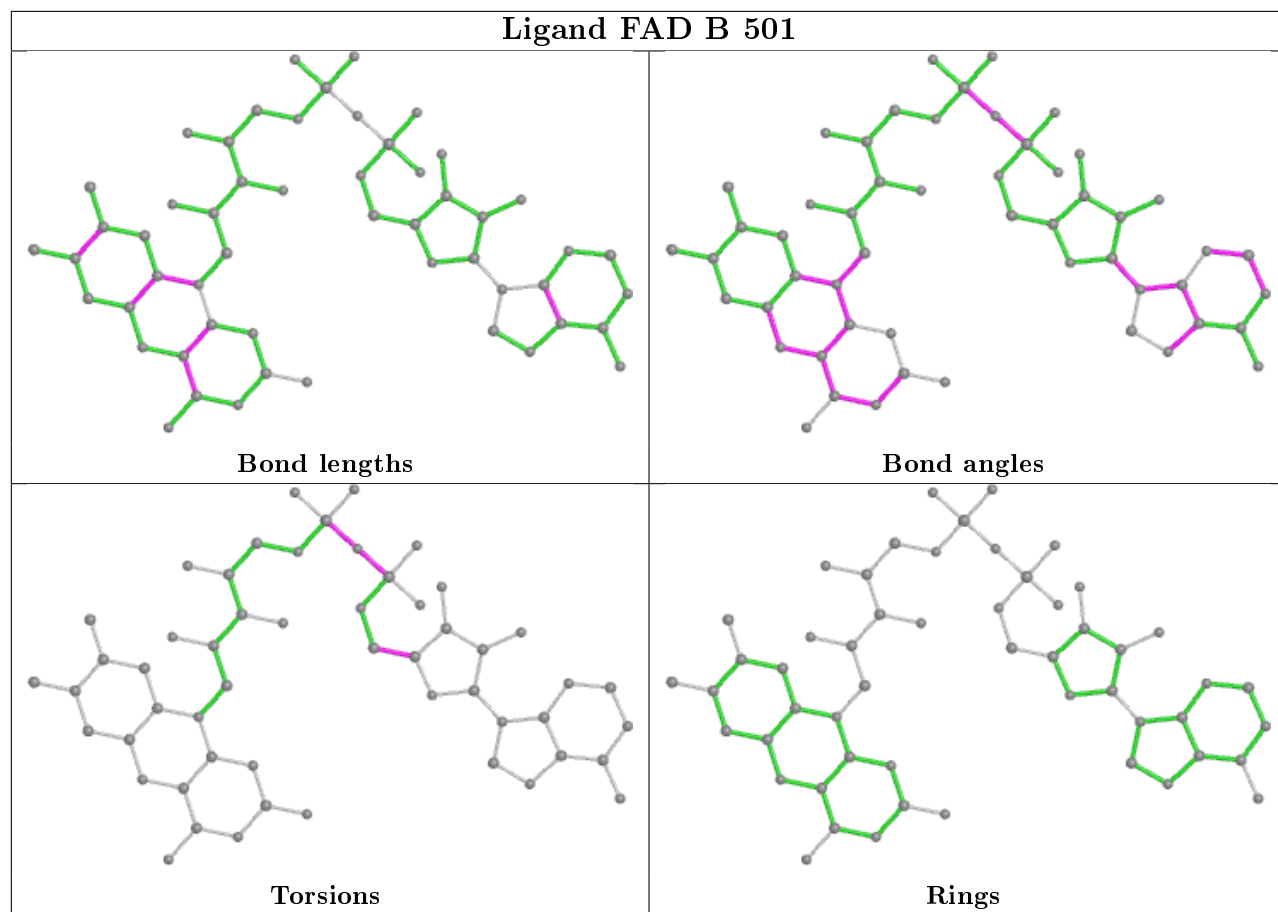


Ligand 2JR B 509

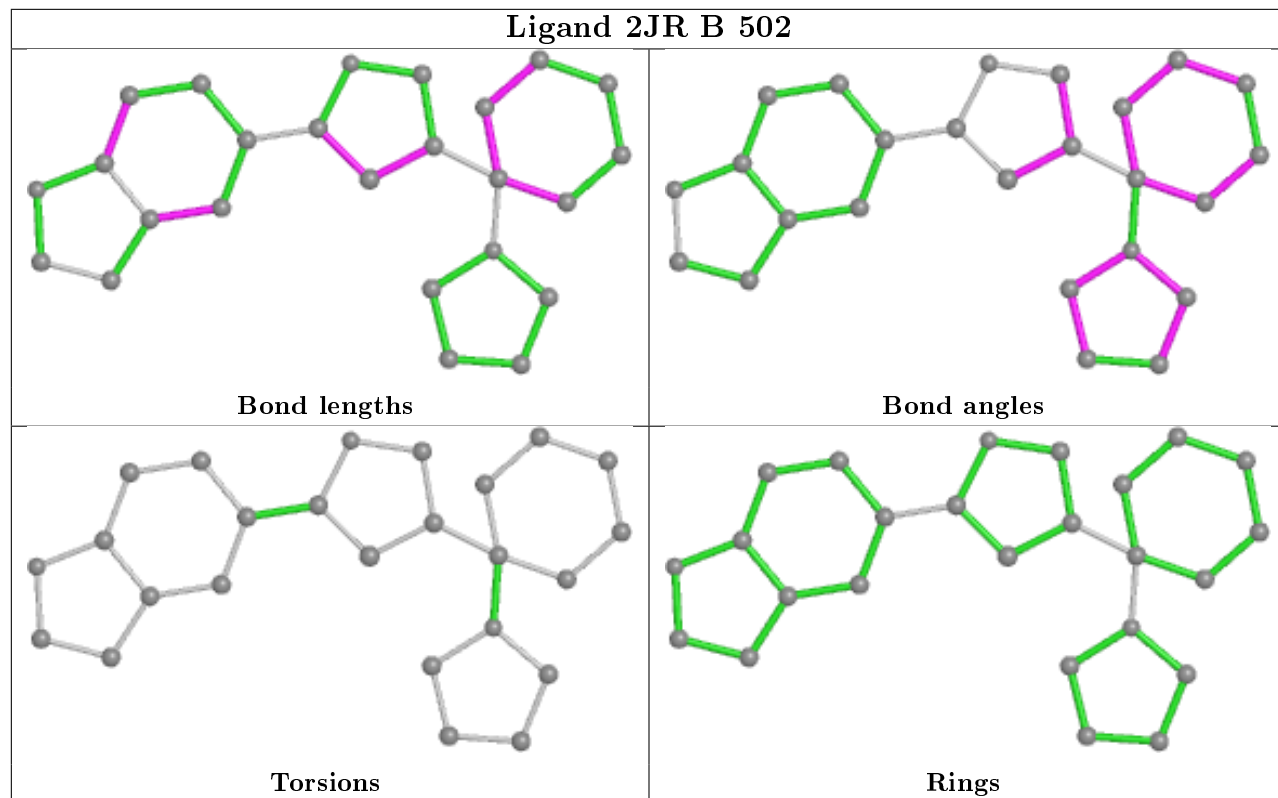




Ligand FAD B 501



Ligand 2JR B 502



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	485/495 (97%)	0.50	41 (8%) 10 10	44, 68, 97, 125	0
1	B	485/495 (97%)	0.38	9 (1%) 66 69	43, 61, 91, 113	0
All	All	970/990 (97%)	0.44	50 (5%) 27 29	43, 64, 95, 125	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	SER	6.1
1	A	156	ILE	4.6
1	A	350	PHE	4.5
1	A	345	LEU	4.1
1	A	323	TYR	3.8
1	A	20	GLY	3.8
1	A	301	VAL	3.8
1	A	141	ALA	3.7
1	A	309	VAL	3.7
1	A	302	LYS	3.6
1	A	303	LEU	3.4
1	A	349	VAL	3.3
1	A	482	GLU	3.3
1	A	114	PHE	3.3
1	A	390	ALA	3.3
1	A	479	VAL	3.1
1	A	311	VAL	3.1
1	A	347	ASP	3.0
1	A	24	ALA	3.0
1	A	355	ARG	2.9
1	A	476	TYR	2.9
1	B	472	ARG	2.9
1	A	487	LEU	2.8
1	A	317	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	322	ILE	2.7
1	A	386	PHE	2.7
1	A	331	ARG	2.6
1	A	359	HIS	2.6
1	A	377	LEU	2.5
1	A	158	LEU	2.4
1	B	57	CYS	2.4
1	A	389	VAL	2.4
1	A	30	ARG	2.4
1	A	356	LYS	2.3
1	B	388	LYS	2.3
1	A	480	LYS	2.3
1	A	123	PHE	2.3
1	B	477	TYR	2.3
1	A	10	ILE	2.3
1	A	251	THR	2.2
1	B	468	LEU	2.2
1	A	353	LYS	2.1
1	B	275	THR	2.1
1	A	425	LEU	2.1
1	A	27	TYR	2.1
1	B	415	ILE	2.1
1	A	352	ASN	2.1
1	A	385	GLU	2.1
1	B	478	TYR	2.0
1	B	479	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

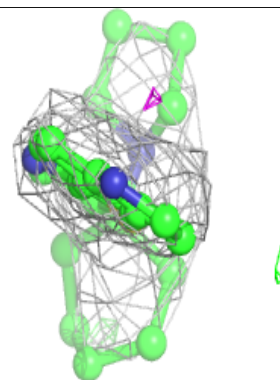
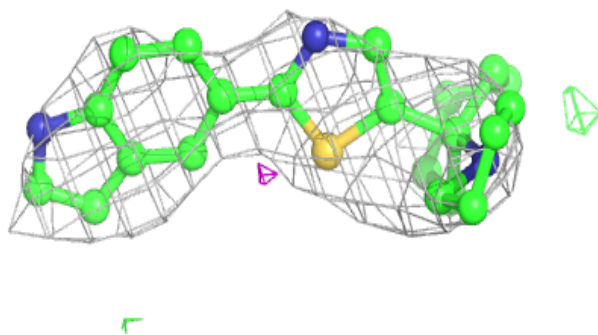
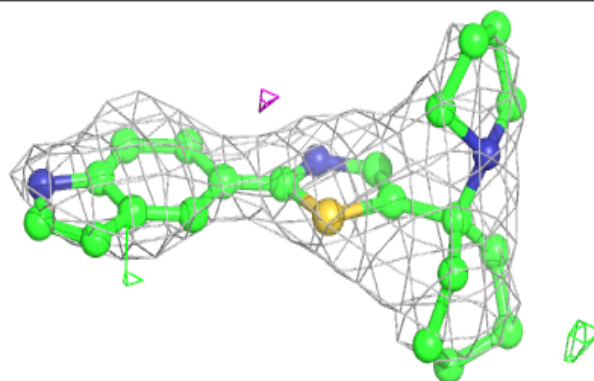
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	505	5/5	0.83	0.14	116,119,124,124	0
3	2JR	A	502	25/25	0.86	0.39	126,132,135,136	0
4	SO4	B	505	5/5	0.87	0.23	110,111,113,115	0
4	SO4	B	504	5/5	0.88	0.14	106,107,112,114	0
4	SO4	B	507	5/5	0.88	0.27	120,121,123,123	0
3	2JR	B	502	25/25	0.90	0.22	86,92,94,95	0
4	SO4	B	503	5/5	0.93	0.18	96,98,100,102	0
3	2JR	B	509	25/25	0.93	0.23	70,80,85,85	25
2	FAD	A	501	53/53	0.95	0.15	54,64,69,71	0
4	SO4	B	506	5/5	0.95	0.15	109,110,113,114	0
5	EPE	B	508	15/15	0.96	0.13	58,60,63,63	0
4	SO4	A	503	5/5	0.96	0.10	77,78,81,84	0
4	SO4	A	504	5/5	0.97	0.16	91,92,97,98	0
2	FAD	B	501	53/53	0.97	0.20	43,48,52,53	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.

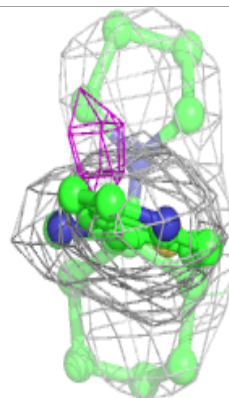
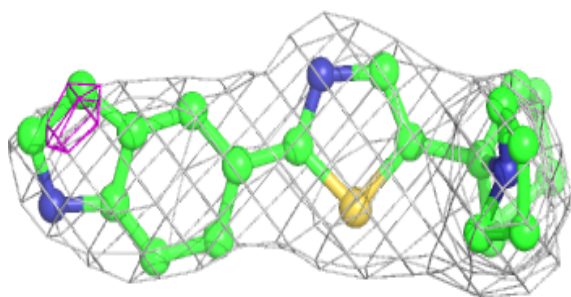
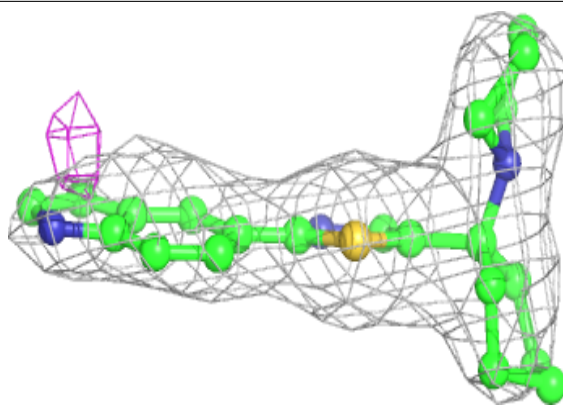
Electron density around 2JR A 502:

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

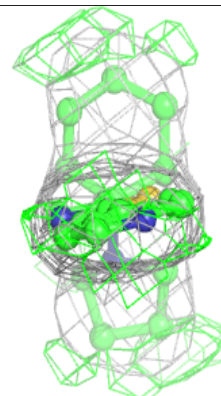
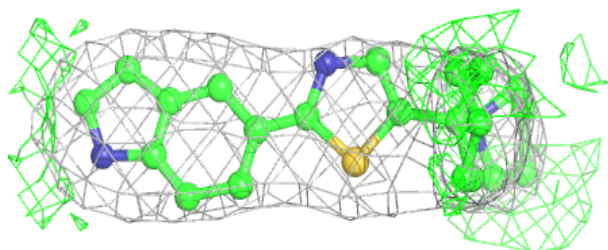
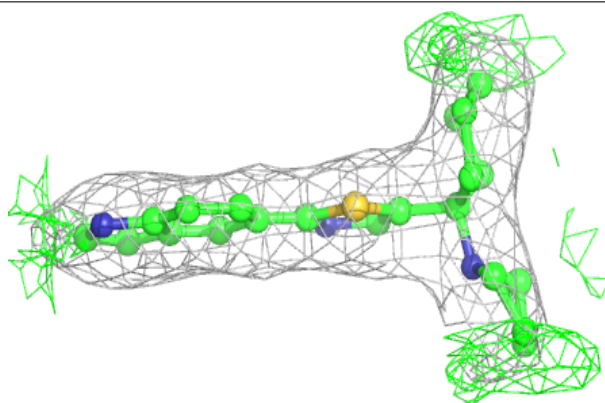


Electron density around 2JR B 502:

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

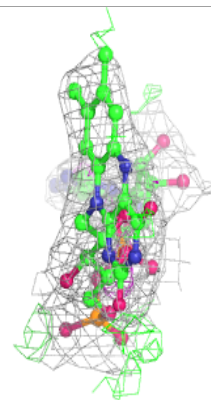
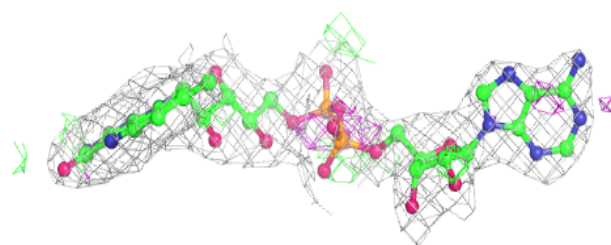
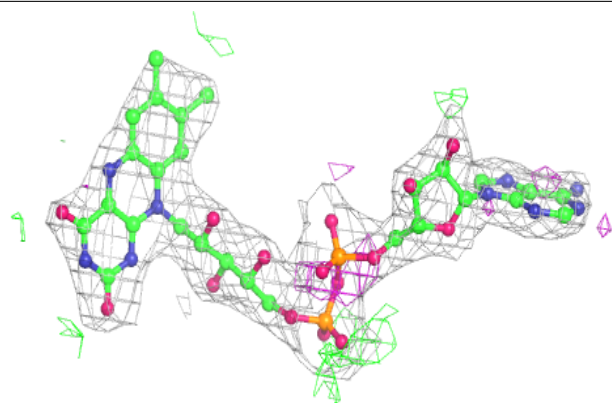
**Electron density around 2JR B 509:**

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

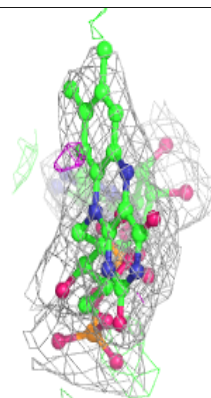
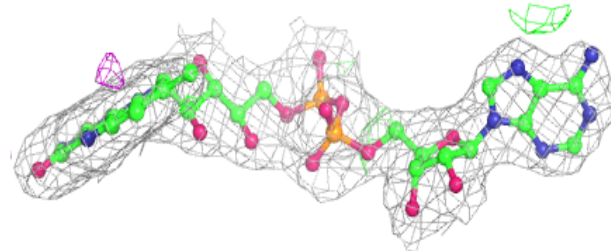
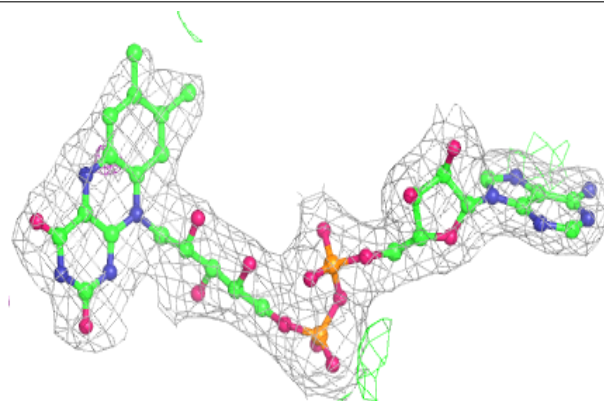


Electron density around FAD A 501:

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

**Electron density around FAD 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)



6.5 Other polymers

There are no such residues in this entry.