



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:57 AM EDT

PDB ID : 1YRX / pdb_00001yrx
Title : Structure of a novel photoreceptor: the BLUF domain of AppA from Rhodobacter sphaeroides
Authors : Anderson, S.; Dragnea, V.; Masuda, S.; Ybe, J.; Moffat, K.; Bauer, C.
Deposited on : 2005-02-05
Resolution : 2.30 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

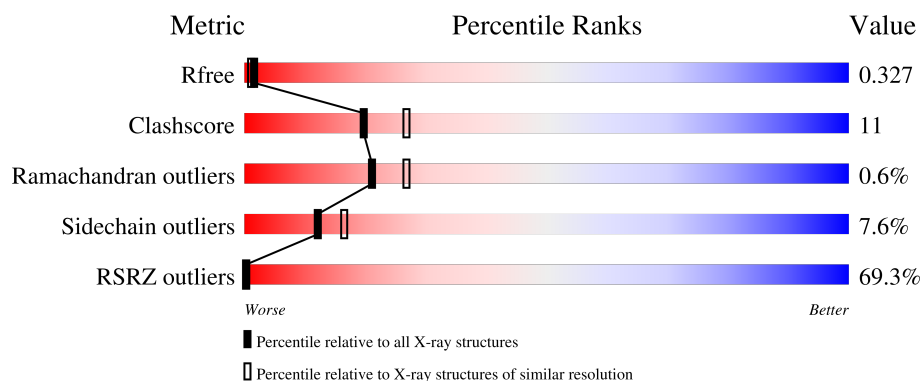
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	121	76% 78%16%••
1	B	121	66% 64%26%6%•
1	C	121	58% 75%19%•5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2962 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.

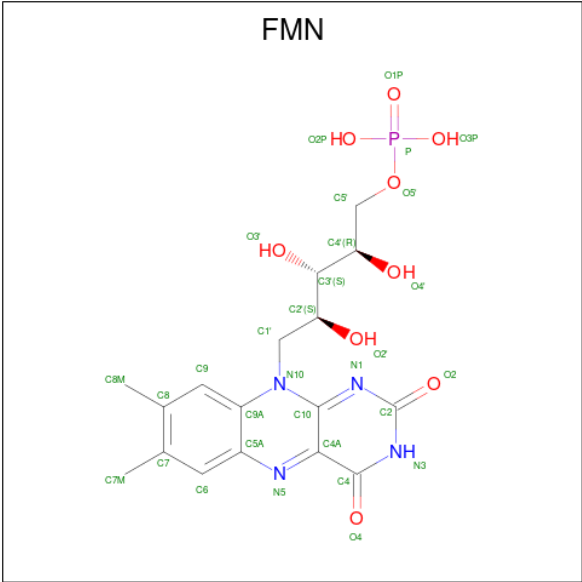
- Molecule 1 is a protein called hypothetical protein Rsph03001874.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			918	570	172	169	7			
1	B	116	Total	C	N	O	S	0	0	0
			909	565	170	167	7			
1	C	115	Total	C	N	O	S	0	0	0
			869	543	155	164	7			

There are 12 discrepancies between the modelled and reference sequences:

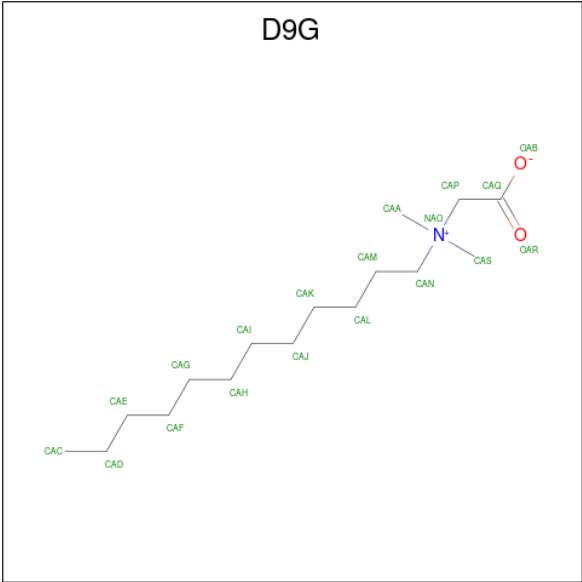
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ALA	-	cloning artifact	UNP Q53119
A	14	GLY	-	cloning artifact	UNP Q53119
A	15	HIS	-	cloning artifact	UNP Q53119
A	16	MET	-	cloning artifact	UNP Q53119
B	13	ALA	-	cloning artifact	UNP Q53119
B	14	GLY	-	cloning artifact	UNP Q53119
B	15	HIS	-	cloning artifact	UNP Q53119
B	16	MET	-	cloning artifact	UNP Q53119
C	13	ALA	-	cloning artifact	UNP Q53119
C	14	GLY	-	cloning artifact	UNP Q53119
C	15	HIS	-	cloning artifact	UNP Q53119
C	16	MET	-	cloning artifact	UNP Q53119

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is N-DODECYL-N,N-DIMETHYLGLYCINATE (CCD ID: D9G) (formula: $C_{16}H_{33}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 19 16 1 2	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 6 6	0	0
3	C	1	Total C N O 19 16 1 2	0	0
3	C	1	Total C 10 10	0	0
3	C	1	Total C 10 10	0	0

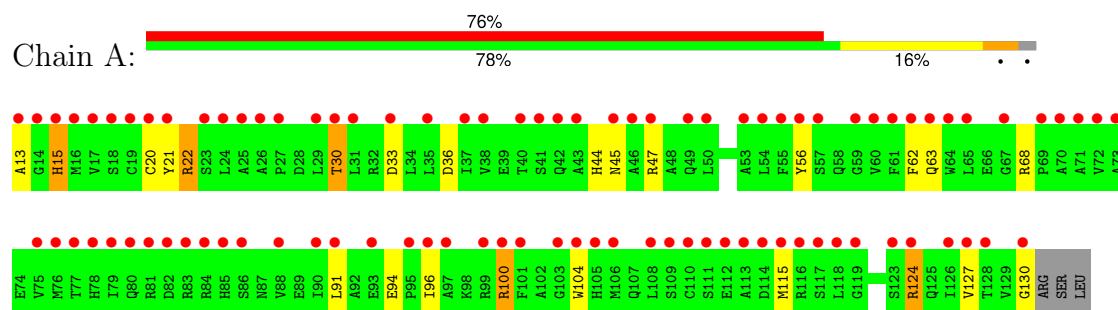
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	30	Total O 30 30	0	0
4	C	21	Total O 21 21	0	0

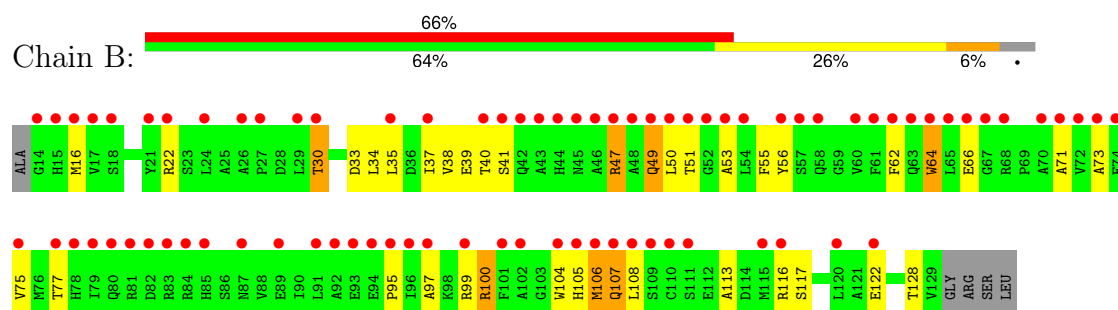
3 Residue-property plots [i](#)

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: hypothetical protein Rsph03001874



• Molecule 1: hypothetical protein Rsph03001874



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.67Å 98.67Å 127.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.30) 95.4 (50.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.29Å)	Xtriage
Refinement program	XTALVIEW, REFMAC 5.1	Depositor
R, R_{free}	0.241 , 0.273 0.311 , 0.327	Depositor DCC
R_{free} test set	1387 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2962	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, D9G

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	0.89	0/935	0.94	0/1265
1	B	1.01	4/926 (0.4%)	1.04	0/1253
1	C	0.60	0/885	0.84	0/1203
All	All	0.85	4/2746 (0.1%)	0.94	0/3721

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	ALA	C-O	12.11	1.40	1.23
1	B	97	ALA	C-N	8.64	1.44	1.33
1	B	47	ARG	C-N	6.14	1.42	1.33
1	B	49	GLN	CD-NE2	5.96	1.45	1.33

There are no bond angle outliers.

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	918	0	896	26	1
1	B	909	0	888	28	0
1	C	869	0	823	15	1
2	A	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	19	1	0
2	C	31	0	19	0	0
3	A	37	0	67	0	0
3	C	39	0	71	1	0
4	A	46	0	0	5	0
4	B	30	0	0	3	0
4	C	21	0	0	1	0
All	All	2962	0	2802	65	1

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 11.

All (65) 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:104:TRP:HZ3	4:B:226:HOH:O	1.33	1.11
1:A:100:ARG:HH11	1:A:100:ARG:HG3	1.27	0.97
1:B:30:THR:HG22	1:B:33:ASP:H	1.34	0.92
1:A:30:THR:HG21	4:A:345:HOH:O	1.71	0.89
1:B:37:ILE:O	1:B:41:SER:HB2	1.79	0.81
1:A:100:ARG:HH11	1:A:100:ARG:CG	1.94	0.80
1:A:22:ARG:HG2	1:A:91:LEU:HD11	1.63	0.79
1:A:115:MET:HE2	1:A:115:MET:HA	1.65	0.78
1:C:110:CYS:SG	1:C:115:MET:HE3	2.26	0.75
1:A:20:CYS:SG	1:A:62:PHE:CE2	2.80	0.74
1:B:62:PHE:CZ	1:B:64:TRP:CZ3	2.79	0.70
1:C:115:MET:HA	1:C:115:MET:HE2	1.79	0.64
1:A:130:GLY:HA3	4:A:350:HOH:O	1.97	0.63
1:A:30:THR:HG23	4:A:325:HOH:O	1.98	0.62
1:B:34:LEU:O	1:B:38:VAL:HG23	1.99	0.62
1:A:30:THR:HG22	1:A:33:ASP:H	1.66	0.61
1:C:21:TYR:CE1	1:C:63:GLN:HB3	2.36	0.60
1:A:100:ARG:NH1	4:A:346:HOH:O	2.35	0.59
1:B:113:ALA:O	1:B:117:SER:HB3	2.02	0.59
1:A:22:ARG:NH2	1:B:100:ARG:O	2.36	0.58
1:B:55:PHE:HD1	1:B:107:GLN:HG2	1.68	0.58
1:B:62:PHE:CZ	1:B:64:TRP:HZ3	2.20	0.58
1:C:34:LEU:HD22	1:C:106:MET:HE1	1.86	0.57
1:A:100:ARG:HG3	1:A:100:ARG:NH1	2.08	0.57
1:B:55:PHE:CD1	1:B:107:GLN:HG2	2.39	0.57
1:B:62:PHE:HZ	1:B:64:TRP:CZ3	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:GLY:O	1:C:104:TRP:HA	2.04	0.56
1:C:124:ARG:HH11	1:C:124:ARG:HB2	1.71	0.55
1:A:13:ALA:HB3	1:A:15:HIS:CE1	2.43	0.54
1:A:124:ARG:HD2	1:A:124:ARG:C	2.34	0.53
1:C:33:ASP:O	1:C:37:ILE:HG13	2.08	0.52
1:B:51:THR:OG1	1:B:66:GLU:HG3	2.08	0.52
1:A:21:TYR:CE1	1:A:63:GLN:HB3	2.45	0.52
1:B:73:ALA:HB2	4:B:220:HOH:O	2.10	0.52
1:A:91:LEU:HD23	1:B:100:ARG:HG3	1.94	0.50
1:A:20:CYS:SG	1:A:62:PHE:CZ	3.03	0.50
1:B:38:VAL:HG22	1:B:106:MET:SD	2.51	0.50
1:C:58:GLN:HG3	1:C:58:GLN:O	2.12	0.49
1:C:125:GLN:NE2	4:C:309:HOH:O	2.46	0.48
1:A:100:ARG:HB3	1:B:22:ARG:HH12	1.79	0.48
1:B:35:LEU:O	1:B:39:GLU:HG2	2.14	0.47
1:B:117:SER:HA	4:B:224:HOH:O	2.15	0.47
1:B:53:ALA:HA	1:B:105:HIS:O	2.16	0.46
1:B:106:MET:HE3	1:B:106:MET:HA	1.98	0.46
1:B:56:TYR:HB3	1:B:108:LEU:HD23	1.99	0.45
1:B:49:GLN:O	1:B:99:ARG:NH2	2.50	0.45
1:A:56:TYR:CD2	1:A:56:TYR:C	2.95	0.45
1:A:45:ASN:HD22	1:A:104:TRP:CD1	2.35	0.44
1:C:111:SER:OG	1:C:114:ASP:OD1	2.30	0.44
1:A:44:HIS:HD2	1:A:47:ARG:NH1	2.15	0.44
1:C:120:LEU:HD21	3:C:301:D9G:HAJ2	1.99	0.43
1:A:68:ARG:NH2	1:C:33:ASP:OD1	2.51	0.43
1:B:16:MET:O	1:B:95:PRO:HA	2.19	0.43
1:B:50:LEU:HD13	1:B:75:VAL:HG11	2.00	0.43
1:B:56:TYR:HB3	1:B:108:LEU:CD2	2.49	0.43
1:B:40:THR:HG21	2:B:202:FMN:H4'	2.00	0.42
1:B:71:ALA:O	1:B:75:VAL:HG12	2.19	0.42
1:A:100:ARG:CG	1:A:100:ARG:NH1	2.62	0.42
1:A:96:ILE:HG22	1:A:100:ARG:NH2	2.35	0.41
1:C:124:ARG:HG3	1:C:125:GLN:N	2.35	0.41
1:A:20:CYS:SG	1:A:62:PHE:HE2	2.41	0.41
1:C:124:ARG:HH11	1:C:124:ARG:CB	2.34	0.41
1:B:62:PHE:CE1	1:B:64:TRP:HZ3	2.39	0.41
1:A:44:HIS:HE1	4:A:308:HOH:O	2.03	0.40
1:C:86:SER:O	1:C:87:ASN:C	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:OD1	1:C:32:ARG:NH2[7_555]	2.10	0.10

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	116/121 (96%)	112 (97%)	4 (3%)	0	100	100
1	B	114/121 (94%)	109 (96%)	4 (4%)	1 (1%)	14	17
1	C	113/121 (93%)	106 (94%)	6 (5%)	1 (1%)	14	17
All	All	343/363 (94%)	327 (95%)	14 (4%)	2 (1%)	21	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	ARG
1	C	113	ALA

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	95/99 (96%)	88 (93%)	7 (7%)	13	17
1	B	95/99 (96%)	86 (90%)	9 (10%)	8	10
1	C	88/99 (89%)	83 (94%)	5 (6%)	18	27
All	All	278/297 (94%)	257 (92%)	21 (8%)	12	16

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	22	ARG
1	A	30	THR
1	A	94	GLU
1	A	100	ARG
1	A	124	ARG
1	A	127	VAL
1	B	30	THR
1	B	64	TRP
1	B	77	THR
1	B	100	ARG
1	B	106	MET
1	B	107	GLN
1	B	116	ARG
1	B	122	GLU
1	B	128	THR
1	C	22	ARG
1	C	77	THR
1	C	90	ILE
1	C	124	ARG
1	C	129	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	44	HIS
1	B	58	GLN
1	B	105	HIS
1	C	44	HIS
1	C	63	GLN
1	C	78	HIS
1	C	87	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D9G	C	301	-	18,18,18	1.79	4 (22%)	20,21,21	0.82	1 (5%)
2	FMN	A	201	-	33,33,33	1.19	3 (9%)	48,50,50	1.28	5 (10%)
3	D9G	C	304	-	9,9,18	0.39	0	8,8,21	0.57	0
3	D9G	A	303	-	11,11,18	0.52	0	10,10,21	0.45	0
2	FMN	C	203	-	33,33,33	1.11	2 (6%)	48,50,50	1.35	7 (14%)
2	FMN	B	202	-	33,33,33	1.12	3 (9%)	48,50,50	1.29	9 (18%)
3	D9G	A	302	-	18,18,18	1.76	4 (22%)	20,21,21	0.78	0
3	D9G	A	306	-	5,5,18	0.41	0	4,4,21	0.41	0
3	D9G	C	305	-	9,9,18	0.38	0	8,8,21	0.53	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	D9G	C	301	-	-	11/18/18/18	-
2	FMN	A	201	-	-	2/18/18/18	0/3/3/3
3	D9G	C	304	-	-	4/7/7/18	-
3	D9G	A	303	-	-	4/9/9/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	C	203	-	-	3/18/18/18	0/3/3/3
2	FMN	B	202	-	-	3/18/18/18	0/3/3/3
3	D9G	A	302	-	-	9/18/18/18	-
3	D9G	A	306	-	-	1/3/3/18	-
3	D9G	C	305	-	-	4/7/7/18	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	D9G	CAN-NAO	-4.96	1.40	1.52
2	C	203	FMN	C4A-N5	4.08	1.39	1.30
3	A	302	D9G	CAN-NAO	-3.89	1.43	1.52
2	B	202	FMN	C4A-N5	3.71	1.38	1.30
3	C	301	D9G	CAS-NAO	-3.66	1.41	1.50
3	A	302	D9G	CAS-NAO	-3.61	1.41	1.50
3	A	302	D9G	CAA-NAO	-3.52	1.41	1.50
2	A	201	FMN	C4A-N5	3.38	1.38	1.30
3	A	302	D9G	CAP-CAQ	3.02	1.57	1.52
2	B	202	FMN	C10-N1	2.97	1.39	1.33
2	A	201	FMN	C10-N1	2.89	1.39	1.33
2	A	201	FMN	O2-C2	-2.65	1.19	1.24
3	C	301	D9G	CAA-NAO	-2.58	1.44	1.50
3	C	301	D9G	CAP-CAQ	2.47	1.56	1.52
2	B	202	FMN	C5'-C4'	2.21	1.54	1.51
2	C	203	FMN	C10-N1	2.18	1.37	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	203	FMN	C4-C4A-N5	3.35	122.83	118.21
2	A	201	FMN	C4-N3-C2	-3.18	119.99	125.64
2	C	203	FMN	C4-N3-C2	-3.12	120.11	125.64
2	B	202	FMN	C4-N3-C2	-3.06	120.20	125.64
2	C	203	FMN	C10-C4A-N5	-3.06	118.56	124.81
2	C	203	FMN	C4A-C10-N10	3.05	120.85	116.48
2	B	202	FMN	C10-C4A-N5	-3.02	118.64	124.81
2	A	201	FMN	C4A-C10-N10	2.98	120.75	116.48
2	B	202	FMN	C4A-C10-N10	2.81	120.51	116.48
2	C	203	FMN	C4A-C4-N3	2.73	120.19	113.25
2	A	201	FMN	C10-C4A-N5	-2.69	119.31	124.81
2	B	202	FMN	C4A-C4-N3	2.42	119.41	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	FMN	C4-C4A-N5	2.39	121.50	118.21
2	B	202	FMN	O4-C4-N3	-2.33	115.74	120.11
2	C	203	FMN	C9A-C5A-N5	-2.30	120.01	122.45
3	C	301	D9G	CAM-CAN-NAO	-2.27	110.73	115.35
2	A	201	FMN	C5A-C9A-N10	2.23	119.98	117.97
2	A	201	FMN	C4A-C4-N3	2.23	118.93	113.25
2	B	202	FMN	C9A-C5A-N5	-2.17	120.15	122.45
2	B	202	FMN	C5A-N5-C4A	2.14	121.55	118.09
2	C	203	FMN	C10-N1-C2	2.02	121.22	116.85
2	B	202	FMN	C4A-C10-N1	-2.00	119.68	124.59

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	FMN	C3'-C4'-C5'-O5'
2	A	201	FMN	O4'-C4'-C5'-O5'
2	C	203	FMN	C5'-O5'-P-O3P
3	A	302	D9G	CAM-CAN-NAO-CAA
3	A	302	D9G	CAM-CAN-NAO-CAP
3	C	301	D9G	CAQ-CAP-NAO-CAN
3	C	301	D9G	CAQ-CAP-NAO-CAS
3	C	301	D9G	CAQ-CAP-NAO-CAA
3	C	301	D9G	NAO-CAP-CAQ-OAB
3	C	301	D9G	NAO-CAP-CAQ-OAR
3	A	302	D9G	CAM-CAN-NAO-CAS
3	A	302	D9G	CAG-CAH-CAI-CAJ
3	A	302	D9G	CAL-CAM-CAN-NAO
3	A	303	D9G	CAE-CAF-CAG-CAH
3	C	305	D9G	CAH-CAI-CAJ-CAK
3	A	303	D9G	CAI-CAJ-CAK-CAL
3	C	304	D9G	CAE-CAF-CAG-CAH
3	C	301	D9G	CAD-CAE-CAF-CAG
3	C	301	D9G	CAG-CAH-CAI-CAJ
2	B	202	FMN	O2'-C2'-C3'-C4'
3	C	301	D9G	CAL-CAM-CAN-NAO
2	C	203	FMN	C5'-O5'-P-O1P
3	C	301	D9G	CAK-CAL-CAM-CAN
3	C	301	D9G	CAH-CAI-CAJ-CAK
3	A	306	D9G	CAC-CAD-CAE-CAF
3	C	304	D9G	CAG-CAH-CAI-CAJ
3	A	302	D9G	NAO-CAP-CAQ-OAB

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Mol	Chain	Res	Type	Atoms
3	A	302	D9G	NAO-CAP-CAQ-OAR
3	A	302	D9G	CAF-CAG-CAH-CAI
3	C	305	D9G	CAG-CAH-CAI-CAJ
3	C	304	D9G	CAI-CAJ-CAK-CAL
2	B	202	FMN	O2'-C2'-C3'-O3'
2	C	203	FMN	C5'-O5'-P-O2P
2	B	202	FMN	C1'-C2'-C3'-C4'
3	A	302	D9G	CAE-CAF-CAG-CAH
3	C	301	D9G	CAE-CAF-CAG-CAH
3	A	303	D9G	CAK-CAL-CAM-CAN
3	C	305	D9G	CAE-CAF-CAG-CAH
3	A	303	D9G	CAC-CAD-CAE-CAF
3	C	304	D9G	CAC-CAD-CAE-CAF
3	C	305	D9G	CAC-CAD-CAE-CAF

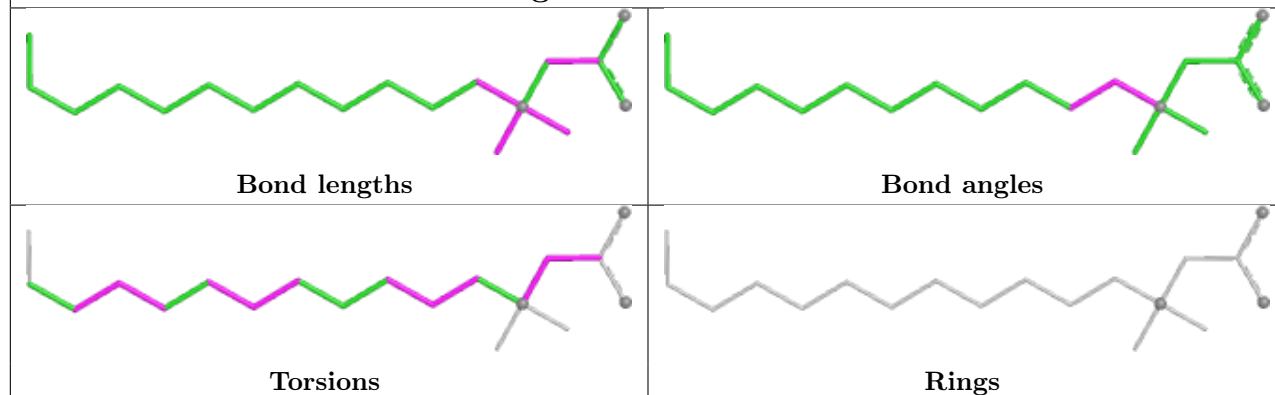
There are no ring outliers.

2 monomers are involved in 2 short contacts:

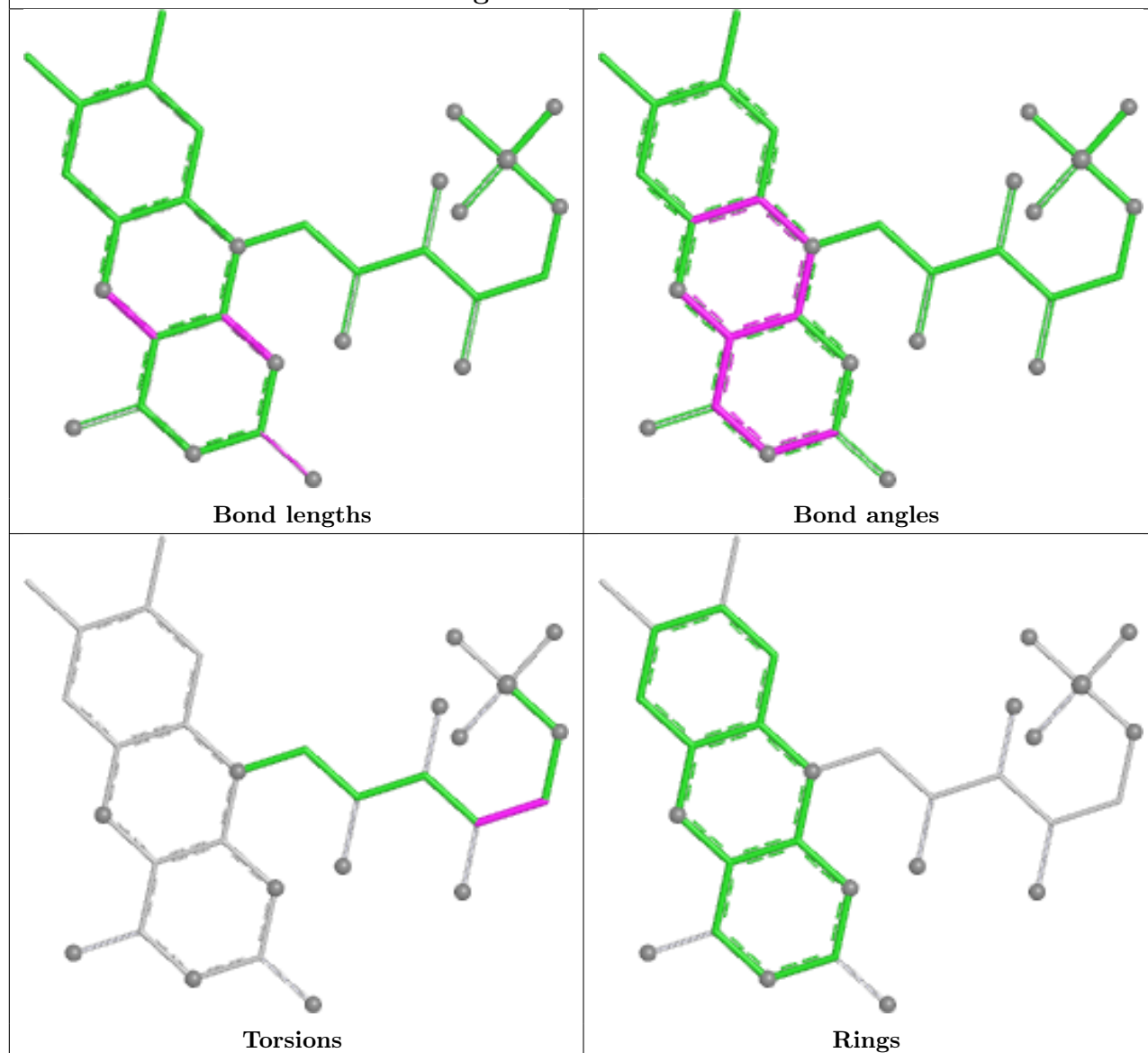
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	D9G	1	0
2	B	202	FMN	1	0

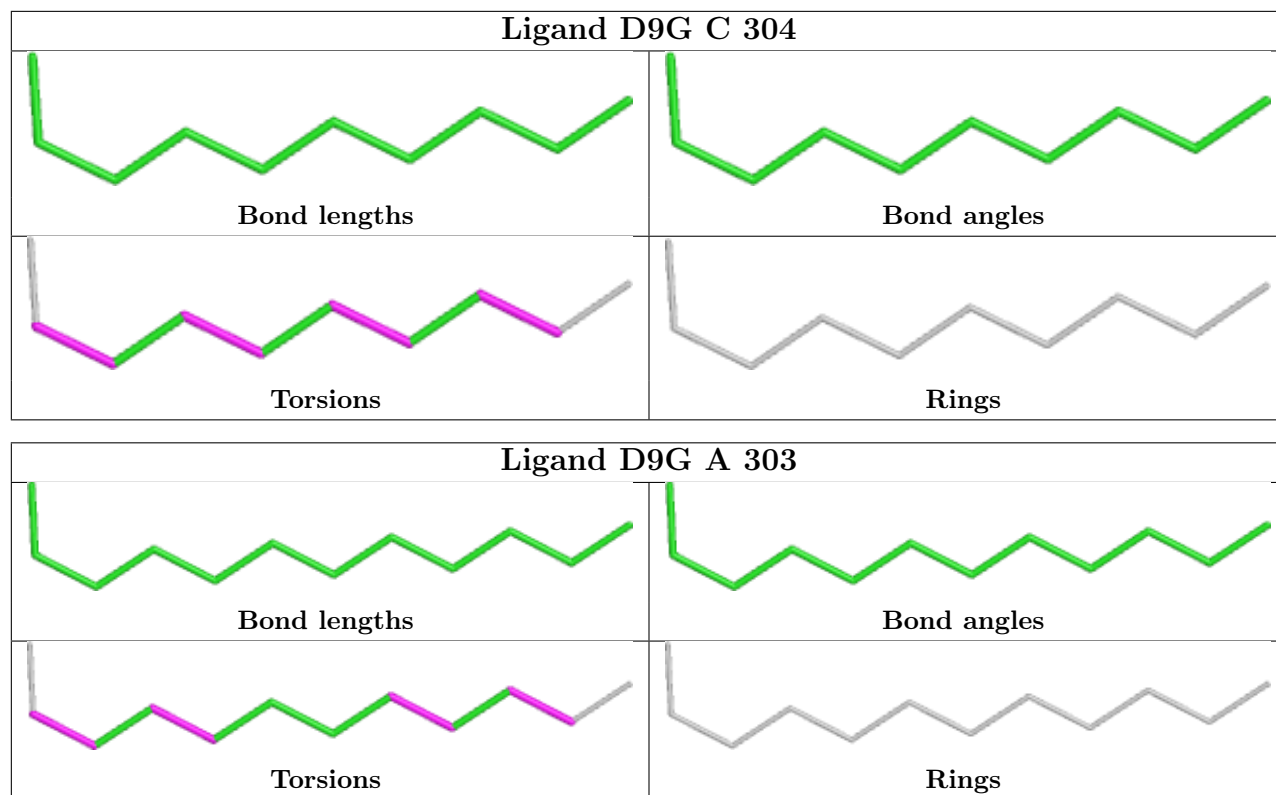
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

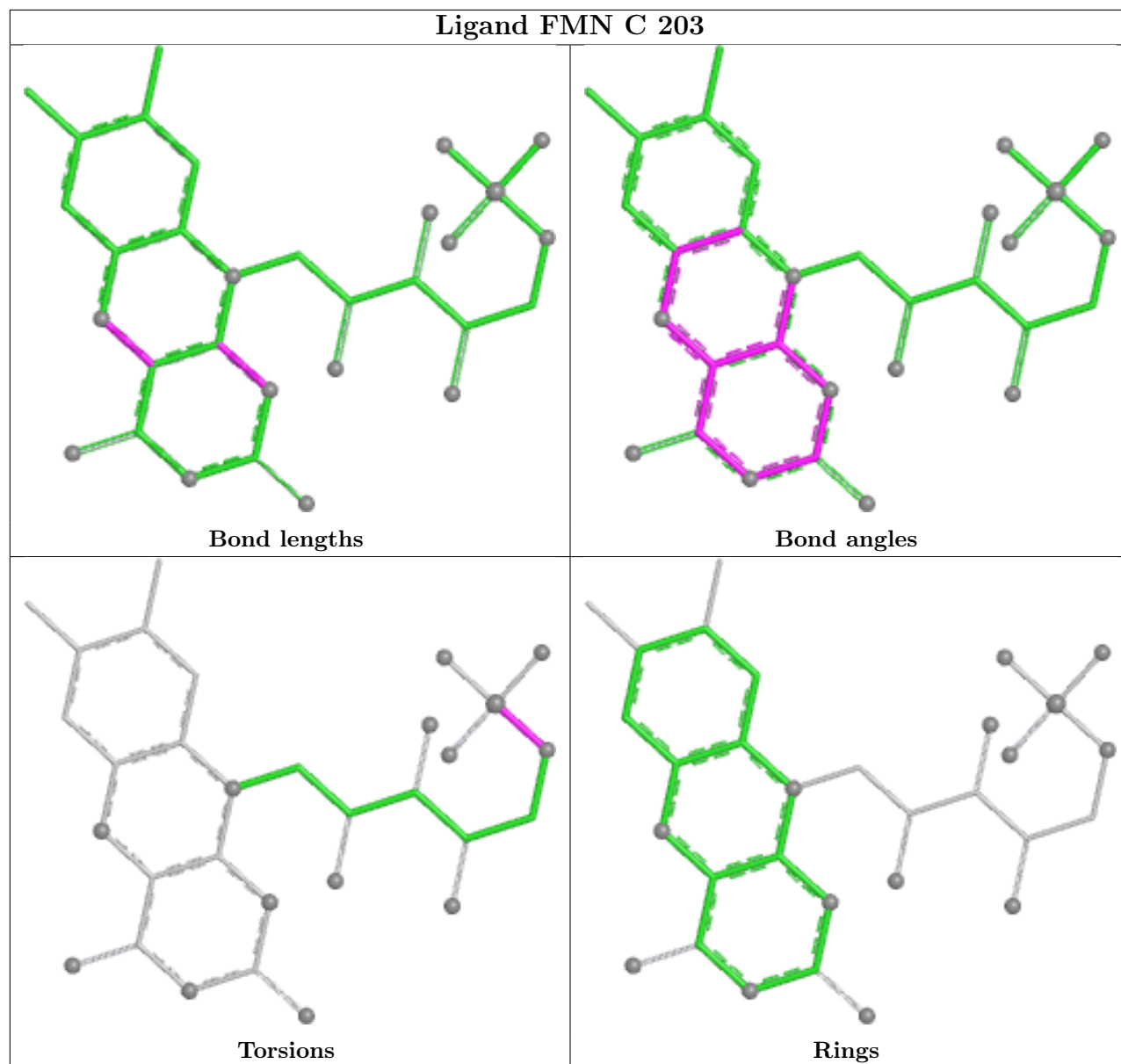
Ligand D9G C 301

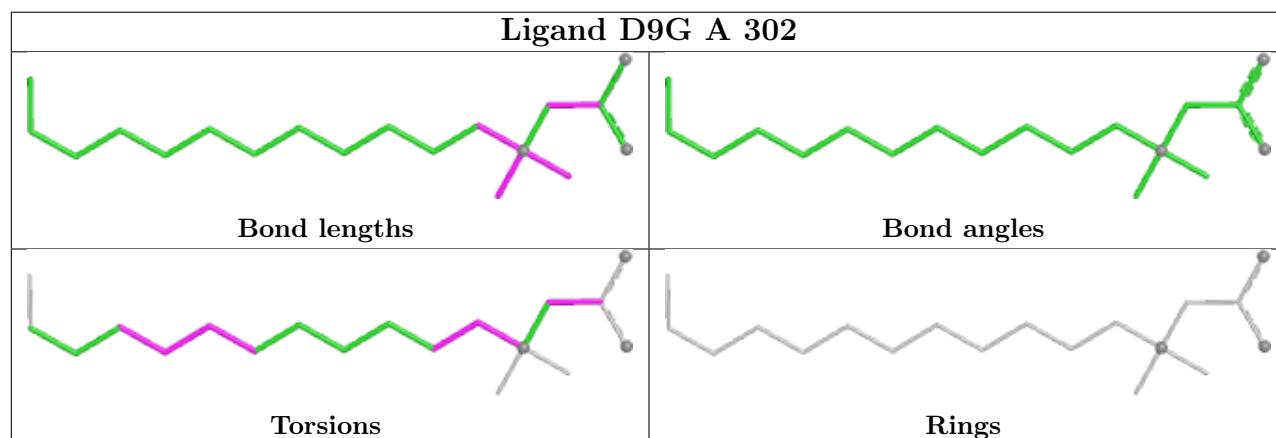
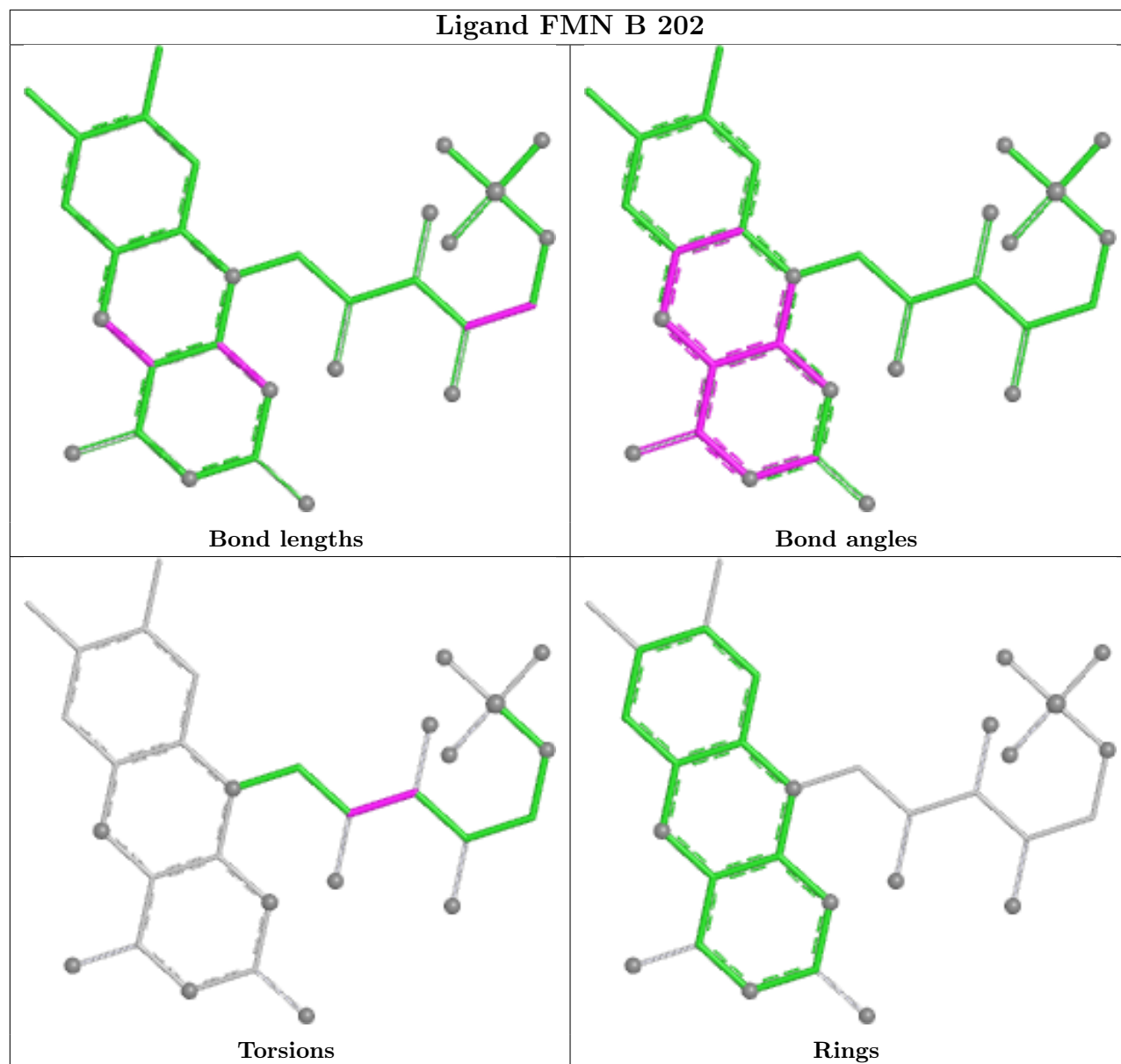


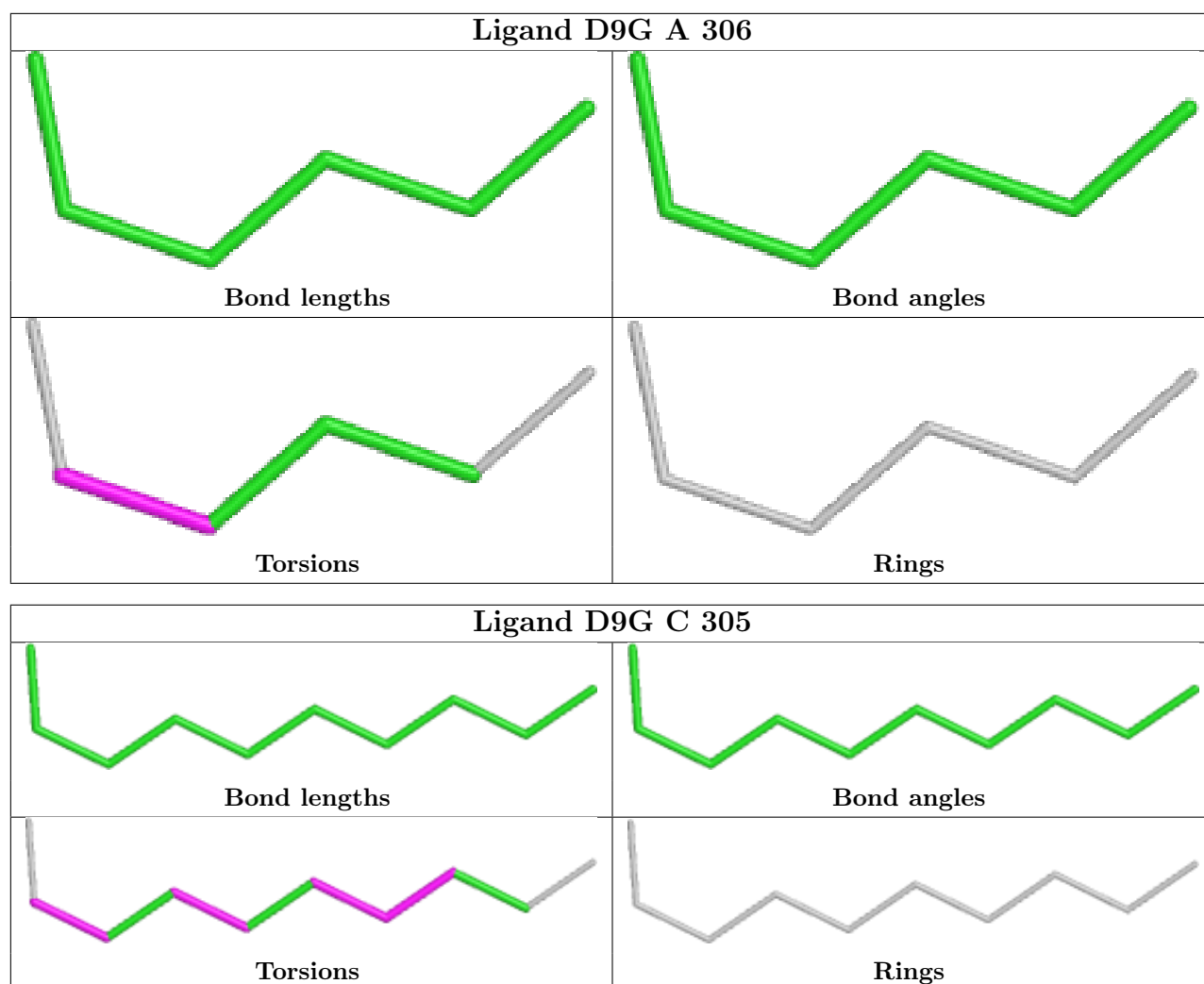
Ligand FMN A 201











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	118/121 (97%)	2.72	92 (77%) 0 0	70, 79, 87, 92	0
1	B	116/121 (95%)	2.66	80 (68%) 0 0	63, 81, 89, 96	0
1	C	115/121 (95%)	2.51	70 (60%) 0 0	65, 77, 85, 107	0
All	All	349/363 (96%)	2.63	242 (69%) 0 0	63, 79, 88, 107	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	VAL	7.0
1	B	70	ALA	6.8
1	C	17	VAL	5.8
1	C	15	HIS	5.8
1	B	75	VAL	5.7
1	B	110	CYS	5.7
1	B	105	HIS	5.4
1	B	46	ALA	5.3
1	A	130	GLY	5.3
1	A	62	PHE	5.2
1	C	95	PRO	5.2
1	C	55	PHE	5.1
1	C	43	ALA	5.1
1	A	110	CYS	5.0
1	C	72	VAL	5.0
1	A	114	ASP	4.7
1	B	62	PHE	4.7
1	A	79	ILE	4.6
1	A	64	TRP	4.5
1	C	77	THR	4.5
1	A	104	TRP	4.5
1	A	108	LEU	4.5
1	B	17	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	61	PHE	4.4
1	C	16	MET	4.4
1	C	67	GLY	4.4
1	A	113	ALA	4.4
1	B	14	GLY	4.4
1	B	30	THR	4.3
1	B	94	GLU	4.3
1	C	50	LEU	4.3
1	C	46	ALA	4.3
1	C	70	ALA	4.3
1	B	73	ALA	4.2
1	B	101	PHE	4.2
1	B	106	MET	4.1
1	A	54	LEU	4.0
1	B	104	TRP	4.0
1	B	71	ALA	4.0
1	B	50	LEU	3.9
1	C	97	ALA	3.9
1	A	20	CYS	3.8
1	A	37	ILE	3.8
1	C	98	LYS	3.8
1	C	90	ILE	3.7
1	A	49	GLN	3.7
1	B	77	THR	3.7
1	B	97	ALA	3.7
1	B	29	LEU	3.6
1	B	83	ARG	3.6
1	C	53	ALA	3.6
1	B	74	GLU	3.6
1	A	95	PRO	3.6
1	B	43	ALA	3.6
1	C	37	ILE	3.6
1	C	62	PHE	3.6
1	A	31	LEU	3.6
1	C	78	HIS	3.6
1	A	21	TYR	3.6
1	B	79	ILE	3.6
1	C	79	ILE	3.6
1	C	129	VAL	3.6
1	B	78	HIS	3.5
1	C	60	VAL	3.5
1	A	70	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	103	GLY	3.5
1	C	30	THR	3.5
1	C	51	THR	3.5
1	A	124	ARG	3.5
1	A	96	ILE	3.5
1	B	24	LEU	3.5
1	A	30	THR	3.5
1	A	75	VAL	3.5
1	B	18	SER	3.5
1	B	64	TRP	3.5
1	A	91	LEU	3.5
1	B	49	GLN	3.5
1	A	72	VAL	3.4
1	A	117	SER	3.4
1	A	119	GLY	3.4
1	C	61	PHE	3.4
1	C	73	ALA	3.4
1	A	41	SER	3.4
1	B	53	ALA	3.4
1	B	65	LEU	3.4
1	B	96	ILE	3.4
1	B	108	LEU	3.4
1	A	35	LEU	3.3
1	A	65	LEU	3.3
1	C	35	LEU	3.3
1	A	101	PHE	3.3
1	A	71	ALA	3.3
1	B	42	GLN	3.3
1	B	45	ASN	3.3
1	A	24	LEU	3.3
1	B	67	GLY	3.2
1	A	29	LEU	3.2
1	B	41	SER	3.2
1	C	64	TRP	3.2
1	A	112	GLU	3.2
1	C	91	LEU	3.2
1	A	26	ALA	3.2
1	A	73	ALA	3.2
1	C	128	THR	3.2
1	A	56	TYR	3.2
1	C	69	PRO	3.2
1	A	55	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	45	ASN	3.1
1	B	92	ALA	3.1
1	A	17	VAL	3.1
1	B	58	GLN	3.1
1	B	72	VAL	3.1
1	A	93	GLU	3.0
1	C	44	HIS	3.0
1	B	82	ASP	3.0
1	A	116	ARG	3.0
1	C	116	ARG	3.0
1	C	71	ALA	3.0
1	A	38	VAL	3.0
1	C	75	VAL	3.0
1	A	46	ALA	3.0
1	B	48	ALA	3.0
1	A	118	LEU	3.0
1	A	84	ARG	3.0
1	C	125	GLN	3.0
1	B	40	THR	3.0
1	A	111	SER	3.0
1	B	115	MET	3.0
1	C	101	PHE	2.9
1	A	97	ALA	2.9
1	A	18	SER	2.9
1	C	92	ALA	2.9
1	A	76	MET	2.9
1	A	86	SER	2.9
1	B	81	ARG	2.9
1	B	35	LEU	2.9
1	B	109	SER	2.8
1	A	90	ILE	2.8
1	B	22	ARG	2.8
1	C	47	ARG	2.8
1	A	25	ALA	2.8
1	A	43	ALA	2.8
1	A	85	HIS	2.8
1	A	82	ASP	2.8
1	C	96	ILE	2.7
1	B	107	GLN	2.7
1	C	93	GLU	2.7
1	B	99	ARG	2.7
1	A	42	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	127	VAL	2.7
1	C	66	GLU	2.7
1	A	50	LEU	2.7
1	C	21	TYR	2.7
1	A	14	GLY	2.7
1	B	52	GLY	2.7
1	B	116	ARG	2.7
1	B	15	HIS	2.6
1	B	27	PRO	2.6
1	C	20	CYS	2.6
1	C	89	GLU	2.6
1	A	33	ASP	2.6
1	B	68	ARG	2.6
1	C	59	GLY	2.6
1	A	106	MET	2.6
1	C	29	LEU	2.6
1	C	48	ALA	2.6
1	A	100	ARG	2.6
1	C	57	SER	2.6
1	A	78	HIS	2.6
1	A	63	GLN	2.6
1	B	54	LEU	2.6
1	A	53	ALA	2.6
1	C	113	ALA	2.6
1	B	87	ASN	2.6
1	B	21	TYR	2.6
1	A	13	ALA	2.5
1	C	56	TYR	2.5
1	C	104	TRP	2.5
1	A	126	ILE	2.5
1	B	84	ARG	2.5
1	A	115	MET	2.5
1	B	63	GLN	2.5
1	A	57	SER	2.4
1	B	47	ARG	2.4
1	A	23	SER	2.4
1	B	60	VAL	2.4
1	C	26	ALA	2.4
1	A	16	MET	2.4
1	C	105	HIS	2.4
1	A	80	GLN	2.4
1	B	93	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	24	LEU	2.4
1	A	15	HIS	2.4
1	B	66	GLU	2.4
1	A	67	GLY	2.3
1	B	120	LEU	2.3
1	C	27	PRO	2.3
1	A	83	ARG	2.3
1	A	105	HIS	2.3
1	A	19	CYS	2.3
1	B	51	THR	2.3
1	B	57	SER	2.3
1	B	122	GLU	2.3
1	C	58	GLN	2.3
1	C	112	GLU	2.3
1	B	102	ALA	2.3
1	A	40	THR	2.3
1	A	77	THR	2.3
1	B	85	HIS	2.3
1	C	109	SER	2.3
1	B	95	PRO	2.2
1	A	47	ARG	2.2
1	A	59	GLY	2.2
1	A	128	THR	2.2
1	B	44	HIS	2.2
1	B	56	TYR	2.2
1	A	109	SER	2.2
1	B	91	LEU	2.2
1	A	81	ARG	2.2
1	B	37	ILE	2.2
1	C	49	GLN	2.2
1	B	26	ALA	2.2
1	C	127	VAL	2.1
1	B	61	PHE	2.1
1	C	103	GLY	2.1
1	B	111	SER	2.1
1	B	89	GLU	2.1
1	C	38	VAL	2.1
1	C	22	ARG	2.1
1	C	68	ARG	2.1
1	C	65	LEU	2.1
1	C	114	ASP	2.1
1	C	84	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	111	SER	2.0
1	B	16	MET	2.0
1	C	94	GLU	2.0
1	B	80	GLN	2.0
1	A	27	PRO	2.0
1	A	88	VAL	2.0
1	A	99	ARG	2.0
1	A	123	SER	2.0
1	A	69	PRO	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](#)

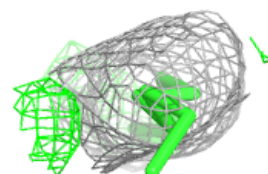
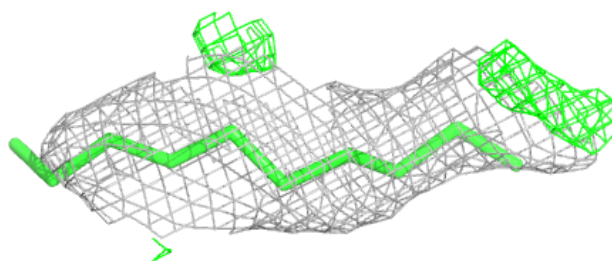
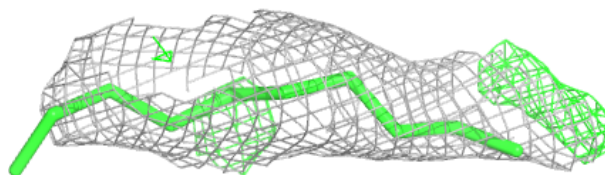
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D9G	C	304	10/19	0.77	0.25	87,89,94,94	0
3	D9G	C	301	19/19	0.79	0.23	84,87,97,97	0
3	D9G	A	303	12/19	0.79	0.29	91,94,97,98	0
3	D9G	C	305	10/19	0.81	0.26	83,84,89,90	0
3	D9G	A	306	6/19	0.82	0.25	80,81,82,85	0
3	D9G	A	302	19/19	0.82	0.20	92,95,103,104	0
2	FMN	B	202	31/31	0.87	0.14	53,64,74,75	5
2	FMN	C	203	31/31	0.87	0.14	59,63,72,74	5
2	FMN	A	201	31/31	0.89	0.12	46,48,69,70	5

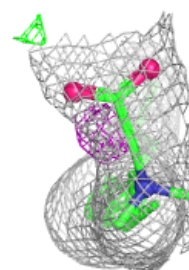
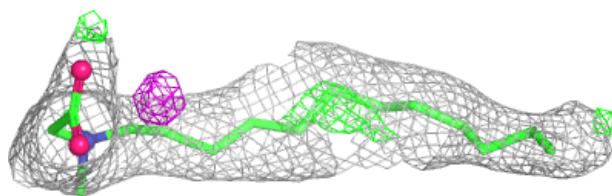
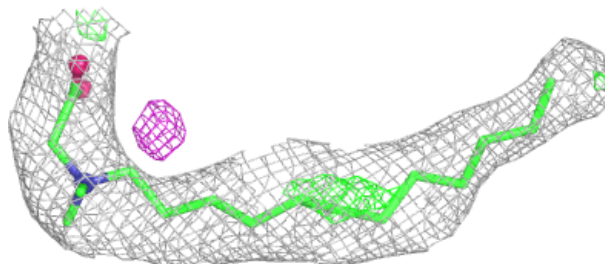
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around D9G C 304:

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

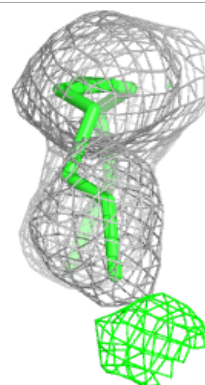
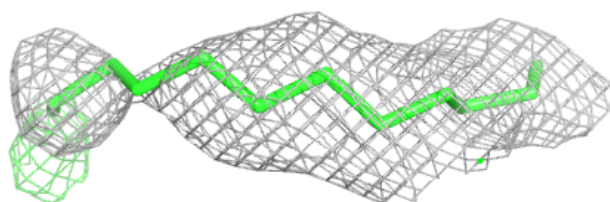
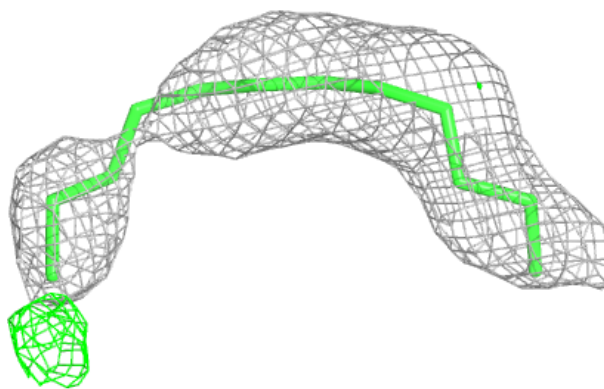
**Electron density around D9G C 301:**

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

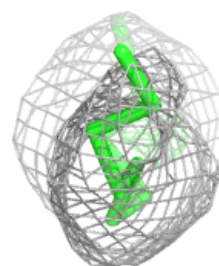
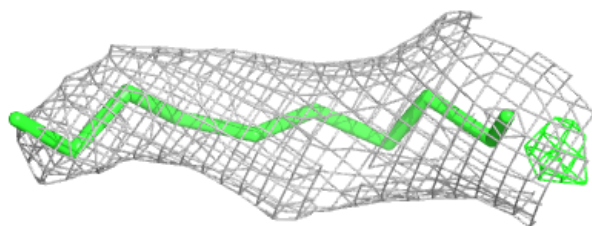
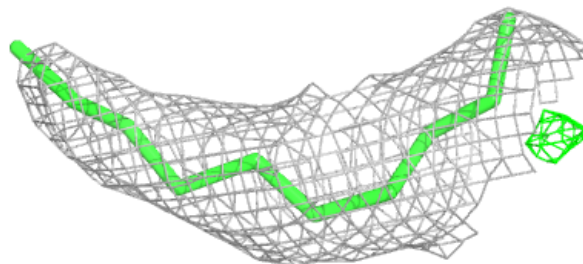


Electron density around D9G A 303:

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

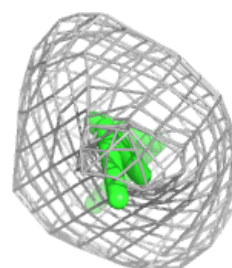
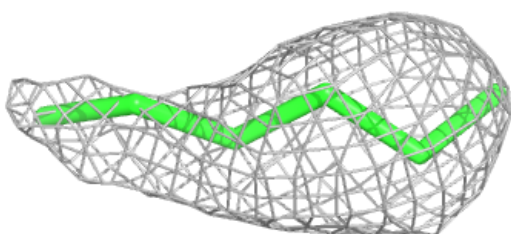
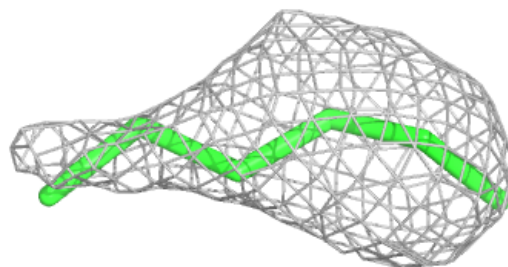
**Electron density around D9G C 305:**

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

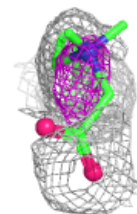
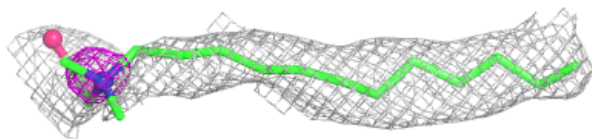
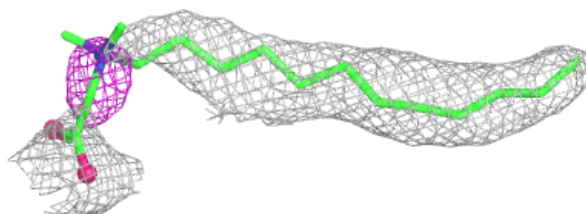


Electron density around D9G A 306:

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

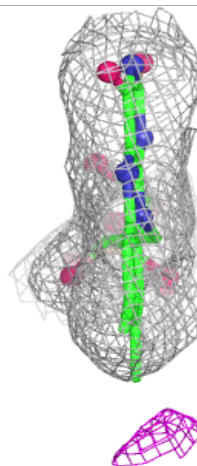
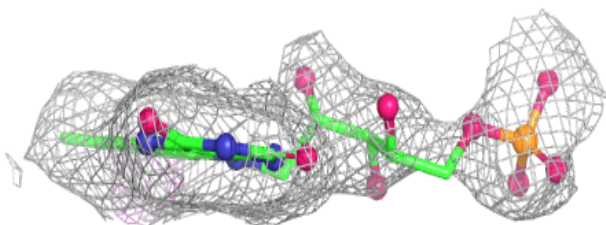
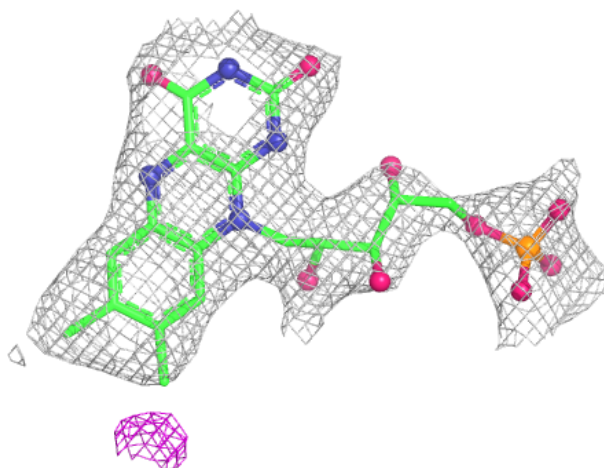
**Electron density around D9G A 302:**

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



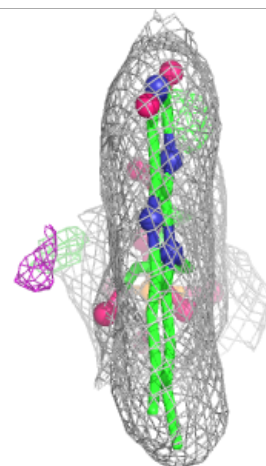
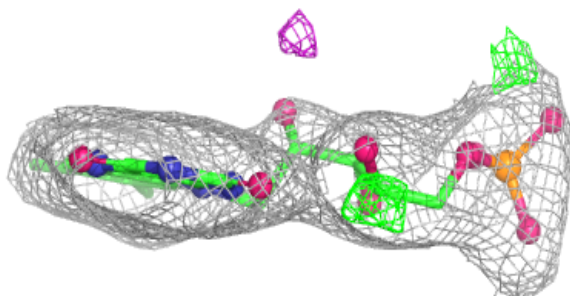
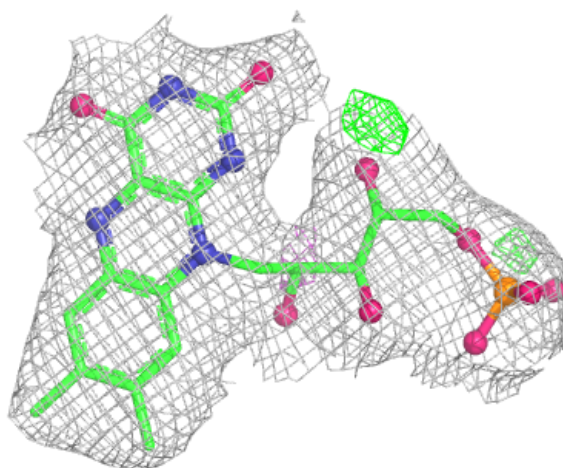
Electron density around FMN B 202:

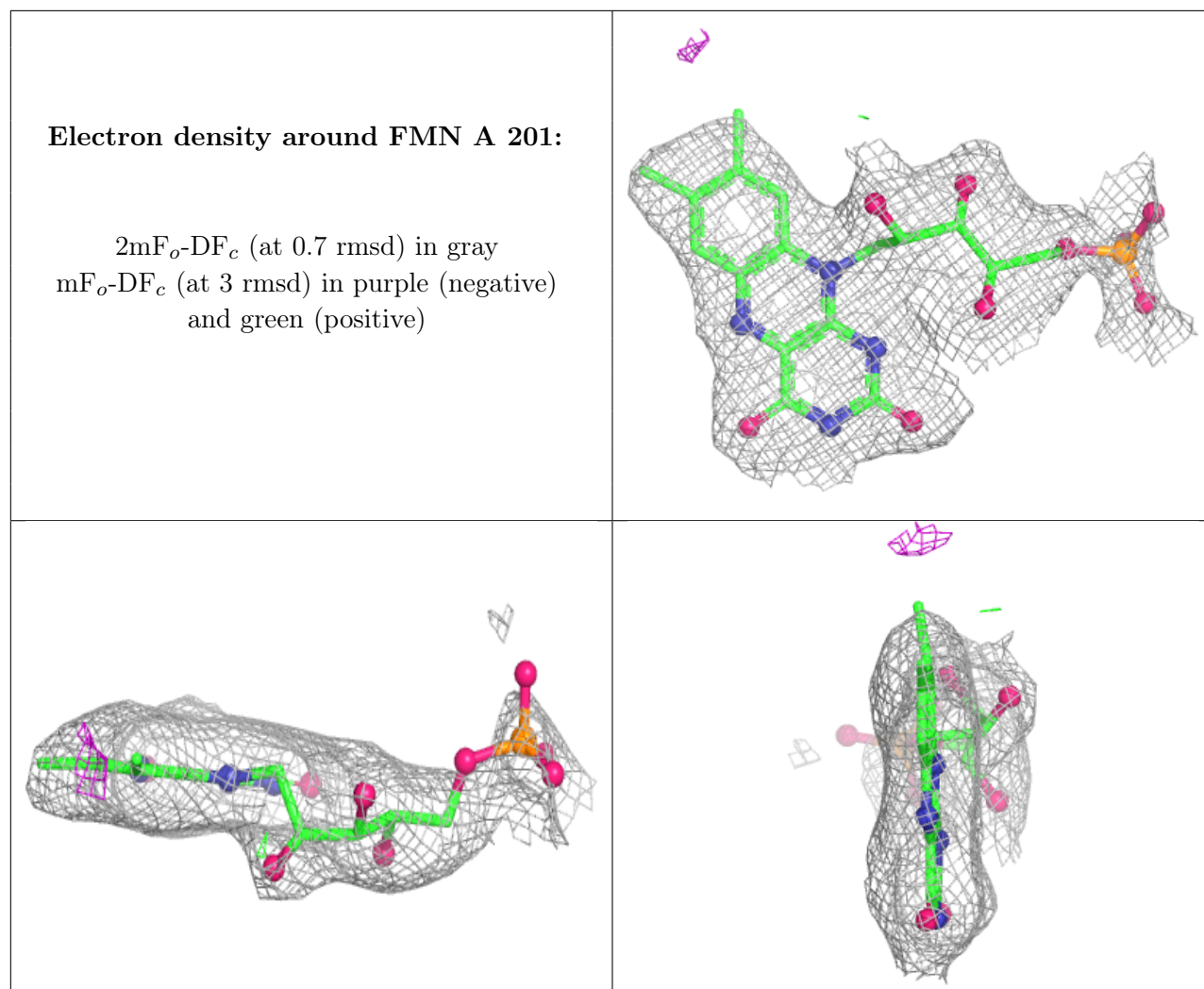
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN C 203:

$2mF_o-DF_c$ (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.