



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:39 PM UTC

PDB ID : 8RX6 / pdb_00008rx6
Title : Mycothione reductase from Mycobacterium tuberculosis in complex with Respi-1093
Authors : Oorts, L.; Osipov, E.M.; Beelen, S.; Strelkov, S.V.
Deposited on : 2024-02-06
Resolution : 3.42 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

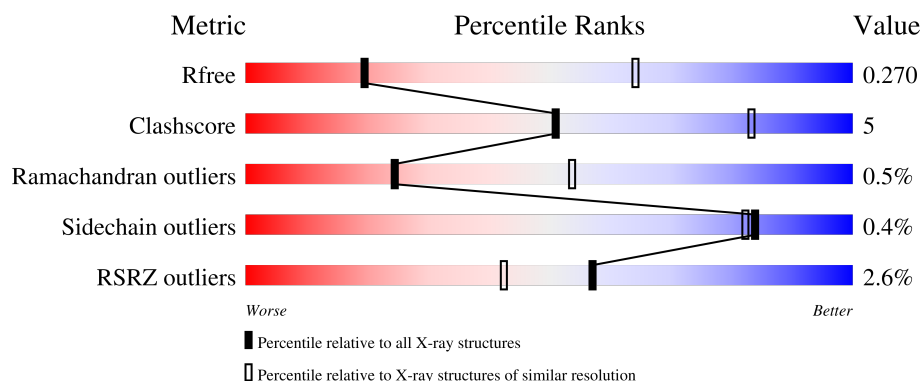
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	459	
1	B	459	
1	C	459	
1	D	459	
1	E	459	

Continued on next page...

Continued from previous page...

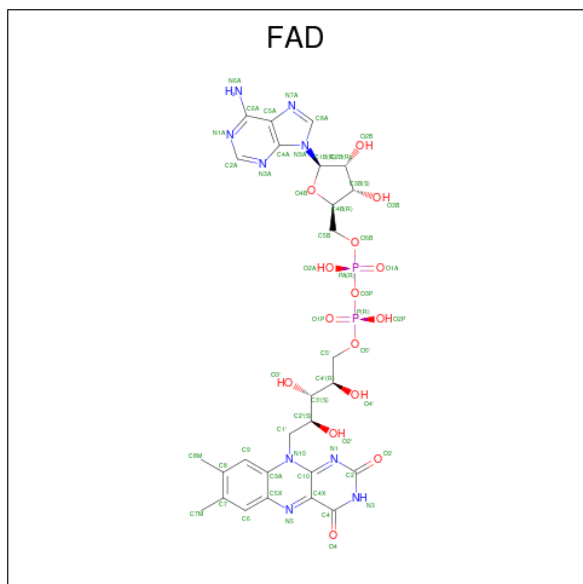
Mol	Chain	Length	Quality of chain
1	F	459	2%87%13%

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 Mycothione reductase.

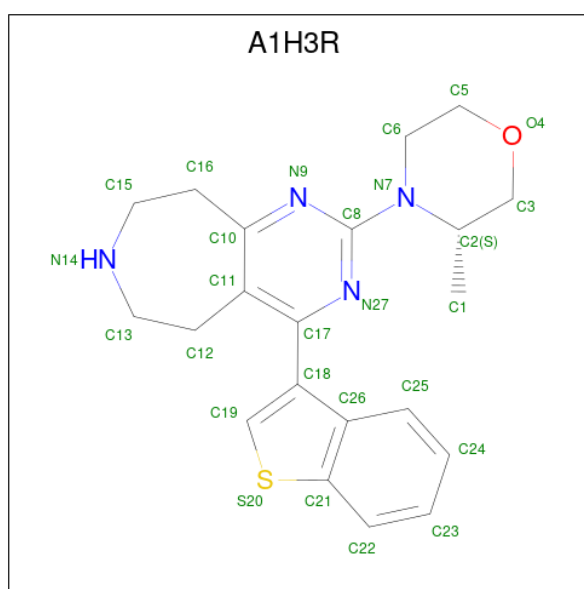
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total 3511	C 2198	N 629	O 667	S 17	14	0	0
1	B	459	Total 3505	C 2195	N 626	O 667	S 17	5	0	0
1	C	459	Total 3511	C 2198	N 629	O 667	S 17	0	0	0
1	D	459	Total 3511	C 2198	N 629	O 667	S 17	21	0	0
1	E	459	Total 3511	C 2198	N 629	O 667	S 17	6	0	0
1	F	459	Total 3505	C 2195	N 626	O 667	S 17	0	0	0

- 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (3 {S})-4-[4-(1-benzothiophen-3-yl)-6,7,8,9-tetrahydro-5 {H}-pyrimido[4,5-d]azepin-2-yl]-3-methyl-morpholine (CCD ID: A1H3R) (formula: C₂₁H₂₄N₄OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	S	0	0
			27	21	4	1	1		
3	E	1	Total	C	N	O	S	0	0
			27	21	4	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	O	0	0
			2	2		

Continued on next page...

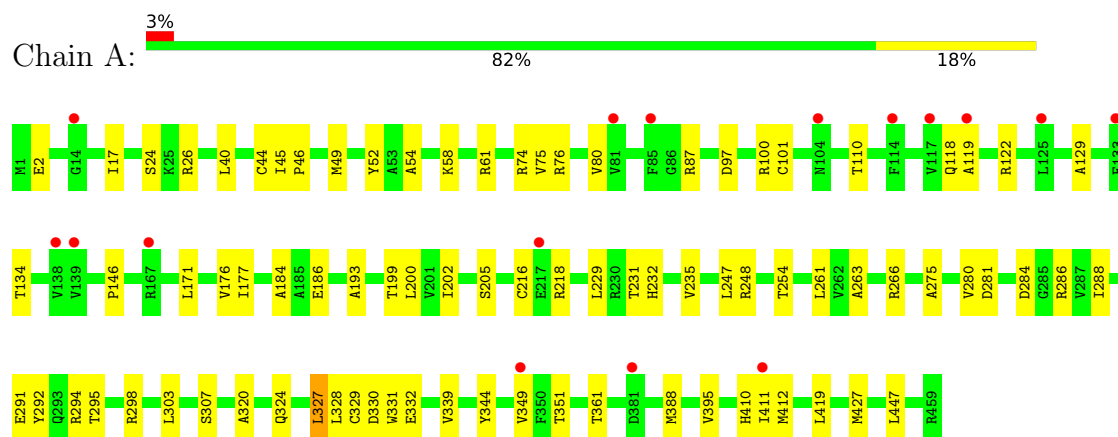
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	O	0	0
			1	1		

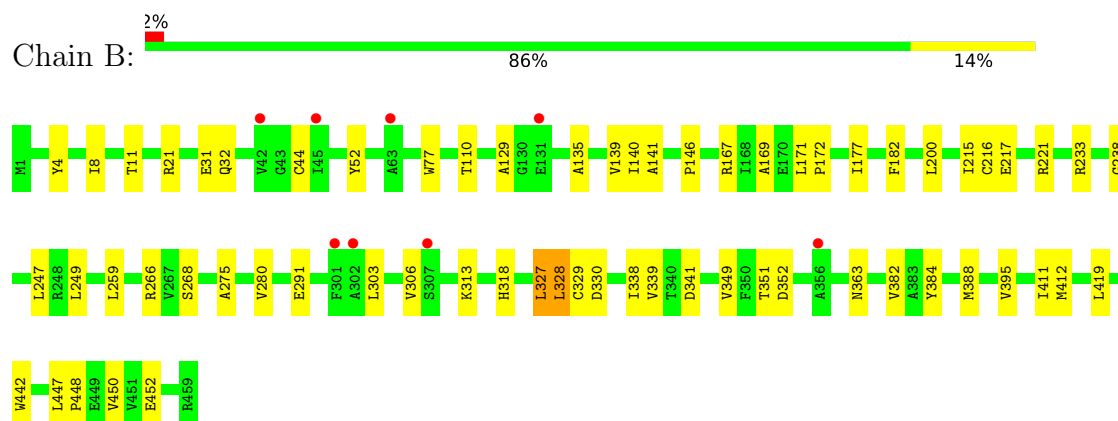
3 Residue-property plots [i](#)

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.

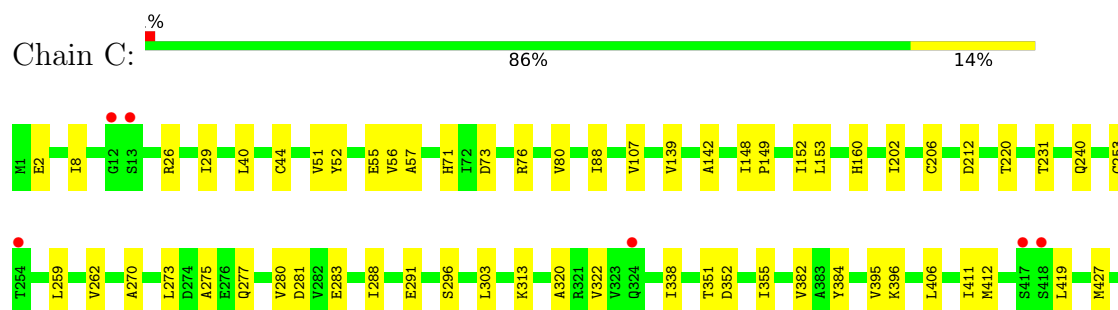
- Molecule 1: Mycothione reductase



- Molecule 1: Mycothione reductase

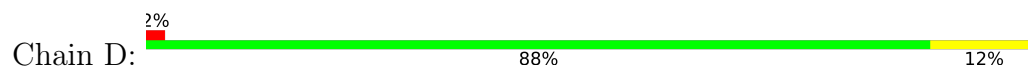


- Molecule 1: Mycothione reductase

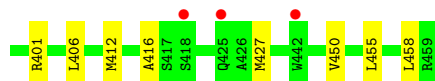
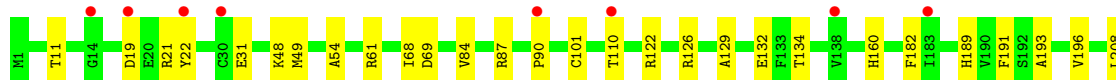
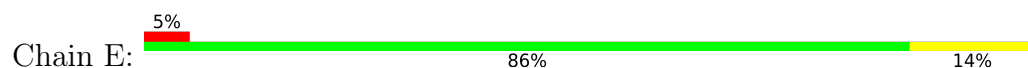




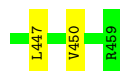
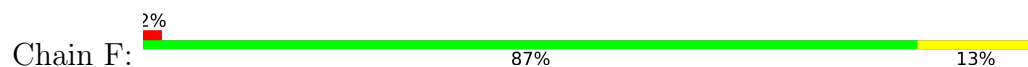
- Molecule 1: Mycothione reductase



- Molecule 1: Mycothione reductase



- Molecule 1: Mycothione reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	175.76 Å 175.76 Å 261.68 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.26 – 3.42 112.26 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (112.26-3.42) 99.4 (112.26-3.42)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.41 Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.233 , 0.270 0.234 , 0.270	Depositor DCC
R_{free} test set	2798 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21429	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2212e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, A1H3R

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	0.09	0/3574	0.26	0/4855
1	B	0.08	0/3568	0.25	0/4848
1	C	0.08	0/3574	0.25	0/4855
1	D	0.11	0/3574	0.28	0/4855
1	E	0.09	0/3574	0.27	0/4855
1	F	0.08	0/3568	0.23	0/4848
All	All	0.09	0/21432	0.26	0/29116

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	3511	0	3473	49	0
1	B	3505	0	3462	39	0
1	C	3511	0	3475	39	0
1	D	3511	0	3475	29	0
1	E	3511	0	3477	42	0
1	F	3505	0	3462	32	0
2	A	53	0	31	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	0	0
2	E	53	0	31	1	0
2	F	53	0	31	2	0
3	D	27	0	0	0	0
3	E	27	0	0	0	0
4	C	2	0	0	0	0
4	F	1	0	0	1	0
All	All	21429	0	21010	219	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 (219) 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:395:VAL:HG23	1:B:411:ILE:HG12	1.58	0.86
1:E:126:ARG:HG2	1:E:132:GLU:HG2	1.68	0.75
1:D:351:THR:HG22	1:D:352:ASP:H	1.52	0.74
1:F:395:VAL:HG23	1:F:411:ILE:HG12	1.73	0.71
1:A:395:VAL:HG23	1:A:411:ILE:HG12	1.74	0.70
1:B:291:GLU:HB2	1:B:339:VAL:HG13	1.72	0.69
1:C:275:ALA:HB1	1:C:280:VAL:HB	1.74	0.68
1:A:294:ARG:NH1	1:A:331:TRP:O	2.27	0.68
1:E:291:GLU:HB2	1:E:339:VAL:HG13	1.77	0.67
1:F:203:ARG:NH2	1:F:264:THR:OG1	2.28	0.66
1:B:233:ARG:HG2	1:B:249:LEU:HD23	1.77	0.65
1:D:395:VAL:HG23	1:D:411:ILE:HG12	1.78	0.65
1:C:419:LEU:HD21	1:C:447:LEU:HG	1.78	0.65
1:A:275:ALA:HB1	1:A:280:VAL:HG13	1.79	0.65
1:A:298:ARG:NH2	1:A:332:GLU:OE1	2.30	0.65
1:C:395:VAL:HG23	1:C:411:ILE:HG12	1.79	0.64
1:E:275:ALA:HB1	1:E:280:VAL:HB	1.80	0.64
1:A:218:ARG:HB2	1:A:412:MET:HE1	1.80	0.64
1:B:167:ARG:NH2	1:C:231:THR:OG1	2.31	0.64
1:C:351:THR:HG22	1:C:352:ASP:H	1.63	0.64
1:E:283:GLU:HG3	1:E:288:ILE:HD11	1.80	0.63
1:E:351:THR:HG22	1:E:352:ASP:H	1.62	0.63
1:E:322:VAL:HA	1:E:338:ILE:HD11	1.81	0.62
1:B:351:THR:HG22	1:B:352:ASP:H	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:GLU:HB2	1:F:339:VAL:HG13	1.82	0.61
1:A:97:ASP:HA	1:A:100:ARG:HG2	1.82	0.61
1:F:8:ILE:HG12	1:F:139:VAL:HB	1.83	0.61
1:B:275:ALA:HB1	1:B:280:VAL:HB	1.83	0.61
1:C:283:GLU:HG2	1:C:288:ILE:HD11	1.82	0.61
1:D:78:ASP:OD1	1:D:78:ASP:N	2.35	0.60
1:E:406:LEU:HB3	1:E:427:MET:HG2	1.83	0.60
1:A:122:ARG:HH21	1:A:134:THR:HG23	1.67	0.59
1:A:303:LEU:HD22	1:A:320:ALA:HA	1.83	0.59
1:D:35:PHE:HB2	1:D:109:ARG:HH12	1.66	0.59
1:E:19:ASP:HB3	1:E:21:ARG:HG2	1.85	0.59
1:A:110:THR:HG21	1:A:129:ALA:HB2	1.85	0.58
1:A:177:ILE:HG12	1:A:261:LEU:HD23	1.85	0.58
1:C:281:ASP:HB3	1:C:288:ILE:HD12	1.84	0.58
1:C:322:VAL:HA	1:C:338:ILE:HD11	1.85	0.58
1:A:349:VAL:HG12	1:A:351:THR:HG23	1.85	0.58
1:E:110:THR:HG21	1:E:129:ALA:HB2	1.86	0.58
1:F:355:ILE:HG12	1:F:412:MET:HG3	1.83	0.58
1:D:126:ARG:NH1	1:D:132:GLU:OE2	2.37	0.57
1:E:327:LEU:C	1:E:329:CYS:H	2.12	0.57
1:C:8:ILE:HG12	1:C:139:VAL:HB	1.85	0.57
1:C:303:LEU:HD22	1:C:320:ALA:HA	1.85	0.57
1:D:202:ILE:HD11	1:D:231:THR:HG22	1.85	0.57
1:E:286:ARG:NH1	1:E:308:SER:O	2.38	0.56
1:E:327:LEU:O	1:E:329:CYS:N	2.38	0.56
1:A:292:TYR:HB2	1:A:294:ARG:HD3	1.86	0.56
1:A:61:ARG:NH1	1:A:193:ALA:O	2.37	0.56
1:A:248:ARG:HG2	1:A:254:THR:HG22	1.88	0.56
1:D:399:THR:HG22	1:D:406:LEU:HD13	1.87	0.56
1:F:303:LEU:HD22	1:F:320:ALA:HA	1.87	0.56
1:A:58:LYS:HE2	1:A:193:ALA:HB2	1.87	0.56
1:A:176:VAL:HG12	1:A:199:THR:HB	1.86	0.56
1:B:327:LEU:C	1:B:329:CYS:H	2.14	0.56
1:A:327:LEU:C	1:A:329:CYS:H	2.14	0.55
1:D:303:LEU:HD22	1:D:320:ALA:HA	1.87	0.55
1:C:270:ALA:HA	1:C:273:LEU:HD12	1.88	0.55
1:C:455:LEU:HA	1:C:458:LEU:HD12	1.87	0.55
1:A:419:LEU:HD11	1:A:447:LEU:HD22	1.87	0.55
1:B:327:LEU:O	1:B:329:CYS:N	2.38	0.55
1:C:149:PRO:HD2	1:C:152:ILE:HD12	1.88	0.55
1:E:182:PHE:HB2	1:E:349:VAL:HG22	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:ALA:HB1	1:F:280:VAL:HB	1.89	0.54
1:C:148:ILE:HG23	1:C:262:VAL:HG11	1.88	0.54
1:A:54:ALA:HB1	1:A:193:ALA:HB3	1.90	0.54
1:F:313:LYS:HE2	2:F:501:FAD:H4'	1.89	0.54
1:C:40:LEU:HG	1:C:88:ILE:HG23	1.90	0.53
1:F:58:LYS:NZ	4:F:601:HOH:O	2.41	0.53
1:A:281:ASP:HB3	1:A:288:ILE:HD12	1.90	0.53
1:E:54:ALA:HB1	1:E:193:ALA:HB3	1.91	0.53
1:E:313:LYS:HD3	2:E:501:FAD:H4'	1.90	0.53
1:B:110:THR:HG21	1:B:129:ALA:HB2	1.90	0.53
1:F:399:THR:HG22	1:F:406:LEU:HA	1.90	0.53
1:F:100:ARG:NH2	1:F:101:CYS:SG	2.81	0.53
1:E:69:ASP:HB2	1:F:74:ARG:HG2	1.91	0.53
1:A:291:GLU:HB2	1:A:339:VAL:HG13	1.90	0.52
1:E:355:ILE:HG12	1:E:412:MET:HG3	1.90	0.52
1:B:221:ARG:HD3	1:E:87:ARG:HD3	1.90	0.52
1:D:213:ASP:OD1	1:D:213:ASP:N	2.43	0.52
1:B:172:PRO:HG3	1:B:259:LEU:HD12	1.92	0.51
1:F:419:LEU:HD11	1:F:447:LEU:HG	1.92	0.51
1:E:122:ARG:NH2	1:E:134:THR:OG1	2.43	0.51
1:D:326:ASN:HB3	1:D:337:MET:HE2	1.93	0.51
1:F:382:VAL:HG21	1:F:450:VAL:HA	1.93	0.51
1:B:217:GLU:HG3	1:E:90:PRO:HB2	1.93	0.51
1:C:51:VAL:O	1:C:55:GLU:HG2	2.10	0.51
1:E:49:MET:HE2	1:E:84:VAL:HG22	1.93	0.51
1:C:160:HIS:CD2	1:C:259:LEU:HD11	2.47	0.50
1:D:54:ALA:HB1	1:D:193:ALA:HB3	1.93	0.50
1:A:200:LEU:HB2	1:A:229:LEU:HD12	1.94	0.50
1:E:455:LEU:HA	1:E:458:LEU:HD12	1.93	0.50
1:C:29:ILE:HG13	1:C:107:VAL:HA	1.93	0.50
1:C:406:LEU:HB2	1:C:427:MET:HG3	1.94	0.50
1:F:228:GLU:OE2	1:F:230:ARG:NH1	2.43	0.50
1:B:382:VAL:HG21	1:B:450:VAL:HA	1.94	0.49
1:C:449:GLU:O	1:C:453:ASN:ND2	2.43	0.49
1:A:327:LEU:O	1:A:329:CYS:N	2.45	0.49
1:A:100:ARG:HG3	1:A:101:CYS:N	2.27	0.49
1:D:275:ALA:HB1	1:D:280:VAL:HB	1.95	0.49
1:C:313:LYS:HE2	2:C:501:FAD:H4'	1.95	0.48
1:D:97:ASP:HA	1:D:100:ARG:HG2	1.95	0.48
1:D:382:VAL:HG11	1:D:450:VAL:HA	1.94	0.48
1:C:76:ARG:O	1:C:80:VAL:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ILE:HB	1:B:200:LEU:HD13	1.95	0.48
1:E:286:ARG:HH12	1:E:309:PRO:HA	1.78	0.48
1:F:271:ASP:OD1	1:F:271:ASP:N	2.47	0.48
1:A:2:GLU:CD	1:A:26:ARG:HH22	2.22	0.47
1:A:17:ILE:O	1:A:324:GLN:NE2	2.45	0.47
1:A:146:PRO:HA	1:A:266:ARG:HG2	1.95	0.47
1:F:118:GLN:OE1	1:F:124:LEU:HB2	2.14	0.47
1:D:8:ILE:HG12	1:D:139:VAL:HB	1.96	0.47
1:C:202:ILE:HD11	1:C:231:THR:HG22	1.96	0.47
1:D:351:THR:HG22	1:D:352:ASP:N	2.25	0.47
1:B:141:ALA:HB2	1:B:303:LEU:HD21	1.96	0.47
1:E:191:PHE:HB3	1:E:196:VAL:HB	1.96	0.47
1:E:382:VAL:HG11	1:E:450:VAL:HA	1.95	0.47
1:E:354:GLN:HG2	1:E:416:ALA:HB3	1.97	0.47
1:E:11:THR:HG23	1:E:31:GLU:HB2	1.97	0.47
1:E:286:ARG:HH12	1:E:308:SER:C	2.22	0.47
1:D:334:THR:HA	1:D:337:MET:HB2	1.98	0.46
1:F:268:SER:HB2	1:F:306:VAL:HA	1.95	0.46
1:A:235:VAL:HG11	1:A:247:LEU:HD22	1.97	0.46
1:C:240:GLN:CD	1:C:240:GLN:H	2.23	0.46
1:E:401:ARG:HB3	1:E:401:ARG:NH1	2.31	0.46
1:F:62:GLY:O	1:F:65:ARG:HG2	2.16	0.46
1:B:447:LEU:N	1:B:448:PRO:HD2	2.31	0.46
1:E:61:ARG:NH1	1:E:193:ALA:O	2.48	0.46
1:A:45:ILE:HG22	1:A:49:MET:HE3	1.98	0.46
1:B:419:LEU:HD21	1:B:447:LEU:HG	1.98	0.46
1:C:57:ALA:HB2	1:D:68:ILE:HD13	1.98	0.46
1:C:384:TYR:CD1	1:C:447:LEU:HD13	2.51	0.46
1:A:74:ARG:HG3	1:A:75:VAL:N	2.31	0.46
1:C:2:GLU:OE1	1:C:26:ARG:NH2	2.49	0.46
1:D:354:GLN:HG2	1:D:416:ALA:HB3	1.97	0.45
1:E:160:HIS:CD2	1:E:259:LEU:HD11	2.50	0.45
1:E:189:HIS:HB2	1:E:351:THR:HG23	1.98	0.45
1:D:160:HIS:CD2	1:D:259:LEU:HD11	2.51	0.45
1:A:76:ARG:O	1:A:80:VAL:HG23	2.17	0.45
1:A:280:VAL:HG23	1:A:295:THR:HB	1.99	0.45
1:B:182:PHE:HB2	1:B:349:VAL:HG22	1.99	0.45
1:B:238:GLY:HA3	1:B:247:LEU:HD23	1.99	0.45
1:C:142:ALA:O	2:C:501:FAD:H8A	2.17	0.45
1:A:286:ARG:NH1	1:A:307:SER:O	2.49	0.44
1:E:382:VAL:HG21	1:E:450:VAL:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:THR:HG23	1:B:31:GLU:HB2	1.99	0.44
1:B:32:GLN:HG2	2:B:501:FAD:C4A	2.48	0.44
1:B:146:PRO:HA	1:B:266:ARG:HG2	1.98	0.44
1:C:355:ILE:HG12	1:C:412:MET:HG3	1.99	0.44
1:C:382:VAL:HG12	1:C:384:TYR:H	1.83	0.44
1:E:314:HIS:CD2	1:E:315:VAL:HG23	2.52	0.44
1:B:327:LEU:C	1:B:329:CYS:N	2.75	0.44
1:B:363:ASN:HB3	1:E:101:CYS:SG	2.58	0.44
1:A:388:MET:HG2	1:B:52:TYR:CZ	2.52	0.44
1:B:77:TRP:CD2	1:B:171:LEU:HD13	2.52	0.44
1:F:77:TRP:CD2	1:F:171:LEU:HD13	2.53	0.44
1:F:140:ILE:HG22	1:F:306:VAL:HG11	1.99	0.44
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.85	0.44
1:B:21:ARG:HD3	1:B:328:LEU:HD11	1.99	0.44
1:B:140:ILE:HG22	1:B:306:VAL:HG11	2.00	0.44
1:B:8:ILE:HG23	1:B:139:VAL:HB	2.00	0.43
1:F:51:VAL:HG11	1:F:350:PHE:HB3	1.99	0.43
1:D:143:GLY:HA2	1:D:305:ASP:HB2	2.00	0.43
1:D:344:TYR:CD1	1:D:427:MET:HE2	2.53	0.43
1:E:327:LEU:C	1:E:329:CYS:N	2.74	0.43
1:F:11:THR:HG23	1:F:31:GLU:HB2	2.01	0.43
1:F:160:HIS:ND1	1:F:259:LEU:HD11	2.33	0.43
1:B:442:TRP:CD1	1:B:452:GLU:HG3	2.54	0.43
1:A:118:GLN:HG3	1:A:119:ALA:H	1.83	0.43
1:B:318:HIS:NE2	1:B:341:ASP:OD2	2.50	0.43
1:A:327:LEU:C	1:A:329:CYS:N	2.76	0.42
1:D:11:THR:HG23	1:D:31:GLU:HB2	2.00	0.42
1:A:186:GLU:HA	1:A:351:THR:HG22	2.00	0.42
1:A:361:THR:HA	1:A:410:HIS:HE2	1.84	0.42
1:B:215:ILE:HG23	1:B:412:MET:HB2	2.01	0.42
1:C:71:HIS:NE2	1:C:73:ASP:OD1	2.52	0.42
1:C:206:CYS:HA	1:C:220:THR:HG21	2.01	0.42
1:C:277:GLN:O	1:C:277:GLN:HG3	2.19	0.42
1:A:184:ALA:HB2	1:A:263:ALA:HB3	2.02	0.42
1:B:169:ALA:HB2	1:C:253:CYS:SG	2.60	0.42
1:D:49:MET:HE2	1:D:84:VAL:HG22	2.02	0.42
1:D:375:LYS:HD2	1:D:457:GLY:HA3	2.02	0.42
1:E:292:TYR:HB2	1:E:294:ARG:HG3	2.01	0.42
1:B:384:TYR:CD2	1:B:447:LEU:HD13	2.54	0.42
1:F:15:ASN:O	1:F:99:ARG:NH2	2.50	0.42
1:B:338:ILE:HD12	1:B:338:ILE:HA	1.95	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:TYR:O	1:B:135:ALA:HA	2.20	0.42
1:C:291:GLU:CD	1:C:291:GLU:H	2.28	0.42
1:A:52:TYR:CZ	1:B:388:MET:HG2	2.55	0.41
1:A:388:MET:HE2	1:A:388:MET:HB3	1.91	0.41
1:C:52:TYR:O	1:C:56:VAL:HG23	2.20	0.41
1:C:212:ASP:OD2	1:C:396:LYS:NZ	2.50	0.41
1:E:290:ASP:OD2	1:E:294:ARG:HB2	2.20	0.41
1:D:171:LEU:HA	1:D:172:PRO:HD3	1.96	0.41
1:D:400:GLU:OE1	1:D:403:SER:OG	2.29	0.41
1:A:87:ARG:HB2	1:F:221:ARG:HG3	2.02	0.41
1:D:359:GLY:HA3	1:D:427:MET:HE1	2.02	0.41
1:F:54:ALA:HB1	1:F:193:ALA:HB3	2.01	0.41
1:B:313:LYS:HE2	2:B:501:FAD:H4'	2.03	0.41
1:E:68:ILE:HD13	1:F:57:ALA:HB2	2.02	0.41
1:E:298:ARG:HA	1:E:331:TRP:CE2	2.56	0.41
1:A:275:ALA:HB1	1:A:280:VAL:CG1	2.50	0.41
1:D:436:MET:HE3	1:D:455:LEU:HD11	2.03	0.41
1:F:142:ALA:O	2:F:501:FAD:H8A	2.21	0.41
1:F:186:GLU:HG2	1:F:350:PHE:O	2.21	0.41
1:B:268:SER:OG	1:B:306:VAL:HA	2.21	0.40
1:A:202:ILE:HD11	1:A:231:THR:HG22	2.02	0.40
1:E:21:ARG:HG3	1:E:22:TYR:CD1	2.56	0.40
1:F:110:THR:HG21	1:F:129:ALA:HB2	2.03	0.40
1:F:111:HIS:CE1	1:F:113:ARG:HG3	2.56	0.40
1:A:205:SER:HB3	1:A:232:HIS:NE2	2.36	0.40
1:C:148:ILE:HB	1:C:153:LEU:HD21	2.03	0.40
1:E:48:LYS:N	1:E:48:LYS:HD3	2.35	0.40
1:A:40:LEU:O	1:A:46:PRO:HD3	2.21	0.40
1:A:45:ILE:O	1:A:49:MET:HG3	2.22	0.40
1:A:344:TYR:CD1	1:A:427:MET:HE2	2.56	0.40
1:C:281:ASP:N	1:C:296:SER:OG	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/459 (100%)	434 (95%)	18 (4%)	5 (1%)	11	37
1	B	457/459 (100%)	435 (95%)	19 (4%)	3 (1%)	18	47
1	C	457/459 (100%)	437 (96%)	20 (4%)	0	100	100
1	D	457/459 (100%)	434 (95%)	22 (5%)	1 (0%)	43	71
1	E	457/459 (100%)	431 (94%)	22 (5%)	4 (1%)	14	41
1	F	457/459 (100%)	437 (96%)	19 (4%)	1 (0%)	43	71
All	All	2742/2754 (100%)	2608 (95%)	120 (4%)	14 (0%)	24	54

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	LEU
1	A	330	ASP
1	B	328	LEU
1	E	328	LEU
1	B	330	ASP
1	A	24	SER
1	B	327	LEU
1	E	208	LEU
1	E	330	ASP
1	F	330	ASP
1	A	327	LEU
1	E	327	LEU
1	A	284	ASP
1	D	331	TRP

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	368/368 (100%)	366 (100%)	2 (0%)	81	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	367/368 (100%)	365 (100%)	2 (0%)	81	80
1	C	368/368 (100%)	367 (100%)	1 (0%)	86	84
1	D	368/368 (100%)	367 (100%)	1 (0%)	86	84
1	E	368/368 (100%)	368 (100%)	0	100	100
1	F	367/368 (100%)	364 (99%)	3 (1%)	73	76
All	All	2206/2208 (100%)	2197 (100%)	9 (0%)	84	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	CYS
1	A	216	CYS
1	B	44	CYS
1	B	216	CYS
1	C	44	CYS
1	D	44	CYS
1	F	44	CYS
1	F	206	CYS
1	F	216	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	415	GLN
1	A	421	GLN
1	A	425	GLN
1	B	137	GLN
1	B	277	GLN
1	B	325	HIS
1	B	342	HIS
1	B	415	GLN
1	B	440	GLN
1	C	118	GLN
1	C	324	GLN
1	D	71	HIS
1	D	239	GLN
1	D	342	HIS
1	D	440	GLN
1	E	41	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	118	GLN
1	E	137	GLN
1	E	440	GLN
1	F	137	GLN
1	F	421	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	FAD	F	501	-	58,58,58	0.29	0	85,89,89	0.27	0
2	FAD	E	501	-	58,58,58	0.29	0	85,89,89	0.27	0
2	FAD	B	501	-	58,58,58	0.29	0	85,89,89	0.28	0
2	FAD	D	501	-	58,58,58	0.28	0	85,89,89	0.27	0
3	A1H3R	D	502	-	31,31,31	0.49	0	30,44,44	0.58	0
2	FAD	A	501	-	58,58,58	0.27	0	85,89,89	0.27	0
3	A1H3R	E	502	-	31,31,31	0.50	0	30,44,44	0.65	0
2	FAD	C	501	-	58,58,58	0.29	0	85,89,89	0.28	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
2	FAD	F	501	-	-	6/34/50/50	0/6/6/6
2	FAD	E	501	-	-	7/34/50/50	0/6/6/6
2	FAD	B	501	-	-	6/34/50/50	0/6/6/6
2	FAD	D	501	-	-	9/34/50/50	0/6/6/6
3	A1H3R	D	502	-	-	0/8/27/27	0/5/5/5
2	FAD	A	501	-	-	7/34/50/50	0/6/6/6
3	A1H3R	E	502	-	-	0/8/27/27	0/5/5/5
2	FAD	C	501	-	-	6/34/50/50	0/6/6/6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	O4'-C4'-C5'-O5'
2	B	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	C5B-O5B-PA-O2A
2	D	501	FAD	C5B-O5B-PA-O2A
2	D	501	FAD	O4'-C4'-C5'-O5'
2	E	501	FAD	C5B-O5B-PA-O2A
2	F	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
2	E	501	FAD	O4B-C4B-C5B-O5B
2	F	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	C3B-C4B-C5B-O5B
2	C	501	FAD	C3B-C4B-C5B-O5B
2	E	501	FAD	C3B-C4B-C5B-O5B
2	F	501	FAD	C3B-C4B-C5B-O5B
2	D	501	FAD	C3B-C4B-C5B-O5B
2	D	501	FAD	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

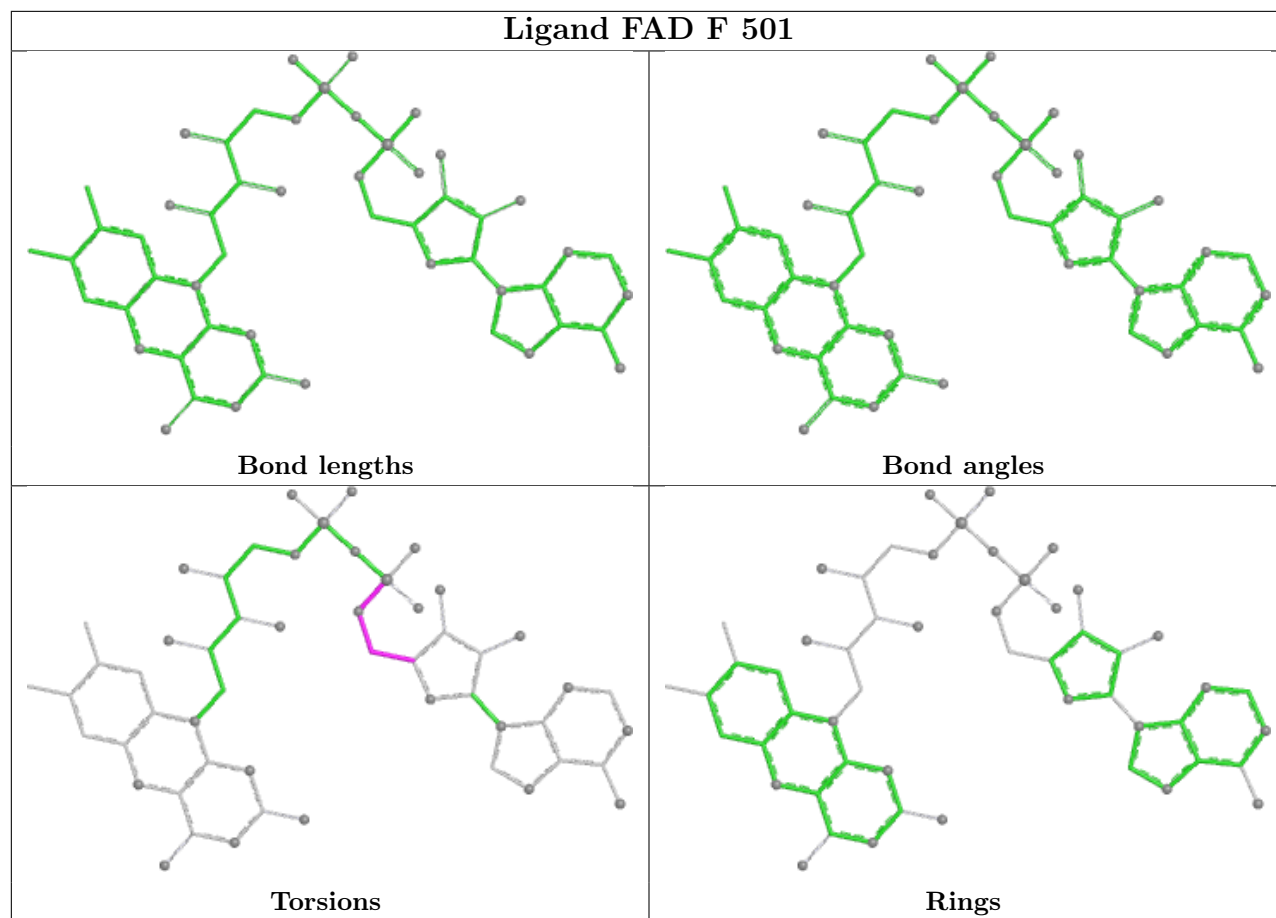
Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C5B-O5B-PA-O3P
2	B	501	FAD	C5B-O5B-PA-O1A
2	B	501	FAD	C5B-O5B-PA-O3P
2	C	501	FAD	C5B-O5B-PA-O1A
2	C	501	FAD	C5B-O5B-PA-O3P
2	D	501	FAD	C5B-O5B-PA-O1A
2	D	501	FAD	C5B-O5B-PA-O3P
2	E	501	FAD	C5B-O5B-PA-O1A
2	E	501	FAD	C5B-O5B-PA-O3P
2	F	501	FAD	C5B-O5B-PA-O1A
2	F	501	FAD	C5B-O5B-PA-O3P
2	D	501	FAD	C2B-C1B-N9A-C8A
2	A	501	FAD	C4B-C5B-O5B-PA
2	B	501	FAD	C4B-C5B-O5B-PA
2	C	501	FAD	C4B-C5B-O5B-PA
2	D	501	FAD	C4B-C5B-O5B-PA
2	E	501	FAD	C4B-C5B-O5B-PA
2	F	501	FAD	C4B-C5B-O5B-PA
2	E	501	FAD	C2B-C1B-N9A-C8A

There are no ring outliers.

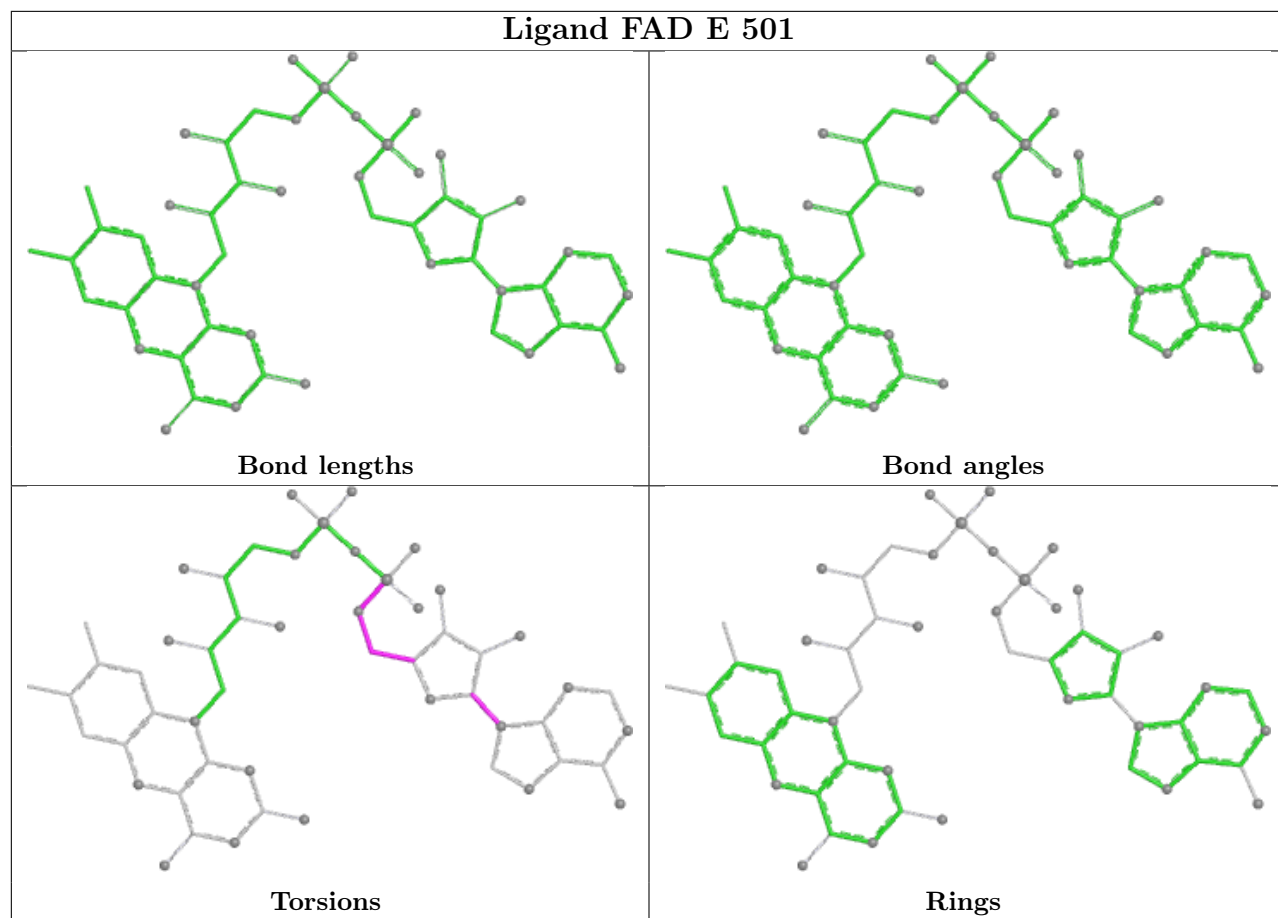
4 monomers are involved in 7 short contacts:

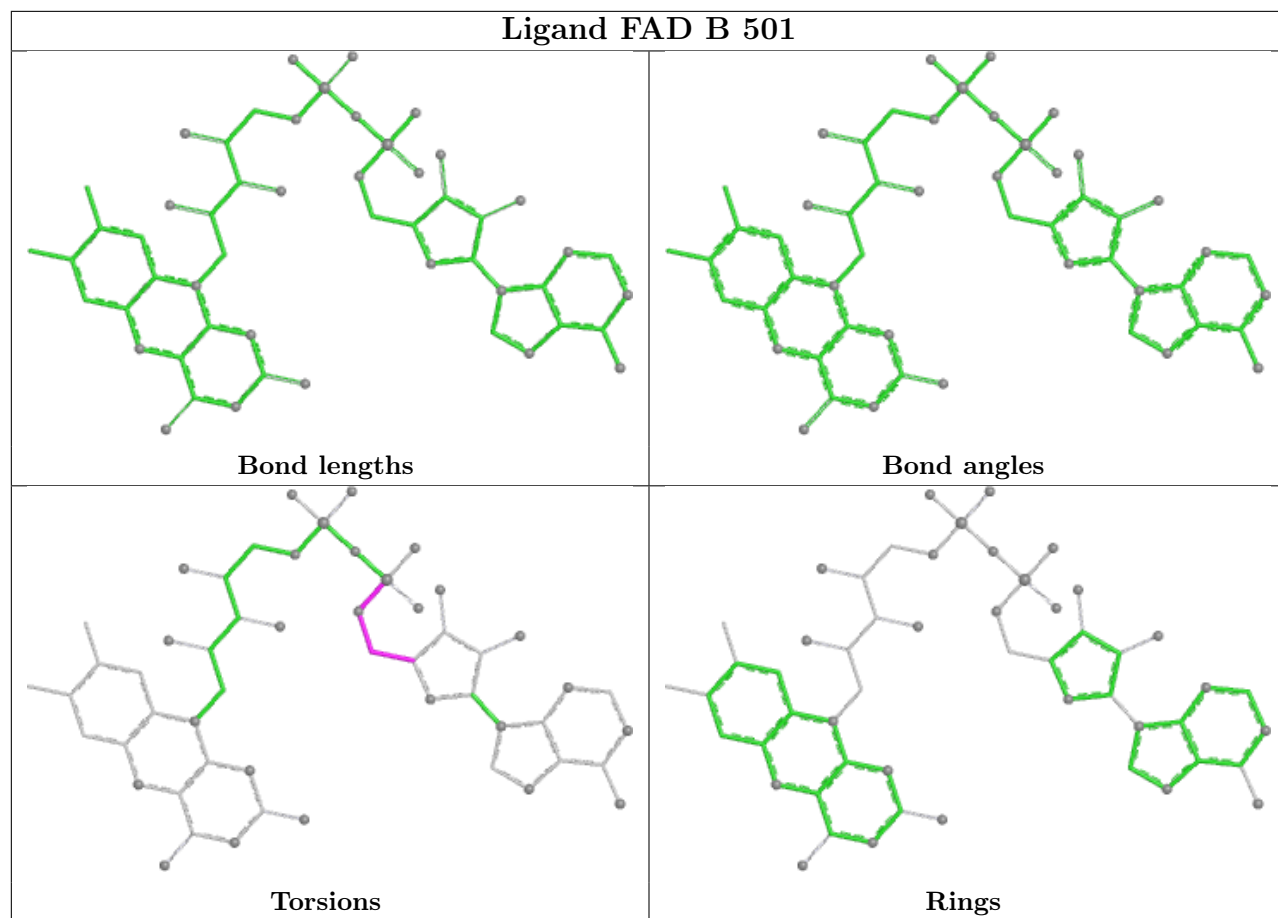
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	FAD	2	0
2	E	501	FAD	1	0
2	B	501	FAD	2	0
2	C	501	FAD	2	0

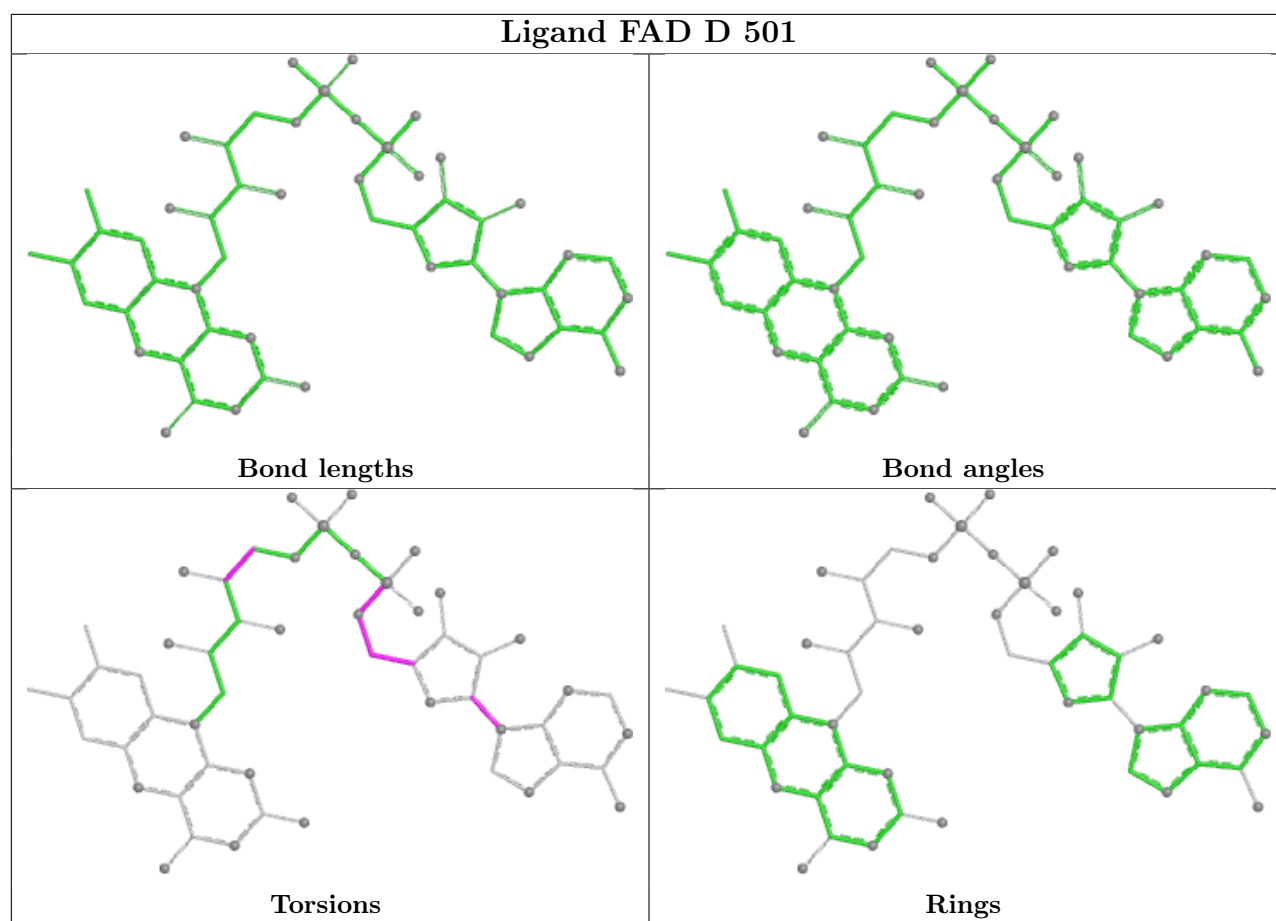
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



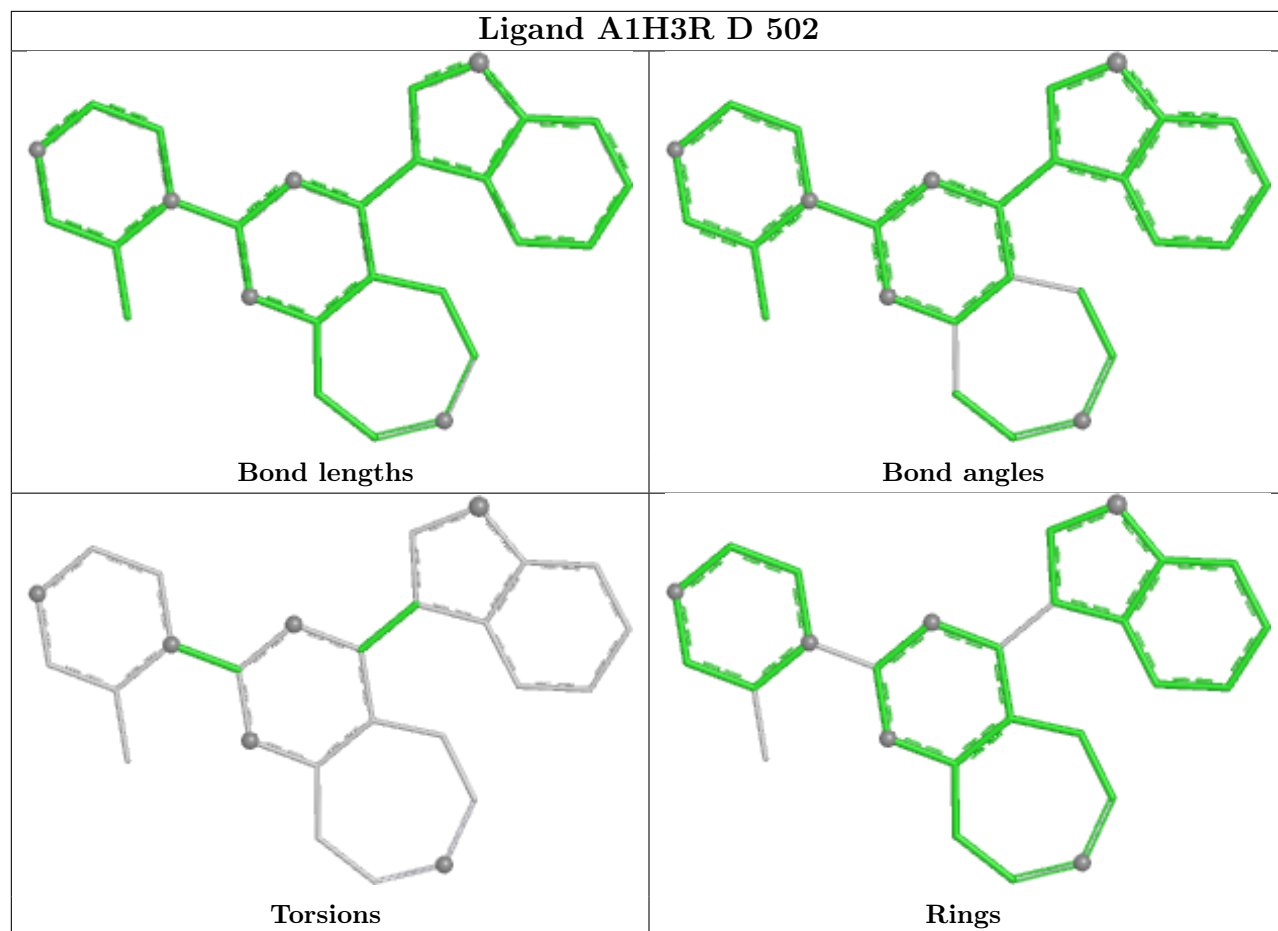
Ligand FAD E 501

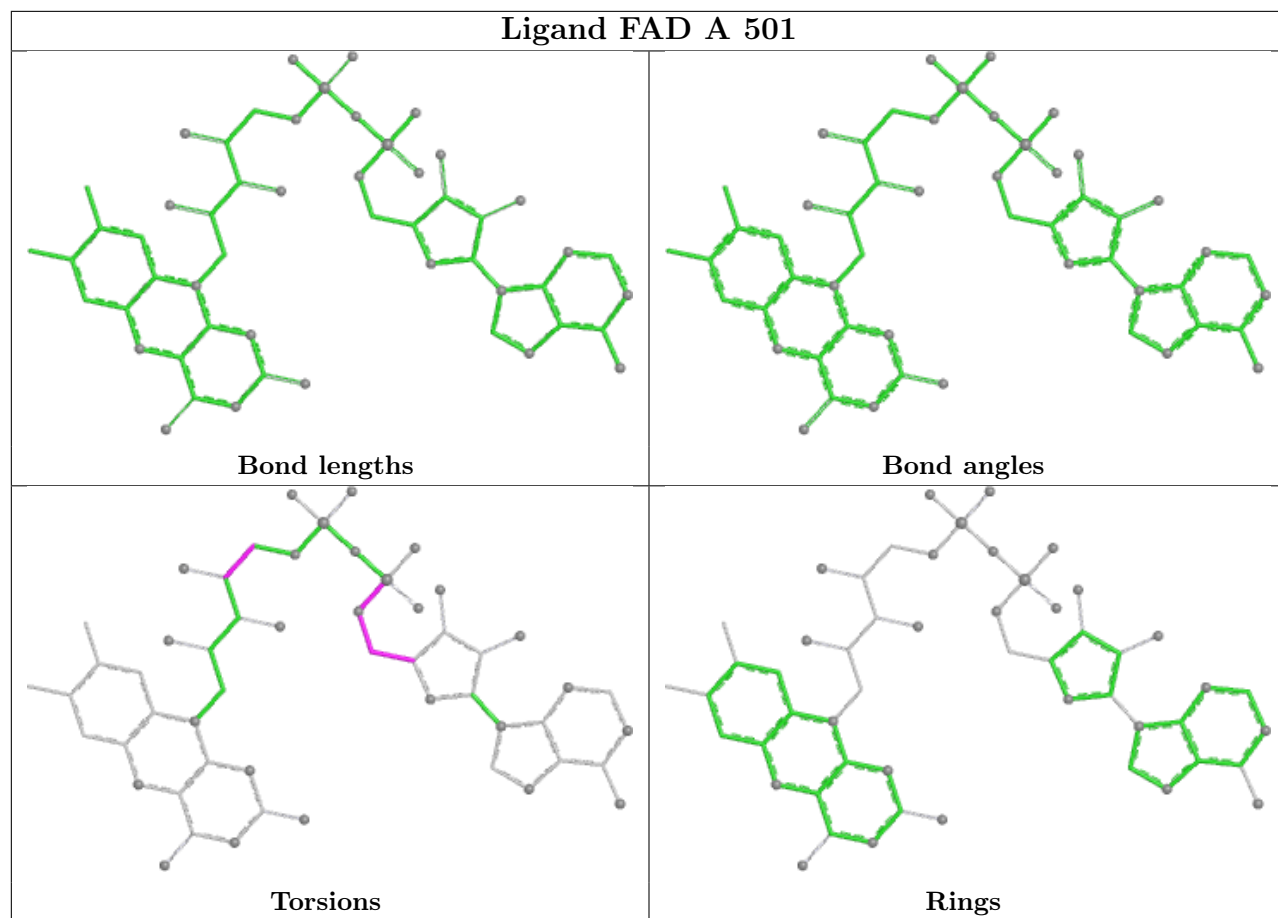




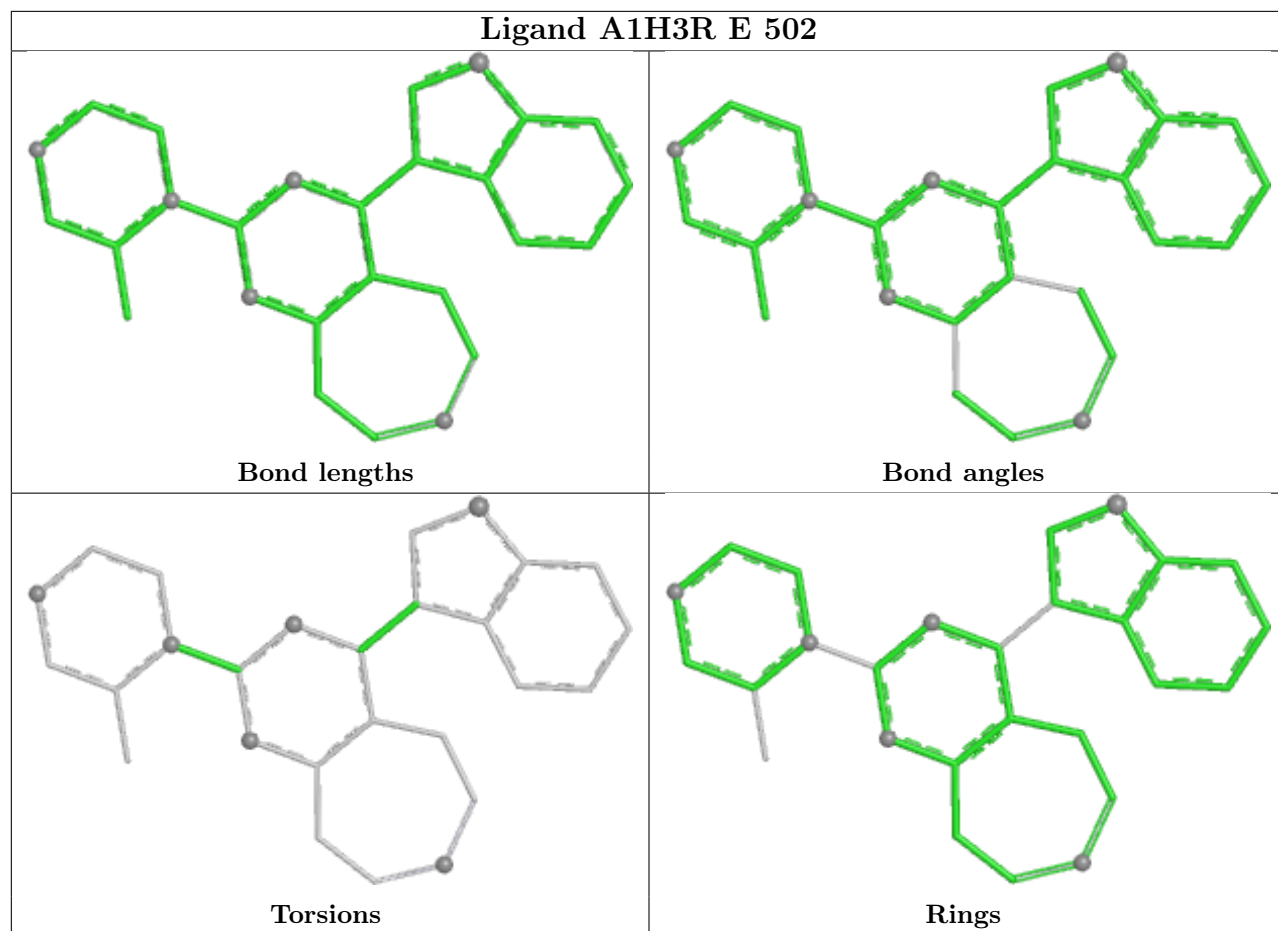


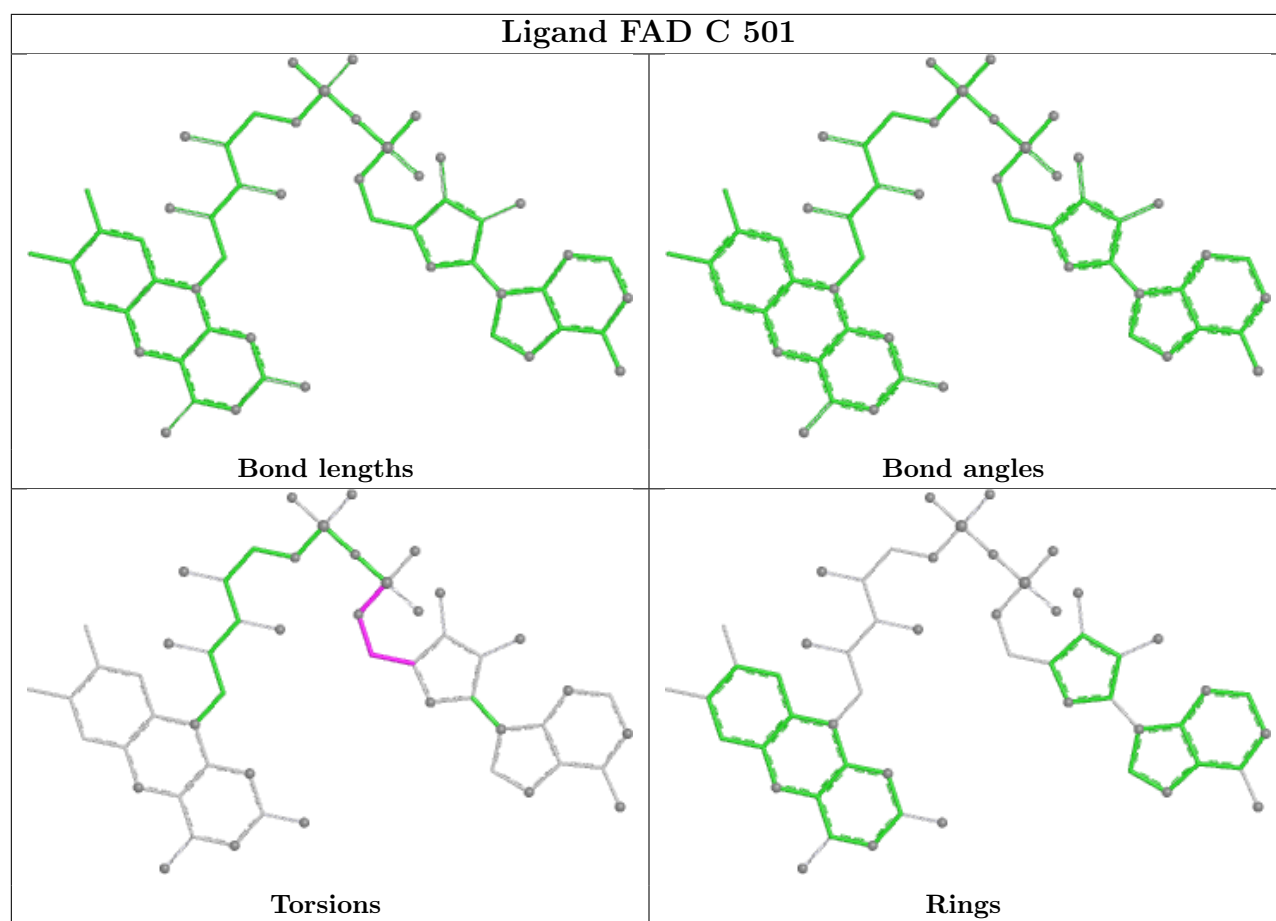
Ligand A1H3R D 502





Ligand A1H3R E 502





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	459/459 (100%)	0.54	16 (3%) 47 34	35, 67, 90, 117	3 (0%)
1	B	459/459 (100%)	0.46	8 (1%) 69 54	36, 66, 89, 108	1 (0%)
1	C	459/459 (100%)	0.36	6 (1%) 75 61	38, 59, 84, 100	0
1	D	459/459 (100%)	0.39	11 (2%) 59 45	29, 59, 86, 101	4 (0%)
1	E	459/459 (100%)	0.51	21 (4%) 37 27	37, 61, 88, 100	1 (0%)
1	F	459/459 (100%)	0.41	9 (1%) 65 50	35, 61, 88, 101	0
All	All	2754/2754 (100%)	0.44	71 (2%) 57 42	29, 62, 87, 117	9 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	357	ALA	5.0
1	F	166	MET	5.0
1	E	302	ALA	5.0
1	A	104	ASN	4.3
1	A	119	ALA	4.2
1	E	22	TYR	4.0
1	F	422	PRO	3.7
1	E	418	SER	3.7
1	E	296	SER	3.6
1	F	314	HIS	3.5
1	D	9	ILE	3.4
1	A	125	LEU	3.3
1	C	418	SER	3.2
1	A	217	GLU	3.1
1	A	133	PHE	3.1
1	E	14	GLY	2.9
1	E	209	ARG	2.9
1	F	84	VAL	2.8
1	A	139	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	30	CYS	2.7
1	C	324	GLN	2.6
1	A	14	GLY	2.6
1	D	459	ARG	2.6
1	B	302	ALA	2.6
1	E	280	VAL	2.6
1	E	348	ALA	2.6
1	D	415	GLN	2.6
1	D	14	GLY	2.6
1	D	10	GLY	2.6
1	C	254	THR	2.5
1	E	425	GLN	2.5
1	E	281	ASP	2.5
1	A	114	PHE	2.4
1	E	30	CYS	2.4
1	F	312	LEU	2.4
1	E	442	TRP	2.4
1	A	381	ASP	2.4
1	C	12	GLY	2.3
1	E	293	GLN	2.3
1	F	340	THR	2.3
1	E	347	ALA	2.3
1	D	19	ASP	2.3
1	D	358	VAL	2.3
1	D	260	LEU	2.3
1	F	44	CYS	2.2
1	A	81	VAL	2.2
1	F	409	ALA	2.2
1	A	138	VAL	2.2
1	A	167	ARG	2.2
1	E	138	VAL	2.2
1	C	417	SER	2.1
1	B	131	GLU	2.1
1	A	85	PHE	2.1
1	B	63	ALA	2.1
1	A	117	VAL	2.1
1	E	110	THR	2.1
1	E	300	VAL	2.1
1	E	19	ASP	2.1
1	B	301	PHE	2.1
1	F	291	GLU	2.1
1	B	307	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	411	ILE	2.1
1	B	45	ILE	2.1
1	D	108	TYR	2.1
1	B	356	ALA	2.1
1	E	90	PRO	2.1
1	A	349	VAL	2.0
1	C	13	SER	2.0
1	D	307	SER	2.0
1	B	42	VAL	2.0
1	E	183	ILE	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](#)

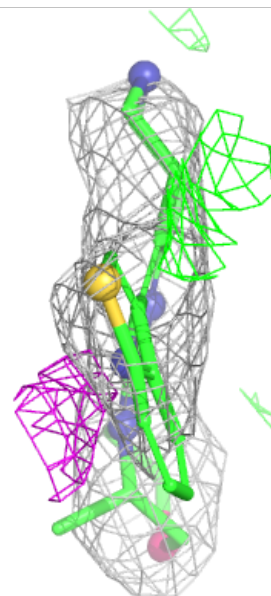
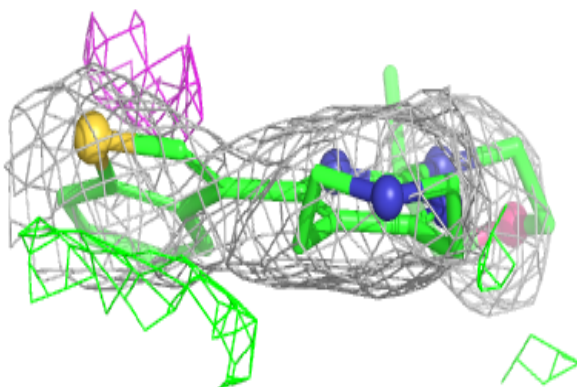
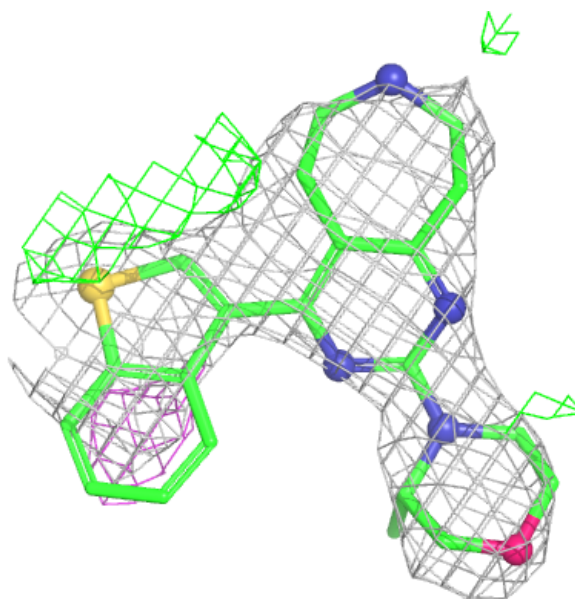
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1H3R	E	502	27/27	0.80	0.22	62,74,80,80	0
3	A1H3R	D	502	27/27	0.86	0.20	61,77,89,95	27
2	FAD	B	501	53/53	0.91	0.11	54,66,78,80	0
2	FAD	E	501	53/53	0.93	0.11	47,61,75,76	0
2	FAD	A	501	53/53	0.93	0.10	53,64,79,84	0
2	FAD	D	501	53/53	0.93	0.11	49,63,79,88	0
2	FAD	F	501	53/53	0.94	0.10	48,62,70,73	0
2	FAD	C	501	53/53	0.95	0.09	48,63,72,74	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.

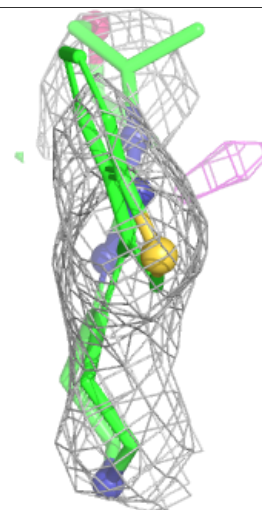
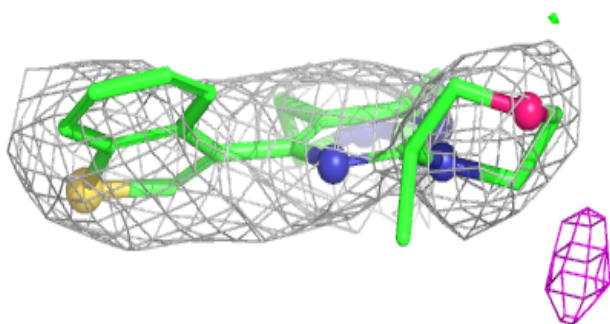
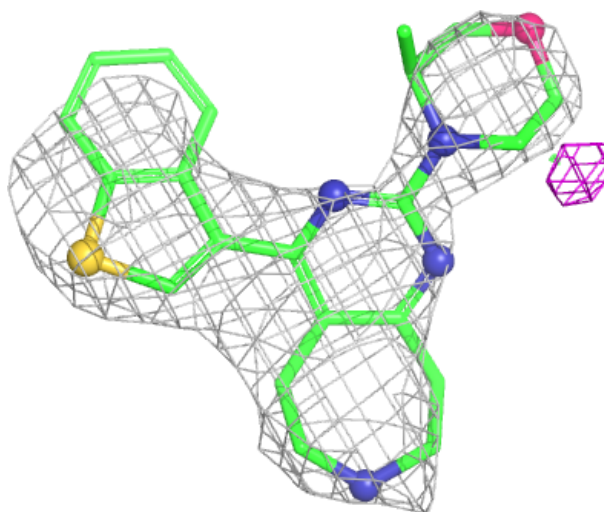
Electron density around A1H3R E 502:

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



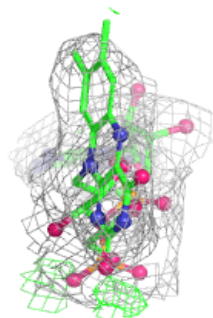
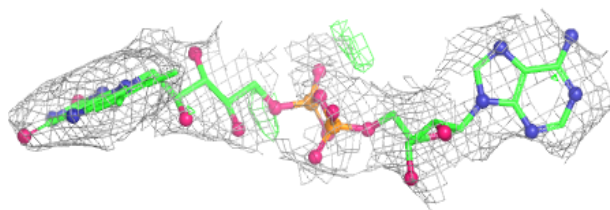
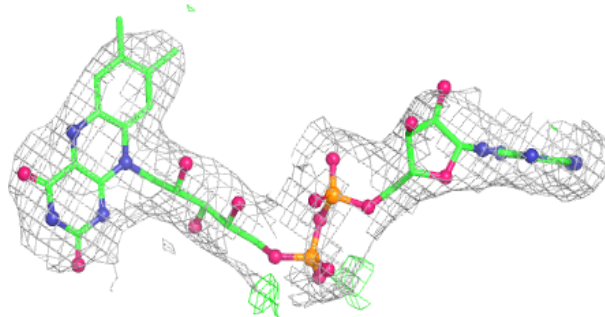
Electron density around A1H3R D 502:

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

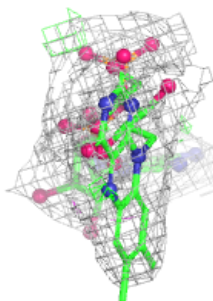
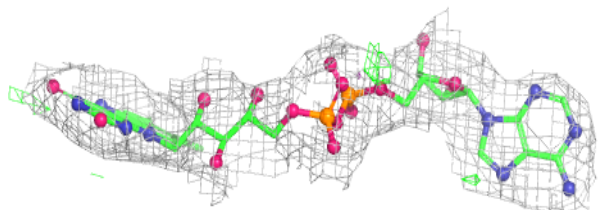
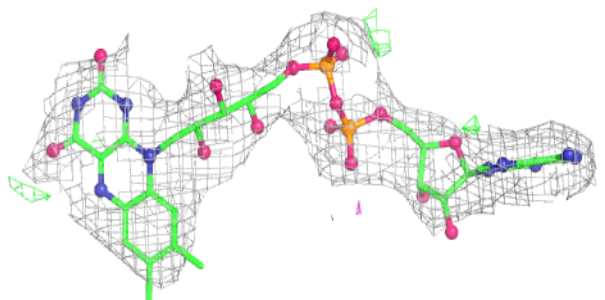


Electron density around FAD B 501:

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

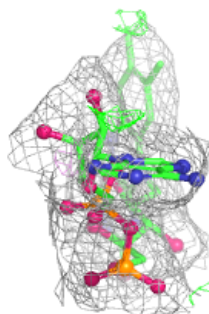
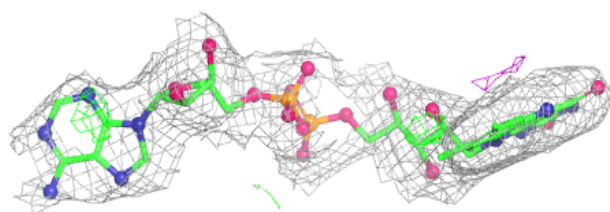
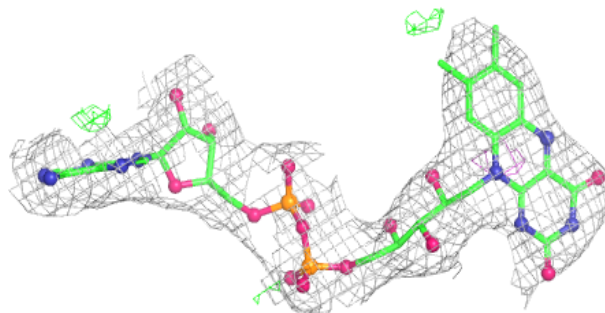
**Electron density around FAD E 501:**

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

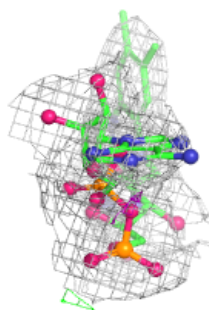
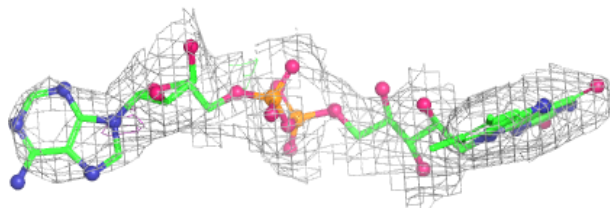
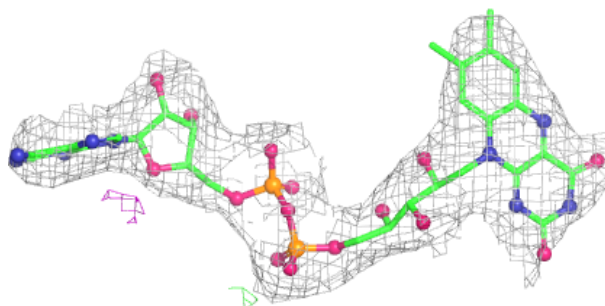


Electron density around FAD A 501:

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

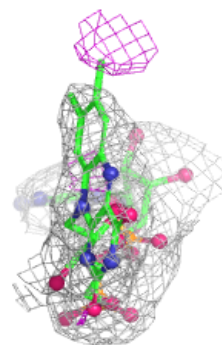
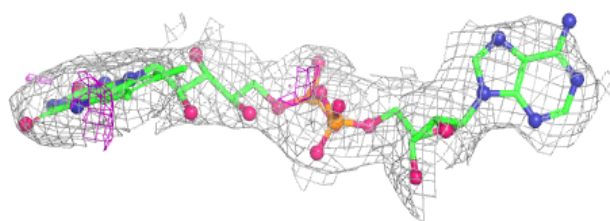
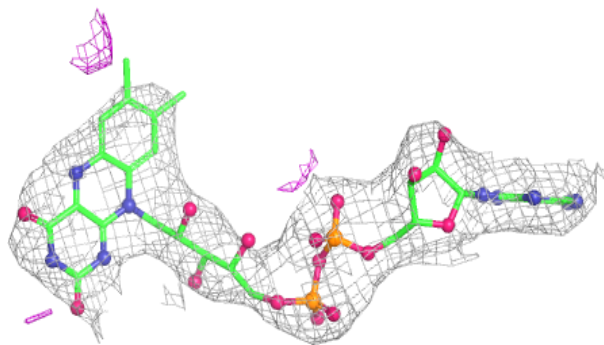
**Electron density around FAD D 501:**

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

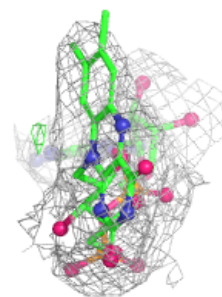
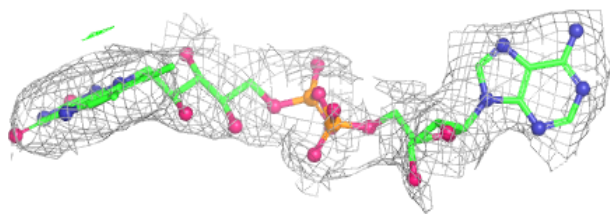
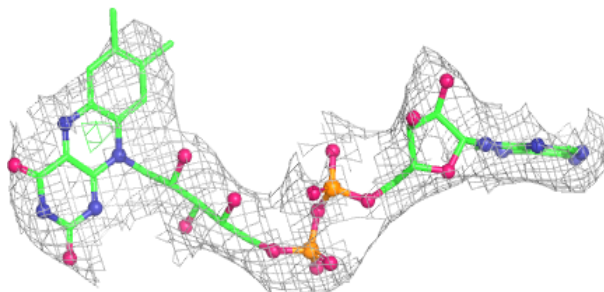


Electron density around FAD F 501:

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

**Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.