



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:28 PM UTC

PDB ID : 9UDD / pdb_00009udd
Title : Crystal structure of MonCI in complex with monoepoxidized farnesyl acetate
Authors : Xiao, H.L.; Guan, Y.Z.; Chen, X.
Deposited on : 2025-04-06
Resolution : 2.10 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

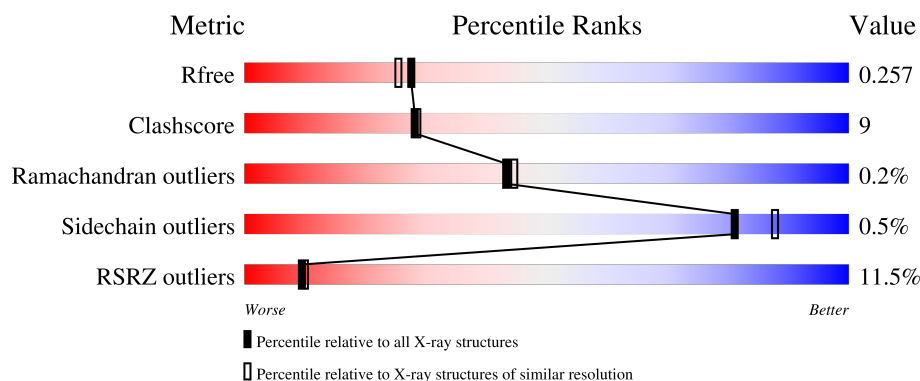
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

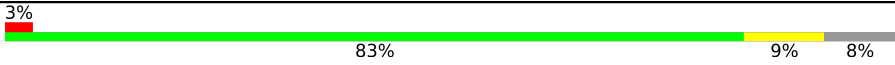
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	511	
1	B	511	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7526 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 MonCI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	1	0
			3592	2245	663	675	9			
1	B	472	Total	C	N	O	S	0	0	0
			3580	2236	662	673	9			

There are 30 discrepancies between the modelled and reference sequences:

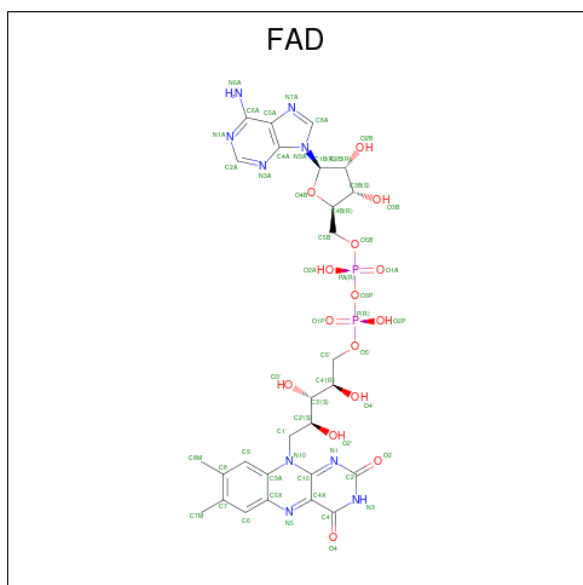
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP Q846W9
A	-13	ASN	-	expression tag	UNP Q846W9
A	-12	HIS	-	expression tag	UNP Q846W9
A	-11	LYS	-	expression tag	UNP Q846W9
A	-10	VAL	-	expression tag	UNP Q846W9
A	-9	HIS	-	expression tag	UNP Q846W9
A	-8	HIS	-	expression tag	UNP Q846W9
A	-7	HIS	-	expression tag	UNP Q846W9
A	-6	HIS	-	expression tag	UNP Q846W9
A	-5	HIS	-	expression tag	UNP Q846W9
A	-4	HIS	-	expression tag	UNP Q846W9
A	-3	ILE	-	expression tag	UNP Q846W9
A	-2	GLU	-	expression tag	UNP Q846W9
A	-1	GLY	-	expression tag	UNP Q846W9
A	0	ARG	-	expression tag	UNP Q846W9
B	-14	MET	-	initiating methionine	UNP Q846W9
B	-13	ASN	-	expression tag	UNP Q846W9
B	-12	HIS	-	expression tag	UNP Q846W9
B	-11	LYS	-	expression tag	UNP Q846W9
B	-10	VAL	-	expression tag	UNP Q846W9
B	-9	HIS	-	expression tag	UNP Q846W9
B	-8	HIS	-	expression tag	UNP Q846W9
B	-7	HIS	-	expression tag	UNP Q846W9
B	-6	HIS	-	expression tag	UNP Q846W9
B	-5	HIS	-	expression tag	UNP Q846W9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP Q846W9
B	-3	ILE	-	expression tag	UNP Q846W9
B	-2	GLU	-	expression tag	UNP Q846W9
B	-1	GLY	-	expression tag	UNP Q846W9
B	0	ARG	-	expression tag	UNP Q846W9

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



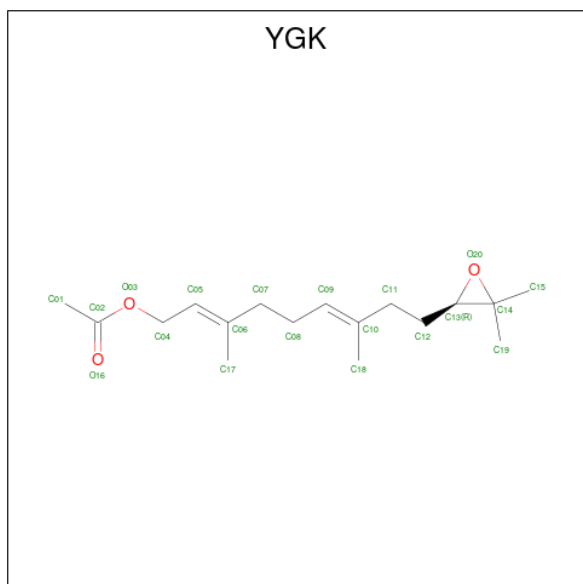
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is Monoepoxidized farnesyl acetate (CCD ID: YGK) (formula: $C_{17}H_{28}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	17	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	187	Total O 187 187	0	0
6	B	28	Total O 28 28	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.83Å 52.44Å 145.51Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	36.34 – 2.10 36.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.34-2.10) 91.4 (36.34-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.196 , 0.231 (Not available) , 0.257	Depositor DCC
R_{free} test set	2870 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7526	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: FAD, GOL, YGK, CL

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	0.44	0/3663	0.66	0/4990
1	B	0.37	0/3650	0.66	0/4972
All	All	0.41	0/7313	0.66	0/9962

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	3592	0	3578	41	0
1	B	3580	0	3570	89	0
2	A	53	0	31	1	0
2	B	53	0	31	5	0
3	A	12	0	16	1	0
4	A	20	0	0	7	0
5	A	1	0	0	0	0
6	A	187	0	0	3	0
6	B	28	0	0	1	0
All	All	7526	0	7226	130	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 9.

All (130) 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:B:184:ARG:HB2	1:B:188:TRP:CZ2	2.07	0.88
1:B:211:ARG:HH21	1:B:291:PRO:HB2	1.41	0.84
1:B:362:ARG:HE	1:B:362:ARG:HA	1.48	0.79
1:B:184:ARG:O	1:B:188:TRP:CD2	2.38	0.77
1:A:208[A]:TYR:OH	1:A:331:ILE:HG13	1.87	0.75
1:B:216:PRO:HG2	1:B:475:VAL:HG13	1.70	0.73
1:A:208[A]:TYR:CE1	1:A:330:PRO:HG2	2.23	0.73
1:A:362:ARG:HD3	1:A:362:ARG:H	1.53	0.72
1:A:5:ARG:NH2	1:B:447:ASN:OD1	2.29	0.65
1:B:48:LYS:C	1:B:48:LYS:HD3	2.22	0.64
1:B:145:GLY:HA2	1:B:155:THR:HG23	1.79	0.64
1:B:189:LEU:HD13	1:B:194:VAL:HG11	1.79	0.64
1:B:212:LEU:HD11	1:B:246:ILE:HD11	1.80	0.64
1:A:362:ARG:NH1	1:A:367:ALA:H	1.95	0.63
1:A:37:ARG:HG3	1:A:162:LEU:HD11	1.79	0.63
1:A:441:GLN:NE2	6:A:602:HOH:O	2.23	0.63
1:B:401:ARG:O	1:B:405:VAL:HG21	2.00	0.62
1:B:407:THR:HG23	1:B:410:ARG:HH11	1.64	0.62
1:B:184:ARG:O	1:B:188:TRP:CE2	2.53	0.62
1:A:208[A]:TYR:CZ	1:A:330:PRO:HG2	2.35	0.62
1:B:54:ARG:HD2	1:B:296:PHE:CE1	2.36	0.61
1:A:214:LYS:NZ	6:A:608:HOH:O	2.33	0.61
1:B:184:ARG:HB2	1:B:188:TRP:CE2	2.38	0.59
1:B:179:THR:OG1	1:B:183:SER:CB	2.51	0.59
1:B:179:THR:OG1	1:B:183:SER:HB2	2.02	0.59
1:B:362:ARG:HA	1:B:362:ARG:NE	2.15	0.58
1:B:211:ARG:HE	1:B:291:PRO:HB3	1.69	0.58
1:B:309:GLU:HB2	1:B:370:LYS:HG2	1.85	0.57
1:A:362:ARG:HH11	1:A:367:ALA:H	1.54	0.56
1:B:317:GLY:H	1:B:365:THR:HG21	1.70	0.56
1:B:195:PRO:HG2	1:B:311:LEU:HD11	1.88	0.56
1:A:242:VAL:HG21	1:A:244:TYR:CZ	2.41	0.55
1:B:189:LEU:HD13	1:B:194:VAL:CG1	2.36	0.55
1:A:197:LEU:HD23	1:A:311:LEU:HD22	1.89	0.55
1:B:95:LEU:HB2	1:B:100:TRP:CZ3	2.42	0.54
1:B:143:LEU:HD11	1:B:188:TRP:CE3	2.43	0.54
1:B:97:GLY:HA3	1:B:231:ASP:HB2	1.88	0.54
1:A:129:ALA:HB3	1:A:132:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HD3	1:A:139:GLU:HG3	1.91	0.52
1:A:102:HIS:HB3	3:A:502:GOL:H12	1.91	0.52
1:B:11:VAL:HB	1:B:34:VAL:HG12	1.91	0.52
1:A:233:ARG:HG2	1:A:390:TYR:CE1	2.44	0.52
1:B:54:ARG:HD2	1:B:296:PHE:CZ	2.45	0.52
1:B:179:THR:OG1	1:B:183:SER:OG	2.26	0.52
1:B:211:ARG:HD3	1:B:213:PHE:CZ	2.45	0.52
1:B:428:SER:O	1:B:432:THR:HG23	2.09	0.51
1:B:184:ARG:O	1:B:188:TRP:CG	2.63	0.51
1:B:212:LEU:HD21	1:B:250:ARG:HB3	1.92	0.51
1:A:208[B]:TYR:CE1	1:A:256:SER:HB3	2.46	0.51
1:A:234:VAL:HG11	1:A:411:LEU:HD11	1.91	0.51
1:B:211:ARG:HH12	1:B:267:GLU:HG3	1.76	0.51
1:B:468:LEU:HB2	1:B:471:GLU:HG3	1.92	0.51
1:B:141:VAL:HB	1:B:158:VAL:HB	1.93	0.51
1:B:143:LEU:HD12	1:B:188:TRP:HB3	1.93	0.50
1:B:85:ARG:NH2	6:B:804:HOH:O	2.41	0.50
1:A:428:SER:O	1:A:432:THR:HG23	2.11	0.50
1:B:223:PHE:CD1	1:B:224:PRO:HD2	2.47	0.50
1:A:426:LYS:HE2	1:A:456:ASP:OD1	2.12	0.49
1:B:11:VAL:HA	1:B:176:ILE:HB	1.94	0.49
1:B:164:SER:O	1:B:166:ARG:N	2.41	0.49
1:A:56:ALA:HB3	4:A:503:YGK:C15	2.43	0.49
1:B:84:ARG:HD2	1:B:220:THR:O	2.13	0.49
1:B:179:THR:C	2:B:700:FAD:H52A	2.38	0.49
1:B:211:ARG:NH2	1:B:291:PRO:HB2	2.20	0.49
1:A:208[B]:TYR:CD1	1:A:256:SER:HB3	2.48	0.48
1:A:233:ARG:HG2	1:A:390:TYR:CZ	2.47	0.48
1:B:48:LYS:HD3	1:B:48:LYS:O	2.13	0.48
1:B:159:VAL:HG11	1:B:170:LEU:HD22	1.94	0.48
1:A:227:ASN:HD21	4:A:503:YGK:C08	2.26	0.47
1:B:272:PRO:HA	1:B:275:GLU:HB2	1.95	0.47
1:B:235:ARG:HG2	1:B:235:ARG:HH21	1.78	0.47
1:B:304:ARG:HH12	1:B:324:SER:HA	1.80	0.47
1:A:208[B]:TYR:OH	4:A:503:YGK:O20	2.28	0.47
1:B:55:HIS:NE2	1:B:298:SER:HB2	2.29	0.47
1:B:212:LEU:HD23	1:B:213:PHE:N	2.30	0.47
1:B:330:PRO:HB3	2:B:700:FAD:C6	2.44	0.47
1:B:46:HIS:CE1	1:B:116:PRO:HG3	2.50	0.47
1:B:15:SER:HB3	2:B:700:FAD:O1P	2.15	0.47
1:A:362:ARG:HH11	1:A:367:ALA:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASP:O	1:B:165:GLY:HA2	2.14	0.46
1:B:9:ALA:O	1:B:32:VAL:HA	2.14	0.46
1:B:229:ALA:HA	1:B:240:PHE:HD1	1.81	0.46
1:B:200:ASP:OD1	1:B:398:THR:HG22	2.16	0.46
1:B:95:LEU:HD13	1:B:100:TRP:CD2	2.52	0.45
1:B:211:ARG:HE	1:B:291:PRO:CB	2.29	0.45
1:B:304:ARG:NH1	1:B:323:ASP:O	2.48	0.45
1:B:135:ARG:HA	1:B:135:ARG:HD3	1.67	0.45
1:A:227:ASN:HD21	4:A:503:YGK:C17	2.29	0.45
1:B:177:ASP:OD2	1:B:185:LEU:HB2	2.17	0.45
1:B:211:ARG:HH21	1:B:291:PRO:CB	2.20	0.45
1:B:423:ARG:NH2	1:B:461:GLU:HG3	2.32	0.45
1:A:275:GLU:HG3	1:A:283:ALA:CB	2.47	0.44
1:A:413:PHE:HZ	1:A:450:LEU:HD21	1.83	0.44
1:B:78:LEU:HD21	1:B:118:LEU:HD12	1.98	0.44
1:B:476:GLY:O	1:B:477:LEU:HD23	2.17	0.44
1:B:212:LEU:HB3	1:B:293:THR:HG23	1.98	0.44
1:B:187:GLN:CD	1:B:187:GLN:N	2.75	0.44
1:A:227:ASN:ND2	4:A:503:YGK:C08	2.81	0.44
1:B:143:LEU:CD2	1:B:175:VAL:HG11	2.48	0.44
1:B:174:LEU:HD21	1:B:176:ILE:HD11	2.00	0.43
1:A:5:ARG:NH1	1:B:445:GLY:O	2.52	0.43
1:A:279:HIS:HE1	1:A:480:ALA:HB1	1.84	0.43
1:B:207:ALA:HB3	1:B:263:LEU:HD11	2.00	0.43
1:A:223:PHE:CG	1:A:224:PRO:HD2	2.54	0.43
1:B:406:ASP:HB3	1:B:409:GLN:HB3	2.01	0.43
1:A:185:LEU:O	1:A:189:LEU:HG	2.19	0.42
1:B:57:HIS:HA	2:B:700:FAD:O4	2.19	0.42
1:B:311:LEU:HG	1:B:313:GLN:H	1.85	0.42
1:A:56:ALA:O	4:A:503:YGK:C15	2.67	0.42
1:B:179:THR:O	2:B:700:FAD:C5B	2.68	0.42
1:B:472:LEU:HA	1:B:472:LEU:HD23	1.82	0.42
1:A:368:LEU:HD23	1:A:368:LEU:HA	1.94	0.42
1:B:233:ARG:HG2	1:B:390:TYR:CD2	2.55	0.42
1:B:257:CYS:SG	1:B:263:LEU:HG	2.59	0.42
1:B:183:SER:CB	1:B:324:SER:OG	2.68	0.41
1:B:269:GLU:HA	1:B:272:PRO:HG2	2.01	0.41
1:A:176:ILE:HD13	1:A:319:LEU:HB2	2.03	0.41
2:A:501:FAD:H9	2:A:501:FAD:H1'1	1.85	0.41
1:B:472:LEU:HD22	1:B:477:LEU:HB2	2.02	0.41
1:A:355:GLN:O	6:A:601:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ALA:HA	1:B:296:PHE:O	2.21	0.41
1:B:243:VAL:HG23	1:B:282:LEU:HD22	2.03	0.41
1:A:208[A]:TYR:CD2	1:A:256:SER:HB3	2.56	0.40
1:B:112:VAL:HG21	1:B:244:TYR:HB3	2.02	0.40
1:B:234:VAL:HG11	1:B:411:LEU:HD11	2.02	0.40
1:B:235:ARG:HA	1:B:235:ARG:HD3	1.86	0.40
1:B:475:VAL:HG12	1:B:475:VAL:O	2.21	0.40
4:A:503:YGK:C11	4:A:503:YGK:C19	2.99	0.40
1:A:346:ILE:O	1:A:350:PHE:HB2	2.22	0.40
1:A:426:LYS:HE2	1:A:456:ASP:CG	2.46	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	469/511 (92%)	458 (98%)	10 (2%)	1 (0%)	43	44
1	B	468/511 (92%)	456 (97%)	11 (2%)	1 (0%)	43	44
All	All	937/1022 (92%)	914 (98%)	21 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	ARG
1	B	165	GLY

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	368/401 (92%)	367 (100%)	1 (0%)	86	91
1	B	367/401 (92%)	364 (99%)	3 (1%)	73	81
All	All	735/802 (92%)	731 (100%)	4 (0%)	81	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	ARG
1	B	189	LEU
1	B	231	ASP
1	B	250	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	46	HIS
1	A	101	GLN
1	A	167	GLN
1	A	227	ASN
1	A	266	HIS
1	A	438	ASN
1	B	46	HIS
1	B	101	GLN
1	B	124	GLN
1	B	136	GLN
1	B	167	GLN
1	B	187	GLN
1	B	222	HIS
1	B	438	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
2	FAD	A	501	-	58,58,58	0.39	0	85,89,89	0.54	1 (1%)
3	GOL	A	502	-	5,5,5	0.95	0	5,5,5	0.97	0
4	YGK	A	503	-	20,20,20	2.14	2 (10%)	27,27,27	2.64	5 (18%)
2	FAD	B	700	-	58,58,58	0.37	0	85,89,89	0.41	0
3	GOL	A	504	-	5,5,5	0.74	0	5,5,5	1.12	1 (20%)

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
2	FAD	A	501	-	-	4/34/50/50	0/6/6/6
3	GOL	A	502	-	-	0/4/4/4	-
4	YGK	A	503	-	-	6/17/25/25	0/1/1/1
2	FAD	B	700	-	-	6/34/50/50	0/6/6/6
3	GOL	A	504	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	YGK	O20-C14	8.86	1.60	1.46
4	A	503	YGK	O20-C13	-2.28	1.41	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	YGK	O20-C13-C14	11.33	68.55	59.92
4	A	503	YGK	C14-O20-C13	-4.37	56.69	60.78
4	A	503	YGK	O20-C13-C12	-3.90	111.08	117.85
4	A	503	YGK	O20-C14-C13	-3.86	54.76	58.95
3	A	504	GOL	C3-C2-C1	-2.22	103.65	111.80
4	A	503	YGK	C12-C13-C14	-2.07	122.15	125.35
2	A	501	FAD	O5'-P-O1P	2.02	116.96	108.94

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5'-O5'-P-O2P
2	A	501	FAD	C5'-O5'-P-O3P
2	B	700	FAD	C5'-O5'-P-O2P
2	B	700	FAD	C5'-O5'-P-O3P
3	A	504	GOL	O1-C1-C2-O2
3	A	504	GOL	O1-C1-C2-C3
4	A	503	YGK	C11-C12-C13-C14
4	A	503	YGK	O16-C02-O03-C04
4	A	503	YGK	C01-C02-O03-C04
4	A	503	YGK	C11-C12-C13-O20
2	A	501	FAD	P-O3P-PA-O1A
2	B	700	FAD	PA-O3P-P-O5'
2	B	700	FAD	P-O3P-PA-O2A
2	A	501	FAD	P-O3P-PA-O2A
4	A	503	YGK	C06-C07-C08-C09
2	B	700	FAD	O3'-C3'-C4'-C5'
2	B	700	FAD	P-O3P-PA-O1A
4	A	503	YGK	C10-C11-C12-C13

There are no ring outliers.

4 monomers are involved in 14 short contacts:

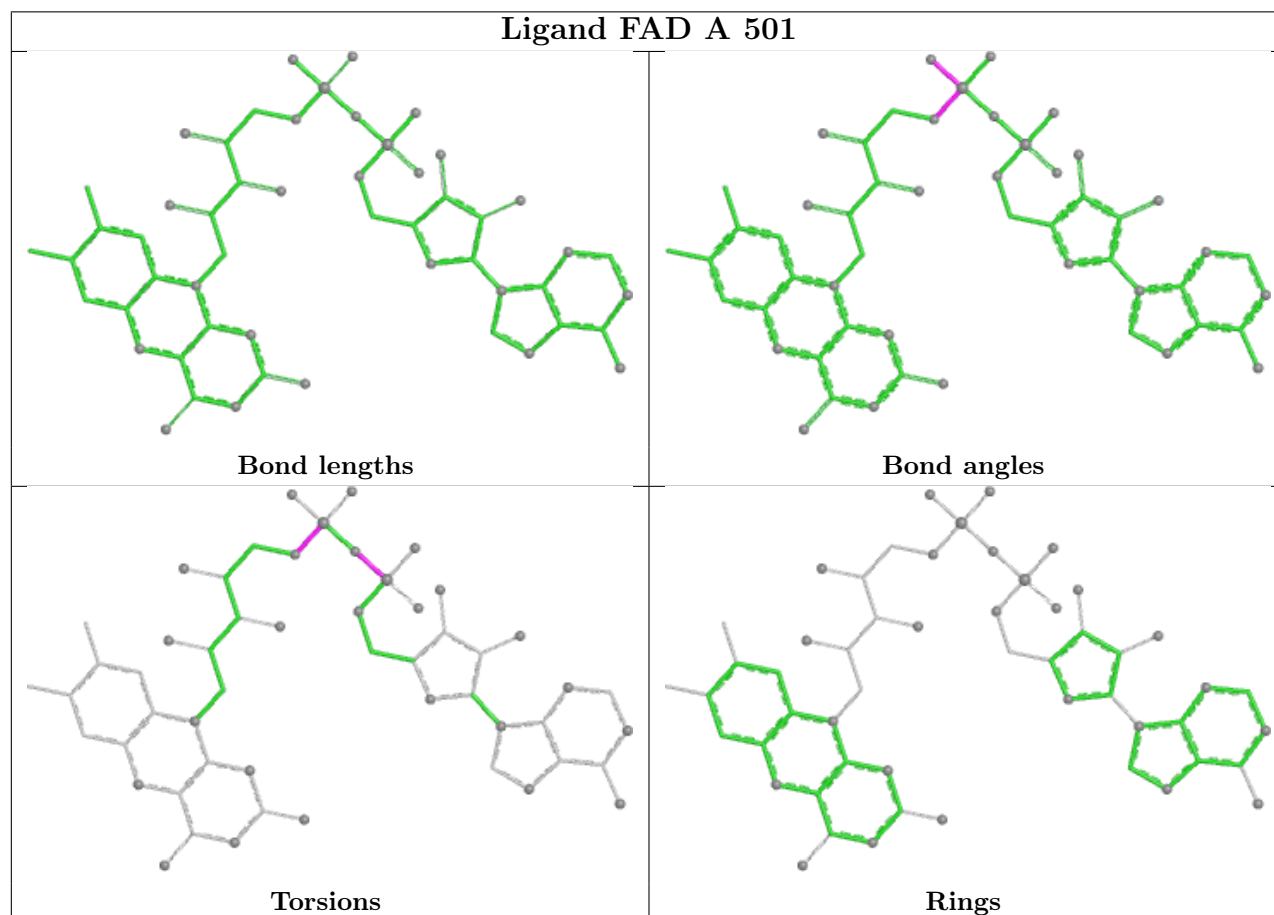
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	1	0

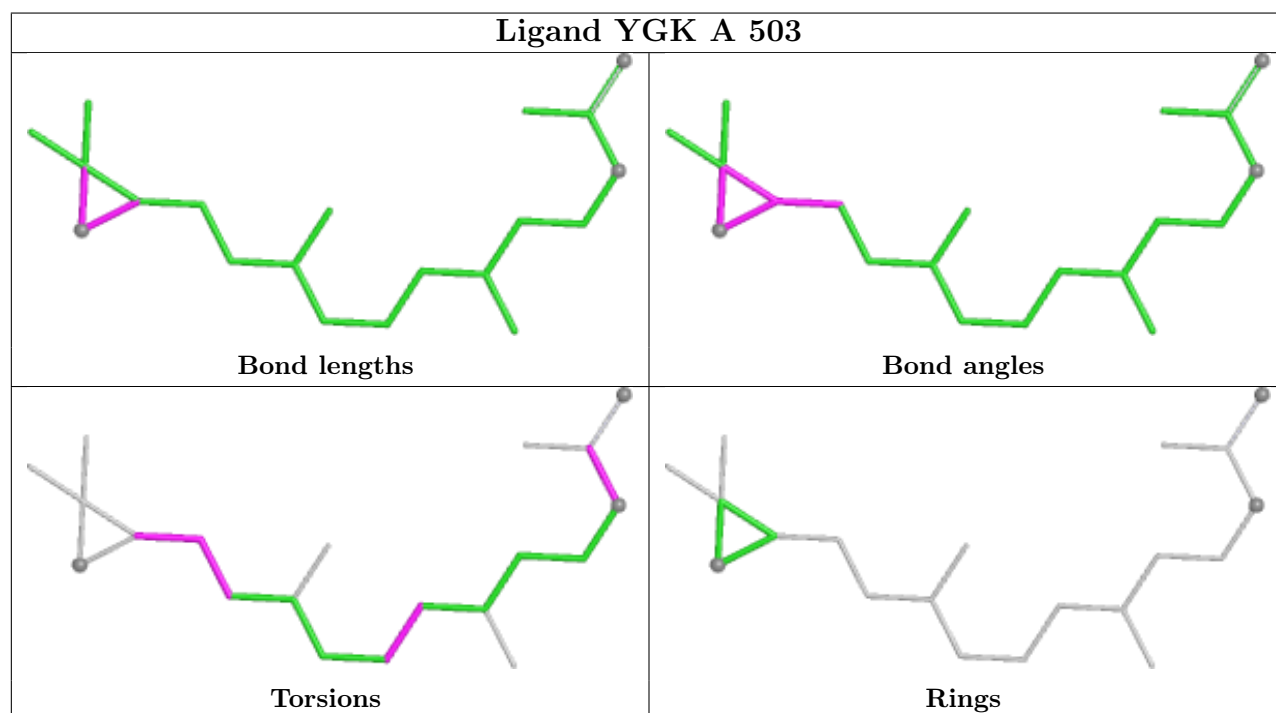
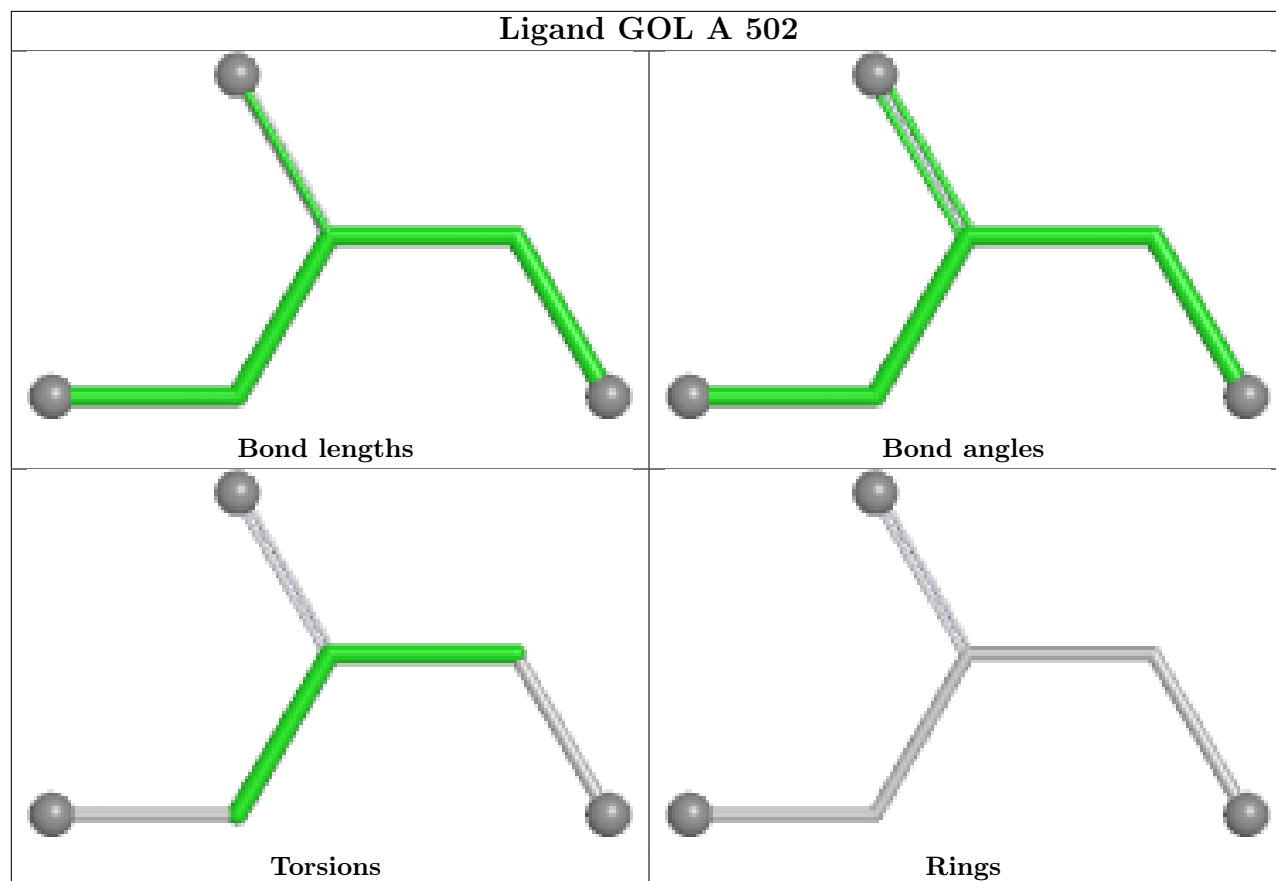
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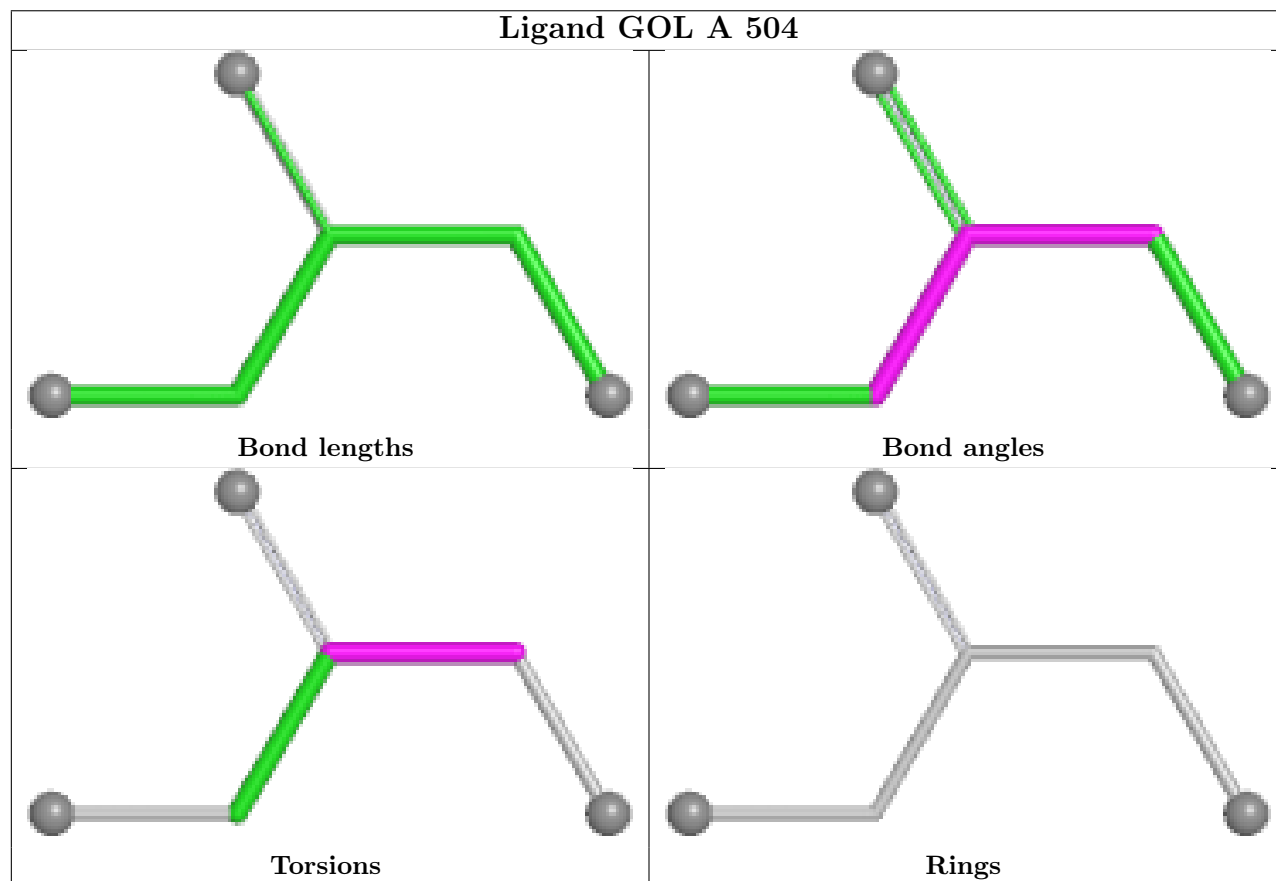
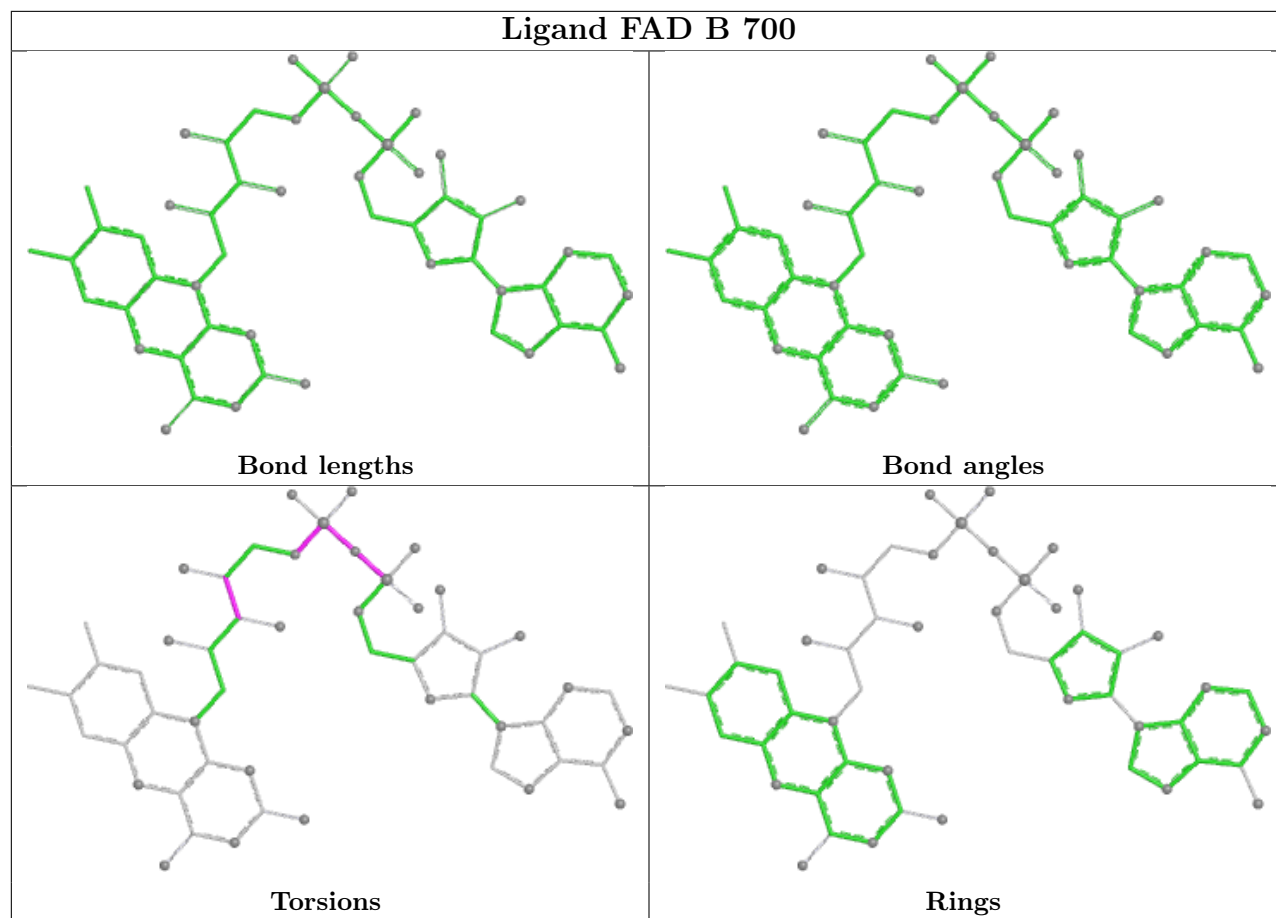
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	1	0
4	A	503	YGK	7	0
2	B	700	FAD	5	0

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](#)

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	472/511 (92%)	0.11	15 (3%)	50 53	18, 39, 67, 125	1 (0%)
1	B	472/511 (92%)	1.19	94 (19%)	3 3	36, 77, 120, 152	0
All	All	944/1022 (92%)	0.65	109 (11%)	9 10	18, 53, 112, 152	1 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	ALA	5.3
1	A	363	ALA	5.2
1	B	363	ALA	5.0
1	B	270	PHE	4.3
1	B	143	LEU	4.3
1	B	192	LEU	4.3
1	A	361	ALA	4.2
1	B	170	LEU	4.2
1	A	480	ALA	4.0
1	B	230	ALA	3.9
1	B	162	LEU	3.7
1	B	480	ALA	3.7
1	B	395	VAL	3.7
1	B	405	VAL	3.6
1	B	306	LEU	3.5
1	B	150	SER	3.4
1	B	409	GLN	3.4
1	A	364	GLY	3.4
1	B	282	LEU	3.4
1	B	295	VAL	3.4
1	A	362	ARG	3.3
1	B	149	GLY	3.3
1	B	204	ALA	3.3
1	B	147	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	148	GLY	3.1
1	B	35	VAL	3.1
1	B	196	ALA	3.1
1	B	127	LEU	3.1
1	A	355	GLN	3.0
1	B	46	HIS	3.0
1	A	451	MET	3.0
1	B	157	VAL	3.0
1	B	197	LEU	3.0
1	B	151	GLY	2.9
1	B	144	THR	2.9
1	A	404	GLY	2.9
1	B	354	VAL	2.9
1	B	38	ASP	2.8
1	B	404	GLY	2.8
1	B	159	VAL	2.8
1	B	367	ALA	2.8
1	B	474	VAL	2.8
1	B	260	GLY	2.8
1	B	292	LEU	2.8
1	B	388	ILE	2.8
1	B	311	LEU	2.7
1	B	44	PRO	2.7
1	B	187	GLN	2.7
1	B	477	LEU	2.7
1	B	232	ASP	2.7
1	B	361	ALA	2.6
1	B	41	PRO	2.6
1	B	296	PHE	2.6
1	B	250	ARG	2.6
1	A	477	LEU	2.6
1	B	364	GLY	2.5
1	B	221	THR	2.5
1	B	216	PRO	2.5
1	B	291	PRO	2.5
1	B	319	LEU	2.5
1	B	133	THR	2.5
1	B	365	THR	2.5
1	B	174	LEU	2.5
1	A	454	ARG	2.5
1	B	213	PHE	2.5
1	B	134	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	475	VAL	2.4
1	B	191	ALA	2.4
1	B	12	LEU	2.4
1	B	209	ALA	2.4
1	B	231	ASP	2.4
1	B	234	VAL	2.4
1	B	451	MET	2.4
1	B	265	THR	2.4
1	B	403	ILE	2.4
1	A	412	ARG	2.4
1	B	158	VAL	2.4
1	B	40	LEU	2.3
1	B	402	LEU	2.3
1	B	441	GLN	2.3
1	B	317	GLY	2.3
1	A	234	VAL	2.3
1	B	10	VAL	2.3
1	B	274	ALA	2.3
1	A	405	VAL	2.3
1	B	48	LYS	2.3
1	B	39	ALA	2.3
1	B	287	ARG	2.2
1	B	266	HIS	2.2
1	A	170	LEU	2.2
1	B	314	TRP	2.2
1	B	407	THR	2.2
1	B	380	TRP	2.1
1	B	140	ALA	2.1
1	B	78	LEU	2.1
1	B	355	GLN	2.1
1	B	175	VAL	2.1
1	B	262	GLN	2.1
1	B	220	THR	2.1
1	B	386	LYS	2.1
1	B	190	ALA	2.1
1	B	185	LEU	2.0
1	B	212	LEU	2.0
1	B	141	VAL	2.0
1	B	126	ALA	2.0
1	B	188	TRP	2.0
1	B	313	GLN	2.0
1	B	82	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	208	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

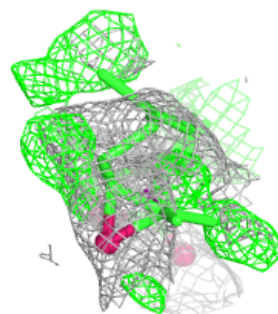
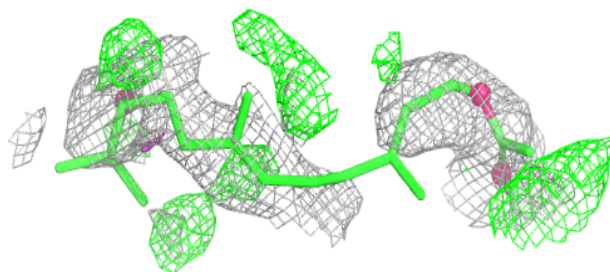
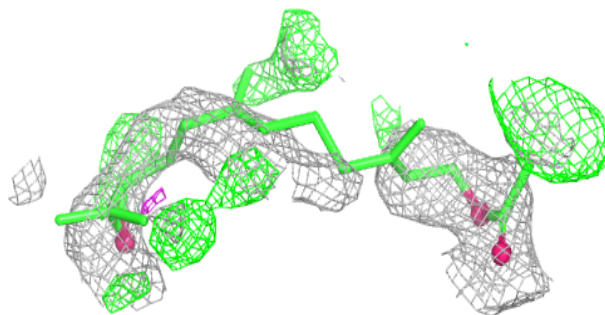
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	YGK	A	503	20/20	0.78	0.27	93,98,104,104	0
3	GOL	A	504	6/6	0.85	0.15	75,76,78,81	0
3	GOL	A	502	6/6	0.87	0.14	70,77,82,84	0
2	FAD	B	700	53/53	0.91	0.10	62,73,96,100	0
2	FAD	A	501	53/53	0.97	0.06	24,31,35,36	0
5	CL	A	505	1/1	0.98	0.09	42,42,42,42	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.

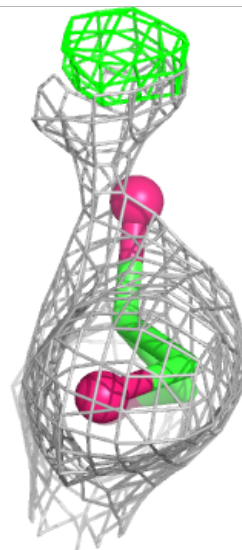
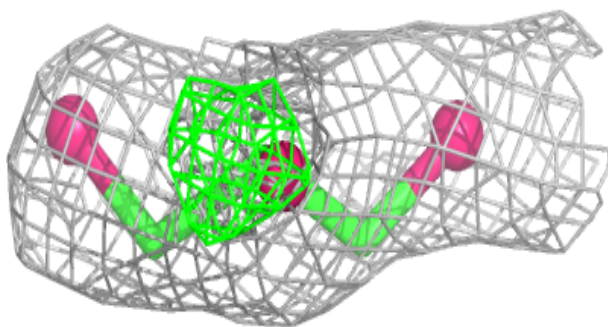
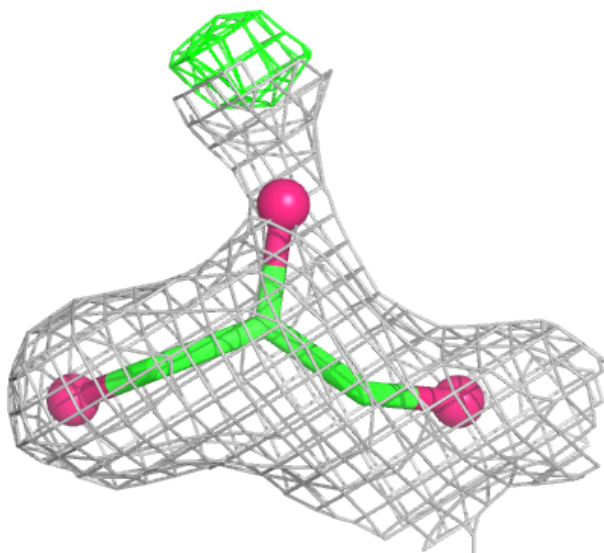
Electron density around YGK A 503:

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



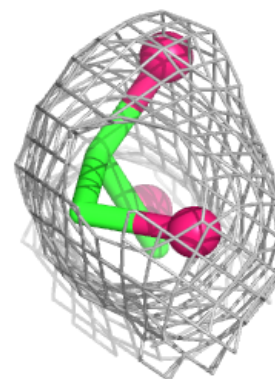
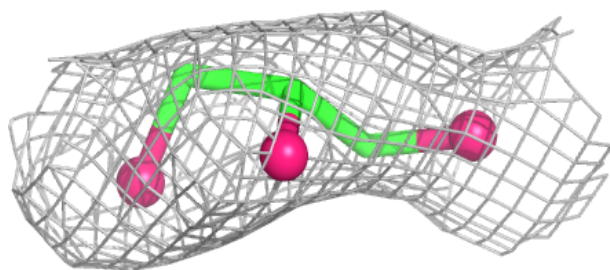
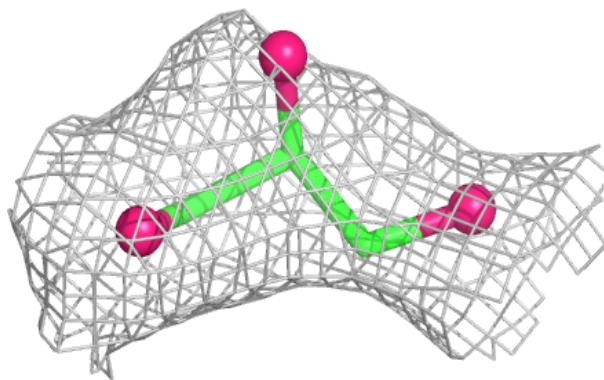
Electron density around GOL A 504:

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and green (positive)

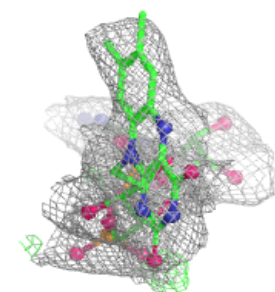
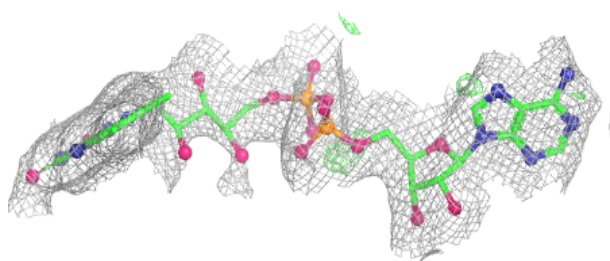
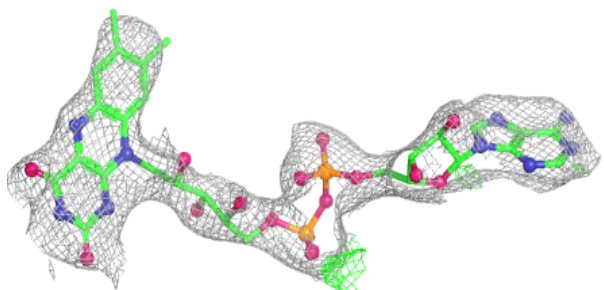


Electron density around GOL A 502:

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and green (positive)

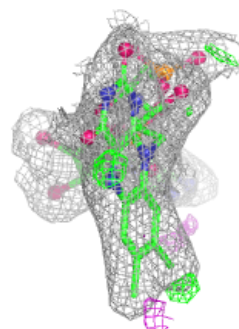
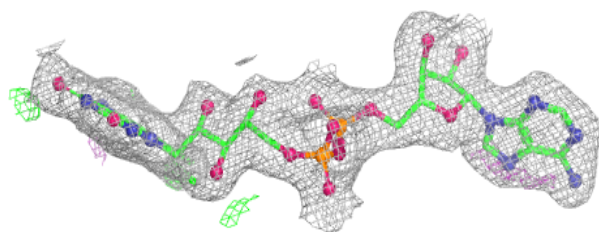
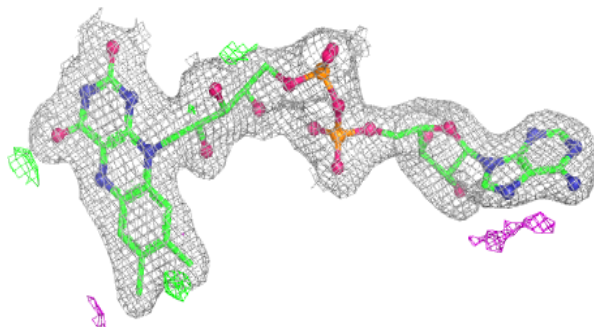
**Electron density around FAD B 700:**

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and green (positive)



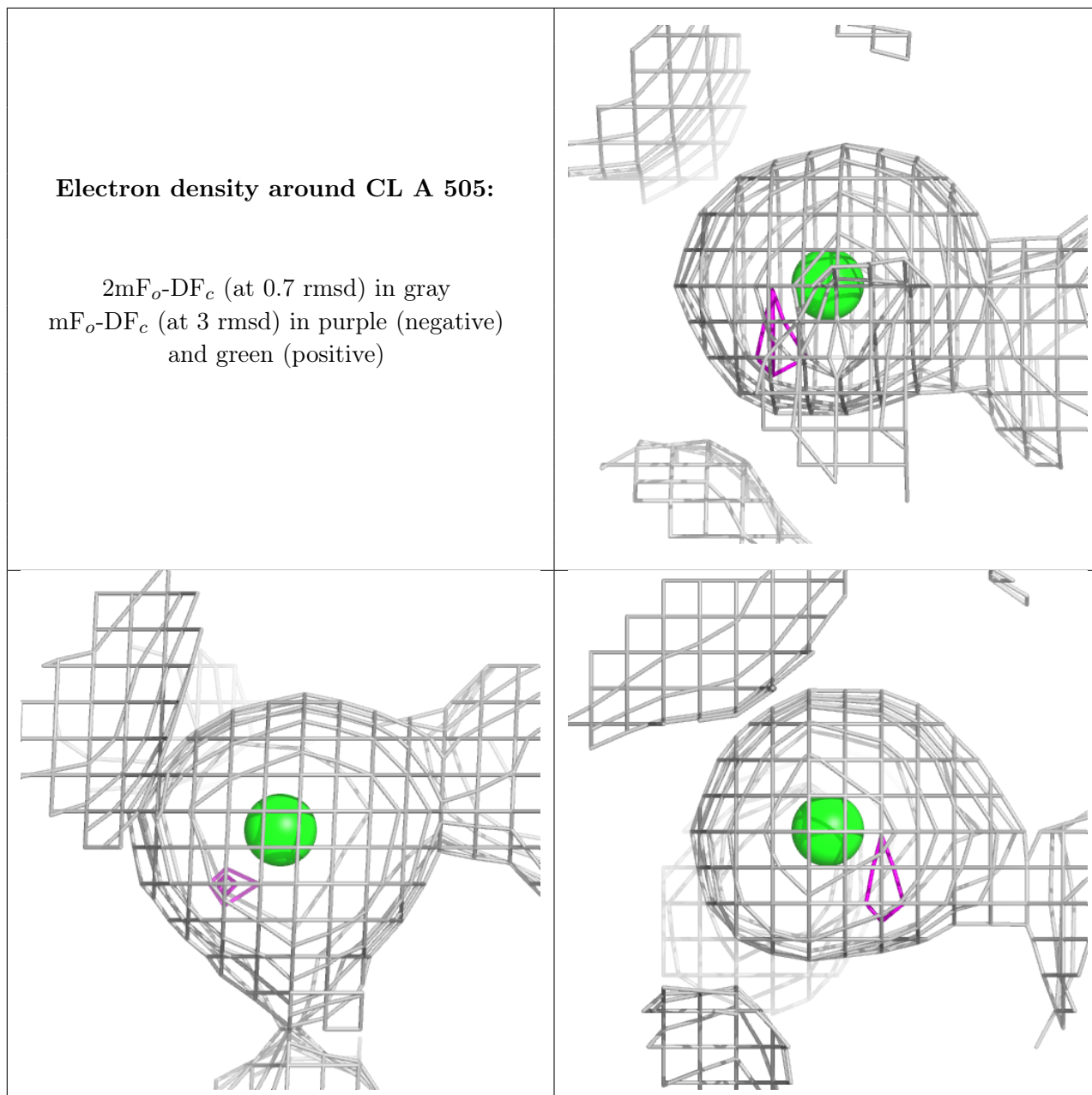
Electron density around FAD A 501:

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



Electron density around CL A 505:

$2mF_o-DF_c$ (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.