



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:34 AM UTC

PDB ID : 8PF5 / pdb_00008pf5
Title : Crystal structure of Trypanosoma brucei trypanothione reductase in complex with 1-(3,4-dichlorobenzyl)-4-(((5-((4-fluorophenethyl)carbamoyl)furan-2-yl)methyl)carbamoyl)-1-(3-phenylpropyl)piperazin-1-ium
Authors : Exertier, C.; Antonelli, L.; Fiorillo, A.; Ilari, A.
Deposited on : 2023-06-15
Resolution : 2.42 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 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)
Xtriage (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

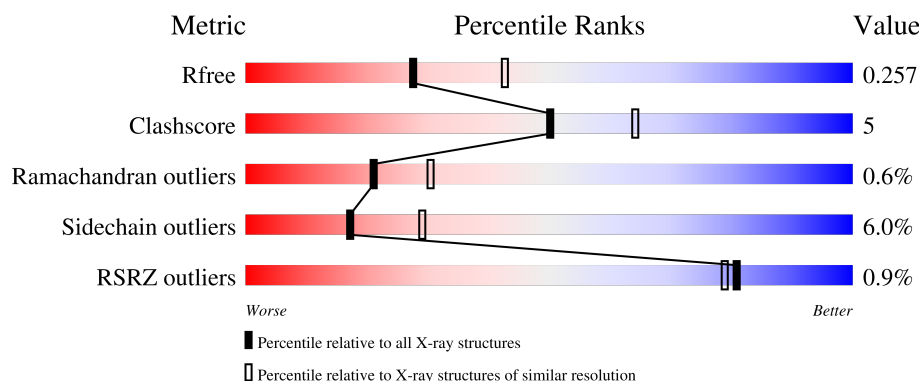
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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 ≥ 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	
2	B	494	
2	C	494	
3	D	495	

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
6	PEG	B	503	-	-	-	X
6	PEG	C	503	-	-	X	-
7	DMS	A	504	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15739 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	488	Total	C	N	O	S	0	1	0
			3711	2360	630	702	19			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0A3L6KZJ1
A	0	HIS	-	expression tag	UNP A0A3L6KZJ1
A	497	ASP	-	expression tag	UNP A0A3L6KZJ1

- Molecule 2 is a protein called Trypanothione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	2	0
			3739	2380	636	703	20			
2	C	488	Total	C	N	O	S	0	3	0
			3732	2376	634	702	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP A0A3L6KZJ1
B	0	HIS	-	expression tag	UNP A0A3L6KZJ1
C	-1	SER	-	expression tag	UNP A0A3L6KZJ1
C	0	HIS	-	expression tag	UNP A0A3L6KZJ1

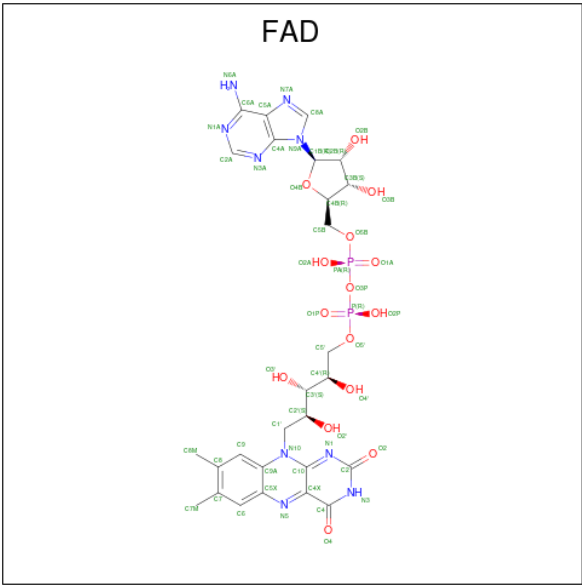
- Molecule 3 is a protein called Trypanothione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	491	Total	C	N	O	S	0	3	0
			3744	2382	638	704	20			

There are 3 discrepancies between the modelled and reference sequences:

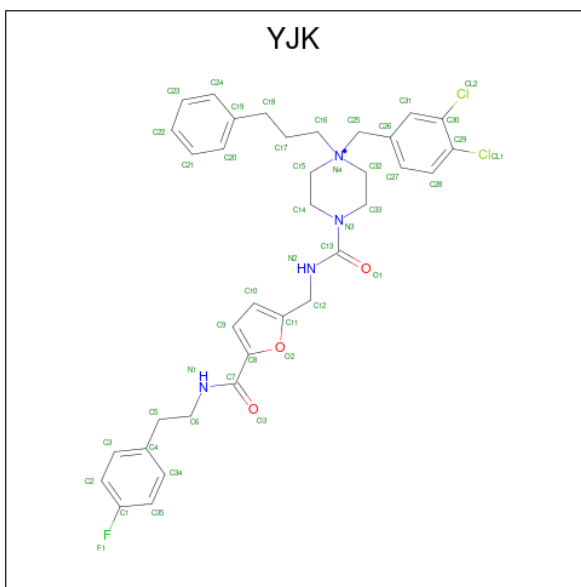
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP A0A3L6KZJ1
D	-1	SER	-	expression tag	UNP A0A3L6KZJ1
D	0	HIS	-	expression tag	UNP A0A3L6KZJ1

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



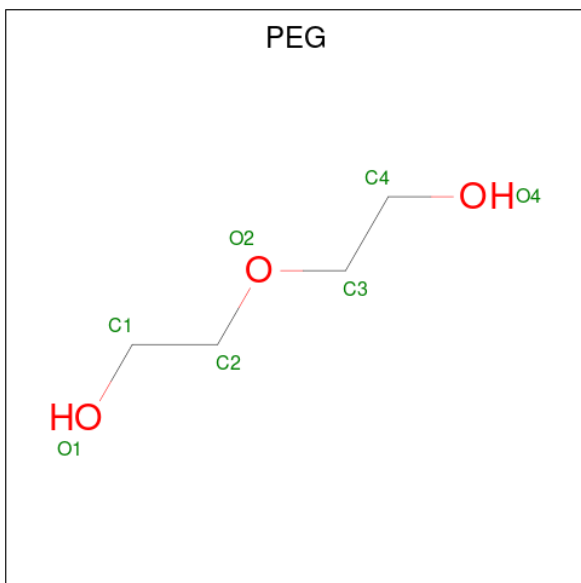
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is 4-[(3,4-dichlorophenyl)methyl]- {N}-[[5-[2-(4-fluorophenyl)ethylcarbamoyl]fu ran-2-yl)methyl]-4-(3-phenylpropyl)-1,4^l-diazinane-1-carboxamide (CCD ID: YJK) (formula: C₃₅H₃₈Cl₂FN₄O₃) (labeled as "Ligand of Interest" by depositor).



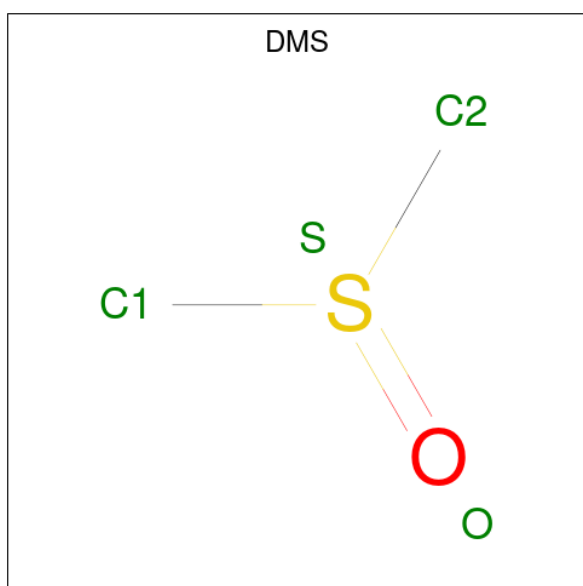
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Cl	F	N	O	0	0
			45	35	2	1	4	3		
5	B	1	Total	C	Cl	F	N	O	0	0
			45	35	2	1	4	3		
5	C	1	Total	C	Cl	F	N	O	24	1
			90	70	4	2	8	6		
5	D	1	Total	C	Cl	F	N	O	0	0
			45	35	2	1	4	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O S 4 2 1 1	0	0
7	D	1	Total C O S 4 2 1 1	0	0

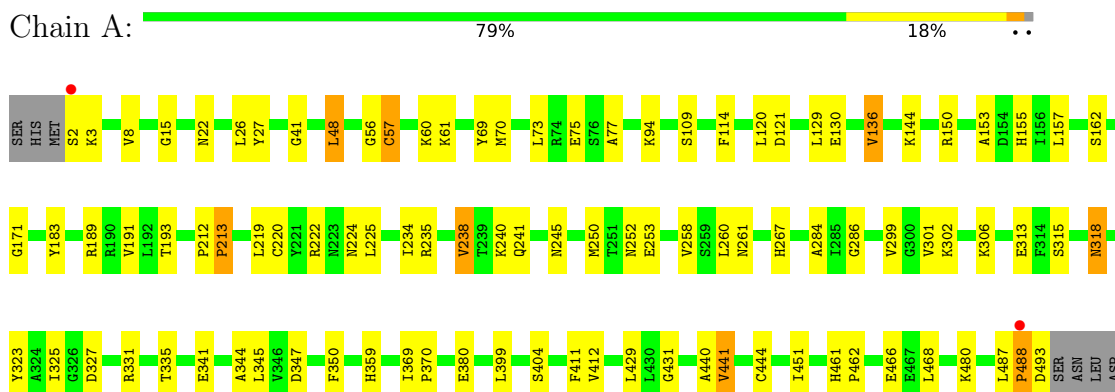
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	91	Total O 91 91	0	0
8	B	80	Total O 80 80	0	0
8	C	68	Total O 68 68	0	0
8	D	101	Total O 101 101	0	0

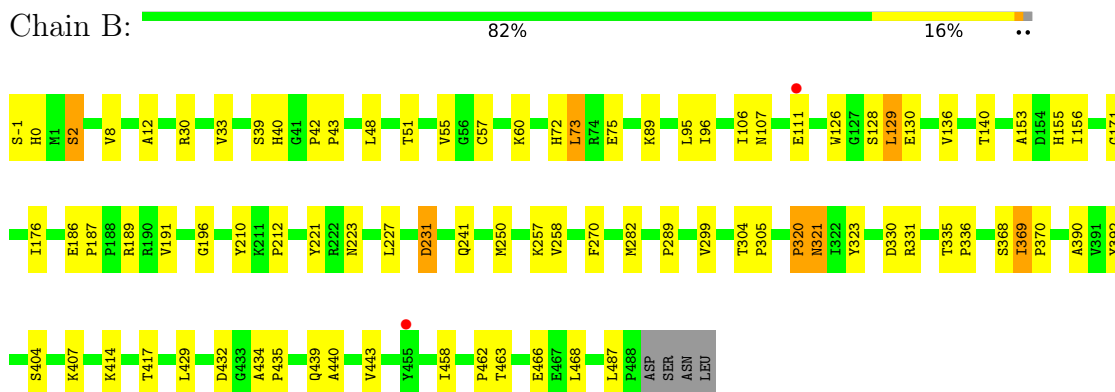
3 Residue-property plots

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.

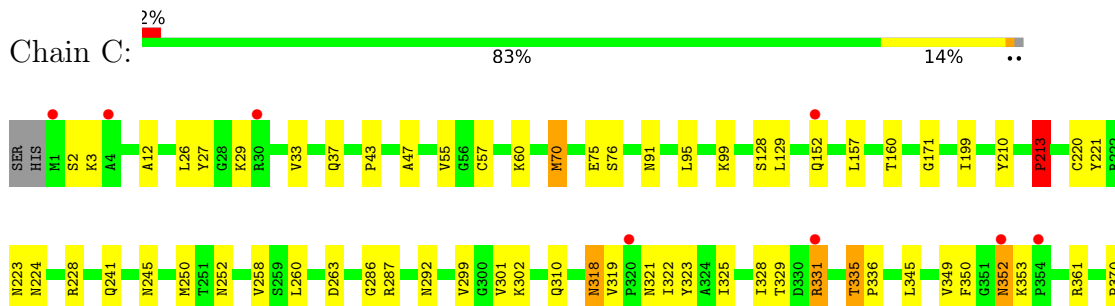
• Molecule 1: Trypanothione reductase

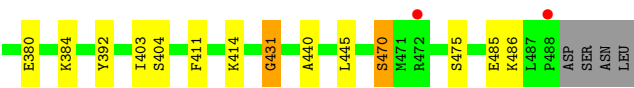


• Molecule 2: Trypanothione reductase

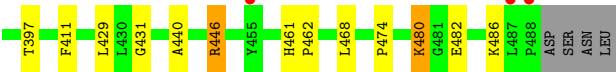
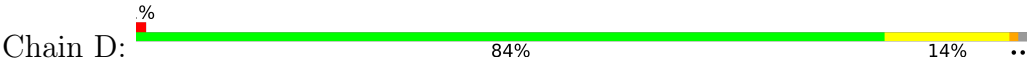


• Molecule 2: Trypanothione reductase





● Molecule 3: Trypanothione reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.96Å 63.31Å 169.11Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	55.83 – 2.42 55.83 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.8 (55.83-2.42) 99.9 (55.83-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.257 0.195 , 0.257	Depositor DCC
R_{free} test set	4052 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15739	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: YJK, FAD, DMS, PEG

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	1.06	0/3791	1.46	7/5142 (0.1%)
2	B	1.05	1/3825 (0.0%)	1.45	5/5188 (0.1%)
2	C	1.05	0/3817	1.41	4/5177 (0.1%)
3	D	1.07	0/3832	1.43	6/5195 (0.1%)
All	All	1.06	1/15265 (0.0%)	1.44	22/20702 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	HIS	CE1-NE2	5.05	1.37	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	91	ASN	CA-C-N	6.08	128.74	120.54
3	D	91	ASN	C-N-CA	6.08	128.74	120.54
2	B	320	PRO	N-CA-C	-5.97	101.71	111.68
2	C	403	ILE	N-CA-C	-5.81	106.05	111.45
3	D	55	VAL	CA-C-N	5.79	126.61	122.16
3	D	55	VAL	C-N-CA	5.79	126.61	122.16
2	C	213	PRO	N-CA-CB	-5.61	97.36	103.25
3	D	42	PRO	N-CA-C	-5.56	105.13	110.47
1	A	15	GLY	CA-C-N	5.45	125.88	119.94
1	A	15	GLY	C-N-CA	5.45	125.88	119.94
2	C	431	GLY	CA-C-O	-5.31	118.03	122.33
2	B	432	ASP	CB-CA-C	5.27	118.32	109.89
3	D	277	ASP	CB-CA-C	5.25	118.41	109.75
2	C	70	MET	N-CA-C	-5.21	104.86	111.11
2	B	368	SER	CA-C-O	-5.17	116.19	121.87
2	B	443	VAL	N-CA-C	-5.14	105.53	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	441	VAL	CA-C-N	5.11	125.65	119.98
1	A	441	VAL	C-N-CA	5.11	125.65	119.98
1	A	77	ALA	CA-C-N	5.08	125.72	120.03
1	A	77	ALA	C-N-CA	5.08	125.72	120.03
2	B	51	THR	N-CA-C	-5.01	105.90	111.36

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	3711	0	3717	51	0
2	B	3739	0	3754	44	0
2	C	3732	0	3749	36	0
3	D	3744	0	3755	32	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
4	C	53	0	31	1	0
4	D	53	0	31	0	0
5	A	45	0	0	1	0
5	B	45	0	0	0	0
5	C	90	0	0	5	0
5	D	45	0	0	0	0
6	A	7	0	10	3	0
6	B	7	0	10	0	0
6	C	14	0	20	6	0
7	A	4	0	6	5	0
7	D	4	0	6	0	0
8	A	91	0	0	0	0
8	B	80	0	0	3	0
8	C	68	0	0	2	0
8	D	101	0	0	3	0
All	All	15739	0	15151	161	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 5.

All (161) 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)
5:C:502[B]:YJK:C18	5:C:502[B]:YJK:C25	2.34	1.05
5:C:502[B]:YJK:C27	5:C:502[B]:YJK:C20	2.42	0.97
1:A:315:SER:OG	7:A:504:DMS:H22	1.82	0.79
1:A:234:ILE:O	1:A:238:VAL:HG12	1.84	0.77
1:A:250:MET:HE2	1:A:253:GLU:HG3	1.67	0.77
2:B:-1:SER:N	8:B:601:HOH:O	2.20	0.75
2:C:157:LEU:HD11	2:C:325:ILE:HG12	1.69	0.73
2:B:221:TYR:CE2	2:B:223:ASN:HB2	2.24	0.73
3:D:411:PHE:CD2	3:D:431:GLY:HA3	2.27	0.69
2:B:8:VAL:HG23	2:B:153:ALA:HB2	1.75	0.69
2:C:440:ALA:HB3	3:D:440:ALA:HB3	1.72	0.69
3:D:370:PRO:HD2	8:D:621:HOH:O	1.93	0.69
2:C:301:VAL:HA	2:C:318:ASN:HD21	1.61	0.66
3:D:341:GLU:OE2	3:D:359:HIS:HE1	1.80	0.65
2:B:289:PRO:HG3	2:B:330:ASP:HB2	1.80	0.63
3:D:136:VAL:HG13	3:D:147:VAL:HG13	1.81	0.63
1:A:171:GLY:HA3	1:A:258:VAL:O	1.98	0.62
1:A:130:GLU:HB2	1:A:136:VAL:CG2	2.30	0.61
5:A:502:YJK:CL1	2:B:106:ILE:HD13	2.38	0.60
2:B:8:VAL:CG2	2:B:153:ALA:HB2	2.32	0.60
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.66	0.60
1:A:70:MET:HE3	1:A:245:ASN:HD21	1.67	0.59
3:D:69:TYR:O	3:D:73:LEU:HG	2.02	0.59
2:B:231:ASP:OD2	2:B:414:LYS:NZ	2.36	0.59
2:B:320:PRO:O	2:B:321:ASN:ND2	2.26	0.59
2:C:286:GLY:N	6:C:503:PEG:H32	2.18	0.59
2:C:287:ARG:HG3	6:C:503:PEG:H31	1.85	0.59
1:A:411:PHE:CD2	1:A:431:GLY:HA3	2.39	0.58
2:C:29:LYS:HE3	2:C:350:PHE:CD1	2.38	0.58
3:D:95:LEU:HD22	3:D:210:TYR:CZ	2.39	0.58
3:D:60:LYS:HD3	3:D:202:GLU:OE1	2.04	0.57
2:C:224:ASN:HD22	2:C:252:ASN:HD21	1.52	0.57
3:D:171:GLY:HA3	3:D:258:VAL:O	2.04	0.56
2:C:160:THR:OG1	2:C:328:ILE:HD12	2.06	0.56
2:C:392:TYR:O	2:C:414:LYS:HA	2.06	0.56
2:B:129:LEU:HD23	2:B:299:VAL:HG21	1.88	0.56
2:B:0:HIS:CD2	8:B:652:HOH:O	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:MET:HE1	2:B:270:PHE:CZ	2.42	0.54
1:A:73:LEU:HD23	2:B:73:LEU:HD22	1.90	0.54
1:A:286:GLY:O	6:A:503:PEG:H12	2.07	0.54
2:C:221:TYR:CE2	2:C:223:ASN:HB2	2.43	0.54
5:C:502[B]:YJK:C33	5:C:502[B]:YJK:C31	2.85	0.54
2:B:95:LEU:HD22	2:B:210:TYR:CZ	2.43	0.54
3:D:429:LEU:HD21	3:D:468:LEU:HD21	1.91	0.53
2:B:0:HIS:HD2	8:B:652:HOH:O	1.89	0.53
1:A:345:LEU:HB2	7:A:504:DMS:H23	1.90	0.53
1:A:261:ASN:HD21	1:A:267:HIS:HB2	1.74	0.52
1:A:315:SER:CB	7:A:504:DMS:H22	2.38	0.52
2:B:390:ALA:HB3	2:B:417:THR:OG1	2.09	0.51
2:C:70:MET:HE3	2:C:245:ASN:HD21	1.76	0.51
3:D:446[A]:ARG:HB3	3:D:446[A]:ARG:HH11	1.74	0.51
2:C:329:THR:OG1	2:C:331:ARG:NH1	2.44	0.50
2:C:241:GLN:OE1	2:C:370:PRO:HG3	2.12	0.50
1:A:157:LEU:HD11	1:A:325:ILE:HG12	1.93	0.50
2:B:75:GLU:HB3	2:B:404:SER:HB2	1.93	0.50
2:B:189:ARG:HA	2:B:212:PRO:HD2	1.93	0.50
2:C:319:VAL:HG11	2:C:322:ILE:HD12	1.94	0.50
1:A:189:ARG:HA	1:A:212:PRO:HD2	1.93	0.49
2:B:250:MET:HE1	2:B:270:PHE:CE2	2.47	0.49
1:A:2:SER:HB2	1:A:150:ARG:O	2.12	0.49
1:A:8:VAL:HG23	1:A:153:ALA:HB2	1.94	0.49
1:A:155:HIS:HB3	1:A:323:TYR:HE2	1.77	0.49
2:C:286:GLY:C	6:C:503:PEG:H31	2.36	0.49
1:A:341:GLU:OE2	1:A:359:HIS:HE1	1.96	0.48
3:D:268:VAL:O	3:D:275:THR:HA	2.13	0.48
1:A:344:ALA:HB3	7:A:504:DMS:S	2.52	0.48
3:D:2:SER:HB2	3:D:150:ARG:O	2.13	0.48
1:A:299:VAL:HG23	1:A:301:VAL:HG23	1.95	0.48
1:A:440:ALA:HB3	2:B:440:ALA:HB3	1.95	0.48
2:C:76:SER:HB3	3:D:69:TYR:CD1	2.49	0.47
1:A:22:ASN:O	1:A:26:LEU:HB2	2.14	0.47
2:C:299:VAL:HG23	2:C:301:VAL:HG23	1.97	0.47
3:D:341:GLU:OE2	3:D:359:HIS:CE1	2.64	0.47
2:B:40:HIS:H	2:B:107:ASN:ND2	2.14	0.46
1:A:219:LEU:C	1:A:219:LEU:HD23	2.40	0.46
2:B:40:HIS:H	2:B:107:ASN:HD21	1.63	0.46
6:C:504:PEG:H42	8:C:628:HOH:O	2.15	0.46
2:C:411:PHE:CD2	2:C:431:GLY:HA3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:TRP:CD1	2:B:140:THR:HA	2.50	0.46
2:B:186:GLU:HB2	2:B:187:PRO:HD2	1.96	0.46
2:B:335:THR:HB	2:B:336:PRO:HD3	1.97	0.46
1:A:466:GLU:HA	2:B:439:GLN:OE1	2.16	0.46
1:A:429:LEU:HD21	1:A:468:LEU:HD21	1.98	0.46
2:C:470:SER:HB3	5:C:502[B]:YJK:CL2	2.53	0.46
3:D:126:TRP:CZ3	3:D:141:ALA:HB2	2.51	0.46
2:C:361[B]:ARG:HD2	2:C:445:LEU:HD23	1.98	0.46
1:A:241:GLN:OE1	1:A:370:PRO:HG3	2.15	0.45
2:B:463:THR:O	2:B:466:GLU:HG2	2.17	0.45
2:B:171:GLY:HA3	2:B:258:VAL:O	2.16	0.45
3:D:249:ILE:HG22	3:D:251:THR:HG23	1.99	0.45
3:D:126:TRP:CE3	3:D:141:ALA:HB2	2.51	0.45
1:A:75:GLU:HB3	1:A:404:SER:HB2	1.98	0.45
1:A:441:VAL:O	1:A:444:CYS:HB2	2.16	0.45
3:D:162:SER:HB3	3:D:327:ASP:HB3	1.99	0.45
3:D:311:VAL:HA	3:D:316:ARG:O	2.17	0.45
2:B:429:LEU:HD21	2:B:468:LEU:HD21	1.99	0.45
2:B:241:GLN:OE1	2:B:370:PRO:CD	2.64	0.45
2:C:26:LEU:O	2:C:27:TYR:CD1	2.70	0.44
1:A:61:LYS:HB2	2:B:462:PRO:HG2	1.99	0.44
2:B:221:TYR:CZ	2:B:223:ASN:HB2	2.52	0.44
1:A:75:GLU:CB	1:A:404:SER:HB2	2.47	0.44
1:A:222:ARG:O	1:A:252:ASN:HA	2.17	0.44
2:B:434:ALA:HB3	2:B:435:PRO:HD3	1.99	0.44
3:D:212:PRO:HB2	3:D:213:PRO:HD2	1.99	0.44
6:C:503:PEG:H22	8:C:605:HOH:O	2.18	0.43
1:A:114:PHE:CE1	1:A:120:LEU:HG	2.54	0.43
2:B:155:HIS:HB3	2:B:323:TYR:HE2	1.82	0.43
1:A:369:ILE:HA	1:A:370:PRO:HA	1.88	0.43
2:B:304:THR:O	2:B:305:PRO:C	2.62	0.43
2:B:392:TYR:O	2:B:414:LYS:HA	2.19	0.43
1:A:56:GLY:O	1:A:57:CYS:C	2.61	0.43
1:A:69:TYR:O	1:A:73:LEU:HG	2.19	0.43
2:C:95:LEU:HD22	2:C:210:TYR:CZ	2.53	0.43
2:C:318:ASN:HD22	2:C:318:ASN:N	2.17	0.43
2:C:37:GLN:OE1	2:C:43:PRO:HD2	2.18	0.43
2:C:171:GLY:HA3	2:C:258:VAL:O	2.19	0.43
2:C:470:SER:CB	5:C:502[B]:YJK:CL2	3.04	0.43
2:C:99:LYS:C	2:C:99:LYS:HD2	2.43	0.43
3:D:40:HIS:HB3	3:D:54:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:220:CYS:HA	3:D:250:MET:O	2.19	0.43
2:C:287:ARG:HD2	4:C:501:FAD:HM82	2.02	0.42
3:D:296:LEU:HD13	3:D:303:LEU:HD21	2.00	0.42
3:D:370:PRO:HG2	8:D:640:HOH:O	2.18	0.42
2:B:96:ILE:HD13	2:B:96:ILE:HA	1.86	0.42
1:A:225:LEU:HD23	1:A:235:ARG:CZ	2.49	0.42
1:A:412:VAL:O	1:A:429:LEU:HA	2.20	0.42
1:A:41:GLY:HA2	1:A:183:TYR:CZ	2.54	0.42
2:B:12:ALA:HB2	2:B:33:VAL:HG12	2.00	0.42
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.87	0.42
2:B:196:GLY:O	2:B:227:LEU:N	2.48	0.42
1:A:27:TYR:CD1	1:A:350:PHE:O	2.72	0.42
1:A:313:GLU:O	7:A:504:DMS:H12	2.19	0.42
2:B:129:LEU:HD11	2:B:156:ILE:HG21	2.00	0.42
2:C:70:MET:CE	2:C:245:ASN:HD21	2.32	0.42
1:A:193:THR:O	1:A:219:LEU:HA	2.20	0.42
2:C:12:ALA:HB2	2:C:33:VAL:HG12	2.01	0.41
3:D:8:VAL:HG22	3:D:32:ALA:HB3	2.02	0.41
1:A:220:CYS:HA	1:A:250:MET:O	2.21	0.41
1:A:488:PRO:C	1:A:493:ASP:N	2.79	0.41
3:D:392:TYR:CZ	3:D:474:PRO:HG3	2.55	0.41
1:A:162:SER:HB3	1:A:327:ASP:HB3	2.03	0.41
3:D:325:ILE:O	3:D:328:ILE:HG22	2.20	0.41
3:D:370:PRO:CD	8:D:621:HOH:O	2.62	0.41
2:B:130:GLU:HB2	2:B:136:VAL:HG23	2.03	0.41
2:B:176:ILE:HG13	2:B:282:MET:HA	2.02	0.41
1:A:461:HIS:HA	1:A:462:PRO:HA	1.77	0.41
2:C:75:GLU:HG2	2:C:404:SER:HB2	2.03	0.41
2:C:263:ASP:OD1	2:C:263:ASP:C	2.63	0.41
3:D:34:VAL:HA	3:D:123:PHE:O	2.21	0.41
1:A:284:ALA:HA	6:A:503:PEG:O1	2.21	0.41
3:D:461:HIS:HA	3:D:462:PRO:HA	1.80	0.41
2:C:220:CYS:HA	2:C:250:MET:O	2.21	0.41
2:C:91:ASN:OD1	2:C:91:ASN:C	2.64	0.40
2:C:199:ILE:HD12	6:C:503:PEG:H42	2.04	0.40
3:D:40:HIS:H	3:D:107:ASN:ND2	2.18	0.40
1:A:487:LEU:O	1:A:488:PRO:C	2.64	0.40
2:B:42:PRO:HA	2:B:43:PRO:HA	1.82	0.40
2:B:369:ILE:HA	2:B:370:PRO:HA	1.90	0.40
1:A:73:LEU:CD2	2:B:73:LEU:HD22	2.51	0.40
1:A:286:GLY:H	6:A:503:PEG:H21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:335:THR:N	2:C:336:PRO:CD	2.84	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	486/495 (98%)	464 (96%)	20 (4%)	2 (0%)	30	42
2	B	490/494 (99%)	468 (96%)	19 (4%)	3 (1%)	21	30
2	C	489/494 (99%)	464 (95%)	20 (4%)	5 (1%)	12	18
3	D	492/495 (99%)	469 (95%)	21 (4%)	2 (0%)	30	42
All	All	1957/1978 (99%)	1865 (95%)	80 (4%)	12 (1%)	21	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	352	ASN
2	C	213	PRO
3	D	480	LYS
1	A	213	PRO
2	B	2	SER
2	C	2	SER
2	C	47	ALA
1	A	48	LEU
2	B	48	LEU
2	C	55	VAL
3	D	55	VAL
2	B	55	VAL

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	402/408 (98%)	377 (94%)	25 (6%)	16	27
2	B	405/407 (100%)	386 (95%)	19 (5%)	23	39
2	C	404/407 (99%)	376 (93%)	28 (7%)	14	23
3	D	404/407 (99%)	378 (94%)	26 (6%)	16	26
All	All	1615/1629 (99%)	1517 (94%)	98 (6%)	17	28

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	57	CYS
1	A	60	LYS
1	A	94	LYS
1	A	109	SER
1	A	121	ASP
1	A	129	LEU
1	A	136	VAL
1	A	144	LYS
1	A	191	VAL
1	A	213	PRO
1	A	224	ASN
1	A	238	VAL
1	A	240	LYS
1	A	260	LEU
1	A	302	LYS
1	A	306	LYS
1	A	318	ASN
1	A	331	ARG
1	A	335	THR
1	A	380	GLU
1	A	399	LEU
1	A	451	ILE
1	A	480	LYS

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Mol	Chain	Res	Type
1	A	488	PRO
2	B	2	SER
2	B	30	ARG
2	B	39	SER
2	B	57	CYS
2	B	60	LYS
2	B	73	LEU
2	B	89	LYS
2	B	111	GLU
2	B	128	SER
2	B	129	LEU
2	B	191	VAL
2	B	231	ASP
2	B	257	LYS
2	B	321	ASN
2	B	331	ARG
2	B	369	ILE
2	B	407	LYS
2	B	458	ILE
2	B	487	LEU
2	C	3	LYS
2	C	57	CYS
2	C	60	LYS
2	C	128	SER
2	C	129	LEU
2	C	152[A]	GLN
2	C	152[B]	GLN
2	C	213	PRO
2	C	228	ARG
2	C	260	LEU
2	C	292	ASN
2	C	302	LYS
2	C	310	GLN
2	C	318	ASN
2	C	321	ASN
2	C	323	TYR
2	C	331	ARG
2	C	335	THR
2	C	345	LEU
2	C	349	VAL
2	C	352	ASN
2	C	353	LYS

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Mol	Chain	Res	Type
2	C	380	GLU
2	C	384	LYS
2	C	470	SER
2	C	475	SER
2	C	485	GLU
2	C	486	LYS
3	D	57	CYS
3	D	60	LYS
3	D	89	LYS
3	D	118	GLU
3	D	129	LEU
3	D	131	SER
3	D	144	LYS
3	D	173	GLU
3	D	191	VAL
3	D	240	LYS
3	D	245	ASN
3	D	260	LEU
3	D	266	LYS
3	D	274	LYS
3	D	302	LYS
3	D	306	LYS
3	D	328	ILE
3	D	335	THR
3	D	353	LYS
3	D	385	GLU
3	D	397	THR
3	D	446[A]	ARG
3	D	446[B]	ARG
3	D	480	LYS
3	D	482	GLU
3	D	486	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	115	ASN
1	A	152	GLN
1	A	223	ASN
1	A	224	ASN
1	A	245	ASN

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Mol	Chain	Res	Type
1	A	252	ASN
1	A	261	ASN
1	A	318	ASN
1	A	340	ASN
1	A	352	ASN
1	A	359	HIS
2	B	107	ASN
2	B	152	GLN
2	B	252	ASN
2	B	340	ASN
2	B	359	HIS
2	B	419	HIS
2	C	133	ASN
2	C	223	ASN
2	C	224	ASN
2	C	245	ASN
2	C	318	ASN
2	C	402	ASN
3	D	223	ASN
3	D	252	ASN
3	D	292	ASN
3	D	310	GLN
3	D	321	ASN
3	D	340	ASN
3	D	359	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

15 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	FAD	B	501	-	58,58,58	0.80	2 (3%)	85,89,89	0.81	3 (3%)
5	YJK	C	502[A]	-	49,49,49	1.26	1 (2%)	65,67,67	10.36	4 (6%)
6	PEG	B	503	-	6,6,6	0.18	0	5,5,5	0.09	0
6	PEG	C	504	-	6,6,6	0.43	0	5,5,5	0.41	0
6	PEG	A	503	-	6,6,6	0.50	0	5,5,5	0.39	0
5	YJK	C	502[B]	-	49,49,49	0.31	0	65,67,67	0.52	0
6	PEG	C	503	-	6,6,6	0.39	0	5,5,5	0.34	0
7	DMS	D	503	-	3,3,3	0.26	0	3,3,3	0.04	0
4	FAD	D	501	-	58,58,58	0.72	1 (1%)	85,89,89	0.80	2 (2%)
5	YJK	B	502	-	49,49,49	0.35	0	65,67,67	0.66	2 (3%)
7	DMS	A	504	-	3,3,3	0.36	0	3,3,3	0.27	0
4	FAD	C	501	-	58,58,58	0.63	1 (1%)	85,89,89	0.70	1 (1%)
4	FAD	A	501	-	58,58,58	0.55	0	85,89,89	0.73	1 (1%)
5	YJK	D	502	-	49,49,49	0.34	0	65,67,67	0.68	0
5	YJK	A	502	-	49,49,49	0.36	0	65,67,67	1.57	3 (4%)

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	FAD	B	501	-	-	3/34/50/50	0/6/6/6
5	YJK	C	502[A]	-	-	13/31/43/43	0/5/5/5
6	PEG	B	503	-	-	3/4/4/4	-
6	PEG	C	504	-	-	2/4/4/4	-
6	PEG	A	503	-	-	3/4/4/4	-
5	YJK	C	502[B]	-	-	15/31/43/43	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	C	503	-	-	2/4/4/4	-
4	FAD	D	501	-	-	5/34/50/50	0/6/6/6
5	YJK	B	502	-	-	11/31/43/43	1/5/5/5
4	FAD	C	501	-	-	4/34/50/50	0/6/6/6
4	FAD	A	501	-	-	5/34/50/50	0/6/6/6
5	YJK	D	502	-	-	9/31/43/43	0/5/5/5
5	YJK	A	502	-	-	14/31/43/43	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502[A]	YJK	C13-N3	-8.42	1.21	1.36
4	B	501	FAD	PA-O3P	-2.67	1.56	1.59
4	D	501	FAD	C2-N3	-2.52	1.33	1.39
4	B	501	FAD	C2-N3	-2.38	1.33	1.39
4	C	501	FAD	PA-O3P	2.14	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502[A]	YJK	N2-C13-N3	72.75	161.78	117.66
5	C	502[A]	YJK	O1-C13-N3	-40.29	65.47	121.67
5	A	502	YJK	N2-C13-N3	10.25	123.87	117.66
5	C	502[A]	YJK	C14-N3-C13	-5.46	102.00	121.83
5	C	502[A]	YJK	C33-N3-C13	4.48	138.10	121.83
5	A	502	YJK	C12-N2-C13	4.18	125.34	120.81
4	B	501	FAD	C2B-C1B-N9A	2.72	120.05	113.30
5	A	502	YJK	O1-C13-N3	-2.70	117.90	121.67
5	B	502	YJK	C14-C15-N4	2.52	111.37	108.73
4	D	501	FAD	O2P-P-O3P	-2.47	100.58	107.27
5	B	502	YJK	C33-C32-N4	2.27	111.11	108.73
4	A	501	FAD	O5'-C5'-C4'	2.11	115.00	109.36
4	B	501	FAD	C4-N3-C2	-2.10	121.91	125.64
4	D	501	FAD	O2P-P-O1P	2.08	122.11	112.44
4	B	501	FAD	C4X-C4-N3	2.05	118.48	113.25
4	C	501	FAD	C4-N3-C2	-2.05	122.00	125.64

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	YJK	N3-C13-N2-C12
5	A	502	YJK	O1-C13-N2-C12
5	A	502	YJK	C26-C25-N4-C15
5	A	502	YJK	C26-C25-N4-C16
5	A	502	YJK	C26-C25-N4-C32
5	B	502	YJK	N3-C13-N2-C12
5	B	502	YJK	O1-C13-N2-C12
5	B	502	YJK	O1-C13-N3-C14
5	B	502	YJK	O1-C13-N3-C33
5	B	502	YJK	N4-C25-C26-C27
5	C	502[A]	YJK	N3-C13-N2-C12
5	C	502[A]	YJK	N2-C13-N3-C14
5	C	502[A]	YJK	N2-C13-N3-C33
5	C	502[A]	YJK	C16-C17-C18-C19
5	C	502[A]	YJK	C26-C25-N4-C15
5	C	502[B]	YJK	N2-C13-N3-C33
5	C	502[B]	YJK	O1-C13-N3-C33
5	C	502[B]	YJK	C26-C25-N4-C15
5	C	502[B]	YJK	C26-C25-N4-C16
5	C	502[B]	YJK	C26-C25-N4-C32
5	D	502	YJK	N3-C13-N2-C12
5	D	502	YJK	O1-C13-N2-C12
5	D	502	YJK	N2-C13-N3-C33
5	D	502	YJK	C16-C17-C18-C19
5	D	502	YJK	C26-C25-N4-C15
5	D	502	YJK	C26-C25-N4-C16
5	D	502	YJK	C26-C25-N4-C32
5	A	502	YJK	N4-C16-C17-C18
5	C	502[B]	YJK	N4-C16-C17-C18
5	B	502	YJK	N4-C25-C26-C31
5	C	502[A]	YJK	N4-C16-C17-C18
5	C	502[A]	YJK	C26-C25-N4-C16
5	C	502[A]	YJK	C26-C25-N4-C32
5	A	502	YJK	C17-C16-N4-C15
5	A	502	YJK	C17-C16-N4-C32
5	D	502	YJK	N4-C16-C17-C18
6	B	503	PEG	C1-C2-O2-C3
5	A	502	YJK	C17-C16-N4-C25
6	A	503	PEG	O2-C3-C4-O4
5	C	502[A]	YJK	O1-C13-N3-C33
5	D	502	YJK	O1-C13-N3-C33
6	B	503	PEG	O1-C1-C2-O2
6	C	503	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	B	502	YJK	C16-C17-C18-C19
5	B	502	YJK	N4-C16-C17-C18
6	A	503	PEG	O1-C1-C2-O2
5	B	502	YJK	N2-C13-N3-C33
6	C	504	PEG	O2-C3-C4-O4
5	C	502[B]	YJK	N3-C13-N2-C12
5	C	502[B]	YJK	C16-C17-C18-C19
4	A	501	FAD	PA-O3P-P-O5'
4	B	501	FAD	PA-O3P-P-O5'
4	D	501	FAD	PA-O3P-P-O5'
6	A	503	PEG	C4-C3-O2-C2
4	A	501	FAD	O4B-C4B-C5B-O5B
5	C	502[B]	YJK	O1-C13-N3-C14
6	B	503	PEG	C4-C3-O2-C2
6	C	504	PEG	C1-C2-O2-C3
4	A	501	FAD	P-O3P-PA-O2A
4	C	501	FAD	P-O3P-PA-O2A
4	D	501	FAD	P-O3P-PA-O2A
5	A	502	YJK	C10-C11-C12-N2
5	B	502	YJK	C10-C11-C12-N2
5	A	502	YJK	O2-C11-C12-N2
5	C	502[A]	YJK	O2-C11-C12-N2
4	B	501	FAD	P-O3P-PA-O2A
5	C	502[A]	YJK	C10-C11-C12-N2
4	A	501	FAD	C3B-C4B-C5B-O5B
5	C	502[B]	YJK	O2-C11-C12-N2
4	D	501	FAD	O4B-C4B-C5B-O5B
5	A	502	YJK	C17-C18-C19-C20
5	A	502	YJK	C17-C18-C19-C24
5	C	502[B]	YJK	O1-C13-N2-C12
5	C	502[B]	YJK	N2-C13-N3-C14
5	C	502[B]	YJK	C17-C18-C19-C24
4	A	501	FAD	P-O3P-PA-O1A
4	C	501	FAD	PA-O3P-P-O5'
5	B	502	YJK	O2-C11-C12-N2
5	C	502[B]	YJK	C17-C18-C19-C20
4	C	501	FAD	P-O3P-PA-O1A
4	D	501	FAD	P-O3P-PA-O1A
6	C	503	PEG	O1-C1-C2-O2
4	D	501	FAD	C3B-C4B-C5B-O5B
5	A	502	YJK	N2-C13-N3-C33
5	C	502[A]	YJK	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
5	C	502[A]	YJK	C17-C18-C19-C24
4	B	501	FAD	PA-O3P-P-O2P
4	C	501	FAD	PA-O3P-P-O2P
5	C	502[B]	YJK	C17-C16-N4-C25

All (1) ring outliers are listed below:

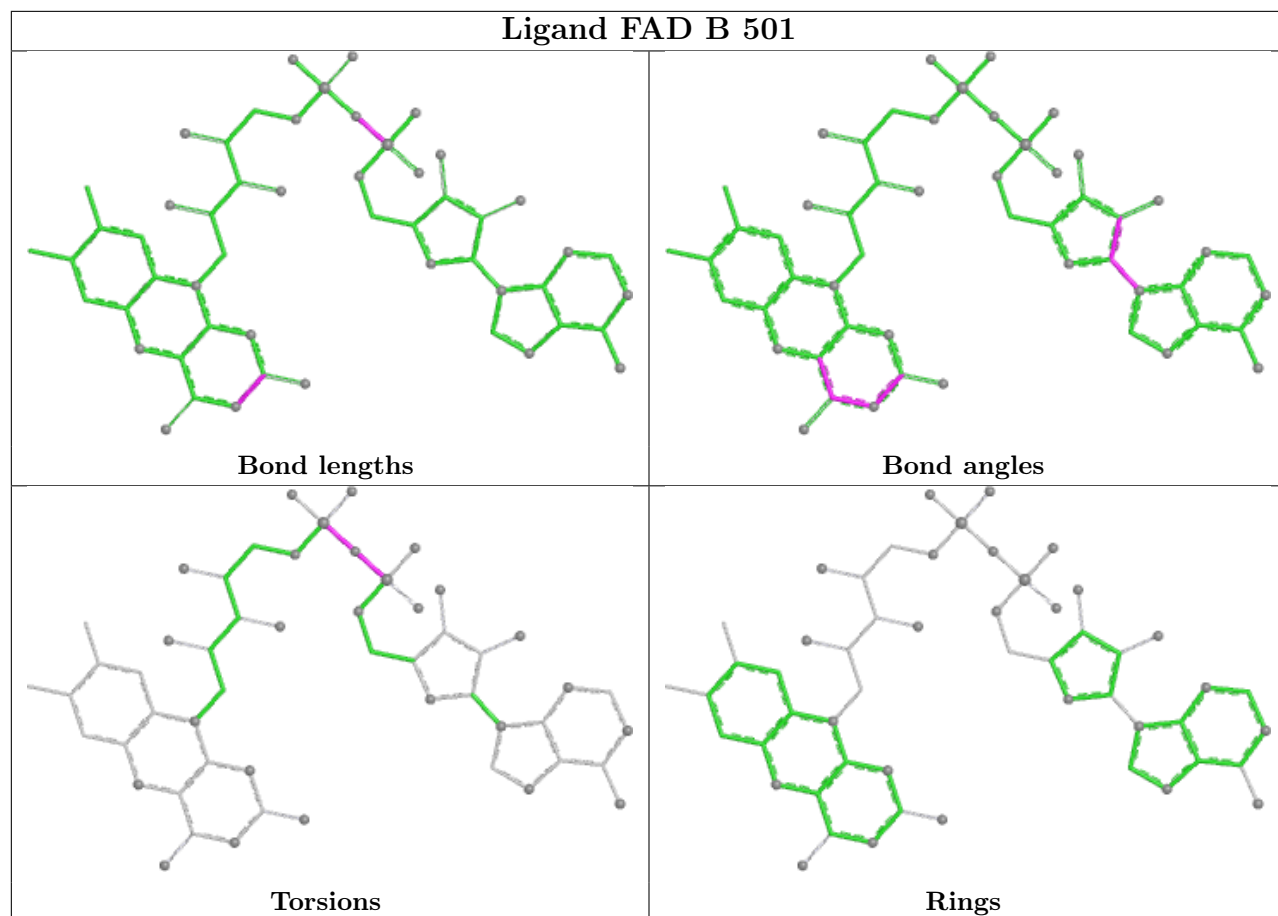
Mol	Chain	Res	Type	Atoms
5	B	502	YJK	C14-C15-C32-C33-N3-N4

7 monomers are involved in 21 short contacts:

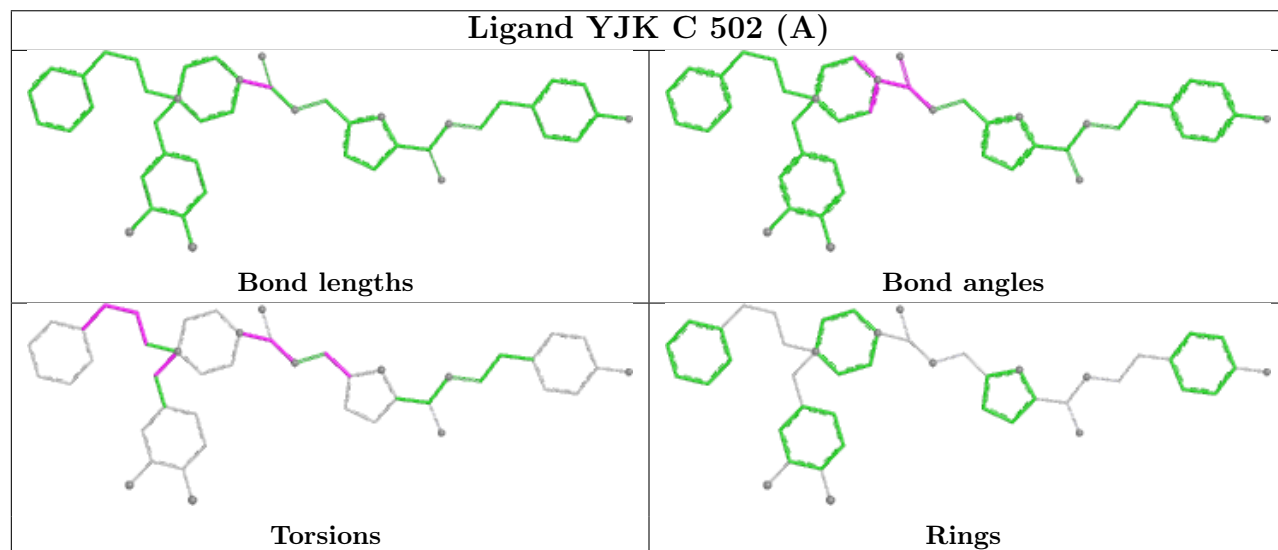
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	504	PEG	1	0
6	A	503	PEG	3	0
5	C	502[B]	YJK	5	0
6	C	503	PEG	5	0
7	A	504	DMS	5	0
4	C	501	FAD	1	0
5	A	502	YJK	1	0

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.

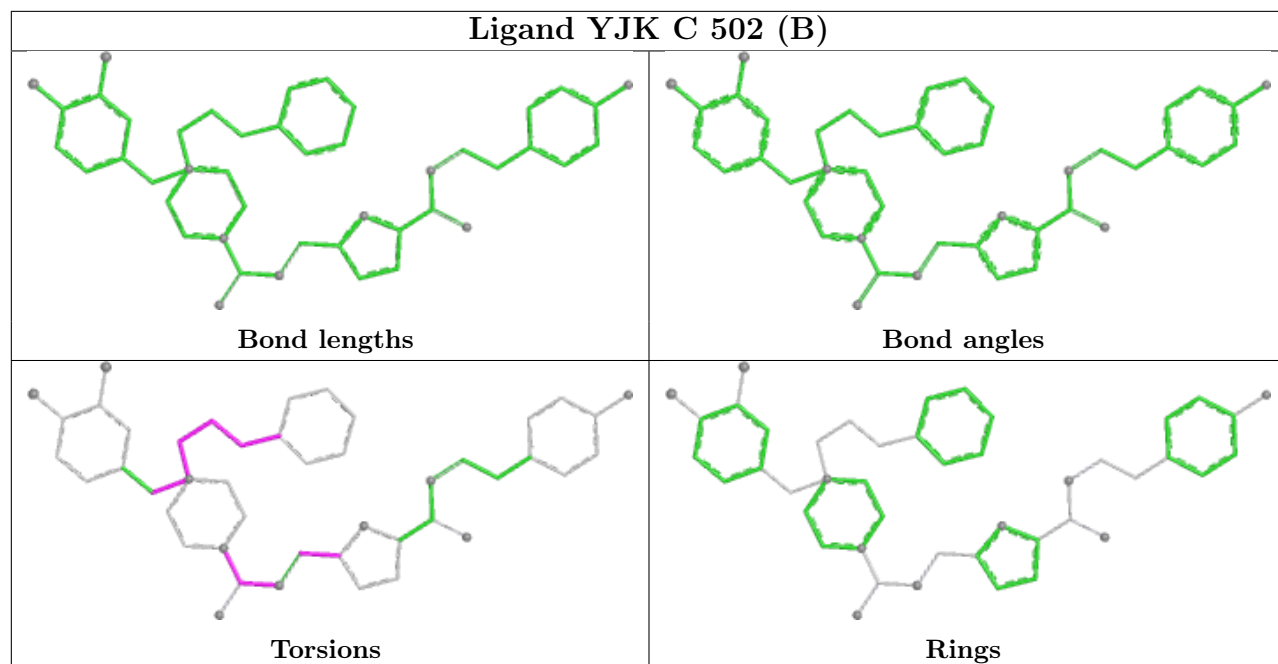
Ligand FAD B 501



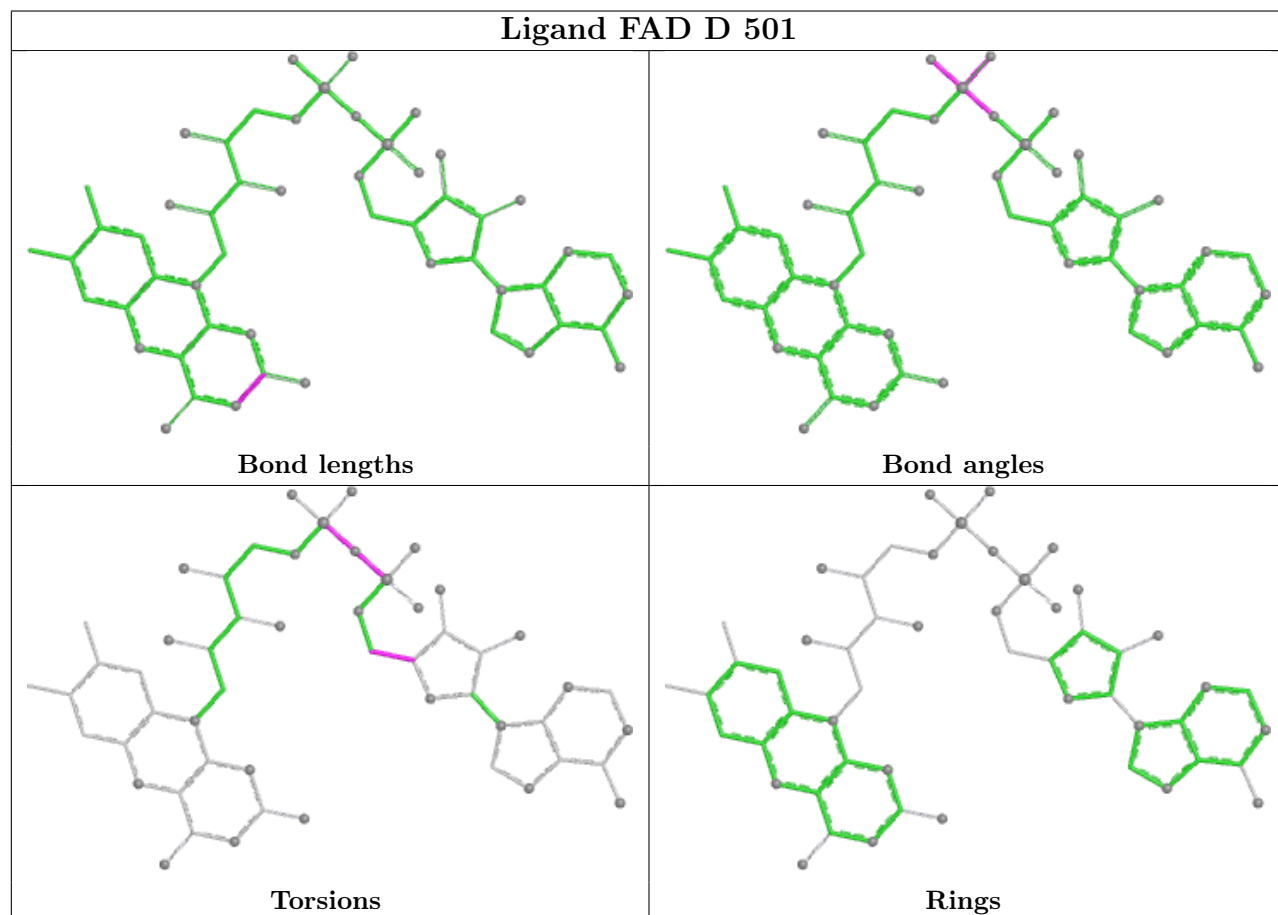
Ligand YJK C 502 (A)



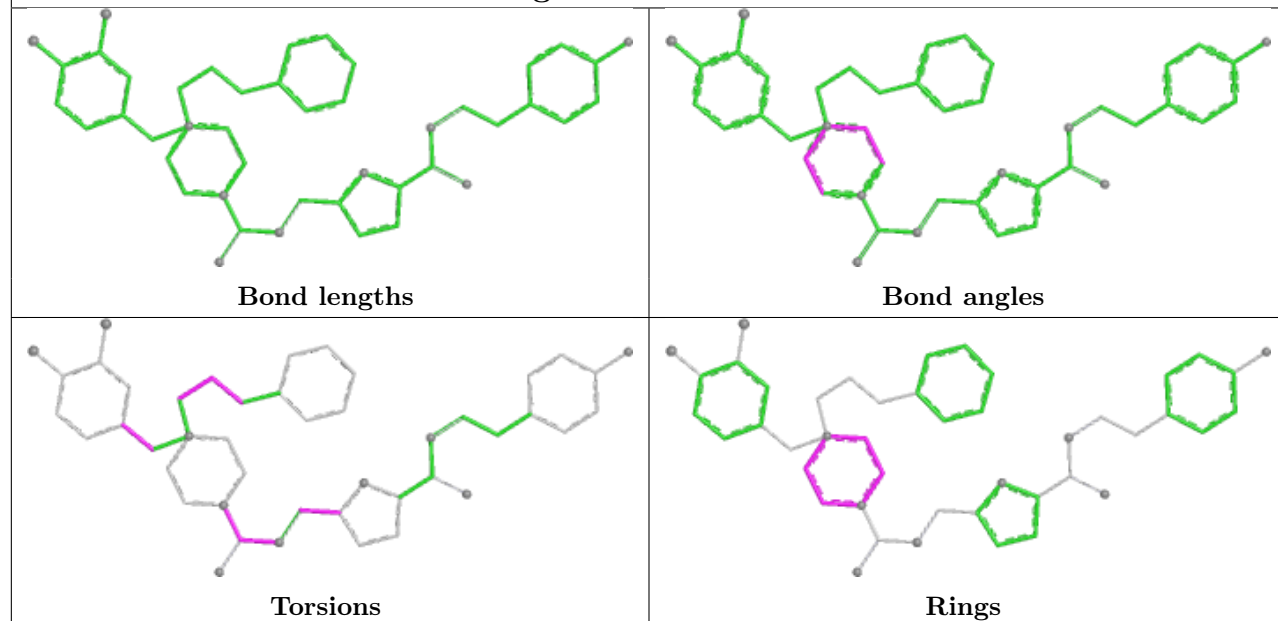
Ligand YJK C 502 (B)



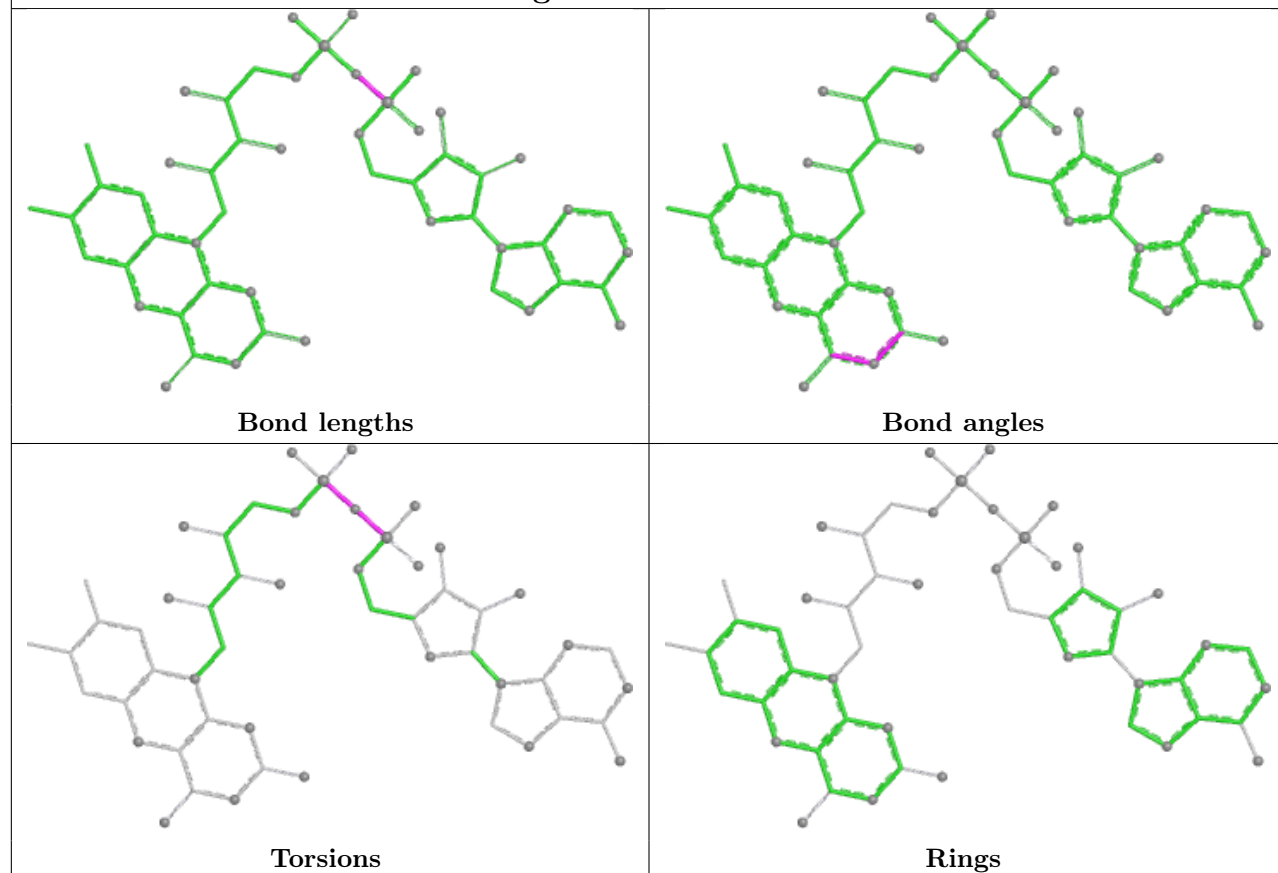
Ligand FAD D 501



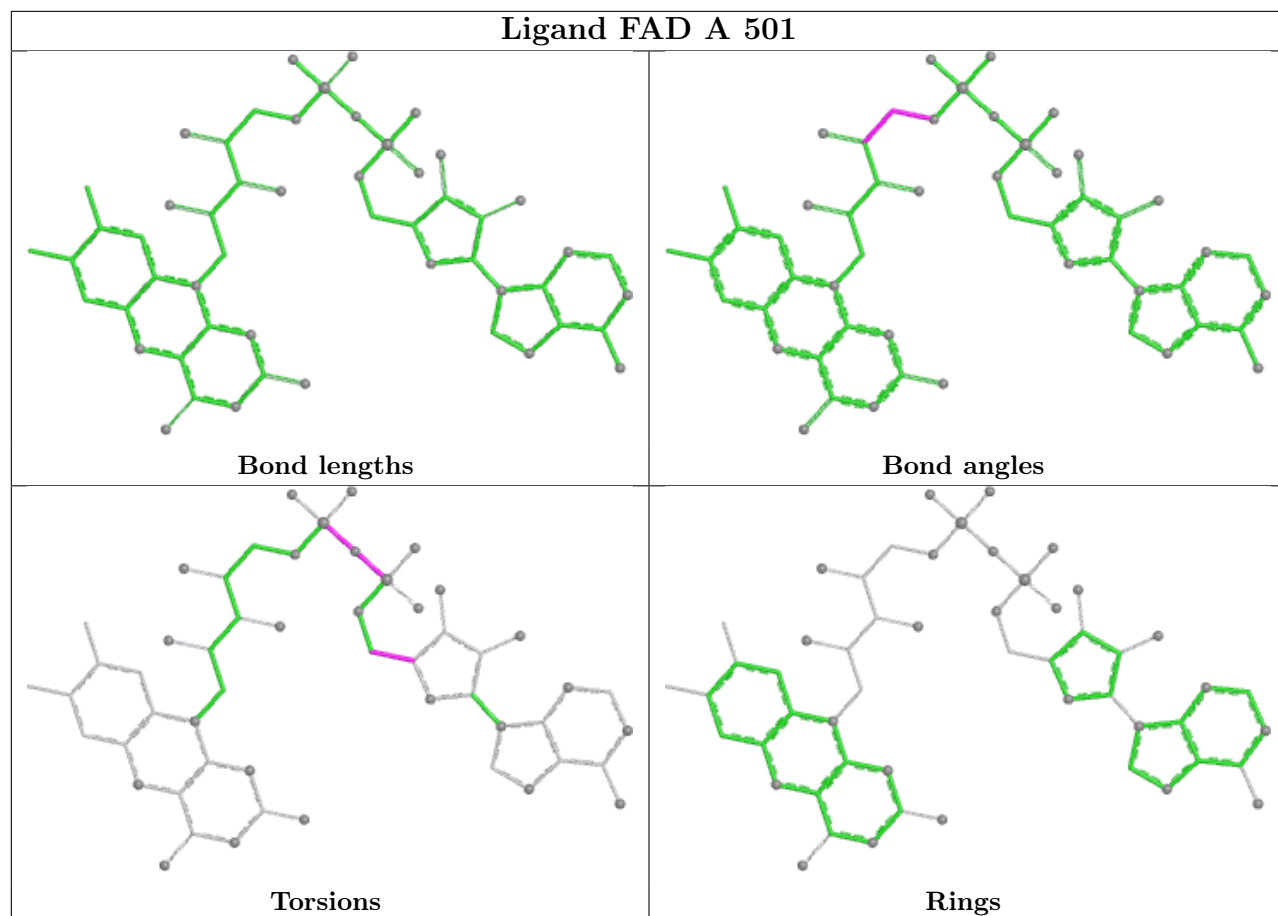
Ligand YJK B 502



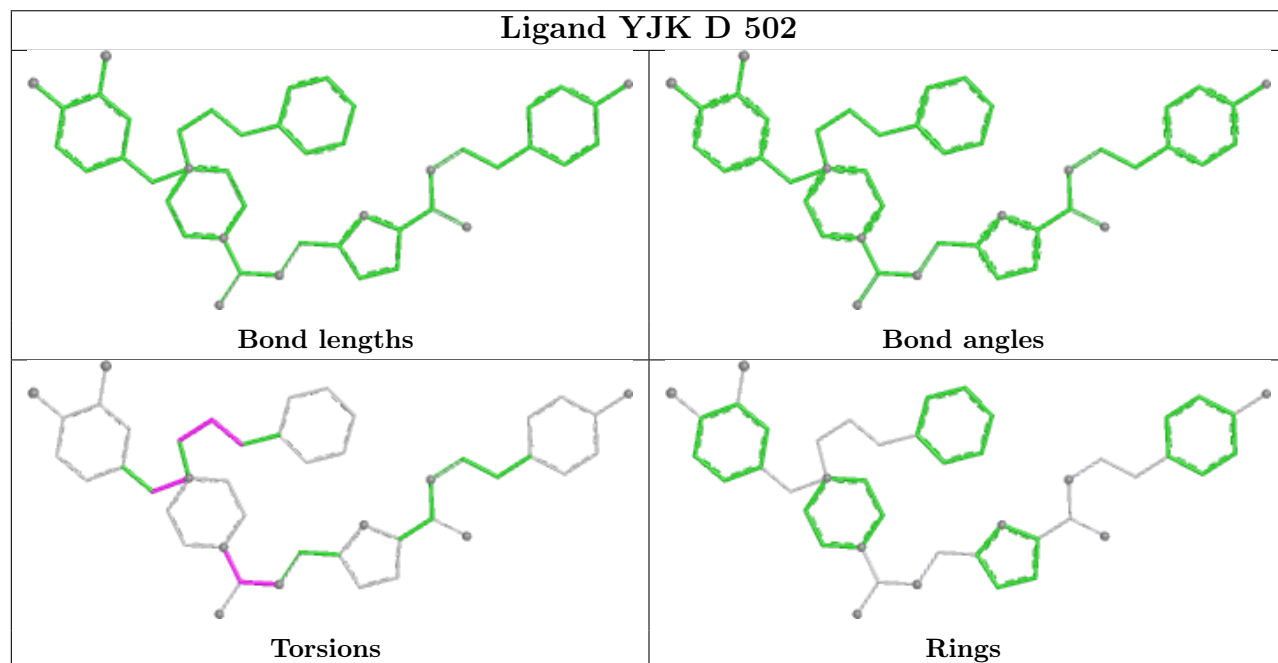
Ligand FAD C 501

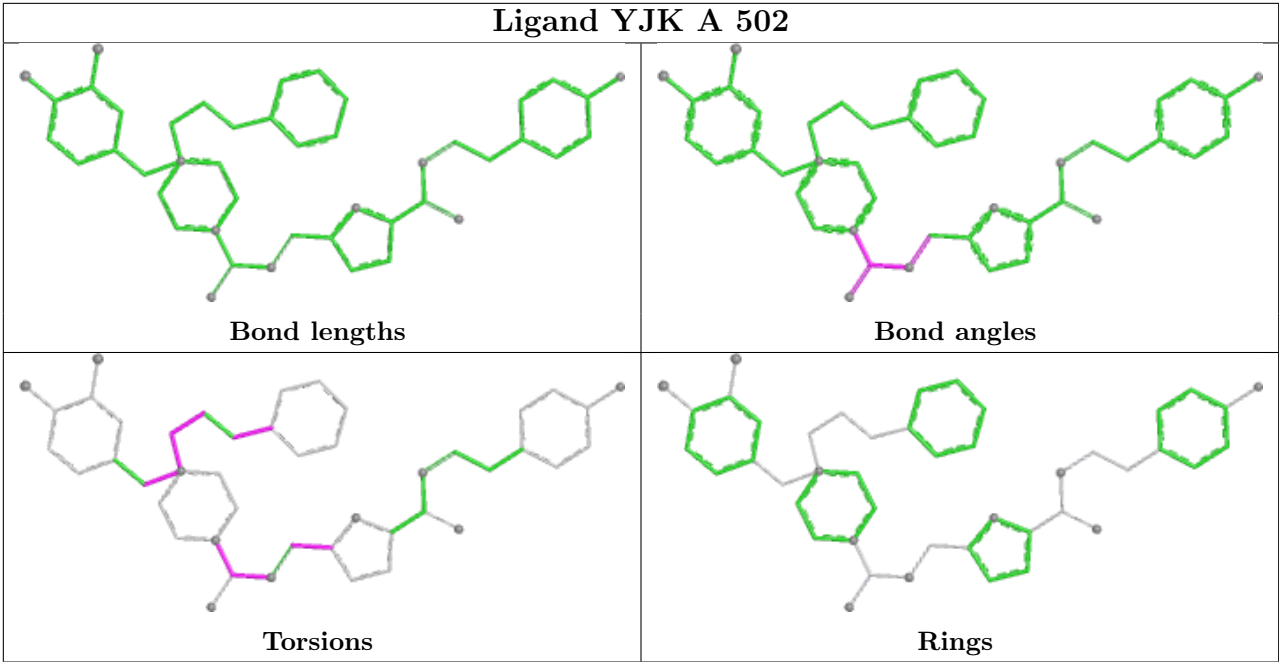


Ligand FAD A 501



Ligand YJK D 502





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	488:PRO	C	493:ASP	N	2.79

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	488/495 (98%)	-0.19	2 (0%) 88 87	23, 39, 65, 93	1 (0%)
2	B	490/494 (99%)	-0.26	2 (0%) 88 87	24, 36, 57, 85	2 (0%)
2	C	488/494 (98%)	0.04	10 (2%) 65 61	24, 44, 82, 112	3 (0%)
3	D	491/495 (99%)	-0.16	4 (0%) 82 80	26, 39, 62, 99	3 (0%)
All	All	1957/1978 (98%)	-0.14	18 (0%) 81 79	23, 39, 71, 112	9 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	455[A]	TYR	3.7
2	C	152[A]	GLN	3.0
3	D	488	PRO	2.9
2	C	488	PRO	2.8
2	C	30	ARG	2.8
2	C	354	PRO	2.5
1	A	2	SER	2.5
1	A	488	PRO	2.3
2	C	352	ASN	2.3
2	C	1	MET	2.3
2	C	4	ALA	2.2
3	D	487	LEU	2.2
2	C	320	PRO	2.2
2	B	455[A]	TYR	2.2
2	B	111	GLU	2.1
2	C	472	ARG	2.1
2	C	331	ARG	2.1
3	D	353	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

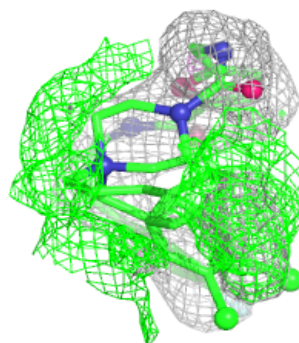
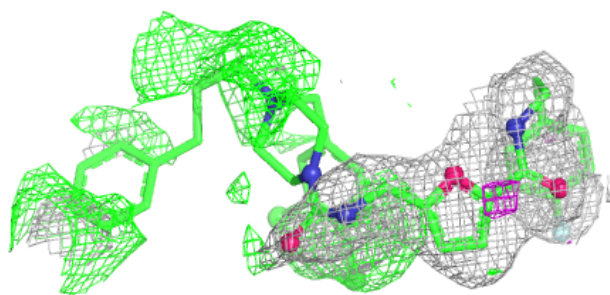
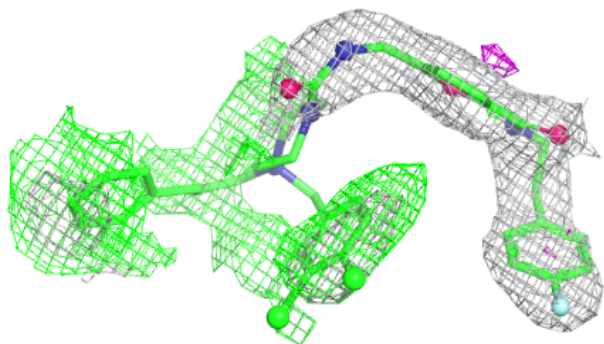
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	B	503	7/7	0.62	0.44	40,41,43,44	7
7	DMS	A	504	4/4	0.71	0.32	76,78,81,95	0
5	YJK	A	502	45/45	0.75	0.39	43,59,69,72	24
5	YJK	B	502	45/45	0.75	0.31	44,72,85,87	24
5	YJK	D	502	45/45	0.79	0.33	50,63,81,89	24
7	DMS	D	503	4/4	0.79	0.23	99,102,107,108	0
6	PEG	C	504	7/7	0.80	0.18	53,61,66,68	0
6	PEG	C	503	7/7	0.84	0.17	40,50,56,59	0
6	PEG	A	503	7/7	0.84	0.18	43,44,56,60	0
5	YJK	C	502[B]	45/45	0.87	0.16	53,76,96,98	45
5	YJK	C	502[A]	45/45	0.87	0.16	44,56,67,76	45
4	FAD	C	501	53/53	0.96	0.06	29,35,44,48	0
4	FAD	A	501	53/53	0.97	0.06	24,32,45,47	0
4	FAD	B	501	53/53	0.97	0.06	23,28,32,37	0
4	FAD	D	501	53/53	0.98	0.05	25,29,35,40	0

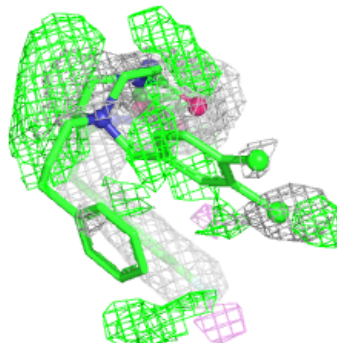
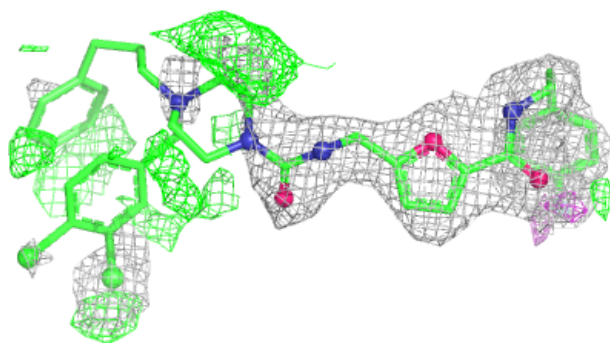
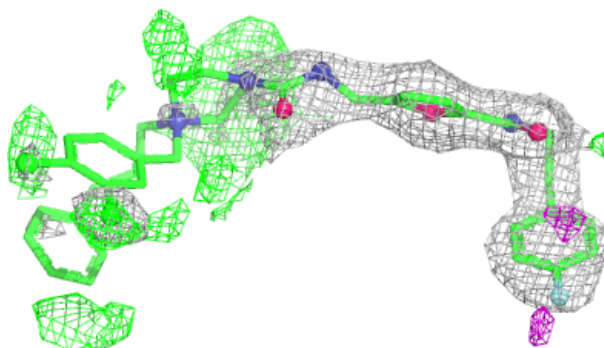
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YJK 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)

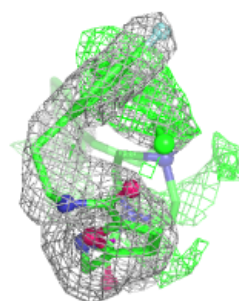
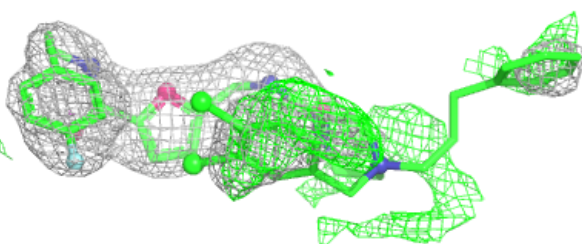
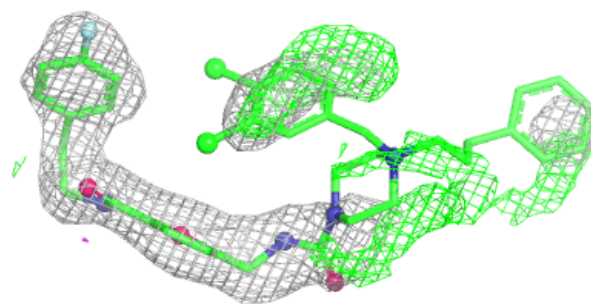
**Electron density around YJK B 502:**

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

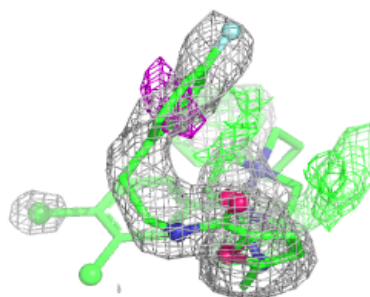
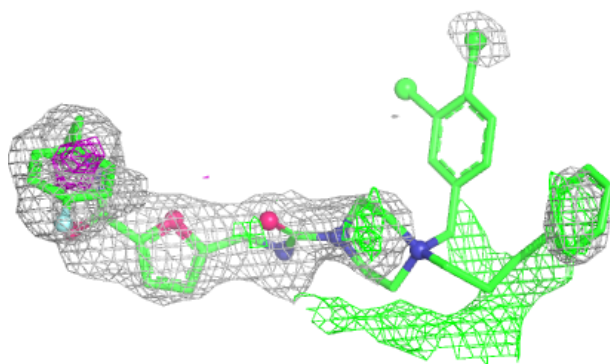
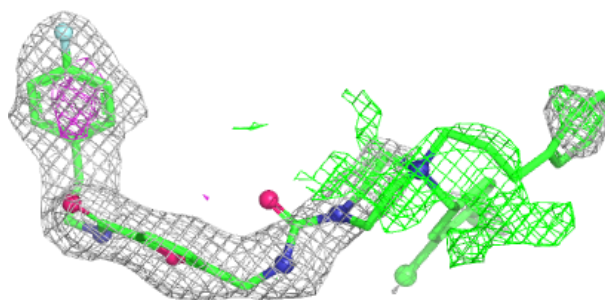


Electron density around YJK D 502:

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

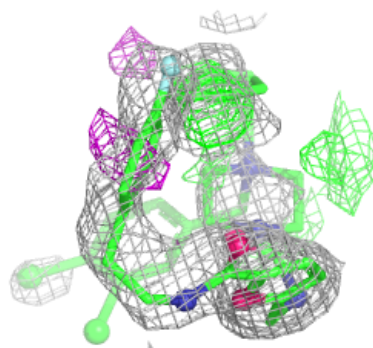
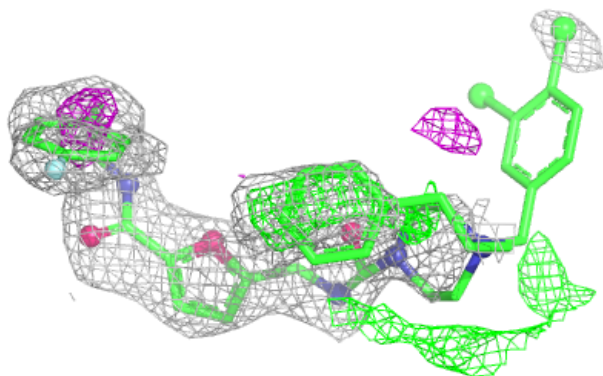
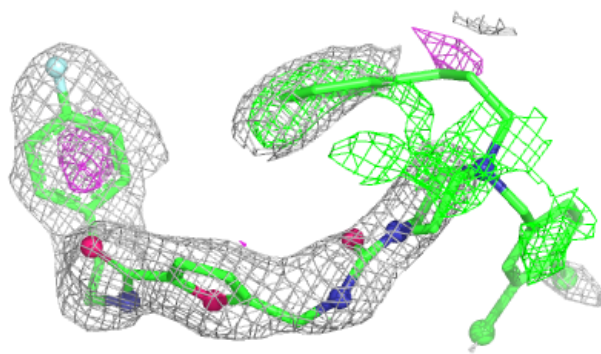
**Electron density around YJK C 502 (B):**

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

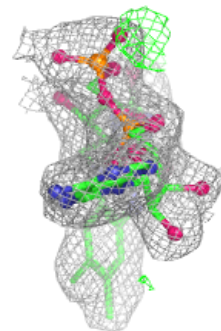
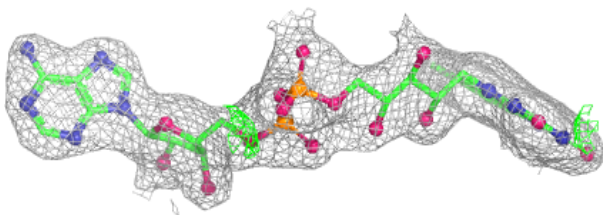
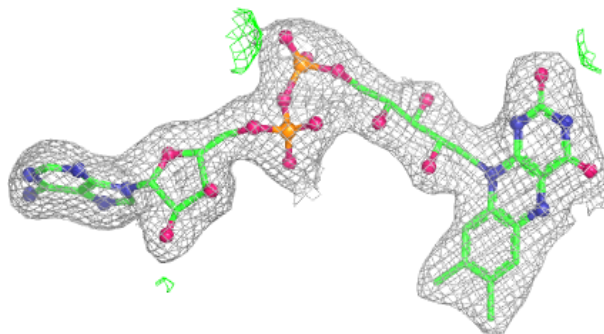


Electron density around YJK C 502 (A):

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

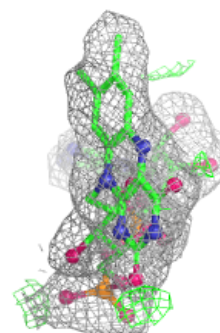
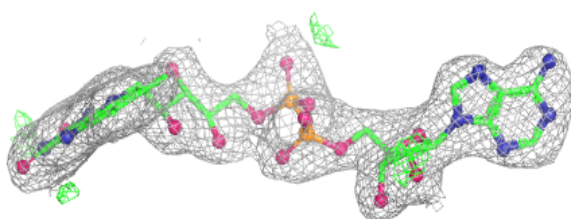
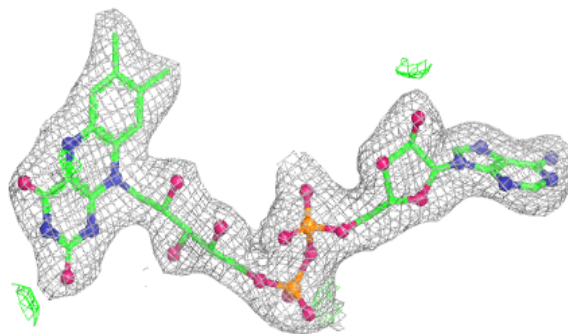
**Electron density around FAD C 501:**

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

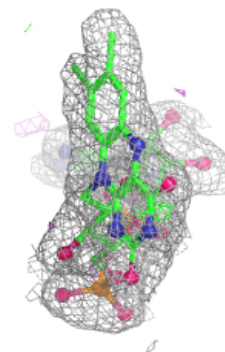
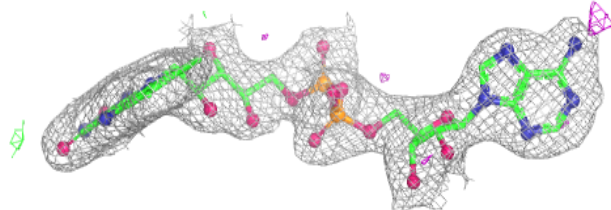
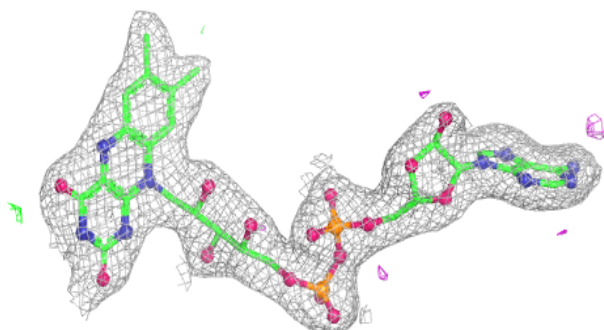


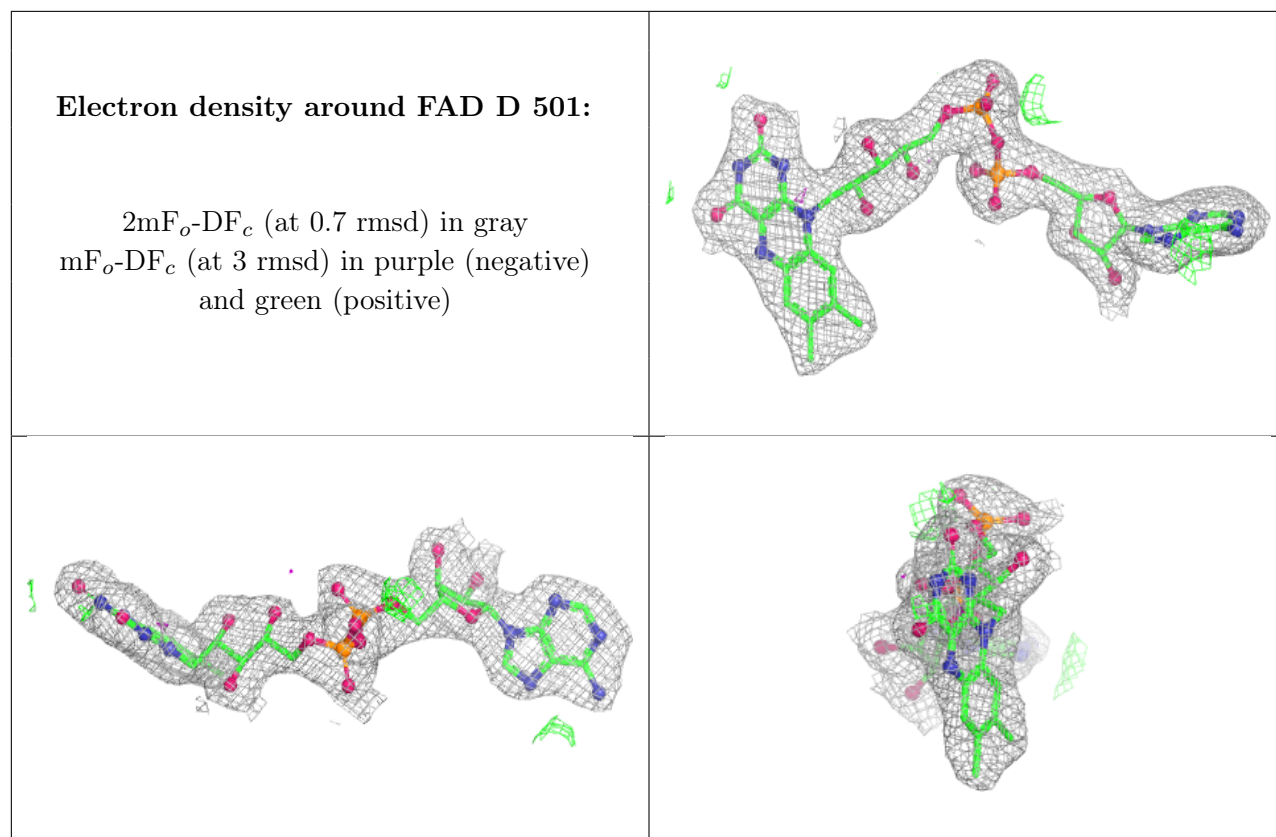
Electron density around FAD A 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.