



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:30 AM UTC

PDB ID : 4TMB / pdb_00004tmb
Title : CRYSTAL STRUCTURE of OLD YELLOW ENZYME from CANDIDA MACEDONIENSIS AKU4588
Authors : Horita, S.; Kataoka, M.; Kitamura, N.; Nakagawa, T.; Miyakawa, T.; Ohtsuka, J.; Nagata, K.; Shimizu, S.; Tanokura, M.
Deposited on : 2014-05-31
Resolution : 1.80 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

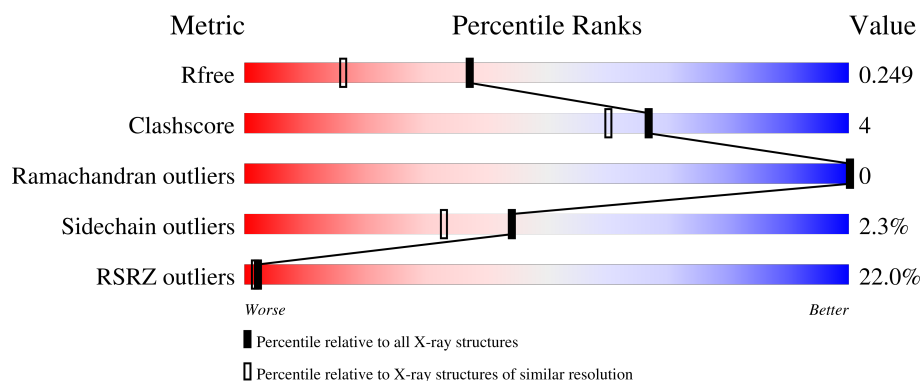
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	403	2% 87% 8% • •
1	B	403	83% 9% 7%
1	C	403	% 86% 8% • 5%
1	D	403	81% 87% 7% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13296 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 Old yellow enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3138	2010	531	592	5			
1	B	374	Total	C	N	O	S	0	0	0
			2991	1910	509	567	5			
1	C	381	Total	C	N	O	S	0	0	0
			3044	1944	518	576	6			
1	D	383	Total	C	N	O	S	0	0	0
			3062	1955	521	580	6			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

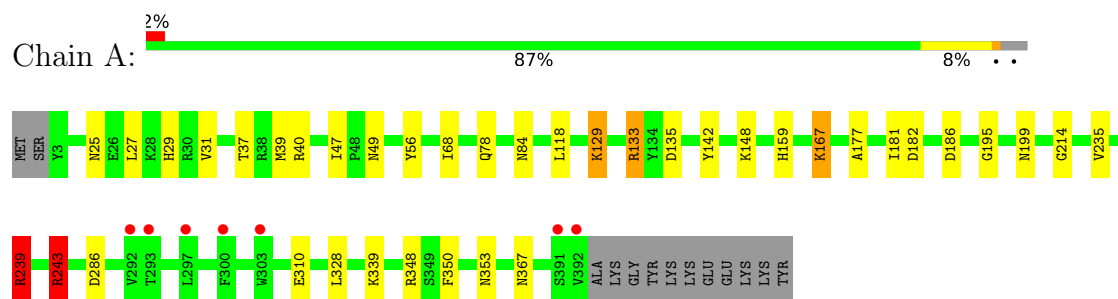
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total	O	0	0
			247	247		
3	B	263	Total	O	0	0
			263	263		
3	C	178	Total	O	0	0
			178	178		
3	D	249	Total	O	0	0
			249	249		

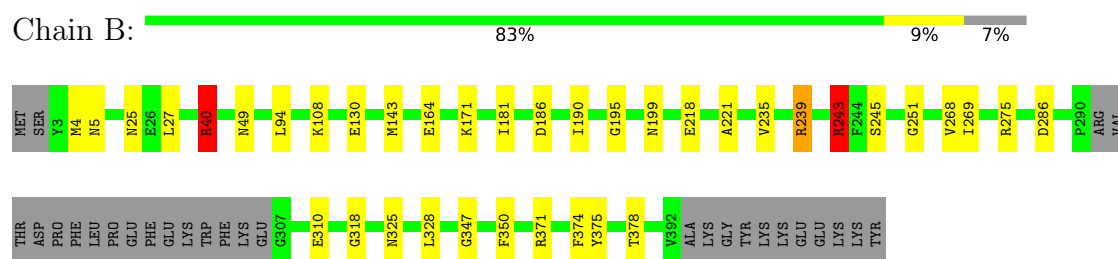
3 Residue-property plots [i](#)

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.

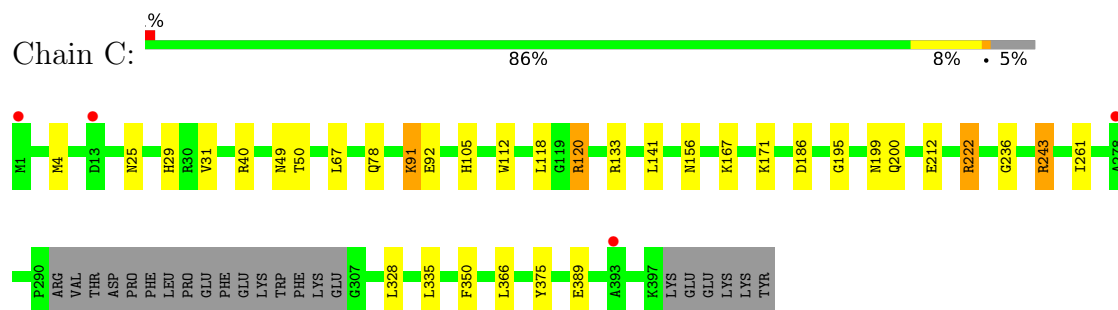
- Molecule 1: Old yellow enzyme



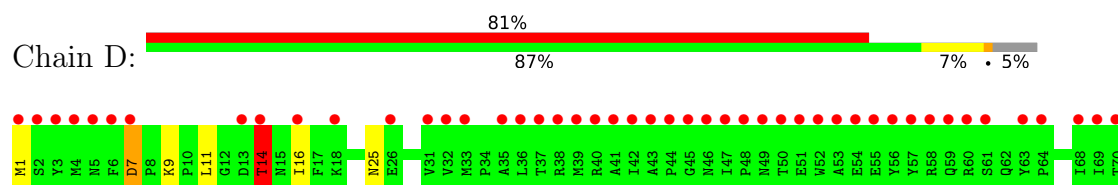
- Molecule 1: Old yellow enzyme



- Molecule 1: Old yellow enzyme



- Molecule 1: Old yellow enzyme



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	287.51Å 59.62Å 100.29Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	19.82 – 1.80 19.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.82-1.80) 98.9 (19.82-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.98 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.210 (Not available) , 0.249	Depositor DCC
R_{free} test set	7432 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13296	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.22	5/3221 (0.2%)	1.16	11/4370 (0.3%)
1	B	1.27	7/3066 (0.2%)	1.21	12/4158 (0.3%)
1	C	1.09	1/3120 (0.0%)	1.11	9/4228 (0.2%)
1	D	1.20	2/3138 (0.1%)	1.12	7/4251 (0.2%)
All	All	1.20	15/12545 (0.1%)	1.15	39/17007 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	322	ARG	CD-NE	-10.10	1.32	1.46
1	A	133	ARG	CD-NE	-6.65	1.36	1.46
1	B	243	ARG	CD-NE	-6.39	1.37	1.46
1	A	68	ILE	C-O	-6.29	1.16	1.24
1	A	214	GLY	N-CA	6.21	1.50	1.45
1	B	245	SER	C-O	6.05	1.30	1.24
1	C	120	ARG	CD-NE	-6.03	1.37	1.46
1	A	239	ARG	CD-NE	-5.99	1.37	1.46
1	B	190	ILE	CA-C	5.95	1.59	1.53
1	D	322	ARG	CZ-NH2	-5.92	1.25	1.33
1	B	239	ARG	CD-NE	-5.68	1.38	1.46
1	B	269	ILE	C-O	-5.50	1.17	1.24
1	B	275	ARG	C-O	-5.42	1.17	1.24
1	B	347	GLY	N-CA	5.35	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	TYR	N-CA	5.03	1.52	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ARG	CD-NE-CZ	13.38	143.14	124.40
1	C	120	ARG	CB-CG-CD	12.06	139.04	111.30
1	B	40	ARG	CG-CD-NE	-11.60	86.49	112.00
1	B	40	ARG	CB-CG-CD	11.57	137.91	111.30
1	A	133	ARG	NE-CZ-NH2	-10.62	109.64	119.20
1	B	40	ARG	NE-CZ-NH2	-10.50	109.75	119.20
1	D	322	ARG	NE-CZ-NH2	-9.15	110.97	119.20
1	C	120	ARG	NE-CZ-NH2	-8.08	111.93	119.20
1	D	322	ARG	NE-CZ-NH1	7.70	129.20	121.50
1	A	239	ARG	NE-CZ-NH2	-7.43	112.51	119.20
1	A	243	ARG	NE-CZ-NH1	7.02	128.52	121.50
1	C	118	LEU	N-CA-C	6.64	119.86	111.69
1	B	40	ARG	NE-CZ-NH1	6.60	128.10	121.50
1	C	120	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	A	133	ARG	CD-NE-CZ	6.46	133.44	124.40
1	A	133	ARG	NE-CZ-NH1	6.41	127.91	121.50
1	B	243	ARG	CB-CG-CD	-6.33	96.74	111.30
1	D	175	ASP	N-CA-C	-6.26	104.38	111.07
1	C	236	GLY	N-CA-C	6.20	119.98	112.48
1	B	5	ASN	N-CA-C	5.80	118.62	108.52
1	D	14	THR	N-CA-CB	-5.77	102.11	110.70
1	C	120	ARG	CD-NE-CZ	5.74	132.43	124.40
1	A	118	LEU	N-CA-C	5.66	118.65	111.69
1	C	50	THR	N-CA-C	5.57	119.33	112.54
1	B	40	ARG	N-CA-CB	5.47	118.58	110.49
1	A	239	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	A	243	ARG	NE-CZ-NH2	-5.45	114.29	119.20
1	C	222	ARG	CB-CG-CD	5.43	123.79	111.30
1	D	322	ARG	CB-CG-CD	-5.42	98.85	111.30
1	D	14	THR	N-CA-C	-5.38	102.22	110.14
1	C	243	ARG	CB-CG-CD	-5.35	98.99	111.30
1	D	7	ASP	CB-CA-C	5.30	115.42	110.17
1	B	318	GLY	CA-C-N	-5.17	114.63	119.85
1	B	318	GLY	C-N-CA	-5.17	114.63	119.85
1	B	325	ASN	N-CA-C	5.16	119.15	112.86
1	A	47	ILE	CA-C-N	-5.08	114.53	119.76
1	A	47	ILE	C-N-CA	-5.08	114.53	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	CB-CG-CD	-5.05	99.68	111.30
1	B	243	ARG	CG-CD-NE	5.05	123.11	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3138	0	3059	25	0
1	B	2991	0	2919	22	0
1	C	3044	0	2979	24	0
1	D	3062	0	2998	18	0
2	A	31	0	19	2	0
2	B	31	0	19	3	0
2	C	31	0	19	3	0
2	D	31	0	19	0	0
3	A	247	0	0	1	0
3	B	263	0	0	3	0
3	C	178	0	0	8	0
3	D	249	0	0	1	0
All	All	13296	0	12031	90	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 4.

All (90) 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:C:120:ARG:HD3	3:C:617:HOH:O	1.51	1.07
1:A:353:ASN:HD21	1:A:367:ASN:H	1.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:HD2	1:A:135:ASP:OD1	1.77	0.84
1:C:4:MET:HE2	3:C:659:HOH:O	1.76	0.84
1:C:212:GLU:O	1:C:222:ARG:NH1	2.11	0.83
1:C:120:ARG:CD	3:C:617:HOH:O	2.18	0.81
1:A:243:ARG:HD3	1:A:286:ASP:CG	2.10	0.76
1:A:78:GLN:HE22	1:A:133:ARG:H	1.36	0.73
1:B:40:ARG:CD	1:B:378:THR:O	2.37	0.73
1:C:195:GLY:H	1:C:199:ASN:HD22	1.37	0.72
1:C:78:GLN:HE22	1:C:133:ARG:H	1.39	0.71
1:A:195:GLY:H	1:A:199:ASN:HD22	1.40	0.70
1:C:25:ASN:HD21	1:C:186:ASP:HB3	1.55	0.70
1:C:375:TYR:CE1	2:C:501:FMN:HM71	2.27	0.69
1:B:130:GLU:OE1	3:B:858:HOH:O	2.10	0.69
1:A:235:VAL:O	1:A:239:ARG:HD3	1.93	0.68
1:A:29:HIS:HD2	1:A:31:VAL:H	1.42	0.67
1:A:133:ARG:HD3	1:A:159:HIS:CD2	2.29	0.67
1:B:40:ARG:HD3	1:B:378:THR:O	1.94	0.66
1:A:353:ASN:HD21	1:A:367:ASN:N	1.91	0.65
1:D:78:GLN:HE22	1:D:133:ARG:H	1.45	0.65
1:D:195:GLY:H	1:D:199:ASN:HD22	1.43	0.65
1:D:235:VAL:O	1:D:239:ARG:HD3	1.97	0.63
1:C:40:ARG:O	1:C:49:ASN:HB2	1.99	0.63
1:A:243:ARG:CD	1:A:286:ASP:CG	2.73	0.62
1:D:121:GLN:HA	1:D:143:MET:HE1	1.82	0.62
1:B:243:ARG:HD2	1:B:286:ASP:CG	2.28	0.59
1:D:7:ASP:OD1	1:D:398:LYS:NZ	2.32	0.58
1:B:195:GLY:H	1:B:199:ASN:HD22	1.48	0.58
1:D:390:GLU:OE1	3:D:601:HOH:O	2.17	0.58
1:D:14:THR:CG2	1:D:16:ILE:H	2.15	0.58
1:C:167:LYS:O	1:C:167:LYS:HE3	2.05	0.57
1:B:371:ARG:HD2	3:B:744:HOH:O	2.05	0.56
1:D:11:LEU:O	1:D:14:THR:HB	2.06	0.55
1:C:105:HIS:HE1	1:C:186:ASP:OD2	1.90	0.55
1:B:235:VAL:O	1:B:239:ARG:HD2	2.08	0.54
1:C:120:ARG:HD2	1:C:200:GLN:HG2	1.90	0.53
1:C:195:GLY:H	1:C:199:ASN:ND2	2.04	0.53
1:A:243:ARG:HD2	1:A:286:ASP:OD1	2.07	0.53
1:C:29:HIS:HD2	1:C:31:VAL:H	1.57	0.53
1:A:243:ARG:HD3	1:A:286:ASP:OD2	2.08	0.53
1:B:243:ARG:HH21	2:B:501:FMN:C2	2.22	0.53
1:B:375:TYR:CE1	2:B:501:FMN:HM71	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ILE:HD12	3:C:636:HOH:O	2.10	0.52
1:D:14:THR:HG23	1:D:16:ILE:H	1.74	0.52
1:C:4:MET:HE3	1:C:366:LEU:CB	2.40	0.52
1:D:195:GLY:H	1:D:199:ASN:ND2	2.08	0.52
1:A:129:LYS:N	1:A:129:LYS:HD3	2.25	0.51
1:B:171:LYS:NZ	1:B:171:LYS:HB3	2.25	0.51
1:B:195:GLY:H	1:B:199:ASN:ND2	2.08	0.51
1:C:243:ARG:NH2	2:C:501:FMN:N1	2.59	0.51
1:D:25:ASN:HD21	1:D:186:ASP:HB3	1.77	0.50
1:B:235:VAL:O	1:B:239:ARG:CD	2.61	0.48
1:D:289:GLU:OE2	1:D:322:ARG:HD2	2.14	0.48
1:C:67:LEU:HD11	1:C:112:TRP:CD1	2.49	0.48
1:C:91:LYS:HE3	1:C:91:LYS:HA	1.95	0.48
1:B:25:ASN:HD21	1:B:186:ASP:HB3	1.78	0.48
1:D:289:GLU:OE2	1:D:322:ARG:CD	2.61	0.48
1:B:4:MET:HE2	1:B:328:LEU:HD21	1.96	0.47
1:B:371:ARG:HD3	1:B:374:PHE:CE2	2.50	0.47
1:C:92:GLU:CD	3:C:752:HOH:O	2.58	0.47
1:B:40:ARG:O	1:B:49:ASN:HB2	2.15	0.47
1:B:164:GLU:HG3	3:B:856:HOH:O	2.15	0.47
1:C:222:ARG:HG3	3:C:718:HOH:O	2.14	0.46
1:D:9:LYS:HE3	1:D:331:ASP:OD1	2.16	0.46
1:A:348:ARG:NH1	2:A:501:FMN:O3P	2.49	0.46
1:A:195:GLY:H	1:A:199:ASN:ND2	2.10	0.45
1:A:25:ASN:HD21	1:A:186:ASP:HB3	1.82	0.45
1:A:235:VAL:O	1:A:239:ARG:CD	2.63	0.45
1:A:40:ARG:O	1:A:49:ASN:HB2	2.16	0.44
1:A:37:THR:O	2:A:501:FMN:H6	2.17	0.44
1:D:221:ALA:HB1	1:D:268:VAL:HG22	1.99	0.44
1:B:143:MET:HE3	1:B:251:GLY:HA2	2.00	0.44
2:C:501:FMN:H1'1	3:C:763:HOH:O	2.17	0.43
1:A:142:TYR:CD1	1:A:148:LYS:HA	2.53	0.43
1:A:167:LYS:HG2	3:A:632:HOH:O	2.18	0.43
1:A:39:MET:HA	1:A:84:ASN:O	2.19	0.42
1:A:29:HIS:CD2	1:A:31:VAL:H	2.30	0.42
1:C:4:MET:HE3	1:C:366:LEU:HB2	2.01	0.42
1:B:243:ARG:HD2	1:B:286:ASP:OD2	2.20	0.41
1:B:243:ARG:NH2	2:B:501:FMN:N1	2.60	0.41
1:C:67:LEU:CD1	1:C:112:TRP:CD1	3.03	0.41
1:C:133:ARG:NH2	3:C:725:HOH:O	2.42	0.41
1:D:14:THR:HG22	1:D:16:ILE:H	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ALA:O	1:A:181:ILE:HG12	2.19	0.41
1:D:142:TYR:CD1	1:D:148:LYS:HA	2.55	0.41
1:B:40:ARG:HD2	1:B:378:THR:O	2.19	0.41
1:B:221:ALA:HB1	1:B:268:VAL:HG22	2.02	0.41
1:A:310:GLU:OE1	1:A:339:LYS:HE2	2.21	0.40
1:D:105:HIS:HE1	1:D:184:GLY:O	2.03	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	388/403 (96%)	379 (98%)	9 (2%)	0	100	100
1	B	370/403 (92%)	358 (97%)	12 (3%)	0	100	100
1	C	377/403 (94%)	366 (97%)	11 (3%)	0	100	100
1	D	379/403 (94%)	370 (98%)	9 (2%)	0	100	100
All	All	1514/1612 (94%)	1473 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	329/340 (97%)	321 (98%)	8 (2%)	43	31
1	B	313/340 (92%)	305 (97%)	8 (3%)	40	28
1	C	318/340 (94%)	310 (98%)	8 (2%)	42	30
1	D	320/340 (94%)	314 (98%)	6 (2%)	50	41
All	All	1280/1360 (94%)	1250 (98%)	30 (2%)	44	33

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	129	LYS
1	A	167	LYS
1	A	182	ASP
1	A	239	ARG
1	A	243	ARG
1	A	328	LEU
1	A	350	PHE
1	B	27	LEU
1	B	94	LEU
1	B	108	LYS
1	B	181	ILE
1	B	218	GLU
1	B	243	ARG
1	B	310	GLU
1	B	350	PHE
1	C	91	LYS
1	C	141	LEU
1	C	156	ASN
1	C	171	LYS
1	C	328	LEU
1	C	335	LEU
1	C	350	PHE
1	C	389	GLU
1	D	1	MET
1	D	14	THR
1	D	129	LYS
1	D	143	MET
1	D	156	ASN
1	D	350	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	25	ASN
1	A	29	HIS
1	A	78	GLN
1	A	107	ASN
1	A	199	ASN
1	A	341	ASN
1	A	353	ASN
1	A	367	ASN
1	B	5	ASN
1	B	25	ASN
1	B	107	ASN
1	B	199	ASN
1	B	309	ASN
1	B	332	GLN
1	B	372	ASN
1	C	25	ASN
1	C	29	HIS
1	C	78	GLN
1	C	156	ASN
1	C	199	ASN
1	C	309	ASN
1	D	24	ASN
1	D	25	ASN
1	D	78	GLN
1	D	107	ASN
1	D	156	ASN
1	D	199	ASN
1	D	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	FMN	C	501	-	33,33,33	2.00	10 (30%)	48,50,50	2.17	15 (31%)
2	FMN	B	501	-	33,33,33	2.22	9 (27%)	48,50,50	1.96	15 (31%)
2	FMN	A	501	-	33,33,33	2.14	13 (39%)	48,50,50	1.53	8 (16%)
2	FMN	D	501	-	33,33,33	1.86	8 (24%)	48,50,50	1.62	11 (22%)

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	FMN	C	501	-	-	1/18/18/18	0/3/3/3
2	FMN	B	501	-	-	1/18/18/18	0/3/3/3
2	FMN	A	501	-	-	1/18/18/18	0/3/3/3
2	FMN	D	501	-	-	1/18/18/18	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FMN	C9A-C5A	5.56	1.50	1.41
2	B	501	FMN	C1'-C2'	5.44	1.60	1.52
2	A	501	FMN	C1'-C2'	5.36	1.60	1.52
2	B	501	FMN	O4-C4	5.14	1.33	1.23
2	C	501	FMN	C9A-C5A	4.78	1.48	1.41
2	B	501	FMN	C8-C7	4.76	1.52	1.40
2	A	501	FMN	C9A-C5A	4.15	1.47	1.41
2	D	501	FMN	C1'-C2'	4.12	1.58	1.52
2	C	501	FMN	C1'-C2'	4.02	1.58	1.52
2	C	501	FMN	O4-C4	3.94	1.31	1.23
2	C	501	FMN	C8-C7	3.86	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FMN	C8-C7	3.74	1.50	1.40
2	B	501	FMN	C4A-N5	3.68	1.38	1.30
2	A	501	FMN	C5A-N5	-3.64	1.32	1.39
2	D	501	FMN	C4A-N5	3.63	1.38	1.30
2	D	501	FMN	C9A-C5A	3.59	1.47	1.41
2	A	501	FMN	C4A-N5	3.40	1.38	1.30
2	D	501	FMN	O4-C4	3.37	1.30	1.23
2	A	501	FMN	O4-C4	3.34	1.29	1.23
2	D	501	FMN	O3'-C3'	3.13	1.50	1.43
2	D	501	FMN	C5A-N5	-3.04	1.33	1.39
2	C	501	FMN	C4A-N5	2.89	1.37	1.30
2	B	501	FMN	C4A-C10	2.81	1.52	1.44
2	C	501	FMN	C4A-C4	2.75	1.54	1.44
2	C	501	FMN	O3'-C3'	2.71	1.49	1.43
2	A	501	FMN	C9A-N10	2.62	1.45	1.41
2	C	501	FMN	C5A-N5	-2.62	1.34	1.39
2	D	501	FMN	C8-C7	2.57	1.47	1.40
2	A	501	FMN	O3'-C3'	2.42	1.48	1.43
2	C	501	FMN	C4'-C3'	2.25	1.57	1.53
2	C	501	FMN	C4A-C10	2.20	1.50	1.44
2	A	501	FMN	C6-C5A	2.19	1.43	1.40
2	A	501	FMN	C10-N1	2.16	1.37	1.33
2	A	501	FMN	O2-C2	2.15	1.28	1.24
2	B	501	FMN	O3'-C3'	2.14	1.48	1.43
2	A	501	FMN	C2-N3	-2.13	1.34	1.39
2	A	501	FMN	C2-N1	-2.07	1.31	1.36
2	D	501	FMN	C9-C8	2.06	1.42	1.39
2	B	501	FMN	C5A-N5	-2.04	1.35	1.39
2	B	501	FMN	C4A-C4	2.01	1.52	1.44

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FMN	O2-C2-N1	-5.91	111.98	121.80
2	C	501	FMN	C4-C4A-N5	5.43	125.70	118.21
2	C	501	FMN	O2-C2-N1	-5.06	113.39	121.80
2	C	501	FMN	C5A-N5-C4A	4.64	125.59	118.09
2	C	501	FMN	O3'-C3'-C4'	4.44	119.02	108.93
2	C	501	FMN	C10-C4A-N5	-4.34	115.95	124.81
2	A	501	FMN	C4-C4A-N5	4.11	123.89	118.21
2	B	501	FMN	C4'-C3'-C2'	-4.01	106.89	113.57
2	A	501	FMN	O2-C2-N1	-3.99	115.17	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FMN	C5A-N5-C4A	3.61	123.93	118.09
2	C	501	FMN	C4A-C10-N1	-3.39	116.27	124.59
2	C	501	FMN	O3P-P-O5'	-3.23	98.26	106.67
2	D	501	FMN	O3'-C3'-C4'	3.16	116.12	108.93
2	B	501	FMN	O2'-C2'-C3'	-3.14	101.90	109.25
2	B	501	FMN	O4-C4-N3	3.07	125.88	120.11
2	D	501	FMN	C4-C4A-N5	3.06	122.43	118.21
2	A	501	FMN	C10-C4A-N5	-3.04	118.60	124.81
2	B	501	FMN	O4-C4-C4A	-3.02	118.57	126.53
2	D	501	FMN	O2-C2-N1	-2.96	116.88	121.80
2	C	501	FMN	C4-N3-C2	-2.93	120.43	125.64
2	B	501	FMN	C5A-C9A-N10	2.89	120.58	117.97
2	C	501	FMN	C4A-C10-N10	2.87	120.59	116.48
2	C	501	FMN	C10-N1-C2	2.81	122.93	116.85
2	A	501	FMN	C4'-C3'-C2'	-2.79	108.92	113.57
2	D	501	FMN	O4-C4-C4A	-2.77	119.21	126.53
2	D	501	FMN	C4'-C3'-C2'	-2.75	108.99	113.57
2	B	501	FMN	C4A-C10-N1	-2.74	117.87	124.59
2	C	501	FMN	N3-C2-N1	2.63	125.09	119.50
2	B	501	FMN	C4-C4A-N5	2.63	121.84	118.21
2	B	501	FMN	N3-C2-N1	2.63	125.08	119.50
2	C	501	FMN	C4'-C3'-C2'	-2.61	109.22	113.57
2	D	501	FMN	C9A-C5A-N5	-2.61	119.69	122.45
2	D	501	FMN	C5A-C9A-N10	2.56	120.28	117.97
2	D	501	FMN	C9-C8-C7	2.54	123.41	119.69
2	B	501	FMN	C10-C4A-N5	-2.52	119.66	124.81
2	B	501	FMN	C4A-C10-N10	2.50	120.06	116.48
2	A	501	FMN	C9A-C5A-N5	-2.40	119.91	122.45
2	B	501	FMN	O3'-C3'-C4'	2.40	114.37	108.93
2	D	501	FMN	C6-C5A-C9A	2.32	122.24	119.05
2	B	501	FMN	O2-C2-N3	2.26	122.92	118.58
2	D	501	FMN	C10-C4A-N5	-2.24	120.24	124.81
2	B	501	FMN	C8M-C8-C9	-2.19	115.71	119.57
2	B	501	FMN	O5'-P-O1P	-2.16	100.60	106.44
2	A	501	FMN	C4A-C10-N1	-2.14	119.35	124.59
2	C	501	FMN	O3P-P-O2P	2.06	115.52	107.80
2	C	501	FMN	C9A-C5A-N5	-2.03	120.31	122.45
2	A	501	FMN	C4A-C10-N10	2.00	119.35	116.48
2	D	501	FMN	C9-C9A-N10	-2.00	119.16	121.85
2	C	501	FMN	O3'-C3'-C2'	-2.00	104.38	108.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

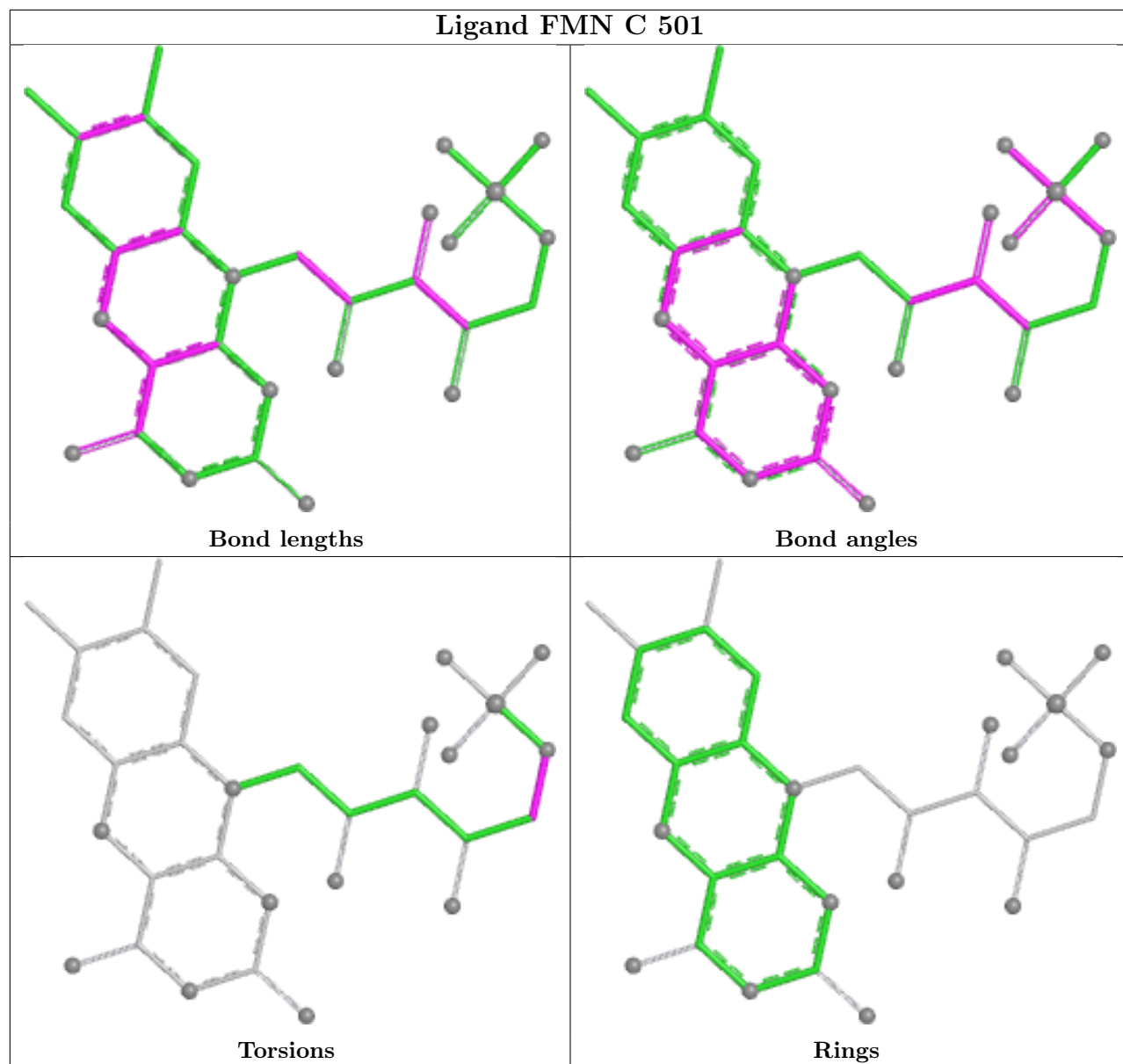
Mol	Chain	Res	Type	Atoms
2	D	501	FMN	C4'-C5'-O5'-P
2	A	501	FMN	C4'-C5'-O5'-P
2	C	501	FMN	C4'-C5'-O5'-P
2	B	501	FMN	C4'-C5'-O5'-P

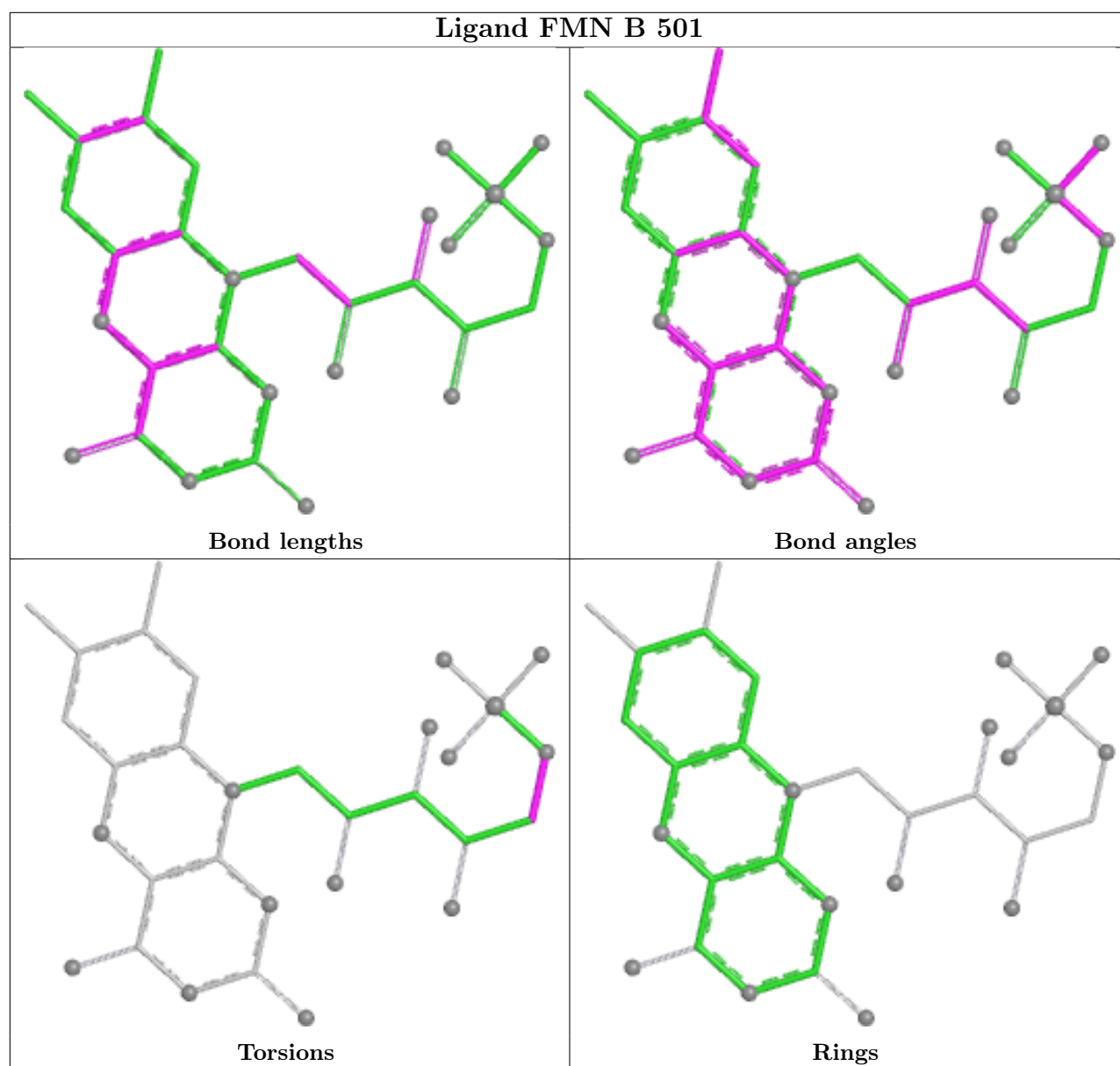
There are no ring outliers.

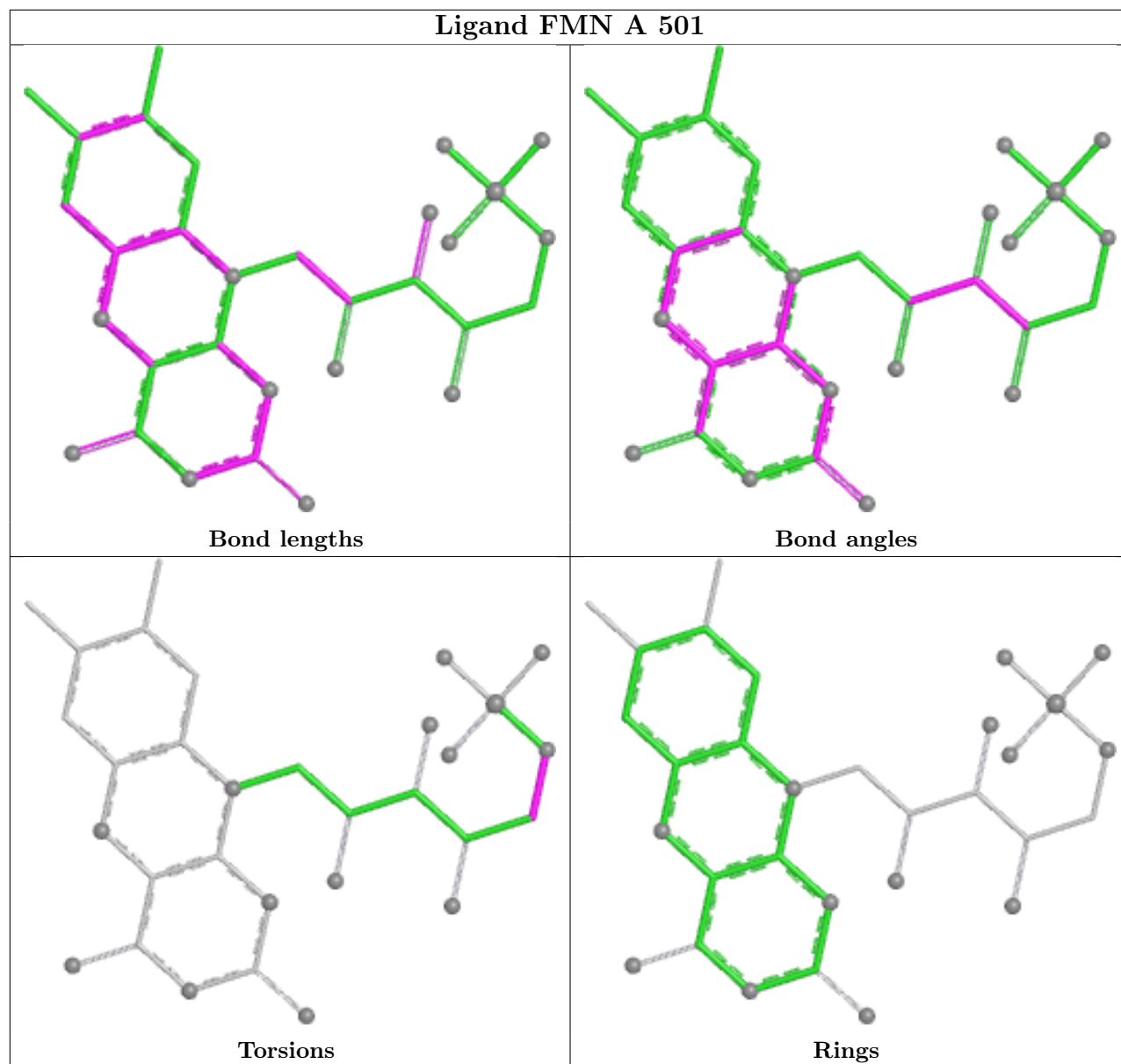
3 monomers are involved in 8 short contacts:

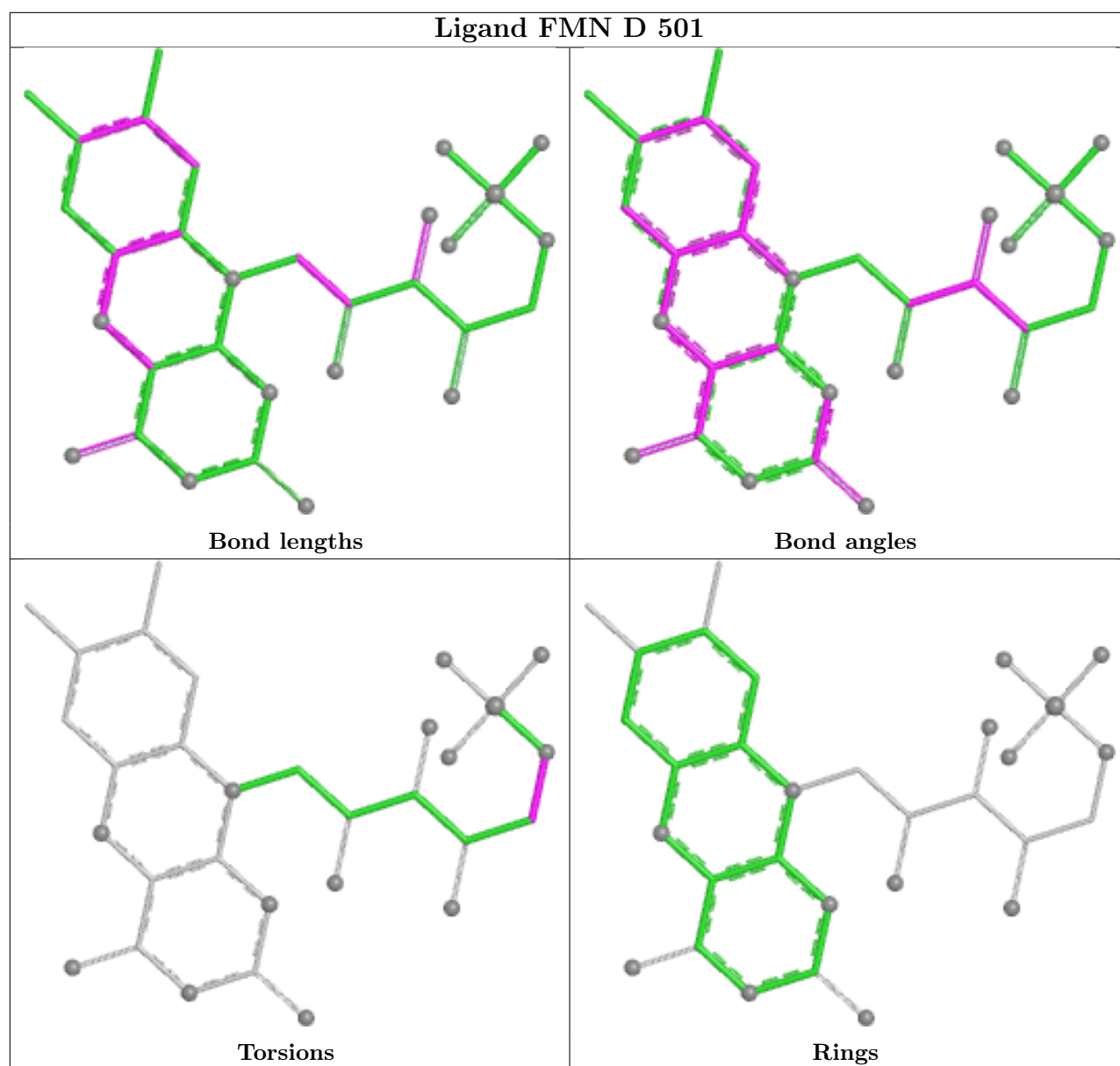
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	FMN	3	0
2	B	501	FMN	3	0
2	A	501	FMN	2	0

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.









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	390/403 (96%)	-0.12	7 (1%) 67 68	12, 17, 34, 56	0
1	B	374/403 (92%)	-0.37	0 100 100	9, 14, 24, 40	0
1	C	381/403 (94%)	0.10	4 (1%) 79 80	12, 23, 36, 47	0
1	D	383/403 (95%)	3.51	325 (84%) 0 0	26, 43, 71, 90	0
All	All	1528/1612 (94%)	0.78	336 (21%) 2 2	9, 21, 56, 90	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	144	GLY	8.6
1	D	151	ALA	8.1
1	D	154	ALA	8.0
1	D	156	ASN	7.9
1	D	134	TYR	7.8
1	D	131	GLY	7.8
1	D	126	VAL	7.7
1	D	205	ILE	7.3
1	D	132	LEU	7.2
1	D	130	GLU	7.0
1	D	157	PRO	7.0
1	D	155	ASN	6.8
1	D	127	LEU	6.7
1	D	89	TRP	6.5
1	D	375	TYR	6.3
1	D	396	TYR	6.2
1	D	41	ALA	6.2
1	D	141	LEU	6.2
1	D	48	PRO	6.2
1	D	378	THR	6.2
1	D	250	PHE	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	152	LEU	6.1
1	D	142	TYR	6.1
1	D	140	ASP	6.0
1	D	212	GLU	6.0
1	D	373	THR	6.0
1	D	91	LYS	6.0
1	D	207	ASN	5.9
1	D	159	HIS	5.9
1	D	208	ASN	5.8
1	D	376	THR	5.8
1	D	160	GLY	5.8
1	D	372	ASN	5.8
1	D	85	VAL	5.7
1	D	210	THR	5.7
1	D	195	GLY	5.7
1	D	377	PHE	5.7
1	D	371	ARG	5.6
1	D	196	TYR	5.6
1	D	213	TYR	5.6
1	D	182	ASP	5.5
1	D	118	LEU	5.5
1	D	139	ASP	5.5
1	D	206	SER	5.5
1	D	397	LYS	5.4
1	D	124	PRO	5.4
1	D	52	TRP	5.3
1	D	51	GLU	5.3
1	D	42	ILE	5.3
1	D	135	ASP	5.3
1	D	86	PRO	5.2
1	D	161	ILE	5.2
1	D	381	GLY	5.2
1	D	50	THR	5.2
1	D	382	TYR	5.2
1	D	143	MET	5.1
1	D	251	GLY	5.1
1	D	122	ALA	5.1
1	D	374	PHE	5.1
1	D	128	LYS	5.1
1	D	43	ALA	5.1
1	D	257	GLU	5.0
1	D	45	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	148	LYS	5.0
1	D	138	THR	5.0
1	D	253	MET	5.0
1	D	74	PHE	4.9
1	D	81	GLY	4.9
1	D	214	GLY	4.9
1	D	325	ASN	4.9
1	D	393	ALA	4.9
1	D	158	GLN	4.8
1	D	46	ASN	4.8
1	D	385	TYR	4.8
1	D	392	VAL	4.8
1	D	84	ASN	4.8
1	D	123	TRP	4.7
1	D	204	PRO	4.7
1	D	147	GLU	4.7
1	D	119	GLY	4.7
1	D	1	MET	4.7
1	D	380	GLU	4.7
1	D	150	ARG	4.7
1	D	384	ASP	4.7
1	D	149	GLU	4.6
1	D	255	GLY	4.6
1	D	201	PHE	4.6
1	D	162	THR	4.6
1	D	369	TYR	4.6
1	D	2	SER	4.6
1	D	79	SER	4.6
1	D	83	PRO	4.6
1	D	37	THR	4.6
1	D	47	ILE	4.6
1	D	163	LYS	4.5
1	D	49	ASN	4.5
1	D	261	ILE	4.5
1	D	260	GLY	4.5
1	A	293	THR	4.5
1	D	77	ALA	4.5
1	D	193	ALA	4.5
1	D	262	VAL	4.5
1	D	217	ILE	4.5
1	D	352	ALA	4.5
1	D	169	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	254	SER	4.5
1	D	53	ALA	4.5
1	D	197	LEU	4.4
1	D	358	TYR	4.4
1	D	368	LYS	4.4
1	D	72	GLY	4.4
1	D	90	SER	4.4
1	D	116	TRP	4.4
1	D	328	LEU	4.3
1	D	121	GLN	4.3
1	D	215	GLY	4.3
1	D	39	MET	4.2
1	D	137	ALA	4.2
1	D	145	GLU	4.2
1	D	245	SER	4.2
1	D	221	ALA	4.2
1	D	94	LEU	4.2
1	D	203	ASP	4.2
1	D	129	LYS	4.1
1	D	399	GLU	4.1
1	D	252	THR	4.1
1	D	146	GLU	4.1
1	D	383	THR	4.1
1	D	198	LEU	4.1
1	D	100	ILE	4.0
1	D	117	VAL	4.0
1	D	351	ILE	4.0
1	D	265	TYR	4.0
1	D	76	SER	4.0
1	D	324	GLY	4.0
1	D	323	VAL	4.0
1	D	370	ASP	4.0
1	D	224	THR	4.0
1	D	133	ARG	4.0
1	D	219	ASN	4.0
1	D	387	SER	4.0
1	D	209	ARG	4.0
1	D	248	GLY	3.9
1	D	307	GLY	3.9
1	D	259	PRO	3.9
1	D	92	GLU	3.9
1	D	125	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	153	LYS	3.9
1	D	6	PHE	3.9
1	D	348	ARG	3.8
1	D	164	GLU	3.8
1	D	395	GLY	3.8
1	D	288	VAL	3.8
1	D	58	ARG	3.8
1	D	366	LEU	3.8
1	D	258	ASN	3.8
1	D	367	ASN	3.8
1	D	216	SER	3.8
1	D	244	PHE	3.8
1	D	211	ASP	3.7
1	D	233	ASP	3.7
1	D	388	TYR	3.7
1	D	379	LYS	3.7
1	D	120	ARG	3.7
1	D	5	ASN	3.7
1	D	95	ALA	3.6
1	D	82	TYR	3.6
1	D	200	GLN	3.6
1	D	247	TYR	3.6
1	D	269	ILE	3.6
1	D	73	THR	3.6
1	D	349	SER	3.6
1	D	36	LEU	3.6
1	D	40	ARG	3.6
1	D	167	LYS	3.6
1	D	249	THR	3.6
1	D	190	ILE	3.5
1	D	353	ASN	3.5
1	D	194	ASN	3.5
1	D	35	ALA	3.5
1	D	38	ARG	3.5
1	D	68	ILE	3.4
1	D	166	ILE	3.4
1	D	264	GLN	3.4
1	D	101	PHE	3.4
1	D	4	MET	3.4
1	D	398	LYS	3.4
1	D	32	VAL	3.4
1	D	97	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	93	GLN	3.3
1	D	346	TYR	3.3
1	D	268	VAL	3.3
1	D	44	PRO	3.3
1	D	218	GLU	3.3
1	D	290	PRO	3.3
1	D	78	GLN	3.3
1	D	87	GLY	3.3
1	D	136	SER	3.3
1	D	103	ALA	3.3
1	D	111	VAL	3.3
1	D	177	ALA	3.3
1	D	390	GLU	3.3
1	D	55	GLU	3.2
1	D	56	TYR	3.2
1	D	223	PHE	3.2
1	D	88	ILE	3.2
1	D	386	PRO	3.2
1	D	173	TYR	3.2
1	D	391	SER	3.2
1	D	3	TYR	3.1
1	D	26	GLU	3.1
1	D	59	GLN	3.1
1	D	183	ALA	3.1
1	D	170	ILE	3.1
1	D	80	GLY	3.1
1	D	202	LEU	3.1
1	D	356	LEU	3.1
1	D	227	VAL	3.1
1	D	176	ALA	3.1
1	D	199	ASN	3.0
1	D	102	ASN	3.0
1	D	242	ILE	3.0
1	D	228	VAL	3.0
1	D	98	LYS	3.0
1	D	274	LYS	3.0
1	D	340	PRO	3.0
1	D	222	ARG	3.0
1	D	165	GLU	3.0
1	D	115	LEU	2.9
1	D	394	LYS	2.9
1	D	7	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	354	PRO	2.9
1	D	230	ALA	2.9
1	D	13	ASP	2.9
1	D	389	GLU	2.9
1	D	113	VAL	2.9
1	D	178	LYS	2.9
1	C	1	MET	2.9
1	D	104	ILE	2.9
1	D	70	THR	2.8
1	D	267	TYR	2.8
1	D	168	GLN	2.8
1	D	339	LYS	2.8
1	D	181	ILE	2.8
1	D	287	LEU	2.8
1	D	364	LEU	2.8
1	D	345	GLY	2.8
1	D	191	HIS	2.8
1	D	174	VAL	2.8
1	D	171	LYS	2.8
1	D	220	ARG	2.8
1	D	243	ARG	2.8
1	D	357	VAL	2.8
1	D	180	ALA	2.7
1	D	185	ALA	2.7
1	D	347	GLY	2.7
1	D	175	ASP	2.7
1	D	308	THR	2.7
1	D	335	LEU	2.7
1	D	277	ARG	2.7
1	D	350	PHE	2.7
1	D	18	LYS	2.6
1	D	256	GLY	2.6
1	D	239	ARG	2.6
1	D	69	ILE	2.6
1	D	278	ALA	2.6
1	D	327	ALA	2.6
1	D	33	MET	2.6
1	D	184	GLY	2.6
1	D	57	TYR	2.5
1	D	54	GLU	2.5
1	D	96	GLU	2.5
1	D	229	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	179	LYS	2.5
1	C	393	ALA	2.5
1	A	392	VAL	2.5
1	D	71	GLU	2.5
1	D	329	ASP	2.5
1	D	266	ALA	2.5
1	D	232	VAL	2.5
1	D	172	GLU	2.5
1	D	330	PRO	2.5
1	D	341	ASN	2.4
1	D	225	LEU	2.4
1	D	14	THR	2.4
1	D	263	ALA	2.4
1	A	292	VAL	2.4
1	D	359	ARG	2.4
1	D	107	ASN	2.4
1	D	317	LYS	2.4
1	D	312	ILE	2.4
1	D	322	ARG	2.4
1	D	231	VAL	2.4
1	D	310	GLU	2.4
1	D	272	LEU	2.3
1	D	326	TYR	2.3
1	D	226	GLU	2.3
1	D	365	PRO	2.3
1	D	60	ARG	2.3
1	D	331	ASP	2.3
1	D	360	LEU	2.3
1	C	278	ALA	2.3
1	D	285	ILE	2.3
1	D	270	GLY	2.3
1	C	13	ASP	2.3
1	D	313	TYR	2.3
1	D	75	PRO	2.3
1	D	246	PRO	2.3
1	D	321	LEU	2.3
1	D	106	GLU	2.2
1	D	61	SER	2.2
1	D	355	ASP	2.2
1	D	108	LYS	2.2
1	A	300	PHE	2.2
1	D	235	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	320	VAL	2.2
1	A	297	LEU	2.2
1	D	187	GLY	2.2
1	D	192	SER	2.2
1	A	303	TRP	2.2
1	D	64	PRO	2.2
1	D	316	TRP	2.1
1	D	286	ASP	2.1
1	D	110	PHE	2.1
1	D	332	GLN	2.1
1	D	99	LYS	2.1
1	D	16	ILE	2.1
1	D	315	ILE	2.1
1	A	391	SER	2.1
1	D	241	SER	2.1
1	D	31	VAL	2.1
1	D	112	TRP	2.1
1	D	234	ALA	2.1
1	D	333	ALA	2.1
1	D	284	PHE	2.0
1	D	63	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	C	501	31/31	0.86	0.11	20,27,32,33	0
2	FMN	B	501	31/31	0.92	0.09	14,18,22,24	0

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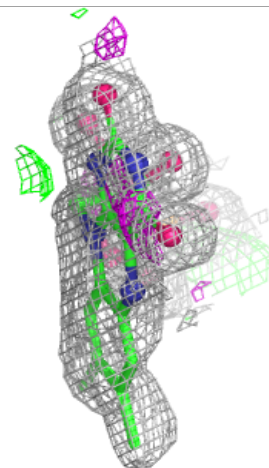
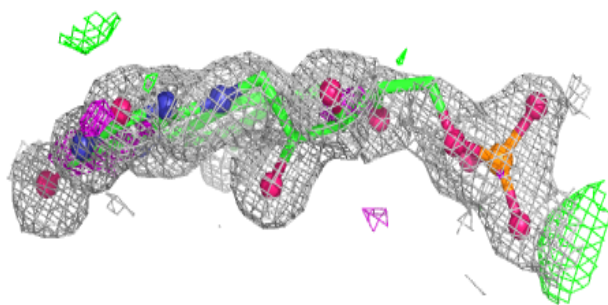
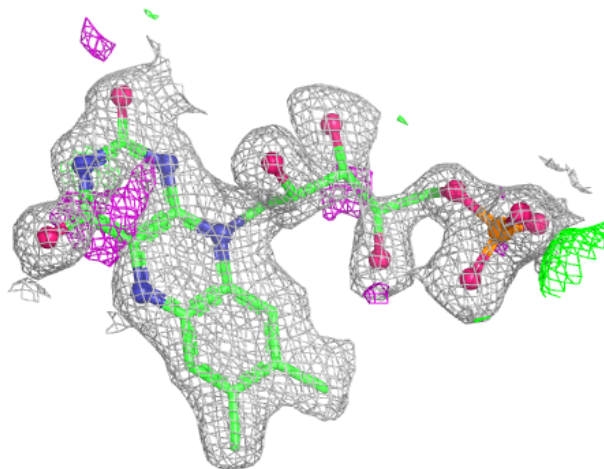
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	A	501	31/31	0.93	0.08	15,20,23,24	0
2	FMN	D	501	31/31	0.93	0.08	17,19,22,23	0

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.

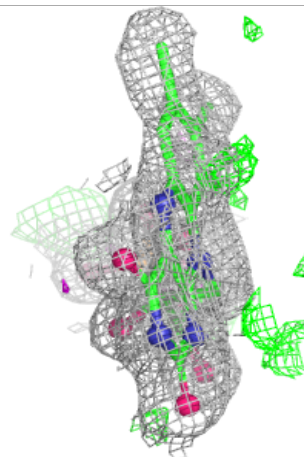
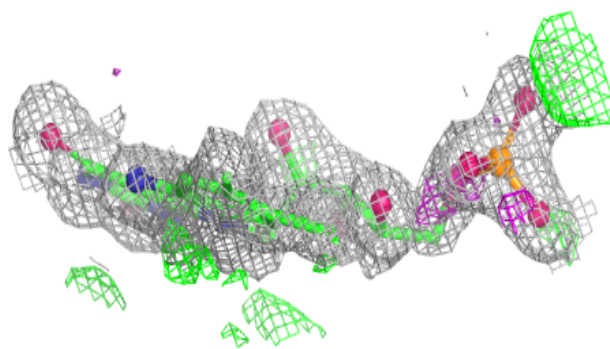
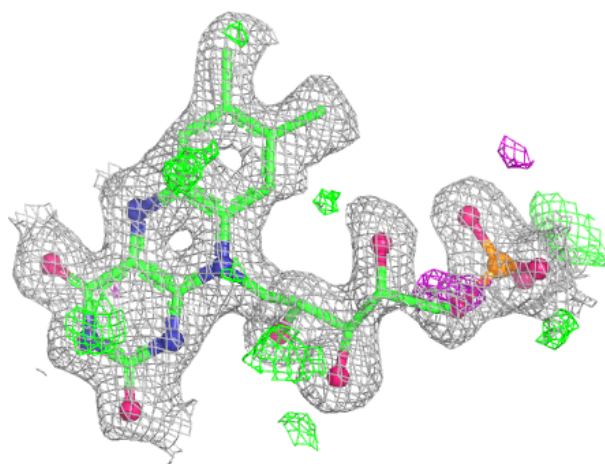
Electron density around FMN C 501:

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



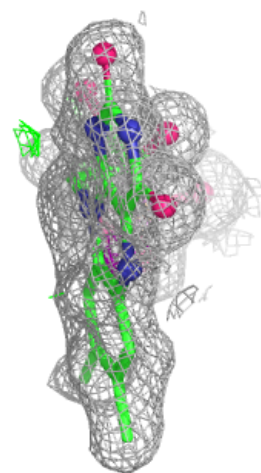
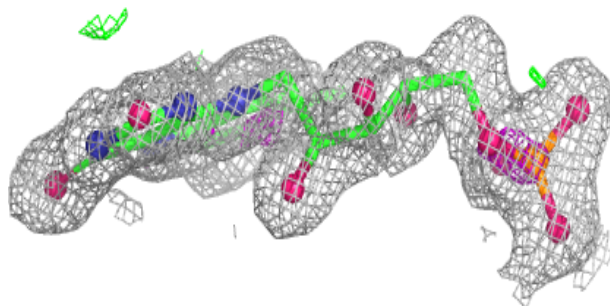
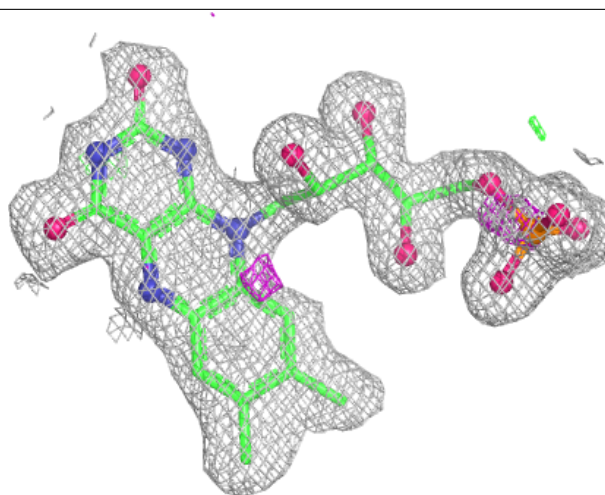
Electron density around FMN B 501:

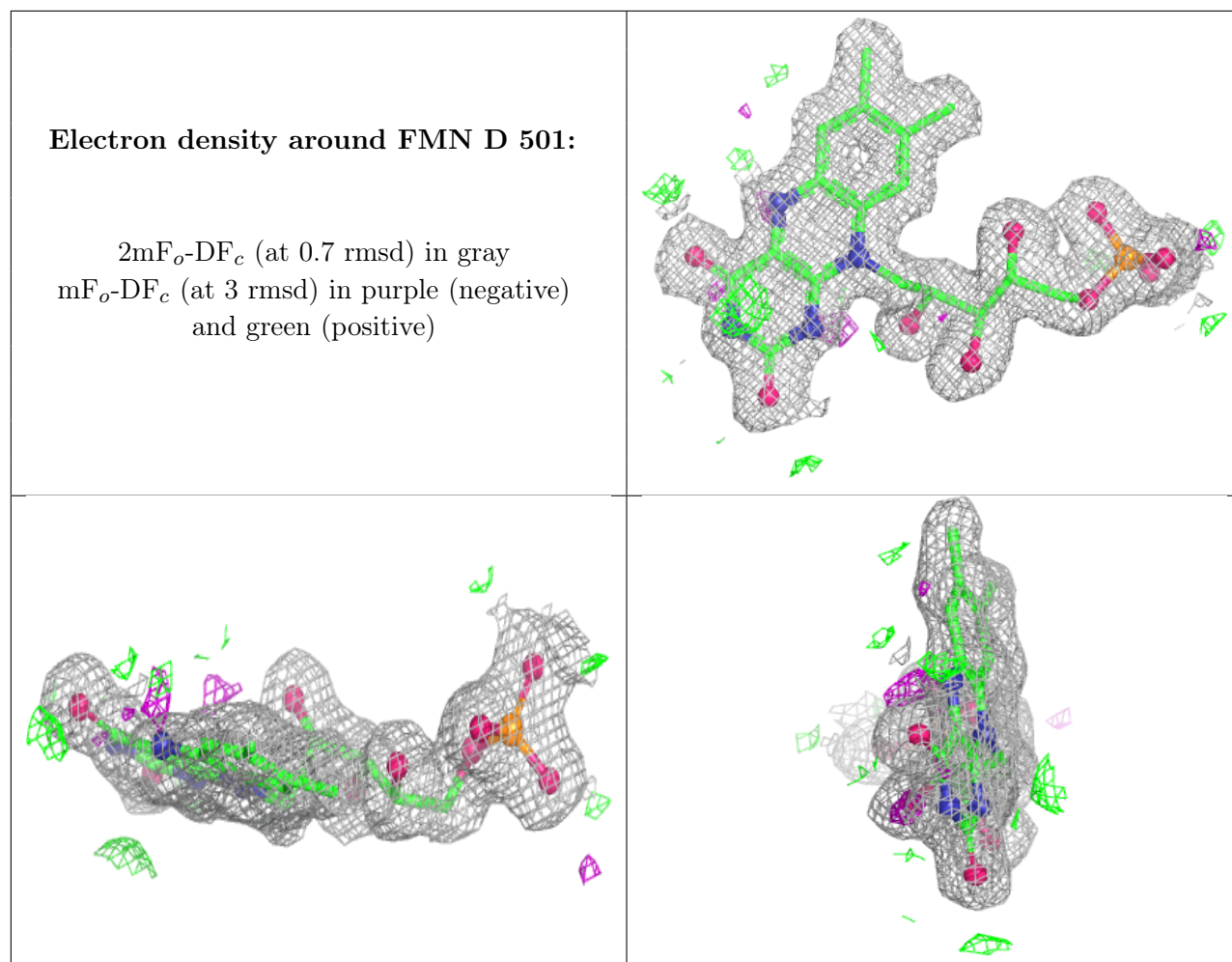
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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 ⓘ

There are no such residues in this entry.