



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:16 AM UTC

PDB ID : 7BN7 / pdb_00007bn7
Title : Crystal structure of ene-reductase OYE2 from *S. cerevisiae*
Authors : Robescu, M.S.; Bergantino, E.; Hall, M.; Cendron, L.
Deposited on : 2021-01-21
Resolution : 2.45 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

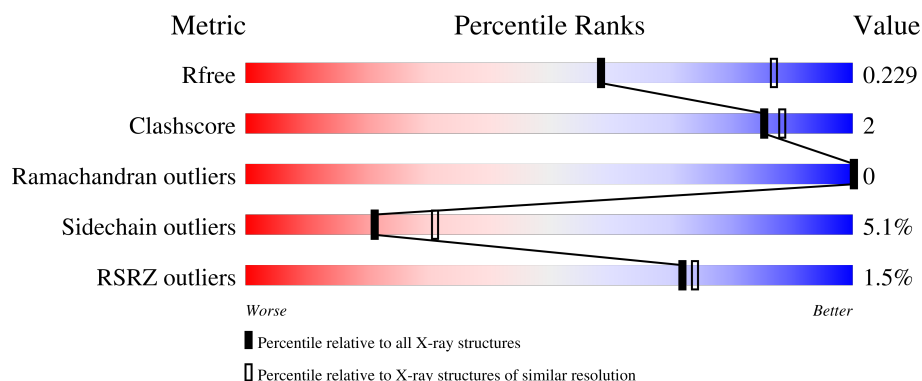
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	400	% 90% 7% ..
1	B	400	2% 88% 9% ..
1	C	400	% 90% 8% ..
1	D	400	2% 89% 9% .

2 Entry composition [i](#)

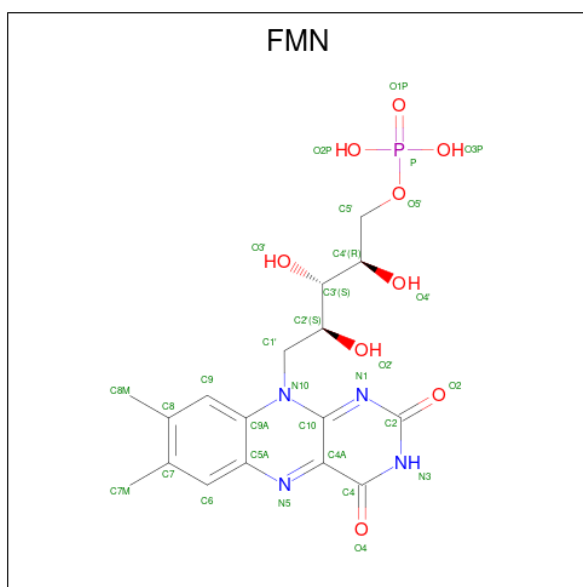
There are 4 unique types of molecules in this entry. The entry contains 13087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OYE2 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3154	2013	548	589	4			
1	B	394	Total	C	N	O	S	0	0	0
			3136	2000	545	587	4			
1	C	396	Total	C	N	O	S	0	1	0
			3163	2018	550	591	4			
1	D	396	Total	C	N	O	S	0	0	0
			3154	2013	548	589	4			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total	O	0	0
			99	99		
4	B	77	Total	O	0	0
			77	77		

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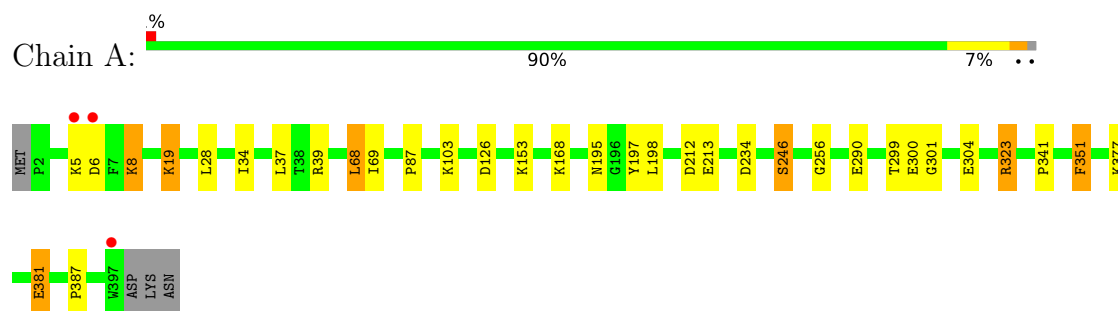
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	66	Total 66	O 66	0	0
4	D	84	Total 84	O 84	0	0

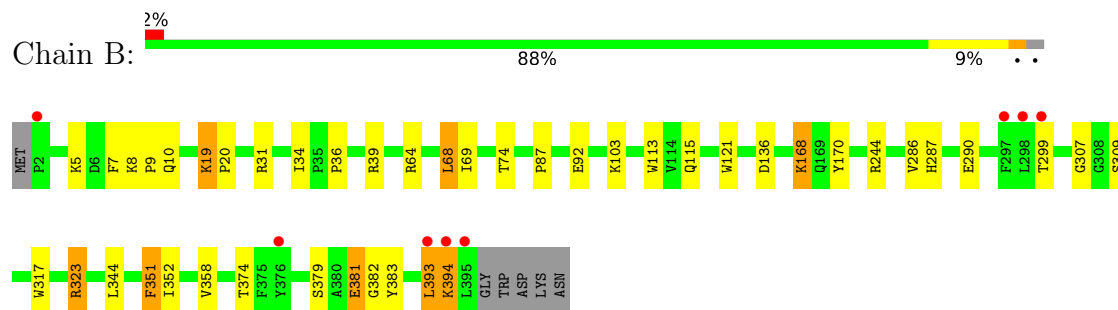
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

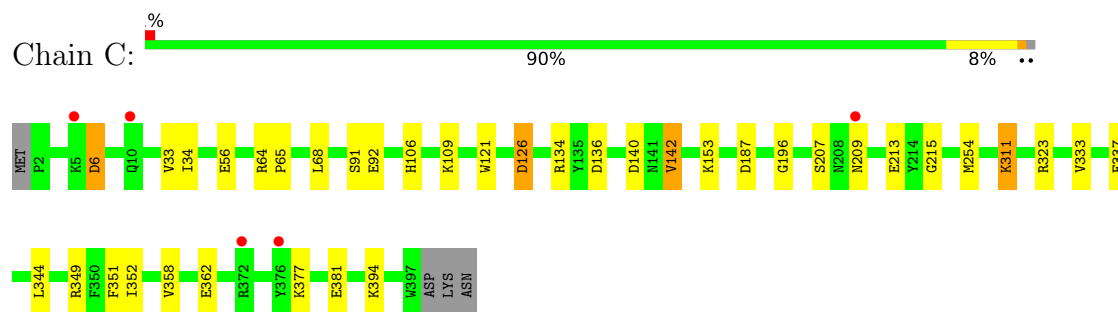
• Molecule 1: OYE2 isoform 1



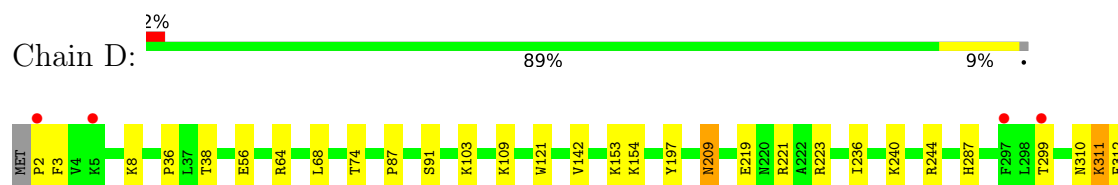
• Molecule 1: OYE2 isoform 1

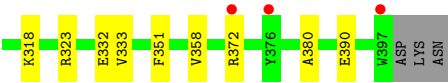


• Molecule 1: OYE2 isoform 1



• Molecule 1: OYE2 isoform 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.29Å 131.97Å 138.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.45 49.19 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.19-2.45) 93.0 (49.19-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.189 , 0.226 0.192 , 0.229	Depositor DCC
R_{free} test set	3607 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 20.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13087	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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, GOL

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	0.85	3/3238 (0.1%)	1.13	9/4393 (0.2%)
1	B	0.81	0/3218	1.10	5/4365 (0.1%)
1	C	0.81	2/3247 (0.1%)	1.10	6/4405 (0.1%)
1	D	0.86	4/3238 (0.1%)	1.12	6/4393 (0.1%)
All	All	0.84	9/12941 (0.1%)	1.11	26/17556 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	215	GLY	N-CA	7.08	1.51	1.45
1	D	236	ILE	N-CA	6.47	1.52	1.46
1	D	310	ASN	C-O	-5.69	1.16	1.24
1	A	301	GLY	C-O	-5.60	1.16	1.24
1	D	311	LYS	C-O	-5.41	1.17	1.24
1	A	387	PRO	C-O	-5.39	1.17	1.23
1	C	311	LYS	C-O	-5.10	1.17	1.24
1	A	300	GLU	C-O	-5.02	1.17	1.23
1	D	312	PHE	C-O	-5.01	1.17	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	LYS	CB-CA-C	8.22	117.84	110.44
1	A	387	PRO	N-CA-C	7.18	123.66	111.68
1	A	19	LYS	CB-CA-C	6.95	117.86	109.31
1	D	312	PHE	CA-CB-CG	6.81	120.61	113.80
1	C	142	VAL	N-CA-CB	6.46	118.36	111.00
1	B	87	PRO	N-CA-C	6.38	121.27	111.57
1	B	393	LEU	N-CA-C	-6.38	104.41	111.36
1	A	87	PRO	N-CA-C	6.22	121.02	111.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	GLY	CA-C-N	5.92	127.54	120.14
1	A	256	GLY	C-N-CA	5.92	127.54	120.14
1	D	380	ALA	N-CA-C	-5.89	105.58	112.89
1	A	126	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	304	GLU	CB-CA-C	5.68	119.51	110.19
1	B	74	THR	CB-CA-C	5.68	119.22	110.14
1	D	87	PRO	N-CA-C	5.52	120.85	111.03
1	C	126	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	394	LYS	N-CA-C	-5.45	102.82	110.50
1	C	33	VAL	CA-C-N	-5.44	118.67	122.59
1	C	33	VAL	C-N-CA	-5.44	118.67	122.59
1	D	209	ASN	CA-CB-CG	5.41	118.01	112.60
1	D	74	THR	CB-CA-C	5.32	119.33	109.70
1	A	212	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	209	ASN	N-CA-C	-5.29	106.05	112.88
1	A	341	PRO	N-CA-C	5.24	120.13	114.68
1	D	219	GLU	CB-CG-CD	5.17	121.40	112.60
1	C	92	GLU	CB-CG-CD	5.03	121.14	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3154	0	3070	12	0
1	B	3136	0	3057	21	0
1	C	3163	0	3077	10	0
1	D	3154	0	3070	9	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	3	0
3	A	6	0	8	2	0
3	B	12	0	16	3	0
3	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	8	3	0
4	A	99	0	0	0	0
4	B	77	0	0	1	0
4	C	66	0	0	0	0
4	D	84	0	0	4	0
All	All	13087	0	12390	55	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 2.

All (55) 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:A:195:ASN:ND2	3:A:502:GOL:H11	2.15	0.61
1:B:64:ARG:HG2	1:B:358:VAL:HG11	1.83	0.61
1:D:240:LYS:NZ	4:D:606:HOH:O	2.36	0.59
1:C:106:HIS:HE1	1:C:187:ASP:OD2	1.88	0.56
1:D:197:TYR:OH	3:D:502:GOL:H31	2.06	0.55
2:D:501:FMN:C10	3:D:502:GOL:H2	2.37	0.55
1:B:379:SER:HB2	1:B:381:GLU:HG2	1.90	0.54
1:B:34:ILE:HG12	1:B:351:PHE:CE2	2.45	0.52
2:D:501:FMN:C4A	3:D:502:GOL:H2	2.39	0.52
1:C:64:ARG:HD2	1:C:65:PRO:HD2	1.90	0.52
1:B:290:GLU:OE2	1:B:323:ARG:HD2	2.10	0.51
1:B:34:ILE:HD12	1:B:69:ILE:HG12	1.91	0.51
1:B:68:LEU:HD21	1:B:113:TRP:CD1	2.46	0.51
1:A:381:GLU:H	1:A:381:GLU:CD	2.18	0.50
1:A:34:ILE:HG12	1:A:351:PHE:CD2	2.47	0.49
1:C:134:ARG:NH2	1:C:136:ASP:OD2	2.42	0.48
1:A:28:LEU:HD21	1:A:68:LEU:HB2	1.96	0.48
1:C:333:VAL:O	1:C:337:GLU:HG2	2.14	0.47
1:B:383:TYR:HA	4:B:605:HOH:O	2.14	0.47
1:A:195:ASN:HD22	3:A:502:GOL:H11	1.79	0.47
1:D:2:PRO:HB2	1:D:3:PHE:H	1.38	0.47
1:D:64:ARG:HG2	1:D:358:VAL:HG11	1.97	0.47
1:C:64:ARG:HH22	1:C:362:GLU:CD	2.23	0.46
1:C:6:ASP:OD1	1:C:6:ASP:N	2.43	0.46
1:A:34:ILE:HD12	1:A:69:ILE:HG12	1.98	0.46
1:B:36:PRO:HG3	1:B:115:GLN:NE2	2.31	0.45
1:C:349:ARG:O	1:C:352:ILE:HB	2.17	0.45
1:D:244:ARG:HE	1:D:287:HIS:CE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LYS:HB2	1:A:8:LYS:HE2	1.50	0.44
1:C:64:ARG:HG2	1:C:358:VAL:HG11	2.00	0.44
1:B:244:ARG:HA	1:B:287:HIS:O	2.18	0.44
1:B:344:LEU:N	1:B:344:LEU:HD12	2.33	0.44
1:B:374:THR:HB	1:B:382:GLY:HA3	1.99	0.44
1:B:136:ASP:OD2	1:B:170:TYR:OH	2.21	0.43
1:B:309:SER:HB3	3:B:503:GOL:H12	2.00	0.43
1:B:7:PHE:O	1:B:9:PRO:HD3	2.18	0.43
1:A:37:LEU:O	1:A:39:ARG:HG2	2.18	0.43
1:D:221:ARG:O	4:D:601:HOH:O	2.21	0.43
3:B:503:GOL:C1	4:D:629:HOH:O	2.66	0.43
1:A:195:ASN:N	1:A:246:SER:OG	2.43	0.42
3:B:503:GOL:H11	4:D:629:HOH:O	2.19	0.42
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.82	0.41
1:C:344:LEU:HD12	1:C:344:LEU:N	2.35	0.41
1:B:286:VAL:HG23	1:B:317:TRP:CE2	2.56	0.41
1:B:39:ARG:NH1	1:B:352:ILE:HG23	2.34	0.41
1:B:19:LYS:HG2	1:B:20:PRO:HD2	2.02	0.41
1:B:307:GLY:O	1:D:318:LYS:NZ	2.44	0.41
1:A:197:TYR:O	1:A:198:LEU:C	2.64	0.41
1:D:36:PRO:HG2	2:D:501:FMN:C2	2.51	0.41
1:B:19:LYS:HD3	1:B:31:ARG:NH2	2.36	0.41
1:A:34:ILE:HG12	1:A:351:PHE:CE2	2.55	0.40
1:B:168:LYS:HE3	1:B:168:LYS:HB3	1.50	0.40
1:A:290:GLU:OE2	1:A:323:ARG:HD2	2.20	0.40
1:C:196:GLY:HA2	1:C:254:MET:SD	2.61	0.40
1:D:332:GLU:HG2	1:D:333:VAL:N	2.36	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	394/400 (98%)	385 (98%)	9 (2%)	0	100	100
1	B	392/400 (98%)	375 (96%)	17 (4%)	0	100	100
1	C	395/400 (99%)	382 (97%)	13 (3%)	0	100	100
1	D	394/400 (98%)	381 (97%)	13 (3%)	0	100	100
All	All	1575/1600 (98%)	1523 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	326/330 (99%)	310 (95%)	16 (5%)	22	33
1	B	325/330 (98%)	312 (96%)	13 (4%)	28	41
1	C	327/330 (99%)	308 (94%)	19 (6%)	18	27
1	D	326/330 (99%)	307 (94%)	19 (6%)	18	27
All	All	1304/1320 (99%)	1237 (95%)	67 (5%)	21	31

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	ASP
1	A	8	LYS
1	A	19	LYS
1	A	68	LEU
1	A	103	LYS
1	A	153	LYS
1	A	168	LYS
1	A	213	GLU
1	A	234	ASP
1	A	246	SER
1	A	299	THR
1	A	323	ARG

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Mol	Chain	Res	Type
1	A	351	PHE
1	A	377	LYS
1	A	381	GLU
1	B	5	LYS
1	B	10	GLN
1	B	19	LYS
1	B	68	LEU
1	B	92	GLU
1	B	103	LYS
1	B	121	TRP
1	B	168	LYS
1	B	299	THR
1	B	323	ARG
1	B	351	PHE
1	B	381	GLU
1	B	394	LYS
1	C	6	ASP
1	C	34	ILE
1	C	56	GLU
1	C	68	LEU
1	C	91	SER
1	C	109	LYS
1	C	121	TRP
1	C	126	ASP
1	C	140	ASP
1	C	142	VAL
1	C	153	LYS
1	C	207	SER
1	C	213	GLU
1	C	311	LYS
1	C	323	ARG
1	C	351	PHE
1	C	377	LYS
1	C	381	GLU
1	C	394	LYS
1	D	8	LYS
1	D	38	THR
1	D	56	GLU
1	D	68	LEU
1	D	91	SER
1	D	103	LYS
1	D	109	LYS

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Mol	Chain	Res	Type
1	D	121	TRP
1	D	142	VAL
1	D	153	LYS
1	D	154	LYS
1	D	209	ASN
1	D	223	ARG
1	D	299	THR
1	D	311	LYS
1	D	323	ARG
1	D	351	PHE
1	D	372	ARG
1	D	390	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	368	ASN
1	B	159	GLN
1	B	195	ASN
1	B	306	ASN
1	C	176	GLN
1	C	192	HIS
1	C	326	ASN
1	D	47	ASN
1	D	156	ASN
1	D	209	ASN

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

9 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
3	GOL	B	503	-	5,5,5	0.69	0	5,5,5	0.95	0
3	GOL	A	502	-	5,5,5	0.20	0	5,5,5	0.55	0
2	FMN	B	501	-	33,33,33	0.89	1 (3%)	48,50,50	0.67	0
3	GOL	C	502	-	5,5,5	0.67	0	5,5,5	0.82	0
2	FMN	A	501	-	33,33,33	0.85	1 (3%)	48,50,50	0.68	1 (2%)
2	FMN	D	501	-	33,33,33	0.81	0	48,50,50	0.66	0
3	GOL	D	502	-	5,5,5	0.53	0	5,5,5	0.53	0
2	FMN	C	501	-	33,33,33	0.81	0	48,50,50	0.65	0
3	GOL	B	502	-	5,5,5	0.09	0	5,5,5	0.48	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
3	GOL	B	503	-	-	3/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
2	FMN	B	501	-	-	2/18/18/18	0/3/3/3
3	GOL	C	502	-	-	2/4/4/4	-
2	FMN	A	501	-	-	1/18/18/18	0/3/3/3
2	FMN	D	501	-	-	1/18/18/18	0/3/3/3
3	GOL	D	502	-	-	0/4/4/4	-
2	FMN	C	501	-	-	1/18/18/18	0/3/3/3
3	GOL	B	502	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FMN	C2-N3	-2.16	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FMN	C2-N3	-2.09	1.34	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FMN	C4-N3-C2	-2.03	122.03	125.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O1-C1-C2-O2
3	B	502	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	O2-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
3	B	502	GOL	O2-C2-C3-O3
3	C	502	GOL	O2-C2-C3-O3
3	B	503	GOL	C1-C2-C3-O3
2	B	501	FMN	C5'-O5'-P-O1P
2	A	501	FMN	C4'-C5'-O5'-P
2	C	501	FMN	C4'-C5'-O5'-P
2	D	501	FMN	C4'-C5'-O5'-P
2	B	501	FMN	C4'-C5'-O5'-P
3	B	503	GOL	O1-C1-C2-O2

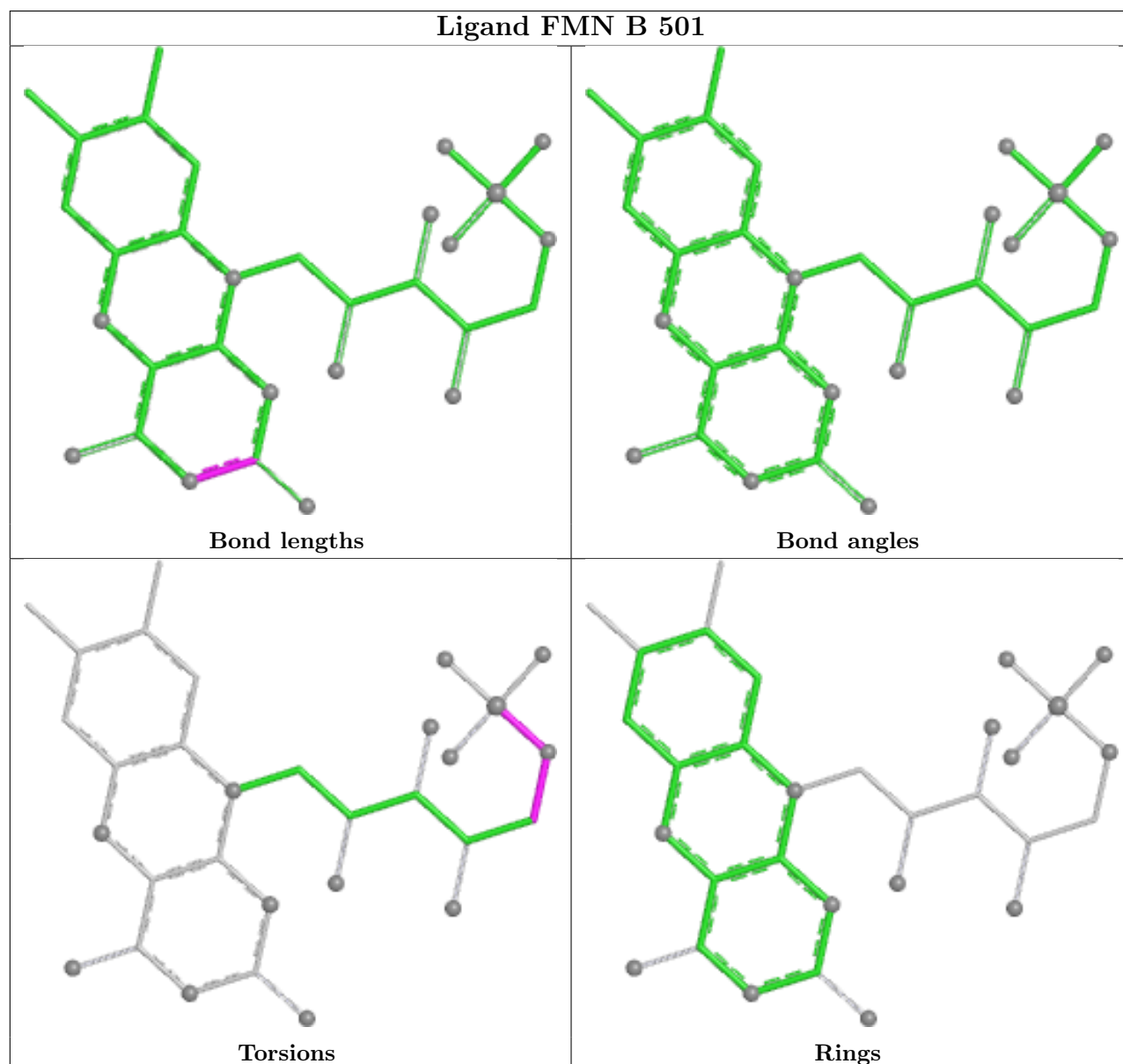
There are no ring outliers.

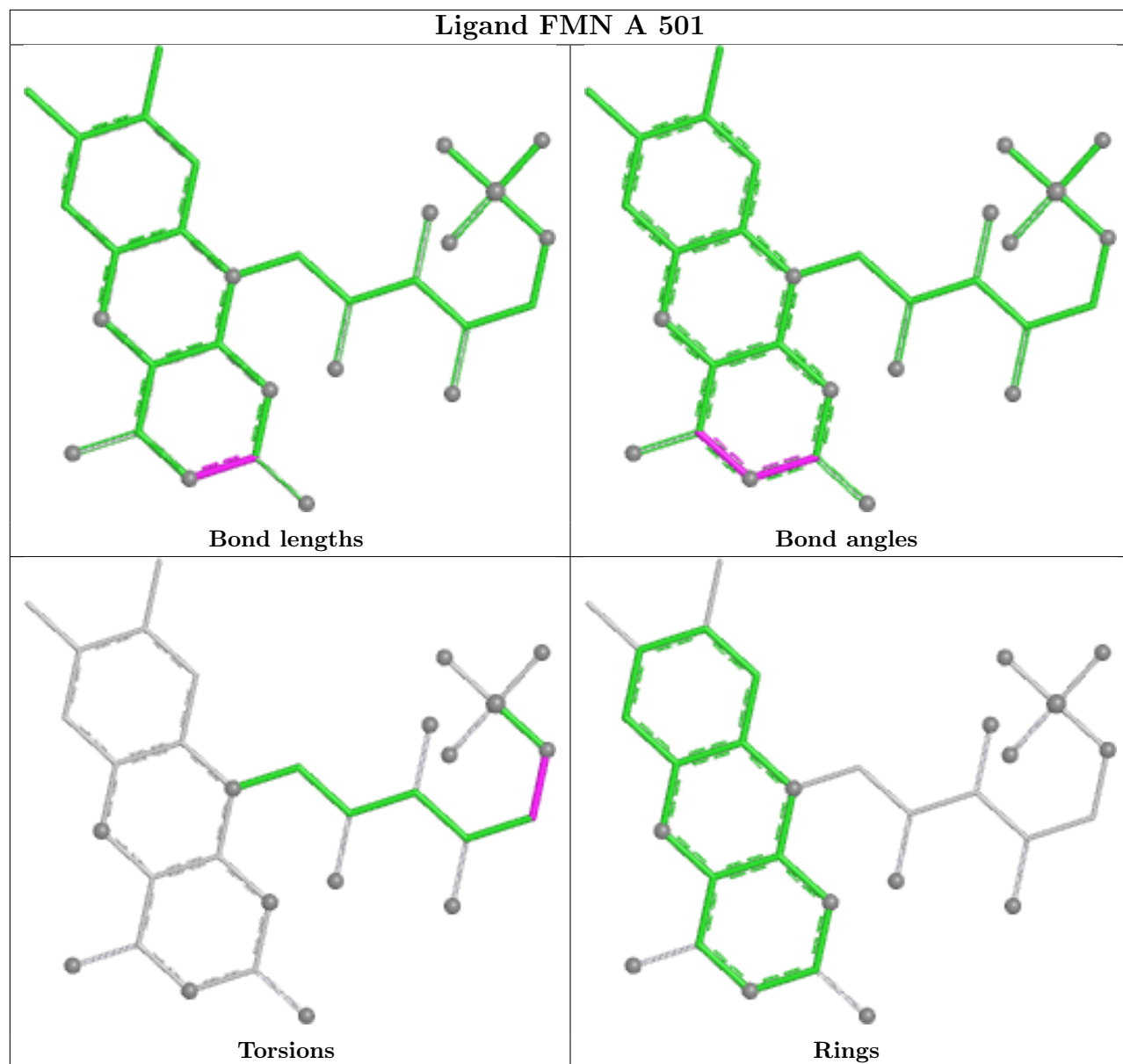
4 monomers are involved in 9 short contacts:

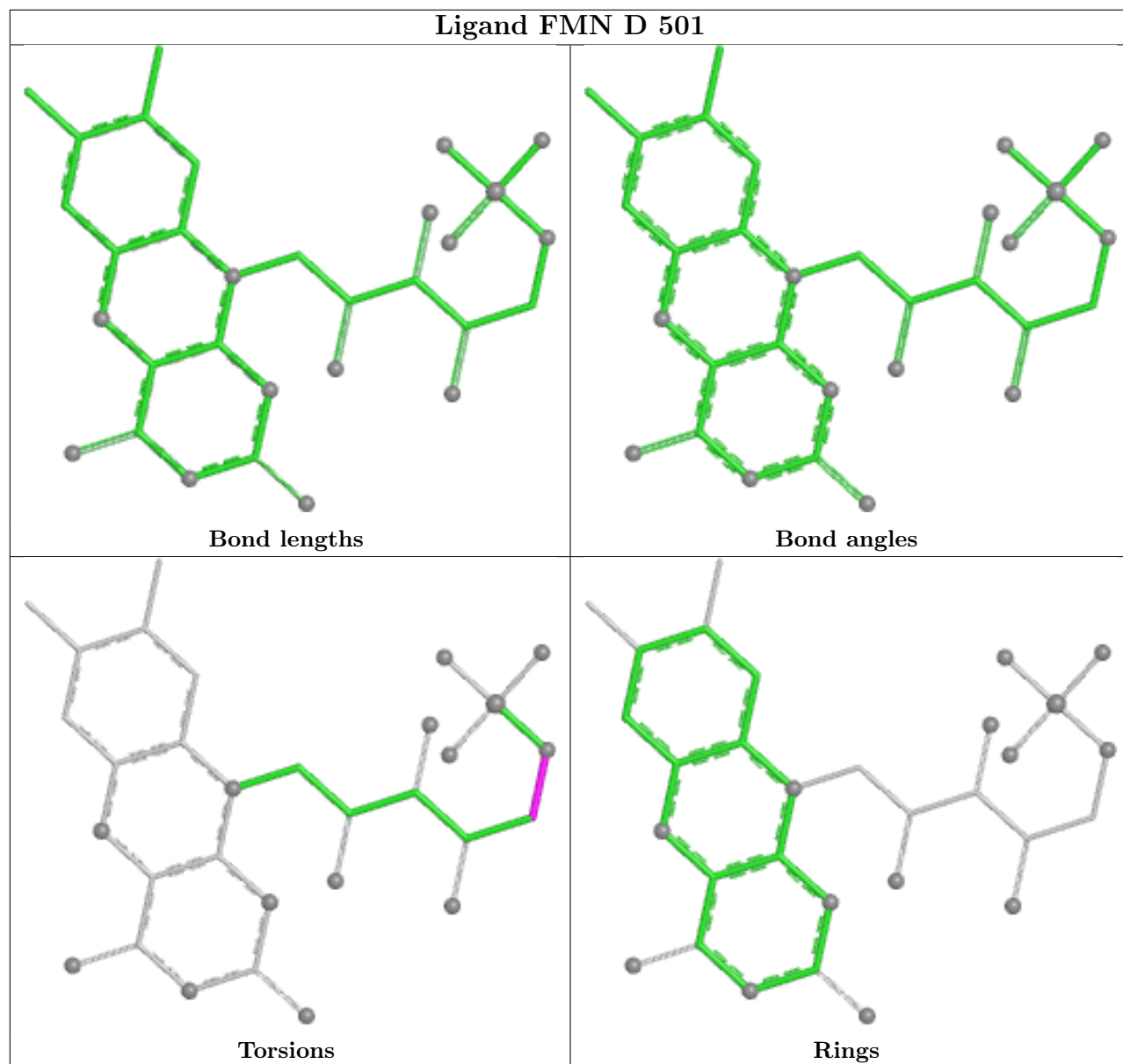
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	GOL	3	0
3	A	502	GOL	2	0
2	D	501	FMN	3	0
3	D	502	GOL	3	0

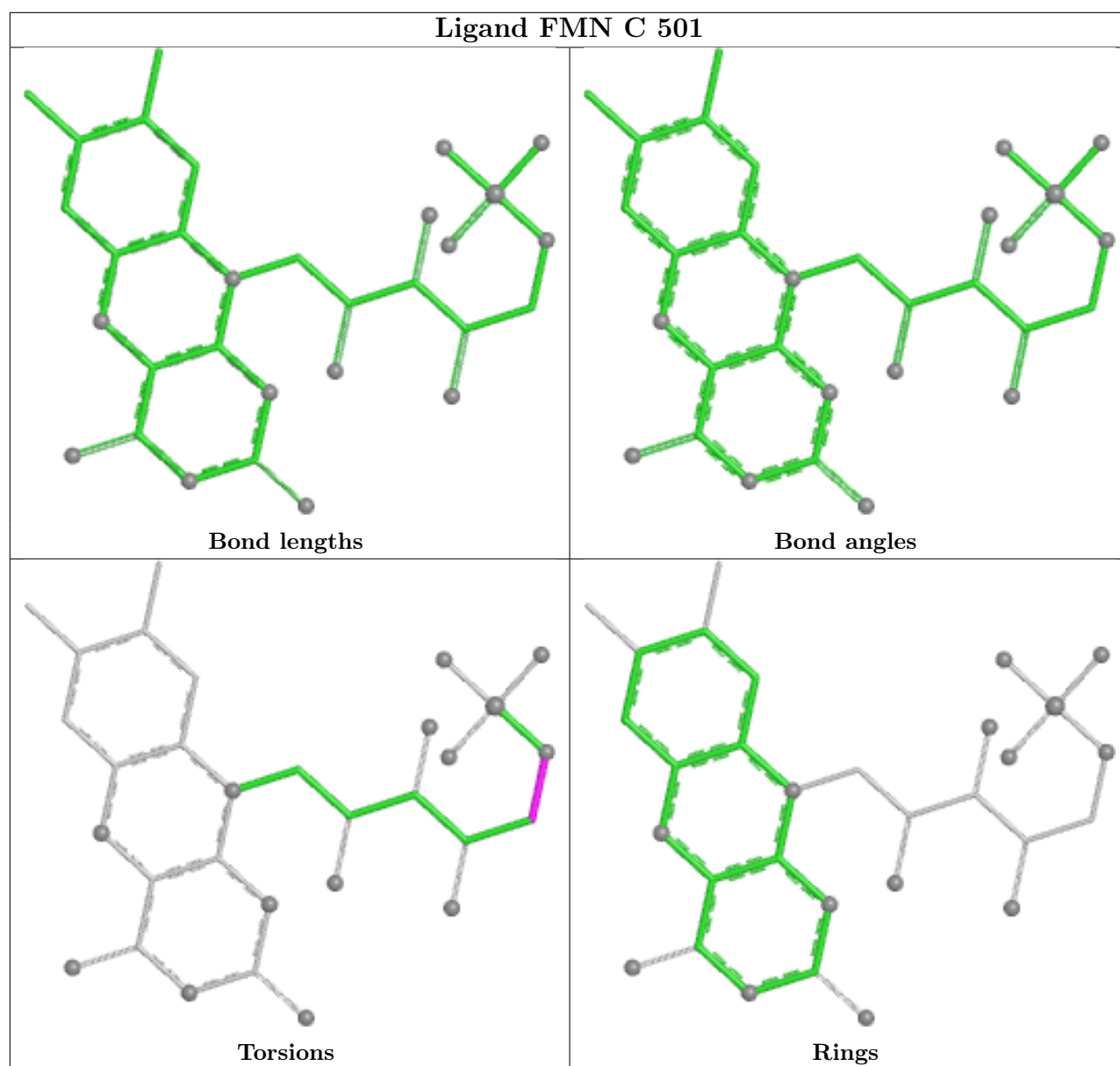
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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	396/400 (99%)	-0.26	3 (0%) 82 83	28, 39, 56, 75	0
1	B	394/400 (98%)	-0.15	8 (2%) 65 66	32, 42, 61, 89	0
1	C	396/400 (99%)	-0.13	5 (1%) 75 77	26, 43, 59, 83	1 (0%)
1	D	396/400 (99%)	-0.18	7 (1%) 67 69	30, 41, 60, 84	0
All	All	1582/1600 (98%)	-0.18	23 (1%) 72 74	26, 41, 59, 89	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	395	LEU	4.8
1	B	297	PHE	3.3
1	A	6	ASP	3.3
1	A	397	TRP	2.8
1	C	10[A]	GLN	2.8
1	B	299	THR	2.7
1	D	299	THR	2.5
1	C	209	ASN	2.5
1	C	372	ARG	2.4
1	D	372	ARG	2.4
1	C	376	TYR	2.4
1	B	2	PRO	2.3
1	D	297	PHE	2.3
1	D	5	LYS	2.3
1	B	393	LEU	2.2
1	D	376	TYR	2.2
1	B	394	LYS	2.2
1	B	298	LEU	2.2
1	A	5	LYS	2.2
1	D	2	PRO	2.1
1	D	397	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	376	TYR	2.0
1	C	5	LYS	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](#)

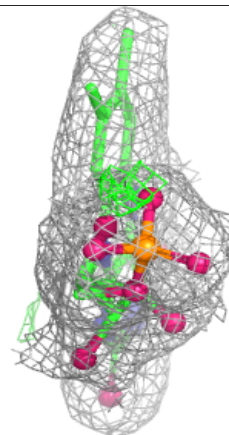
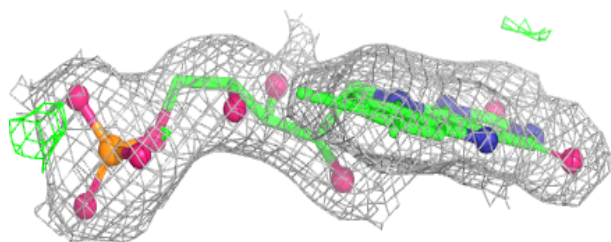
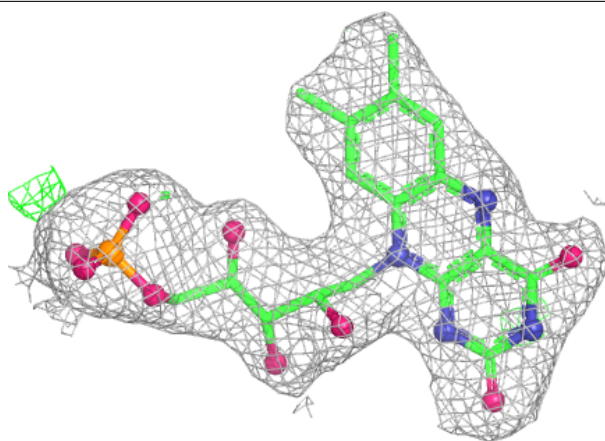
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	B	502	6/6	0.76	0.21	51,54,56,61	0
3	GOL	C	502	6/6	0.81	0.18	44,47,51,53	0
3	GOL	D	502	6/6	0.83	0.15	42,46,47,58	0
3	GOL	A	502	6/6	0.88	0.18	43,49,52,54	0
3	GOL	B	503	6/6	0.88	0.14	40,54,59,60	0
2	FMN	B	501	31/31	0.95	0.08	35,41,45,48	0
2	FMN	C	501	31/31	0.96	0.07	35,41,46,47	0
2	FMN	D	501	31/31	0.97	0.06	37,41,45,48	0
2	FMN	A	501	31/31	0.97	0.07	31,37,41,43	0

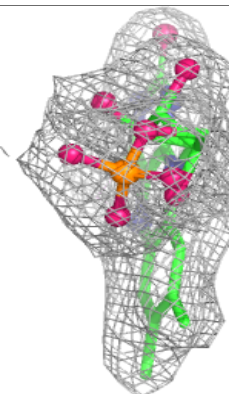
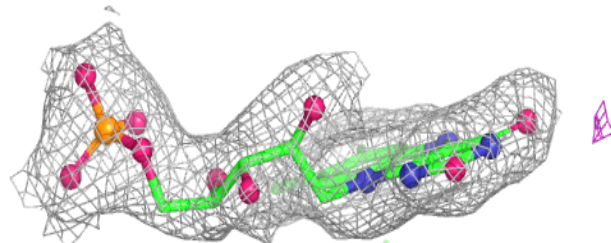
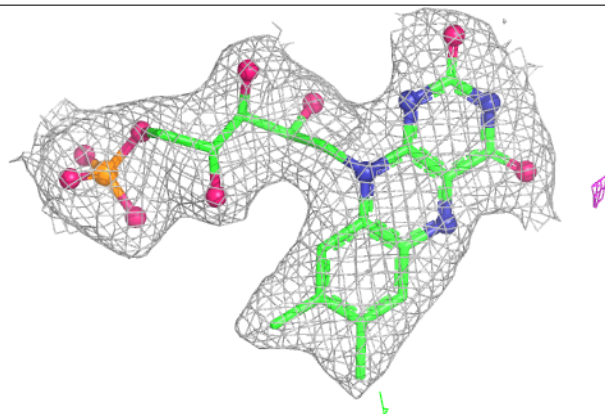
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN 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)

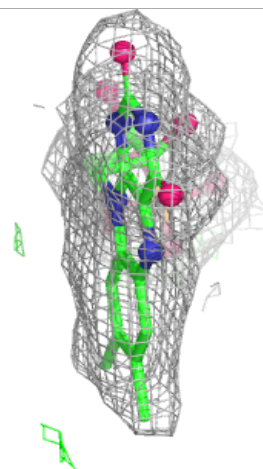
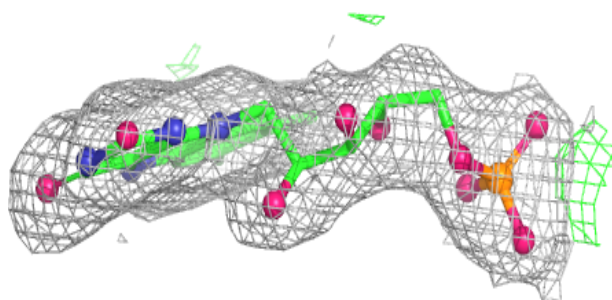
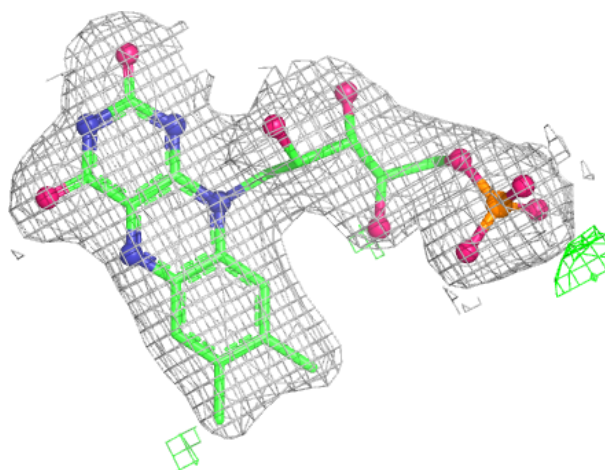
**Electron density around FMN C 501:**

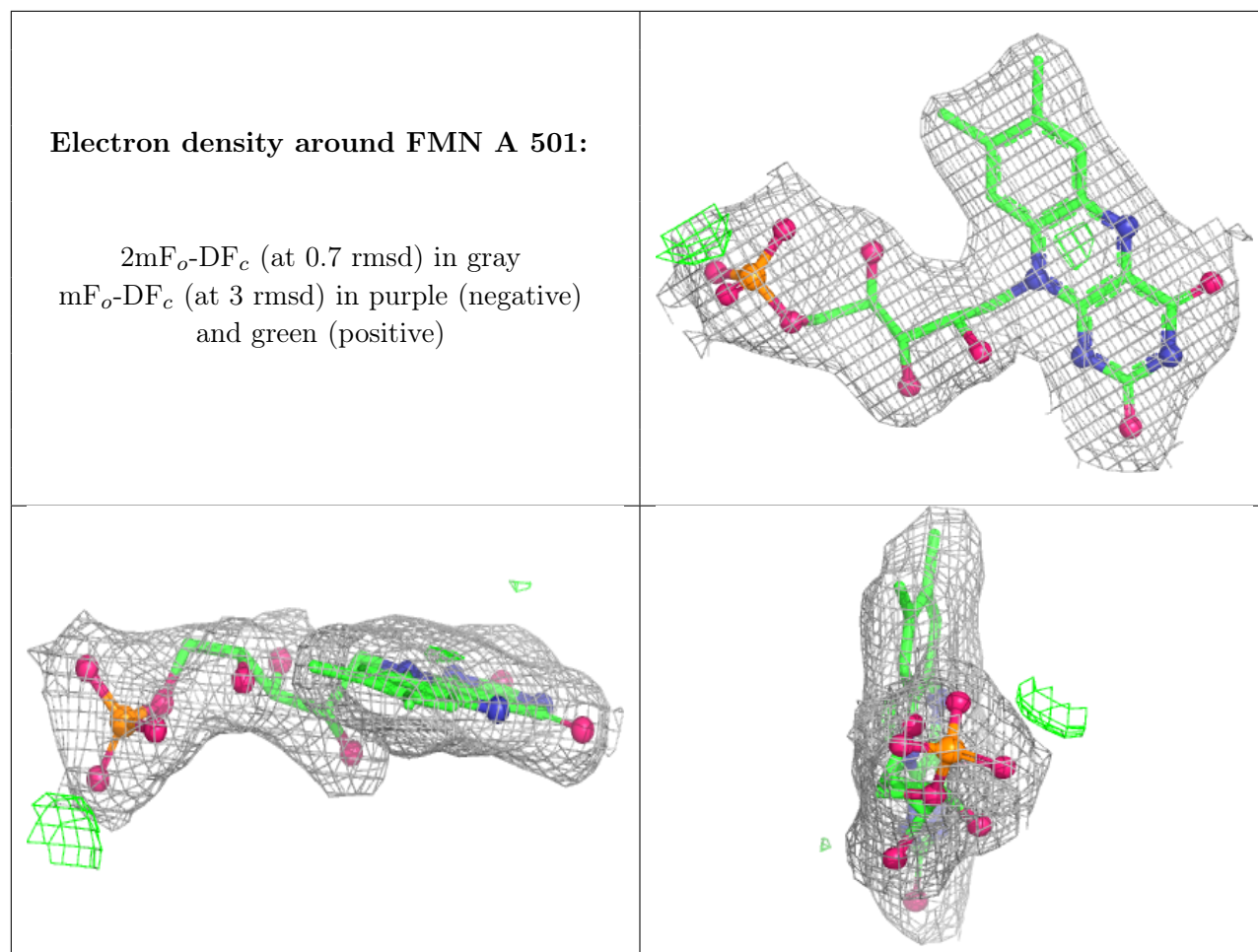
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.