



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2024 – 07:43 pm GMT

PDB ID : 8PF5
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
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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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

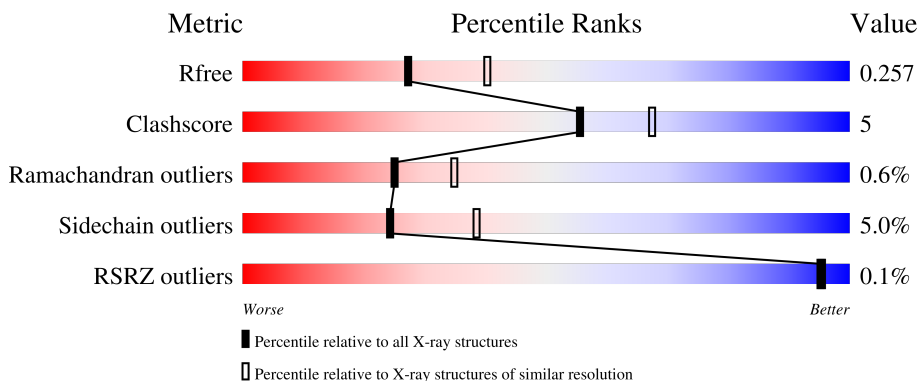
1 Overall quality at a glance

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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (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	81% 16% ..
2	B	494	84% 14% ..
2	C	494	84% 14% ..
3	D	495	85% 13% ..

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	C	503	-	-	X	-
7	DMS	A	504	-	-	X	-

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	488	3711	2360	630	702	19	0	1	0

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
			Total	C	N	O	S			
2	B	490	3739	2380	636	703	20	0	2	0
2	C	488	3732	2376	634	702	20	0	3	0

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

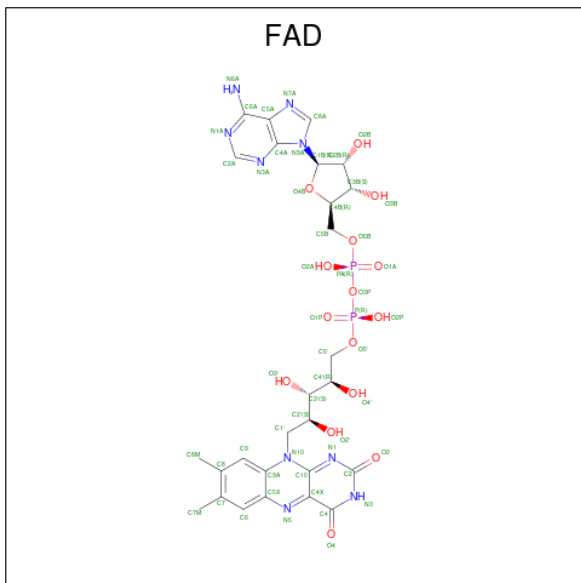
- Molecule 3 is a protein called Trypanothione reductase.

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

There are 3 discrepancies between the modelled and reference sequences:

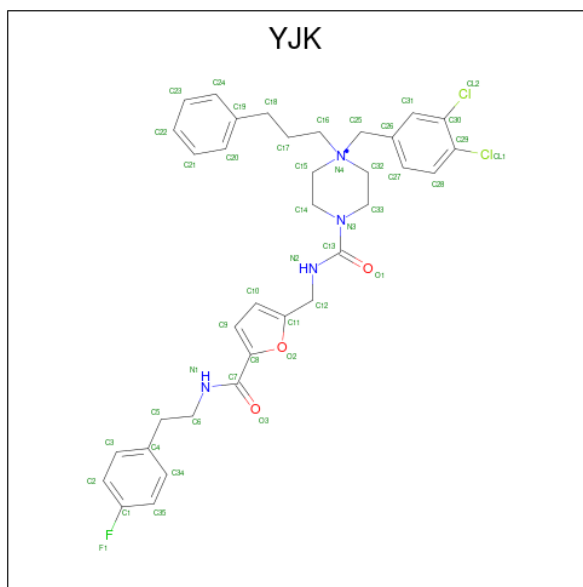
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP A0A3L6KZJ1
D	-1	SER	-	expression tag	UNP A0A3L6KZJ1
D	0	HIS	-	expression tag	UNP A0A3L6KZJ1

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



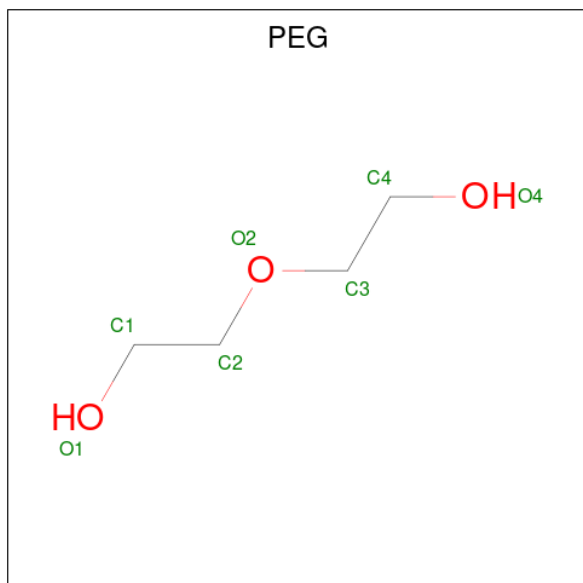
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	53	27	9	15	2	0	0
4	B	1	53	27	9	15	2	0	0
4	C	1	53	27	9	15	2	0	0
4	D	1	53	27	9	15	2	0	0

- Molecule 5 is 4-[(3,4-dichlorophenyl)methyl]-{N}-[[5-[2-(4-fluorophenyl)ethylcarbamoyl]furan-2-yl]methyl]-4-(3-phenylpropyl)-1,4-diazinane-1-carboxamide (three-letter code: YJK) (formula: $C_{35}H_{38}Cl_2FN_4O_3$) (labeled as "Ligand of Interest" by depositor).



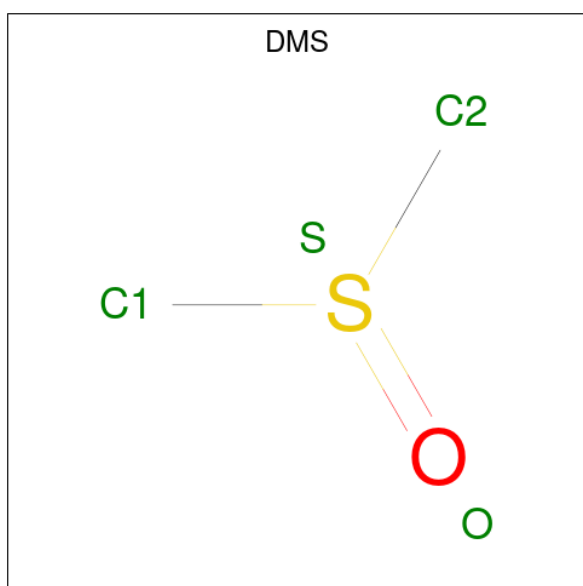
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	Cl	F	N			O	
5	A	1	Total	45	35	2	1	4	3	0	0
5	B	1	Total	45	35	2	1	4	3	0	0
5	C	1	Total	90	70	4	2	8	6	24	1
5	D	1	Total	45	35	2	1	4	3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: 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 (three-letter code: DMS) (formula: C₂H₆OS).



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

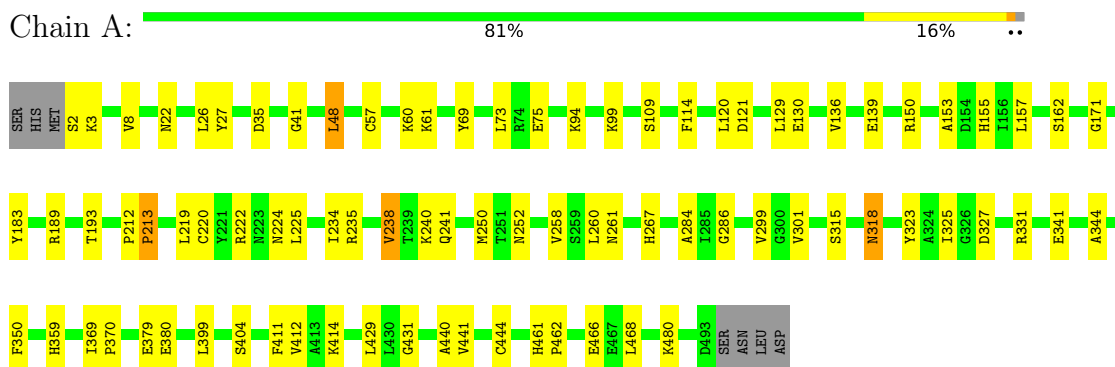
- Molecule 8 is water.

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

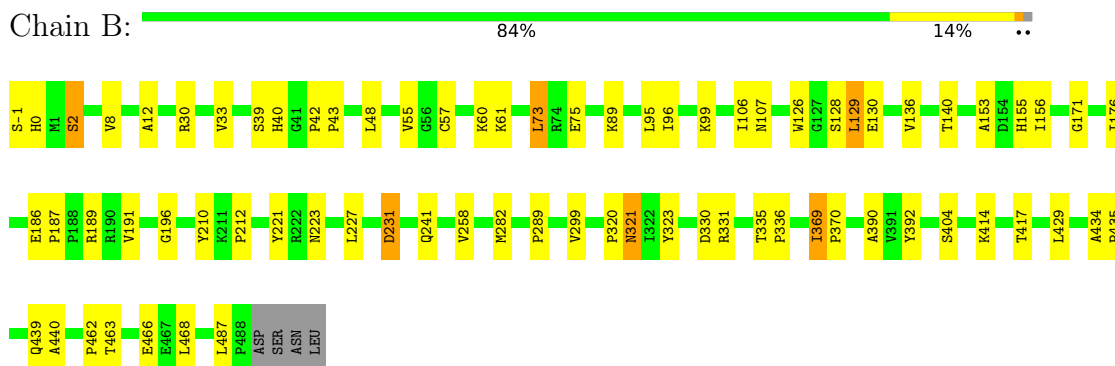
3 Residue-property plots [i](#)

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.

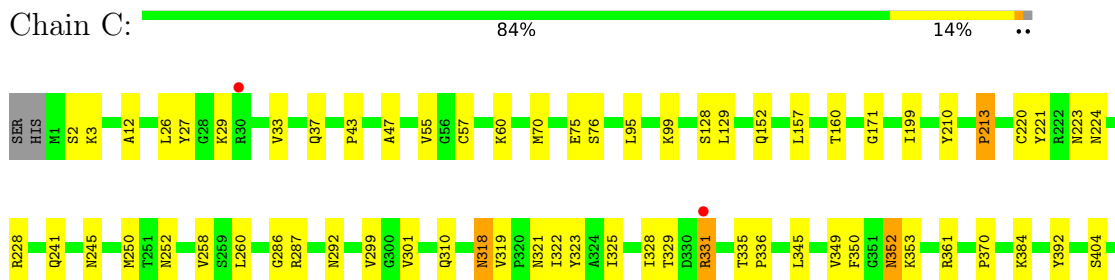
- Molecule 1: Trypanothione reductase



- Molecule 2: Trypanothione reductase



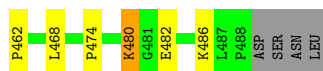
- Molecule 2: Trypanothione reductase





- Molecule 3: Trypanothione reductase

Chain D: 85% 13% ..



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 55.77 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.8 (55.83-2.42) 99.8 (55.77-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.42Å)	Xtrriage
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 (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: PEG, FAD, YJK, DMS

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	0.70	0/3791	0.87	0/5142
2	B	0.70	0/3825	0.88	0/5188
2	C	0.70	0/3817	0.85	0/5177
3	D	0.71	0/3832	0.86	0/5195
All	All	0.70	0/15265	0.86	0/20702

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 [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	3711	0	3717	46	0
2	B	3739	0	3754	41	0
2	C	3732	0	3749	31	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	0	0
4	D	53	0	31	0	0
5	A	45	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	45	0	0	1	0
5	C	90	0	0	5	0
5	D	45	0	0	3	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	4	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	157	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 (157) 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:A:502:YJK:C18	5:A:502:YJK:C32	1.93	1.46
5:C:502[B]:YJK:C18	5:C:502[B]:YJK:C25	2.34	1.05
5:A:502:YJK:C33	5:A:502:YJK:C27	2.38	1.02
5:A:502:YJK:C33	5:A:502:YJK:C26	2.30	1.02
5:C:502[B]:YJK:C27	5:C:502[B]:YJK:C20	2.42	0.97
5:D:502:YJK:C14	5:D:502:YJK:C26	2.57	0.80
1:A:234:ILE:O	1:A:238:VAL:HG12	1.84	0.77
2:B:-1:SER:N	8:B:601:HOH:O	2.20	0.75
1:A:341:GLU:O	7:A:504:DMS:H22	1.88	0.74
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
5:D:502:YJK:C14	5:D:502:YJK:C31	2.76	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:69:TYR:O	3:D:73:LEU:HG	2.02	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
5:D:502:YJK:C27	5:D:502:YJK:C15	2.84	0.55
2:B:0:HIS:CD2	8:B:652:HOH:O	2.60	0.55
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:261:ASN:HD21	1:A:267:HIS:HB2	1.74	0.52
2:B:231:ASP:OD2	2:B:414:LYS:NZ	2.36	0.52
2:B:390:ALA:HB3	2:B:417:THR:OG1	2.09	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
5:A:502:YJK:C32	5:A:502:YJK:C31	2.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:A:502:YJK:C33	5:A:502:YJK:C31	2.89	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
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
1:A:379:GLU:OE1	1:A:414:LYS:NZ	2.48	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:286:GLY:C	6:C:503:PEG:H31	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:392:TYR:O	2:B:414:LYS:HA	2.19	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
3:D:40:HIS:HB3	3:D:54:ASN:OD1	2.19	0.43
3:D:220:CYS:HA	3:D:250:MET:O	2.19	0.43
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
1:A:315:SER:OG	7:A:504:DMS:C2	2.68	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
5:B:502:YJK:C27	5:B:502:YJK:C32	2.97	0.42
1:A:27:TYR:CD1	1:A:350:PHE:O	2.72	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:315:SER:OG	7:A:504:DMS:H21	2.20	0.41
1:A:219:LEU:C	1:A:219:LEU:HD23	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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%)	34 47
2	B	490/494 (99%)	468 (96%)	19 (4%)	3 (1%)	25 35
2	C	489/494 (99%)	464 (95%)	20 (4%)	5 (1%)	15 22
3	D	492/495 (99%)	469 (95%)	21 (4%)	2 (0%)	34 47
All	All	1957/1978 (99%)	1865 (95%)	80 (4%)	12 (1%)	25 35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	352	ASN
2	C	213	PRO

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Mol	Chain	Res	Type
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 [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	402/408 (98%)	382 (95%)	20 (5%)	24	38
2	B	405/407 (100%)	388 (96%)	17 (4%)	30	46
2	C	404/407 (99%)	380 (94%)	24 (6%)	19	30
3	D	404/407 (99%)	382 (95%)	22 (5%)	22	34
All	All	1615/1629 (99%)	1532 (95%)	83 (5%)	24	37

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	35	ASP
1	A	57	CYS
1	A	60	LYS
1	A	94	LYS
1	A	99	LYS
1	A	109	SER
1	A	121	ASP
1	A	129	LEU
1	A	139	GLU
1	A	213	PRO

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Mol	Chain	Res	Type
1	A	224	ASN
1	A	238	VAL
1	A	240	LYS
1	A	260	LEU
1	A	318	ASN
1	A	331	ARG
1	A	380	GLU
1	A	399	LEU
1	A	480	LYS
2	B	2	SER
2	B	30	ARG
2	B	39	SER
2	B	57	CYS
2	B	60	LYS
2	B	61	LYS
2	B	73	LEU
2	B	89	LYS
2	B	99	LYS
2	B	128	SER
2	B	129	LEU
2	B	191	VAL
2	B	231	ASP
2	B	321	ASN
2	B	331	ARG
2	B	369	ILE
2	B	487	LEU
2	C	3	LYS
2	C	57	CYS
2	C	60	LYS
2	C	99	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	310	GLN
2	C	318	ASN
2	C	321	ASN
2	C	323	TYR

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Mol	Chain	Res	Type
2	C	331	ARG
2	C	345	LEU
2	C	349	VAL
2	C	352	ASN
2	C	353	LYS
2	C	384	LYS
2	C	470	SER
2	C	475	SER
3	D	57	CYS
3	D	60	LYS
3	D	71	ASP
3	D	89	LYS
3	D	118	GLU
3	D	129	LEU
3	D	131	SER
3	D	191	VAL
3	D	240	LYS
3	D	260	LEU
3	D	266	LYS
3	D	274	LYS
3	D	302	LYS
3	D	328	ILE
3	D	331	ARG
3	D	353	LYS
3	D	385	GLU
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	152	GLN
1	A	252	ASN
1	A	261	ASN
1	A	318	ASN
1	A	359	HIS
2	B	107	ASN
2	B	152	GLN

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Mol	Chain	Res	Type
2	B	224	ASN
2	C	245	ASN
2	C	252	ASN
2	C	318	ASN
3	D	107	ASN
3	D	252	ASN
3	D	292	ASN
3	D	310	GLN
3	D	321	ASN
3	D	359	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	501	-	53,58,58	0.79	1 (1%)	68,89,89	0.88	2 (2%)
5	YJK	D	502	-	46,49,49	0.75	2 (4%)	59,67,67	0.73	1 (1%)
5	YJK	B	502	-	46,49,49	0.71	2 (4%)	59,67,67	0.84	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DMS	D	503	-	3,3,3	0.26	0	3,3,3	0.05	0
6	PEG	C	504	-	6,6,6	0.43	0	5,5,5	0.41	0
7	DMS	A	504	-	3,3,3	0.37	0	3,3,3	0.26	0
4	FAD	C	501	-	53,58,58	0.60	0	68,89,89	0.79	0
5	YJK	A	502	-	46,49,49	0.67	2 (4%)	59,67,67	2.01	4 (6%)
5	YJK	C	502[B]	-	46,49,49	0.78	2 (4%)	59,67,67	0.65	1 (1%)
5	YJK	C	502[A]	-	46,49,49	1.40	3 (6%)	59,67,67	13.08	5 (8%)
6	PEG	A	503	-	6,6,6	0.50	0	5,5,5	0.40	0
6	PEG	C	503	-	6,6,6	0.39	0	5,5,5	0.35	0
4	FAD	B	501	-	53,58,58	0.80	1 (1%)	68,89,89	0.86	3 (4%)
4	FAD	A	501	-	53,58,58	0.63	0	68,89,89	0.80	2 (2%)
6	PEG	B	503	-	6,6,6	0.17	0	5,5,5	0.09	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
4	FAD	D	501	-	-	5/30/50/50	0/6/6/6
5	YJK	D	502	-	-	11/26/43/43	0/5/5/5
5	YJK	B	502	-	-	11/26/43/43	1/5/5/5
6	PEG	C	504	-	-	2/4/4/4	-
4	FAD	C	501	-	-	4/30/50/50	0/6/6/6
5	YJK	A	502	-	-	13/26/43/43	0/5/5/5
5	YJK	C	502[B]	-	-	14/26/43/43	0/5/5/5
5	YJK	C	502[A]	-	-	11/26/43/43	0/5/5/5
6	PEG	A	503	-	-	3/4/4/4	-
6	PEG	C	503	-	-	2/4/4/4	-
4	FAD	B	501	-	-	3/30/50/50	0/6/6/6
4	FAD	A	501	-	-	5/30/50/50	0/6/6/6
6	PEG	B	503	-	-	3/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502[A]	YJK	C13-N3	-7.80	1.21	1.36
5	C	502[B]	YJK	C10-C11	-3.84	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	YJK	C10-C11	-3.79	1.34	1.39
5	C	502[A]	YJK	C10-C11	-3.79	1.34	1.39
5	B	502	YJK	C10-C11	-3.12	1.35	1.39
5	A	502	YJK	C10-C11	-2.78	1.35	1.39
5	C	502[A]	YJK	C12-C11	-2.65	1.48	1.51
5	C	502[B]	YJK	C12-C11	-2.59	1.48	1.51
5	B	502	YJK	C12-C11	-2.52	1.48	1.51
5	D	502	YJK	C12-C11	-2.49	1.48	1.51
4	D	501	FAD	C2-N3	-2.40	1.33	1.39
5	A	502	YJK	C12-C11	-2.29	1.49	1.51
4	B	501	FAD	C2-N3	-2.27	1.33	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502[A]	YJK	N2-C13-N3	91.73	161.78	117.67
5	C	502[A]	YJK	O1-C13-N3	-40.06	65.47	121.78
5	A	502	YJK	N2-C13-N3	12.90	123.87	117.67
5	C	502[A]	YJK	C14-N3-C13	-5.41	102.00	121.94
5	A	502	YJK	C12-N2-C13	4.99	125.34	120.84
5	C	502[A]	YJK	C33-N3-C13	4.38	138.10	121.94
5	B	502	YJK	C12-C11-C10	3.90	135.48	129.01
5	A	502	YJK	C12-C11-C10	3.40	134.65	129.01
4	D	501	FAD	P-O3P-PA	3.39	144.47	132.83
5	A	502	YJK	O1-C13-N3	-2.76	117.90	121.78
5	C	502[A]	YJK	C12-C11-C10	2.62	133.35	129.01
5	D	502	YJK	C12-C11-C10	2.52	133.19	129.01
5	C	502[B]	YJK	C12-C11-C10	2.48	133.12	129.01
5	B	502	YJK	C14-C15-N4	2.39	111.37	108.75
4	A	501	FAD	C5A-C6A-N6A	2.35	123.92	120.35
4	B	501	FAD	C5A-C6A-N6A	2.24	123.75	120.35
5	B	502	YJK	C33-C32-N4	2.15	111.11	108.75
4	A	501	FAD	O5'-C5'-C4'	2.11	115.00	109.36
4	D	501	FAD	C5A-C6A-N6A	2.11	123.56	120.35
4	B	501	FAD	C4X-C4-N3	2.08	118.48	113.19
4	B	501	FAD	C4-N3-C2	-2.02	121.91	125.64

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	YJK	N3-C13-N2-C12

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Mol	Chain	Res	Type	Atoms
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	B	502	YJK	O3-C7-C8-C9
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
6	B	503	PEG	C1-C2-O2-C3
5	D	502	YJK	N4-C16-C17-C18
5	A	502	YJK	C17-C16-N4-C25
6	A	503	PEG	O2-C3-C4-O4
5	B	502	YJK	N4-C16-C17-C18
5	C	502[A]	YJK	O1-C13-N3-C33
5	D	502	YJK	O1-C13-N3-C33

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Mol	Chain	Res	Type	Atoms
4	A	501	FAD	O4B-C4B-C5B-O5B
5	B	502	YJK	N2-C13-N3-C33
6	B	503	PEG	O1-C1-C2-O2
6	C	503	PEG	O2-C3-C4-O4
5	B	502	YJK	C16-C17-C18-C19
6	A	503	PEG	O1-C1-C2-O2
6	C	504	PEG	O2-C3-C4-O4
5	C	502[B]	YJK	C16-C17-C18-C19
5	C	502[B]	YJK	O1-C13-N3-C14
4	A	501	FAD	PA-O3P-P-O5'
4	B	501	FAD	PA-O3P-P-O5'
4	D	501	FAD	PA-O3P-P-O5'
4	D	501	FAD	O4B-C4B-C5B-O5B
6	A	503	PEG	C4-C3-O2-C2
5	C	502[B]	YJK	N3-C13-N2-C12
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
4	A	501	FAD	C3B-C4B-C5B-O5B
5	C	502[B]	YJK	N2-C13-N3-C14
5	C	502[B]	YJK	O1-C13-N2-C12
4	B	501	FAD	P-O3P-PA-O2A
5	A	502	YJK	C17-C18-C19-C20
5	A	502	YJK	C17-C18-C19-C24
5	A	502	YJK	O1-C13-N3-C33
5	C	502[B]	YJK	C17-C18-C19-C24
4	A	501	FAD	P-O3P-PA-O1A
5	A	502	YJK	N2-C13-N3-C33
5	B	502	YJK	N2-C13-N3-C14
5	D	502	YJK	N2-C13-N3-C14
4	C	501	FAD	PA-O3P-P-O5'
4	D	501	FAD	C3B-C4B-C5B-O5B
5	C	502[B]	YJK	C17-C18-C19-C20
4	C	501	FAD	O4B-C4B-C5B-O5B
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	B	501	FAD	O4B-C4B-C5B-O5B
5	C	502[B]	YJK	C17-C16-N4-C25
5	C	502[A]	YJK	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
5	D	502	YJK	N4-C25-C26-C27
5	C	502[A]	YJK	C17-C18-C19-C24

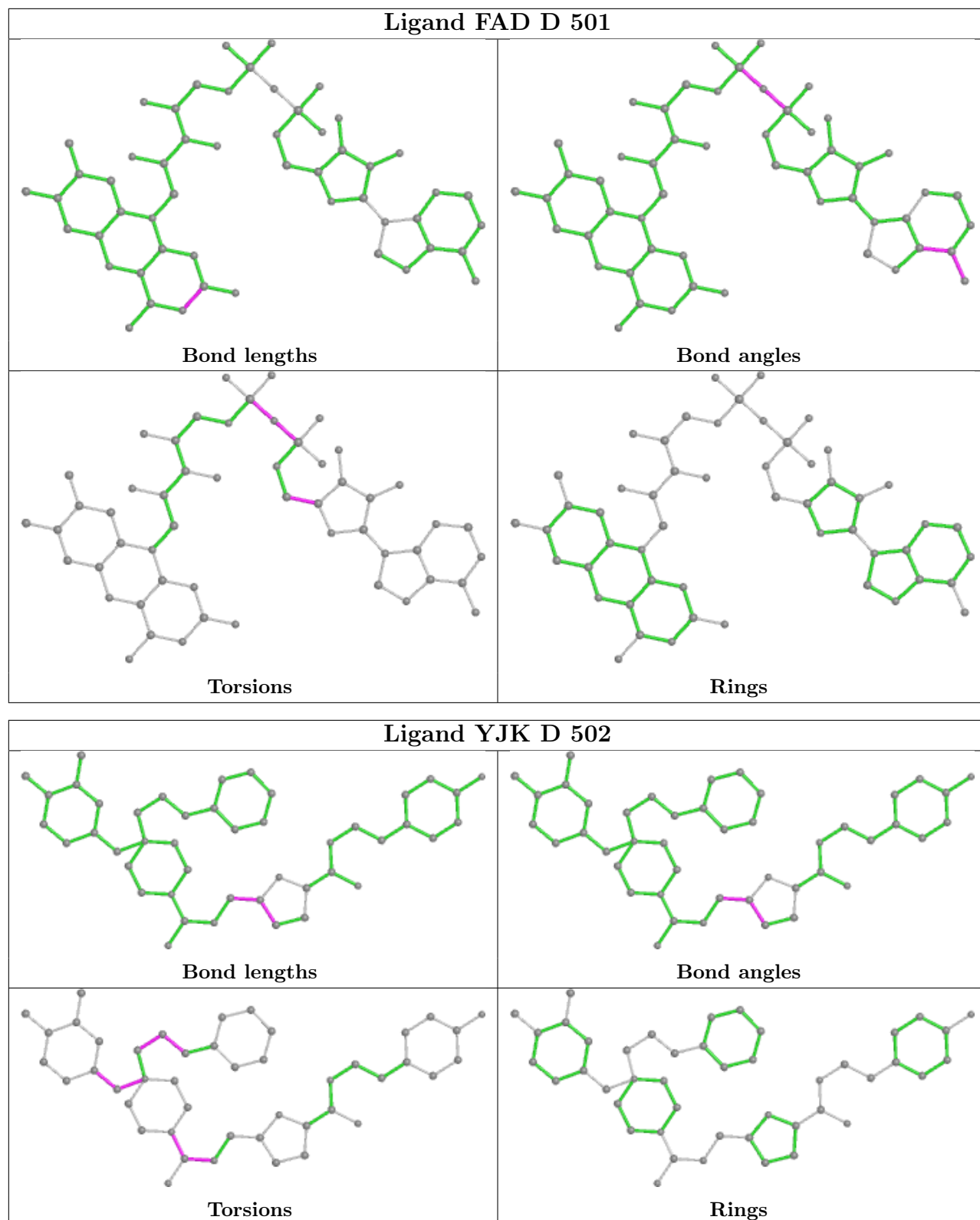
All (1) ring outliers are listed below:

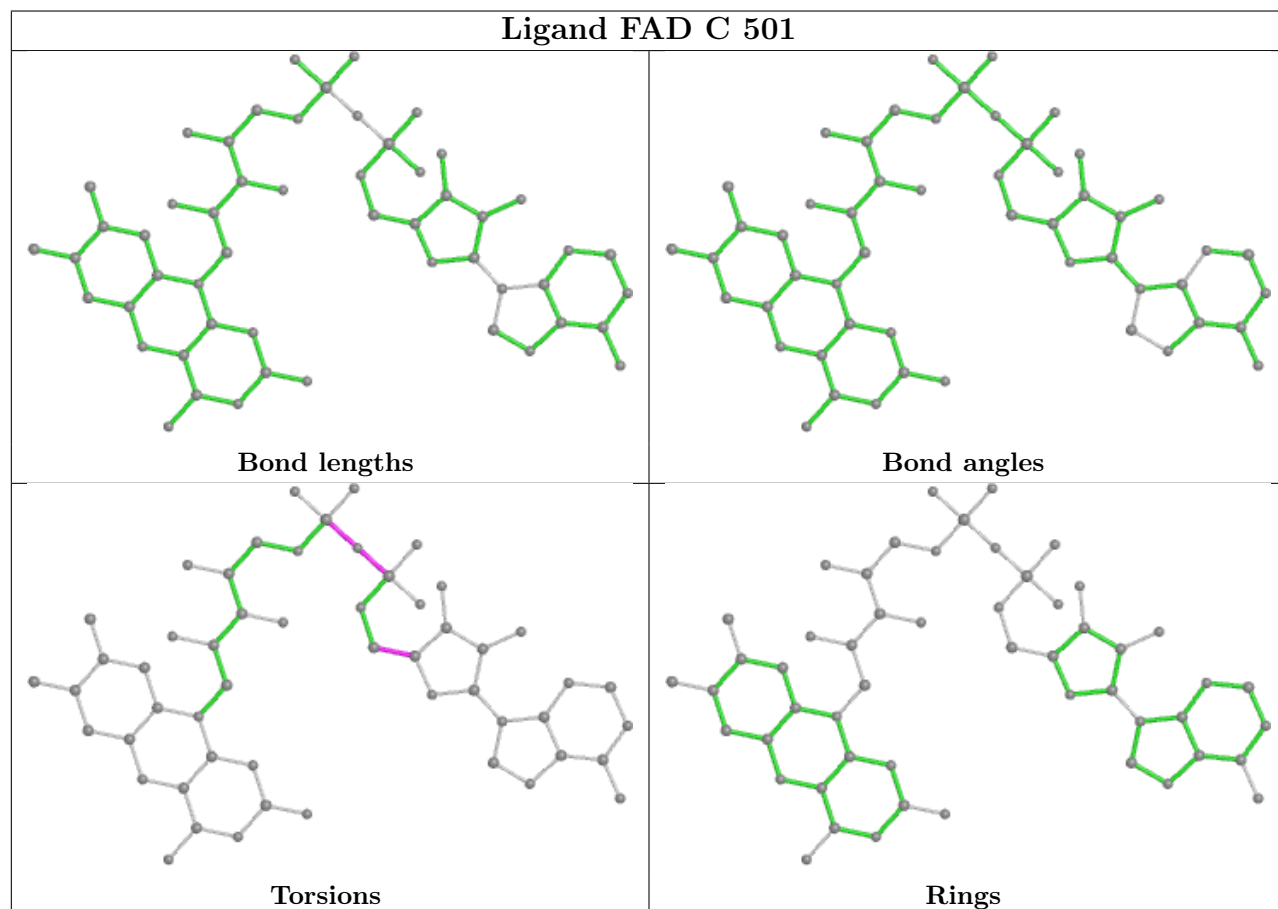
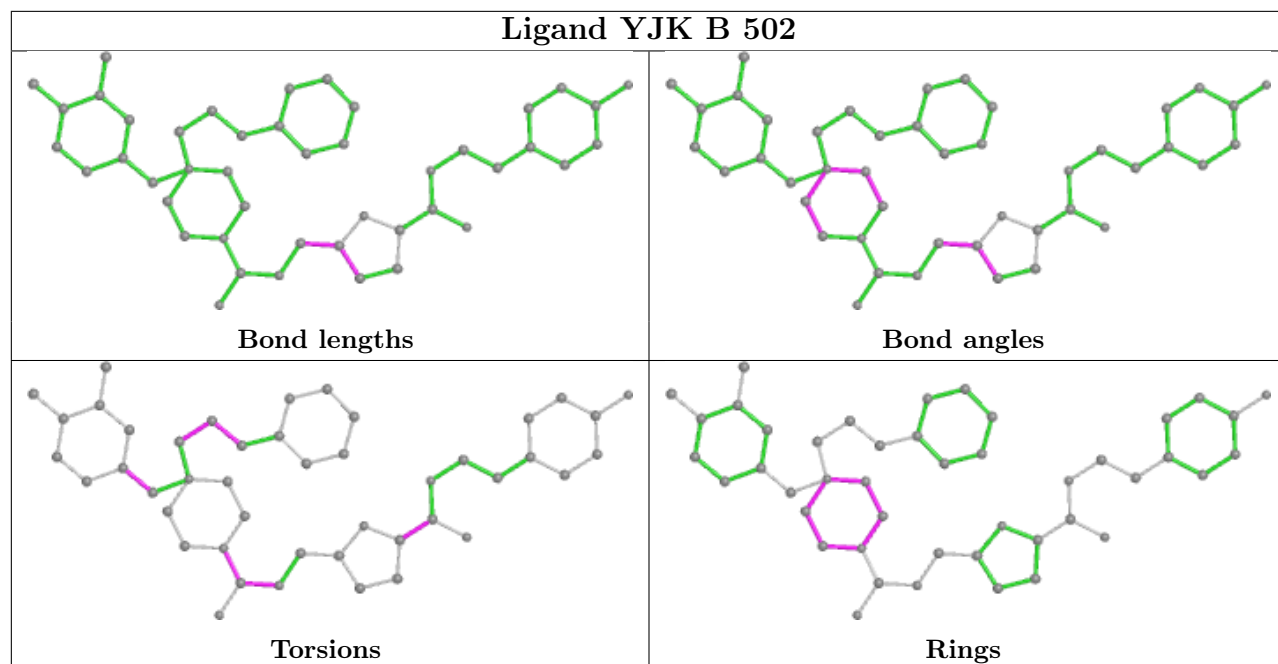
Mol	Chain	Res	Type	Atoms
5	B	502	YJK	C14-C15-C32-C33-N3-N4

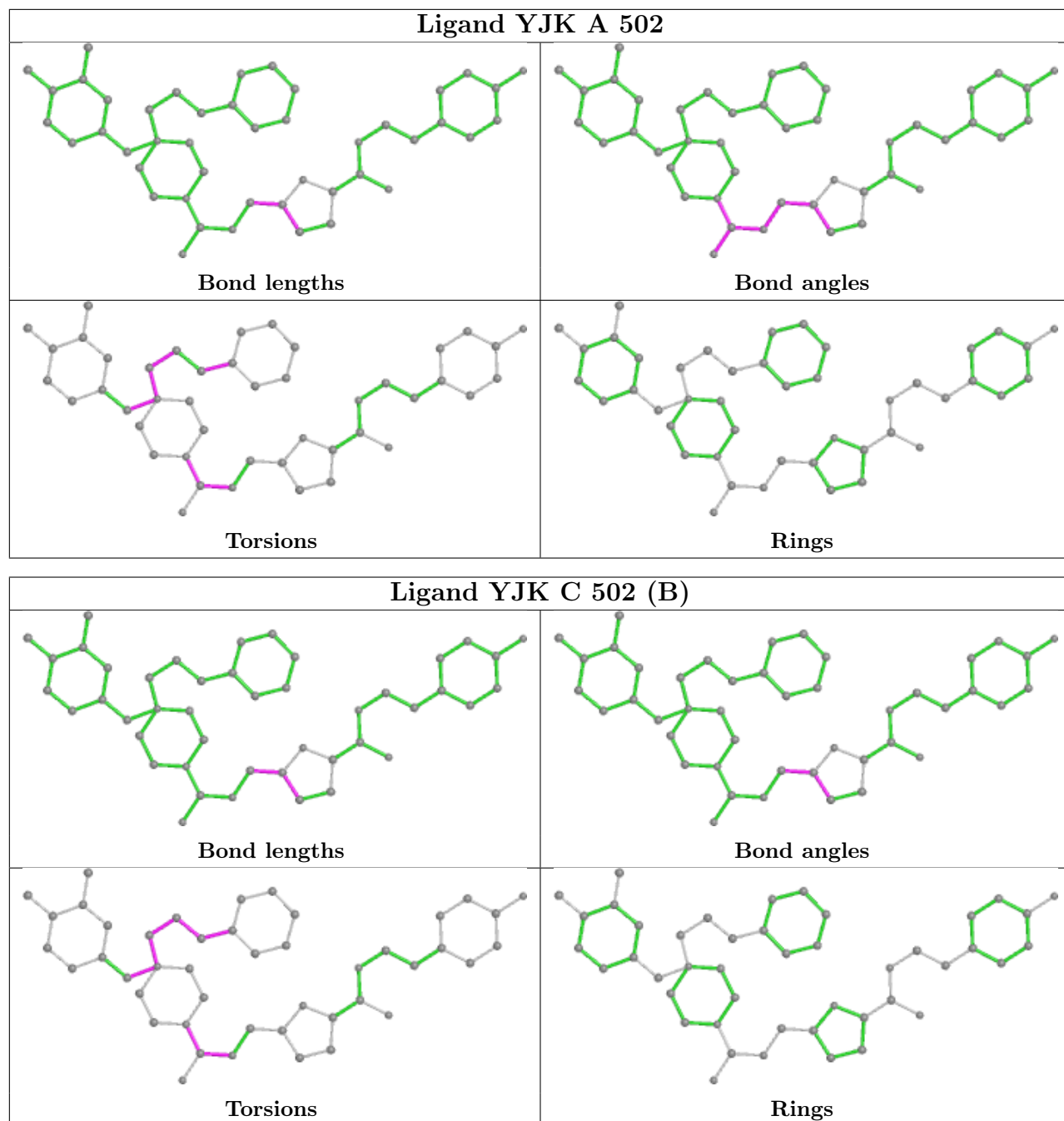
8 monomers are involved in 28 short contacts:

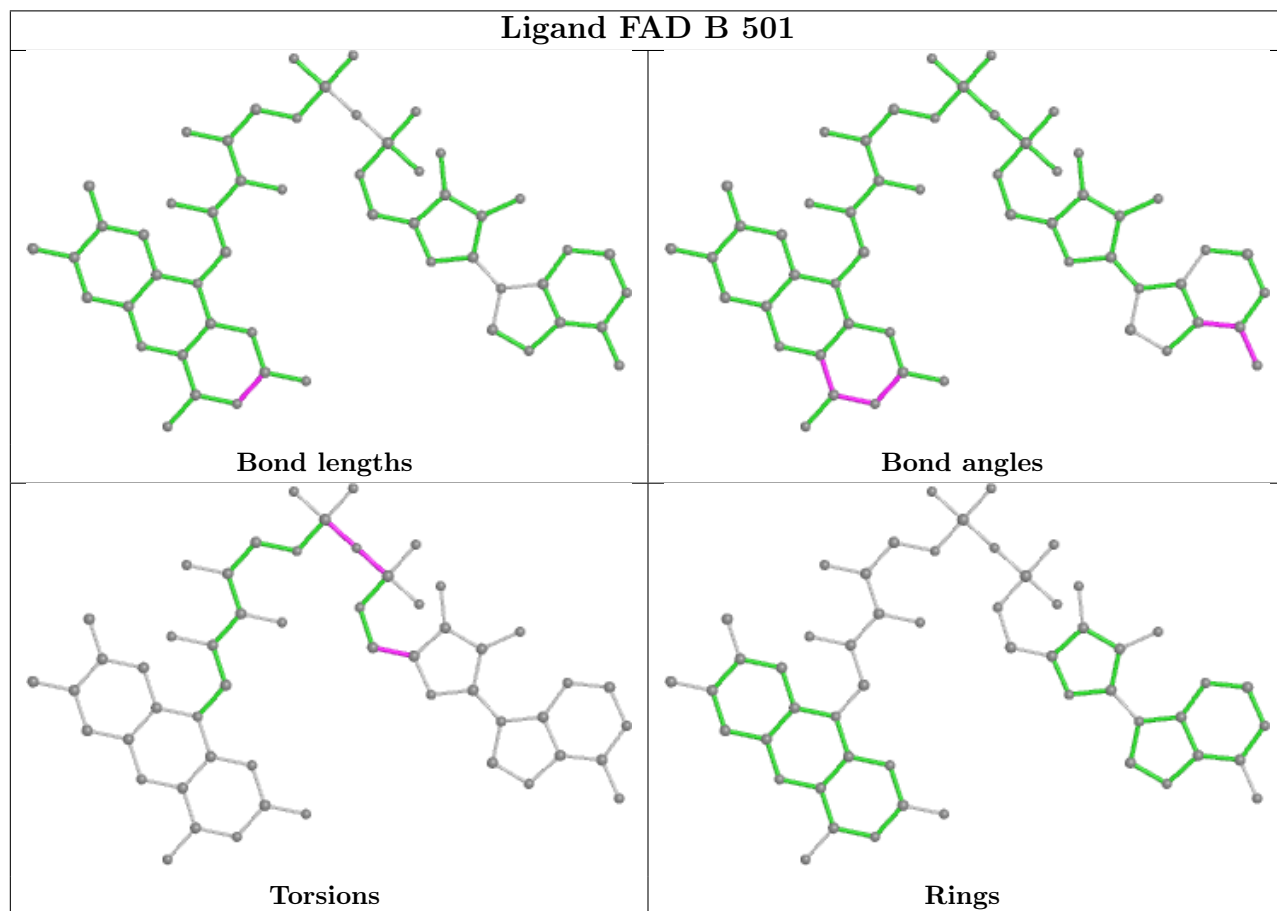
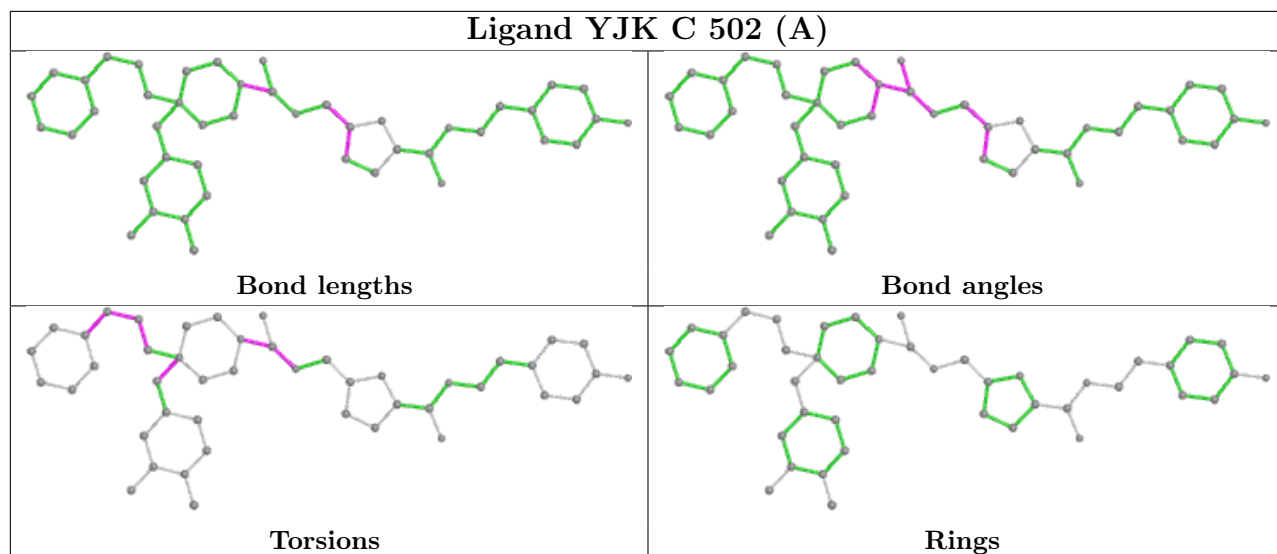
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	YJK	3	0
5	B	502	YJK	1	0
6	C	504	PEG	1	0
7	A	504	DMS	4	0
5	A	502	YJK	6	0
5	C	502[B]	YJK	5	0
6	A	503	PEG	3	0
6	C	503	PEG	5	0

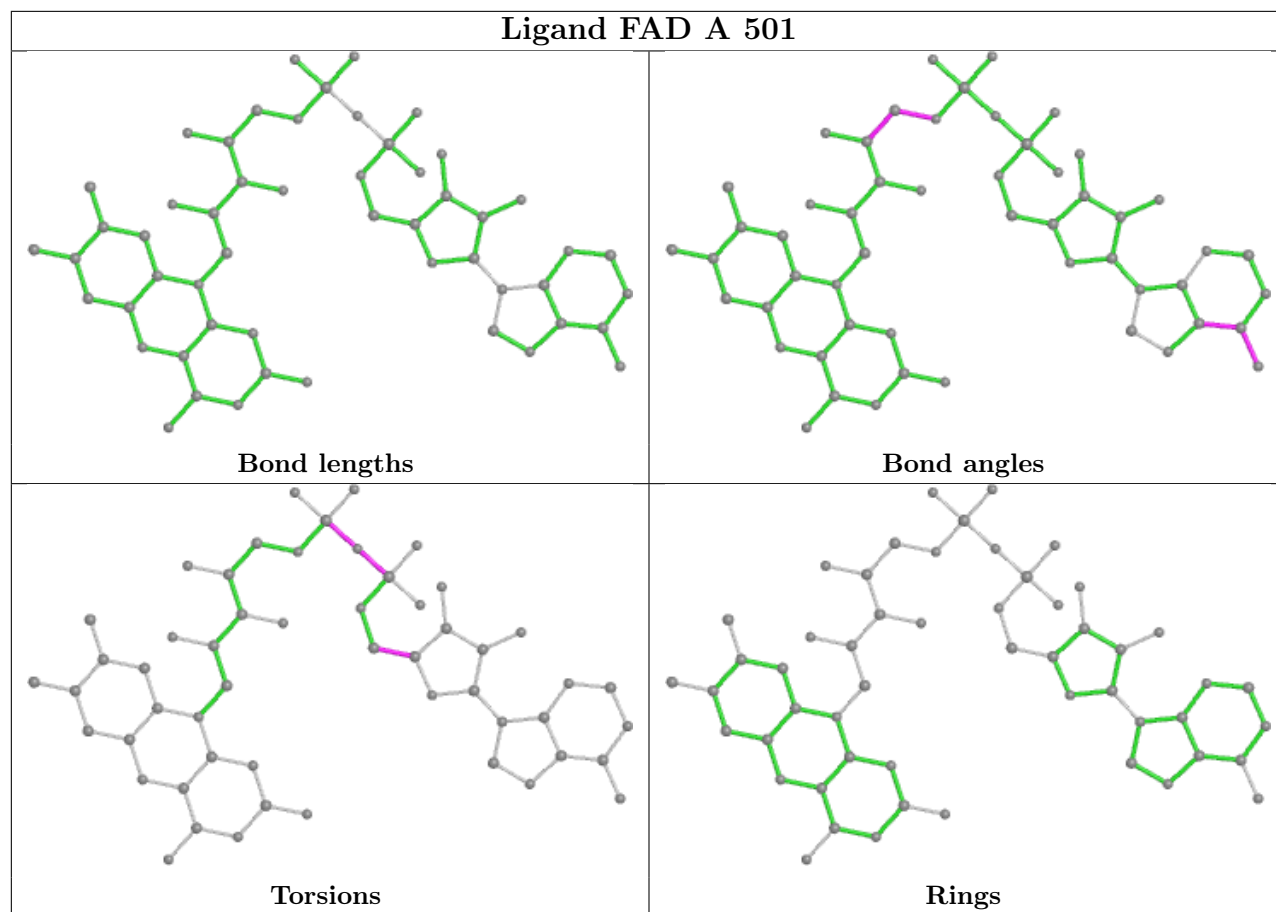
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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%)	-0.54	0 100 100	27, 39, 65, 93	0
2	B	490/494 (99%)	-0.54	0 100 100	24, 36, 57, 85	0
2	C	488/494 (98%)	-0.42	2 (0%) 92 91	26, 44, 82, 112	0
3	D	491/495 (99%)	-0.53	0 100 100	27, 40, 62, 99	0
All	All	1957/1978 (98%)	-0.51	2 (0%) 95 95	24, 39, 71, 112	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	30	ARG	2.3
2	C	331	ARG	2.1

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](#)

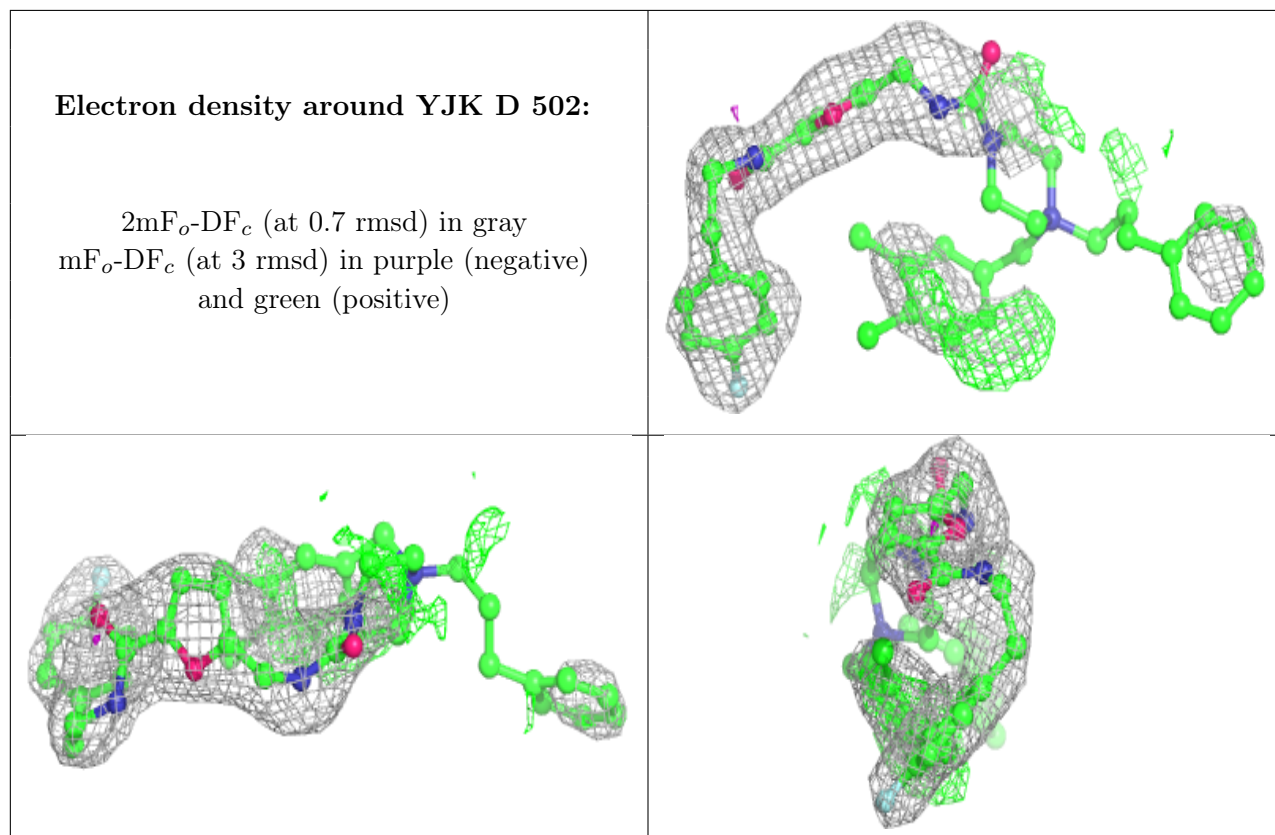
There are no monosaccharides in this entry.

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.

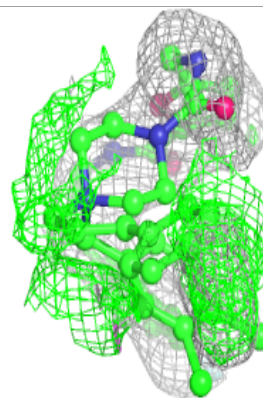
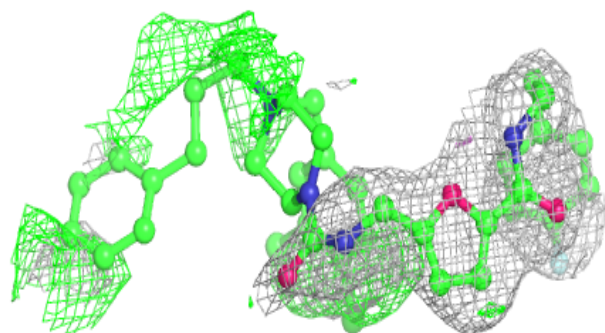
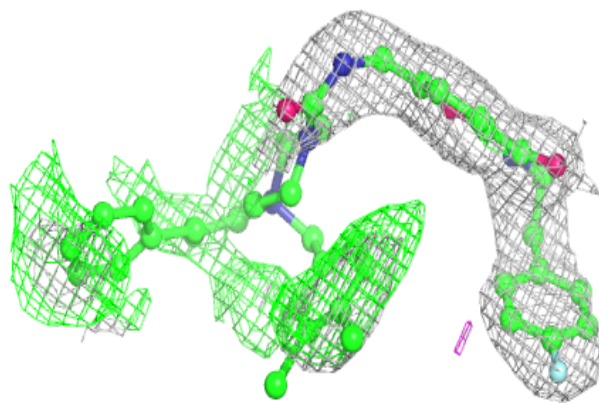
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	DMS	A	504	4/4	0.65	0.38	76,78,81,95	0
6	PEG	C	504	7/7	0.74	0.29	53,61,66,68	0
5	YJK	D	502	45/45	0.83	0.28	50,63,81,89	24
5	YJK	A	502	45/45	0.83	0.32	43,59,69,72	24
5	YJK	B	502	45/45	0.83	0.29	44,72,85,87	24
5	YJK	C	502[B]	45/45	0.84	0.30	53,76,96,98	45
5	YJK	C	502[A]	45/45	0.84	0.30	44,56,67,76	45
6	PEG	C	503	7/7	0.88	0.30	40,50,56,59	0
6	PEG	A	503	7/7	0.89	0.24	43,44,56,60	0
6	PEG	B	503	7/7	0.90	0.55	40,41,43,44	7
7	DMS	D	503	4/4	0.90	0.22	99,102,107,108	0
4	FAD	C	501	53/53	0.97	0.10	29,35,44,48	0
4	FAD	D	501	53/53	0.98	0.11	25,29,35,40	0
4	FAD	B	501	53/53	0.98	0.11	23,28,32,37	0
4	FAD	A	501	53/53	0.98	0.10	24,32,45,47	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.

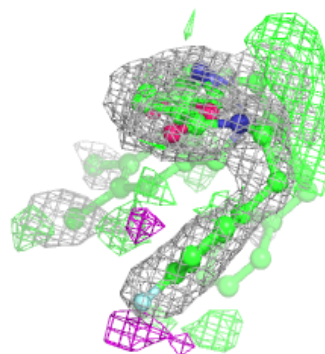
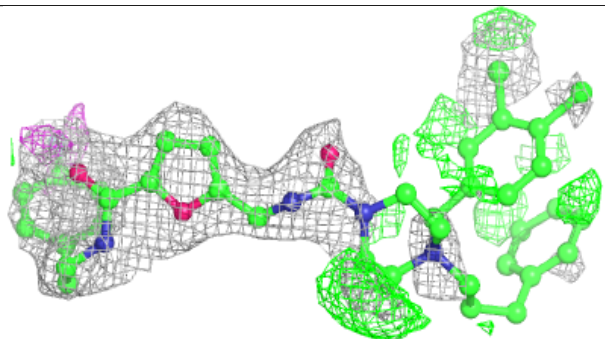
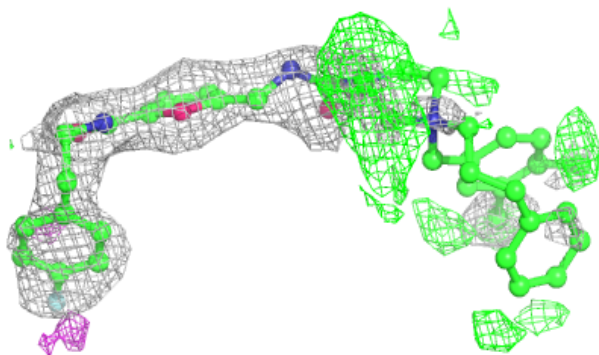


Electron density around YJK A 502:

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

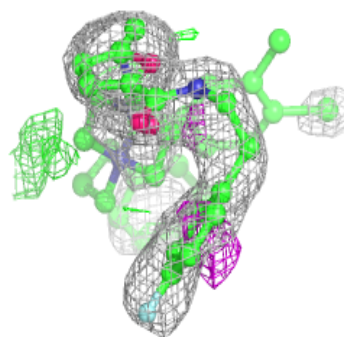
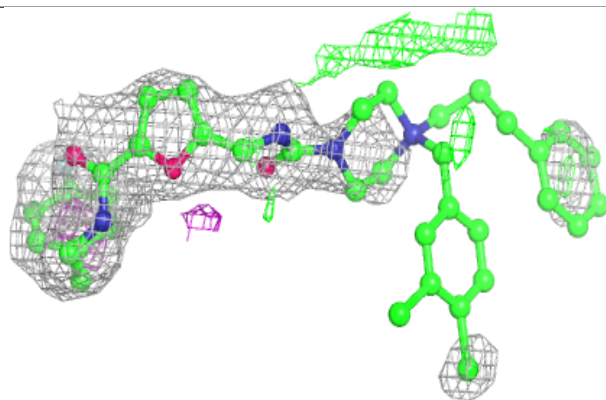
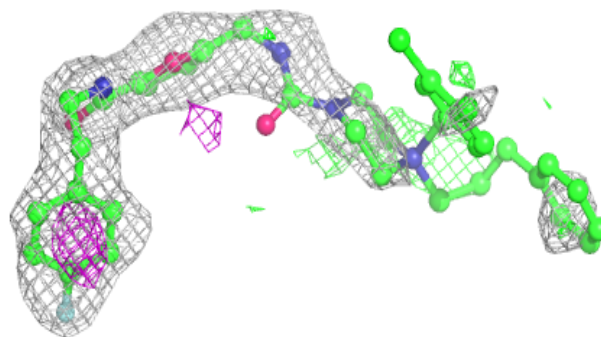
**Electron density around YJK B 502:**

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

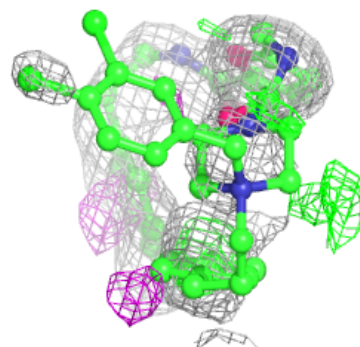
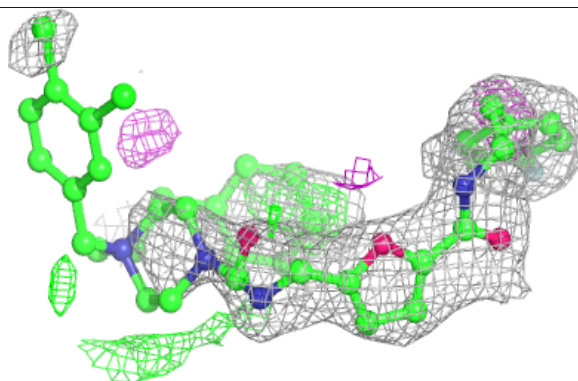
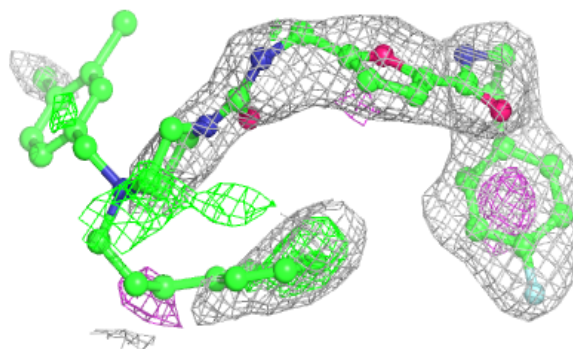


Electron density around YJK C 502 (B):

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

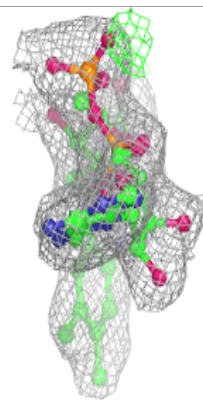
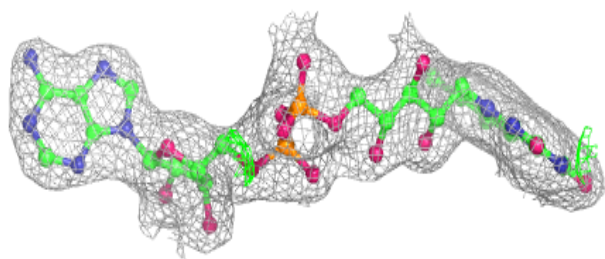
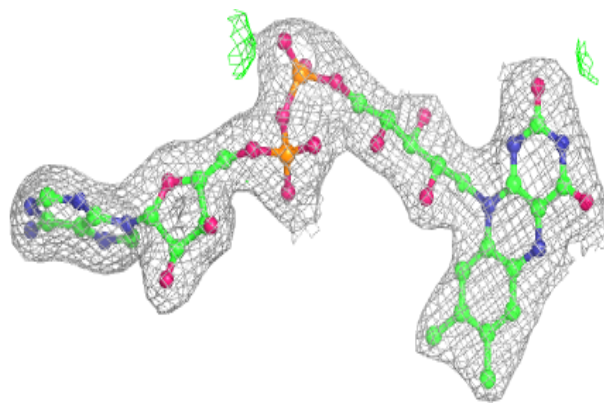
**Electron density around YJK C 502 (A):**

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

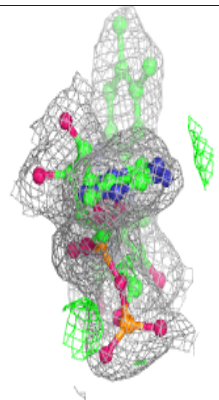
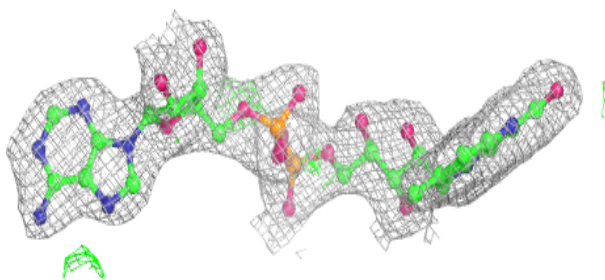
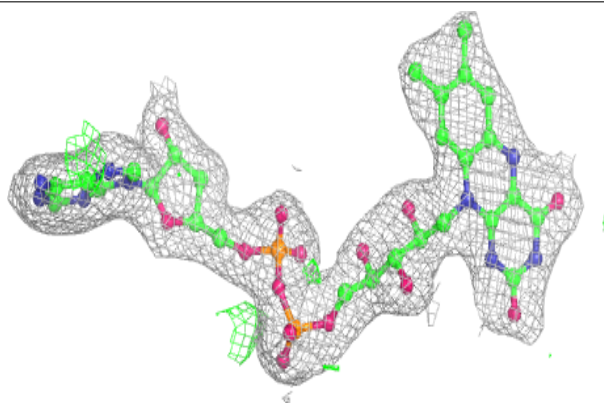


Electron density around FAD C 501:

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

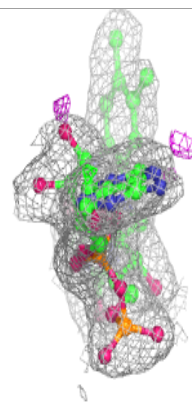
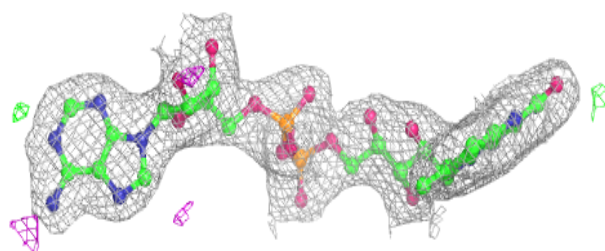
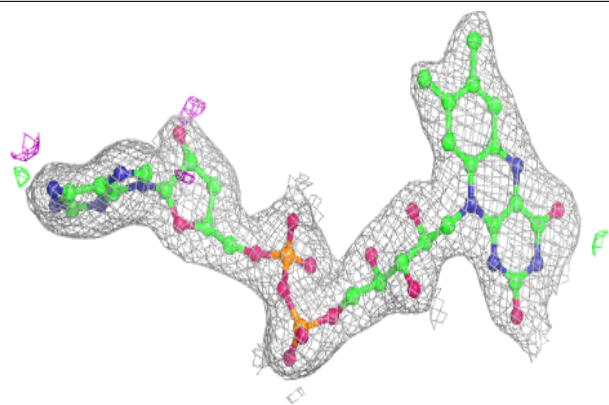
**Electron density around FAD D 501:**

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

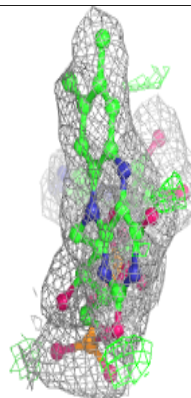
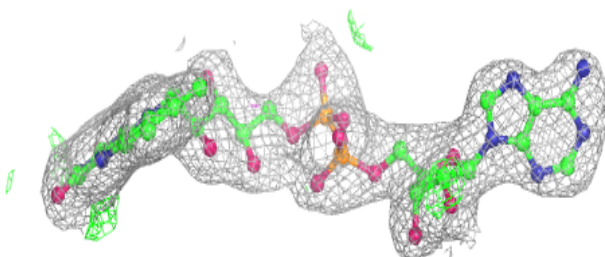
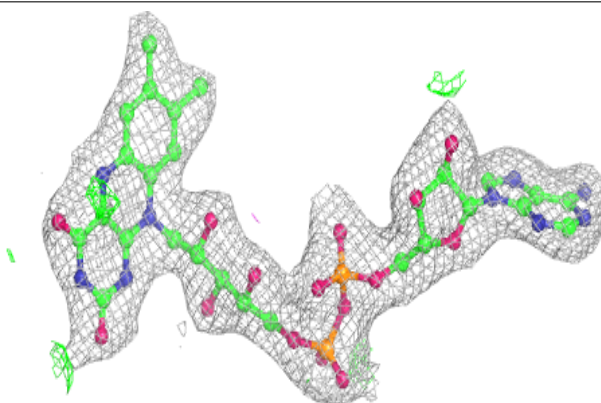


Electron density around FAD B 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.