



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 PM UTC

PDB ID : 6VTY / pdb_00006vty
Title : Crystal structure of Plasmodium falciparum dihydroorotate dehydrogenase bound with Inhibitor DSM483
Authors : Deng, X.; Phillips, M.
Deposited on : 2020-02-13
Resolution : 1.78 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

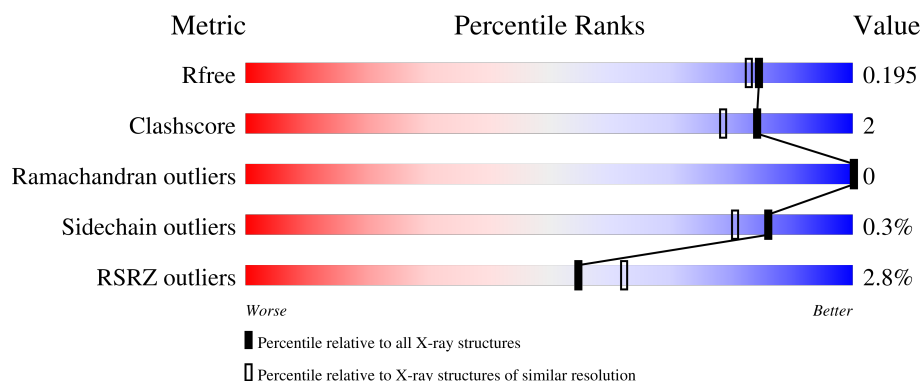
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	431	2% 84% • 13%
1	B	431	2% 79% 7% 14%
1	C	431	3% 81% • 15%
1	D	431	3% 80% 5% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25167 atoms, of which 12193 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 Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	377	Total	C	H	N	O	S	0	1	0
			6025	1916	3031	501	563	14			
1	B	372	Total	C	H	N	O	S	0	2	0
			5972	1894	3012	498	553	15			
1	C	366	Total	C	H	N	O	S	0	7	0
			5947	1880	3012	494	546	15			
1	D	368	Total	C	H	N	O	S	0	3	0
			5914	1875	2986	491	547	15			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	initiating methionine	UNP Q08210
A	140	GLY	-	expression tag	UNP Q08210
A	141	HIS	-	expression tag	UNP Q08210
A	142	HIS	-	expression tag	UNP Q08210
A	143	HIS	-	expression tag	UNP Q08210
A	144	HIS	-	expression tag	UNP Q08210
A	145	HIS	-	expression tag	UNP Q08210
A	146	HIS	-	expression tag	UNP Q08210
A	147	ALA	-	expression tag	UNP Q08210
A	148	GLU	-	expression tag	UNP Q08210
A	149	ASN	-	expression tag	UNP Q08210
A	150	LEU	-	expression tag	UNP Q08210
A	151	TYR	-	expression tag	UNP Q08210
A	152	PHE	-	expression tag	UNP Q08210
A	153	GLN	-	expression tag	UNP Q08210
A	154	GLY	-	expression tag	UNP Q08210
A	155	ALA	-	expression tag	UNP Q08210
A	156	ASP	-	expression tag	UNP Q08210
A	157	PRO	-	expression tag	UNP Q08210
B	139	MET	-	initiating methionine	UNP Q08210
B	140	GLY	-	expression tag	UNP Q08210

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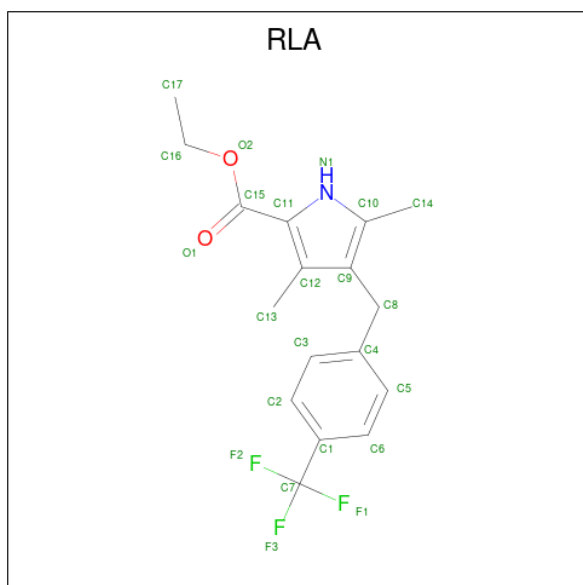
Chain	Residue	Modelled	Actual	Comment	Reference
B	141	HIS	-	expression tag	UNP Q08210
B	142	HIS	-	expression tag	UNP Q08210
B	143	HIS	-	expression tag	UNP Q08210
B	144	HIS	-	expression tag	UNP Q08210
B	145	HIS	-	expression tag	UNP Q08210
B	146	HIS	-	expression tag	UNP Q08210
B	147	ALA	-	expression tag	UNP Q08210
B	148	GLU	-	expression tag	UNP Q08210
B	149	ASN	-	expression tag	UNP Q08210
B	150	LEU	-	expression tag	UNP Q08210
B	151	TYR	-	expression tag	UNP Q08210
B	152	PHE	-	expression tag	UNP Q08210
B	153	GLN	-	expression tag	UNP Q08210
B	154	GLY	-	expression tag	UNP Q08210
B	155	ALA	-	expression tag	UNP Q08210
B	156	ASP	-	expression tag	UNP Q08210
B	157	PRO	-	expression tag	UNP Q08210
C	139	MET	-	initiating methionine	UNP Q08210
C	140	GLY	-	expression tag	UNP Q08210
C	141	HIS	-	expression tag	UNP Q08210
C	142	HIS	-	expression tag	UNP Q08210
C	143	HIS	-	expression tag	UNP Q08210
C	144	HIS	-	expression tag	UNP Q08210
C	145	HIS	-	expression tag	UNP Q08210
C	146	HIS	-	expression tag	UNP Q08210
C	147	ALA	-	expression tag	UNP Q08210
C	148	GLU	-	expression tag	UNP Q08210
C	149	ASN	-	expression tag	UNP Q08210
C	150	LEU	-	expression tag	UNP Q08210
C	151	TYR	-	expression tag	UNP Q08210
C	152	PHE	-	expression tag	UNP Q08210
C	153	GLN	-	expression tag	UNP Q08210
C	154	GLY	-	expression tag	UNP Q08210
C	155	ALA	-	expression tag	UNP Q08210
C	156	ASP	-	expression tag	UNP Q08210
C	157	PRO	-	expression tag	UNP Q08210
D	139	MET	-	initiating methionine	UNP Q08210
D	140	GLY	-	expression tag	UNP Q08210
D	141	HIS	-	expression tag	UNP Q08210
D	142	HIS	-	expression tag	UNP Q08210
D	143	HIS	-	expression tag	UNP Q08210
D	144	HIS	-	expression tag	UNP Q08210

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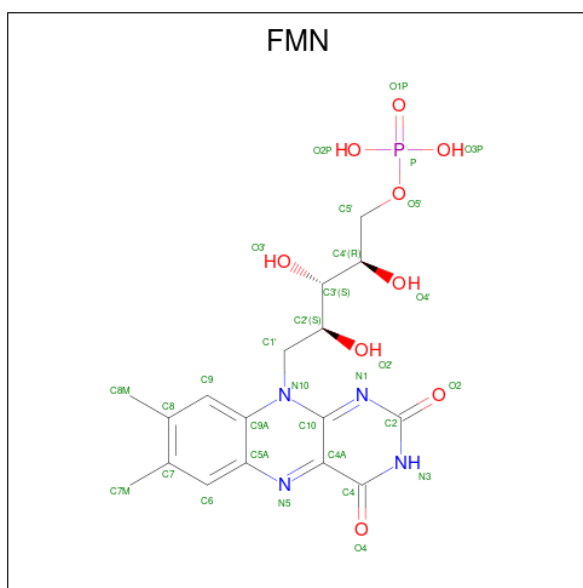
Chain	Residue	Modelled	Actual	Comment	Reference
D	145	HIS	-	expression tag	UNP Q08210
D	146	HIS	-	expression tag	UNP Q08210
D	147	ALA	-	expression tag	UNP Q08210
D	148	GLU	-	expression tag	UNP Q08210
D	149	ASN	-	expression tag	UNP Q08210
D	150	LEU	-	expression tag	UNP Q08210
D	151	TYR	-	expression tag	UNP Q08210
D	152	PHE	-	expression tag	UNP Q08210
D	153	GLN	-	expression tag	UNP Q08210
D	154	GLY	-	expression tag	UNP Q08210
D	155	ALA	-	expression tag	UNP Q08210
D	156	ASP	-	expression tag	UNP Q08210
D	157	PRO	-	expression tag	UNP Q08210

- Molecule 2 is ethyl 3,5-dimethyl-4-{[4-(trifluoromethyl)phenyl]methyl}-1H-pyrrole-2-carboxylate (CCD ID: RLA) (formula: $C_{17}H_{18}F_3NO_2$) (labeled as "Ligand of Interest" by depositor).



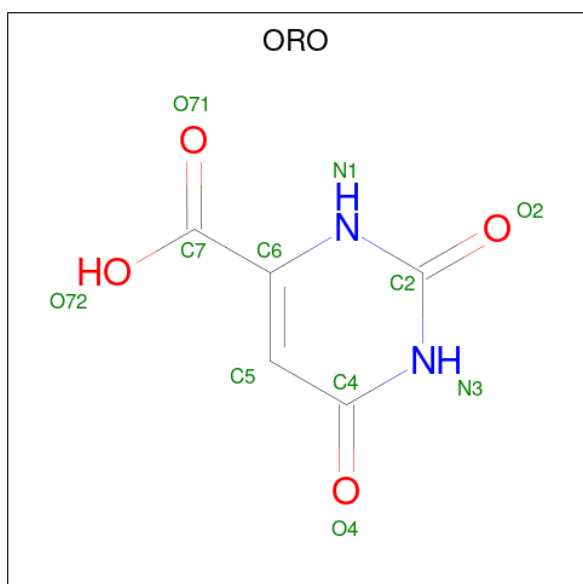
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			40	17	3	17	1	2		
2	B	1	Total	C	F	H	N	O	0	0
			40	17	3	17	1	2		
2	C	1	Total	C	F	H	N	O	0	0
			40	17	3	17	1	2		
2	D	1	Total	C	F	H	N	O	0	0
			40	17	3	17	1	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total 49	C 17	H 18	N 4	O 9	P 1	0	0
3	B	1	Total 49	C 17	H 18	N 4	O 9	P 1	0	0
3	C	1	Total 49	C 17	H 18	N 4	O 9	P 1	0	0
3	D	1	Total 49	C 17	H 18	N 4	O 9	P 1	0	0

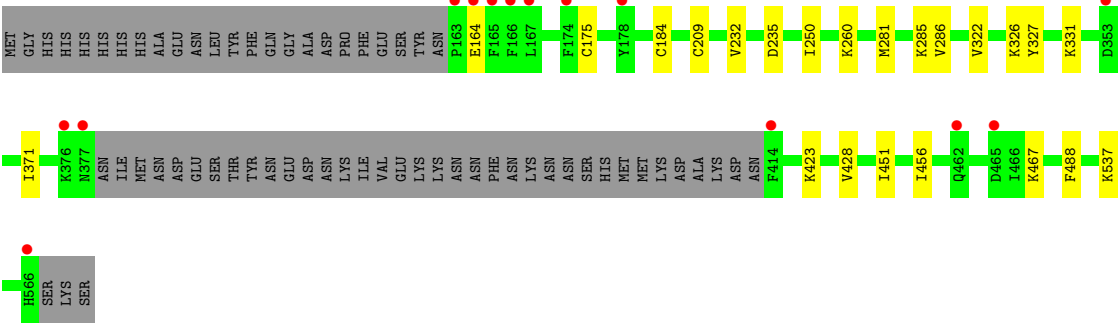
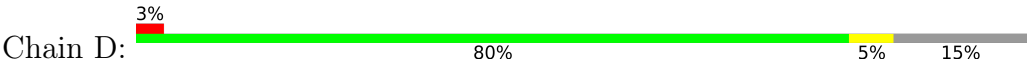
- Molecule 4 is OROTIC ACID (CCD ID: ORO) (formula: $C_5H_4N_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			14	5	3	2	4		
4	B	1	Total	C	H	N	O	0	0
			14	5	3	2	4		
4	C	1	Total	C	H	N	O	0	0
			14	5	3	2	4		
4	D	1	Total	C	H	N	O	0	0
			14	5	3	2	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	283	Total	O	0	0
			283	283		
5	B	196	Total	O	0	0
			196	196		
5	C	253	Total	O	0	0
			253	253		
5	D	165	Total	O	0	0
			165	165		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.09Å 97.52Å 186.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.03 – 1.78 42.03 – 1.78	Depositor EDS
% Data completeness (in resolution range)	92.2 (42.03-1.78) 92.6 (42.03-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.77Å)	Xtriage
Refinement program	PHENIX V1.16	Depositor
R, R_{free}	0.151 , 0.194 0.152 , 0.195	Depositor DCC
R_{free} test set	2002 reflections (1.24%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 48.8	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	0.97	EDS
Total number of atoms	25167	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.82% 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: ORO, RLA, 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	0.88	2/3049 (0.1%)	0.88	1/4106 (0.0%)
1	B	0.86	6/3016 (0.2%)	0.83	1/4059 (0.0%)
1	C	0.93	7/3003 (0.2%)	0.92	1/4039 (0.0%)
1	D	0.76	1/2986 (0.0%)	0.82	0/4018
All	All	0.86	16/12054 (0.1%)	0.86	3/16222 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	CYS	CB-SG	-7.49	1.56	1.81
1	C	236	SER	C-O	-6.21	1.16	1.24
1	B	515	LEU	C-O	-5.88	1.17	1.24
1	B	517	LYS	C-O	-5.66	1.17	1.24
1	B	518	ILE	C-O	-5.64	1.17	1.24
1	D	232	VAL	C-O	-5.63	1.17	1.24
1	C	473	LYS	C-O	-5.59	1.16	1.23
1	C	468	SER	C-O	-5.55	1.16	1.24
1	C	237	ILE	C-O	-5.51	1.18	1.24
1	B	467	LYS	C-O	-5.45	1.17	1.24
1	A	234	ILE	N-CA	-5.37	1.40	1.46
1	A	560	GLU	CB-CG	-5.21	1.36	1.52
1	C	471	ASN	CA-CB	5.16	1.61	1.53
1	C	234	ILE	C-O	-5.14	1.18	1.24
1	C	235	ASP	C-O	-5.07	1.18	1.24
1	B	483	ASP	C-O	-5.05	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	474	GLY	N-CA-C	5.60	118.85	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	SER	CA-CB-OG	-5.46	100.17	111.10
1	B	482	LYS	N-CA-C	5.27	116.71	111.07

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	2994	3031	3031	10	0
1	B	2960	3012	3012	19	0
1	C	2935	3012	3014	11	0
1	D	2928	2986	2986	16	0
2	A	23	17	0	0	0
2	B	23	17	0	0	0
2	C	23	17	0	0	0
2	D	23	17	0	0	0
3	A	31	18	19	1	0
3	B	31	18	19	1	0
3	C	31	18	19	1	0
3	D	31	18	19	0	0
4	A	11	3	3	0	0
4	B	11	3	3	0	0
4	C	11	3	3	0	0
4	D	11	3	3	0	0
5	A	283	0	0	3	0
5	B	196	0	0	3	0
5	C	253	0	0	2	0
5	D	165	0	0	3	0
All	All	12974	12193	12131	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:D:428:VAL:HG23	1:D:451:ILE:CD1	2.01	0.88
1:C:281:MET:HE3	1:C:285:LYS:CG	2.08	0.82
1:C:281:MET:HE3	1:C:285:LYS:HG3	1.62	0.81
1:D:428:VAL:HG23	1:D:451:ILE:HD11	1.61	0.80
1:C:281:MET:HE3	1:C:285:LYS:HG2	1.81	0.61
1:D:281:MET:HE3	1:D:285:LYS:HG2	1.83	0.60
1:B:253:ARG:NH2	5:B:1102:HOH:O	2.35	0.60
1:A:306:HIS:HD2	5:A:1106:HOH:O	1.85	0.59
1:C:281:MET:CE	1:C:285:LYS:HG3	2.33	0.59
1:A:306:HIS:HE1	5:A:1287:HOH:O	1.86	0.58
1:B:264:PHE:CD1	1:B:472:LYS:HE2	2.39	0.57
1:C:331:LYS:HG2	5:C:1227:HOH:O	2.06	0.55
1:D:175:CYS:HB3	1:D:184:CYS:SG	2.46	0.55
1:B:558:LEU:C	1:B:558:LEU:HD23	2.32	0.55
1:B:175:CYS:HB3	1:B:184:CYS:SG	2.47	0.54
1:C:558:LEU:C	1:C:558:LEU:HD23	2.33	0.54
1:D:456:ILE:HG23	1:D:488:PHE:CD2	2.44	0.52
1:B:226:GLY:HA3	3:B:1002:FMN:N5	2.24	0.52
1:D:209[B]:CYS:SG	5:D:1173:HOH:O	2.59	0.50
1:C:331:LYS:HD2	5:C:1293:HOH:O	2.12	0.49
1:D:260:LYS:NZ	5:D:1107:HOH:O	2.45	0.49
1:A:226:GLY:HA3	3:A:1002:FMN:N5	2.28	0.48
1:C:503:ILE:HD12	1:C:503:ILE:N	2.28	0.47
1:D:331:LYS:HG2	5:D:1166:HOH:O	2.13	0.47
1:B:264:PHE:CE1	1:B:472:LYS:HE2	2.50	0.47
1:C:169:ASP:O	1:C:173:LYS:HG2	2.16	0.46
1:B:196:ILE:O	1:B:196:ILE:HG22	2.15	0.46
1:D:250:ILE:HG21	1:D:286:VAL:HG11	1.98	0.45
1:B:503:ILE:HD12	1:B:503:ILE:N	2.31	0.45
1:B:214:HIS:HE1	5:B:1206:HOH:O	1.99	0.45
1:C:460:THR:OG1	1:C:462:GLN:HG2	2.17	0.44
1:B:437:GLU:H	1:B:437:GLU:CD	2.25	0.43
1:D:322:VAL:HG12	1:D:326:LYS:HD2	2.00	0.43
1:A:230:ASN:HB3	1:A:281:MET:HE2	2.00	0.43
1:D:322:VAL:CG1	1:D:326:LYS:HD2	2.48	0.43
1:B:482:LYS:NZ	1:B:516:GLU:OE1	2.50	0.43
1:B:281:MET:HE3	1:B:285:LYS:HB3	2.00	0.42
1:D:281:MET:HE3	1:D:285:LYS:CG	2.48	0.42
1:B:266:ASP:OD2	1:B:269:SER:OG	2.36	0.42
1:A:214:HIS:HE1	5:A:1228:HOH:O	2.02	0.42
1:A:169:ASP:O	1:A:173:LYS:HD3	2.20	0.42
1:B:222:GLY:HA3	1:B:244:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLY:HA3	3:C:1002:FMN:N5	2.34	0.42
1:B:264:PHE:CE2	1:B:472:LYS:HD2	2.55	0.41
1:D:467:LYS:HB2	1:D:467:LYS:HE3	1.87	0.41
1:B:274:ASN:O	1:B:474:GLY:HA3	2.20	0.41
1:D:371:ILE:HG22	1:D:423:LYS:HD2	2.02	0.41
1:A:558:LEU:C	1:A:558:LEU:HD23	2.46	0.41
1:A:373:ASN:HA	1:A:376:LYS:HD3	2.02	0.41
1:D:164:GLU:HG2	1:D:537:LYS:HB2	2.02	0.41
1:D:327:TYR:CE1	1:D:331:LYS:HG3	2.56	0.41
1:A:467:LYS:HZ1	1:B:487:LYS:NZ	2.19	0.41
1:B:229:LYS:NZ	5:B:1111:HOH:O	2.53	0.41
1:A:175:CYS:HB3	1:A:184:CYS:SG	2.61	0.40
1:B:460:THR:OG1	1:B:462:GLN:HG2	2.21	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	374/431 (87%)	368 (98%)	6 (2%)	0	100	100
1	B	370/431 (86%)	361 (98%)	9 (2%)	0	100	100
1	C	369/431 (86%)	361 (98%)	8 (2%)	0	100	100
1	D	367/431 (85%)	360 (98%)	7 (2%)	0	100	100
All	All	1480/1724 (86%)	1450 (98%)	30 (2%)	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	334/383 (87%)	334 (100%)	0	100	100
1	B	331/383 (86%)	329 (99%)	2 (1%)	78	70
1	C	330/383 (86%)	329 (100%)	1 (0%)	86	80
1	D	328/383 (86%)	327 (100%)	1 (0%)	86	80
All	All	1323/1532 (86%)	1319 (100%)	4 (0%)	86	80

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

Mol	Chain	Res	Type
1	B	468	SER
1	B	471	ASN
1	C	235	ASP
1	D	235	ASP

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	306	HIS
1	A	548	HIS
1	B	464	ASN
1	B	494	ASN
1	B	497	ASN
1	C	494	ASN
1	D	195	ASN
1	D	354	ASN
1	D	462	GLN
1	D	464	ASN
1	D	494	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](#)

12 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	RLA	C	1001	-	24,24,24	1.94	7 (29%)	35,35,35	2.60	16 (45%)
3	FMN	C	1002	-	33,33,33	1.20	2 (6%)	48,50,50	1.30	7 (14%)
4	ORO	A	1003	-	11,11,11	1.71	2 (18%)	14,15,15	2.26	6 (42%)
3	FMN	A	1002	-	33,33,33	1.25	5 (15%)	48,50,50	1.22	5 (10%)
3	FMN	D	1002	-	33,33,33	1.10	1 (3%)	48,50,50	1.48	8 (16%)
4	ORO	B	1003	-	11,11,11	1.27	2 (18%)	14,15,15	2.48	6 (42%)
3	FMN	B	1002	-	33,33,33	1.58	7 (21%)	48,50,50	1.27	7 (14%)
4	ORO	C	1003	-	11,11,11	1.14	1 (9%)	14,15,15	1.74	5 (35%)
4	ORO	D	1003	-	11,11,11	1.33	3 (27%)	14,15,15	2.78	6 (42%)
2	RLA	D	1001	-	24,24,24	1.50	3 (12%)	35,35,35	1.97	11 (31%)
2	RLA	B	1001	-	24,24,24	1.83	5 (20%)	35,35,35	1.84	11 (31%)
2	RLA	A	1001	-	24,24,24	1.89	6 (25%)	35,35,35	2.11	16 (45%)

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	RLA	C	1001	-	-	2/17/17/17	0/2/2/2
3	FMN	C	1002	-	-	1/18/18/18	0/3/3/3
4	ORO	A	1003	-	-	2/4/4/4	0/1/1/1
3	FMN	A	1002	-	-	1/18/18/18	0/3/3/3
3	FMN	D	1002	-	-	1/18/18/18	0/3/3/3
4	ORO	B	1003	-	-	4/4/4/4	0/1/1/1
3	FMN	B	1002	-	-	1/18/18/18	0/3/3/3
4	ORO	C	1003	-	-	3/4/4/4	0/1/1/1
4	ORO	D	1003	-	-	2/4/4/4	0/1/1/1
2	RLA	D	1001	-	-	3/17/17/17	0/2/2/2
2	RLA	B	1001	-	-	1/17/17/17	0/2/2/2
2	RLA	A	1001	-	-	2/17/17/17	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	RLA	O2-C15	6.28	1.45	1.33
2	A	1001	RLA	O2-C15	5.88	1.44	1.33
2	C	1001	RLA	O2-C15	5.75	1.44	1.33
2	D	1001	RLA	O2-C15	4.85	1.42	1.33
3	C	1002	FMN	C4A-N5	4.27	1.40	1.30
3	B	1002	FMN	C4A-N5	4.27	1.40	1.30
3	D	1002	FMN	C4A-N5	3.75	1.38	1.30
4	A	1003	ORO	O71-C7	3.67	1.31	1.22
2	C	1001	RLA	C11-C15	3.49	1.54	1.46
2	D	1001	RLA	C11-C15	3.44	1.54	1.46
2	A	1001	RLA	C11-C15	3.42	1.54	1.46
3	A	1002	FMN	C4A-N5	3.26	1.37	1.30
3	B	1002	FMN	C5'-C4'	2.95	1.55	1.51
2	B	1001	RLA	C9-C12	2.76	1.46	1.38
2	A	1001	RLA	C8-C4	2.74	1.56	1.51
3	B	1002	FMN	C9-C8	2.70	1.43	1.39
2	B	1001	RLA	C11-C15	2.68	1.52	1.46
2	A	1001	RLA	C6-C5	2.64	1.43	1.38
2	C	1001	RLA	C8-C4	2.56	1.55	1.51
3	A	1002	FMN	C4A-C10	-2.54	1.36	1.44
3	A	1002	FMN	C4A-C4	-2.49	1.35	1.44
2	A	1001	RLA	C7-C1	2.49	1.54	1.49
3	B	1002	FMN	P-O5'	2.44	1.68	1.60
3	C	1002	FMN	C5'-C4'	2.32	1.55	1.51
4	A	1003	ORO	O4-C4	-2.32	1.20	1.24
2	A	1001	RLA	C6-C1	2.29	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	FMN	C1'-C2'	-2.28	1.49	1.52
4	D	1003	ORO	O71-C7	2.25	1.28	1.22
2	B	1001	RLA	C6-C1	2.25	1.43	1.39
3	A	1002	FMN	C9A-N10	-2.23	1.37	1.41
2	C	1001	RLA	C6-C1	2.22	1.43	1.39
2	C	1001	RLA	C9-C12	2.16	1.44	1.38
4	B	1003	ORO	O72-C7	-2.15	1.24	1.30
4	C	1003	ORO	O71-C7	2.13	1.27	1.22
2	C	1001	RLA	C8-C9	-2.13	1.48	1.51
4	D	1003	ORO	O4-C4	-2.10	1.20	1.24
3	B	1002	FMN	C4A-C4	-2.10	1.36	1.44
3	B	1002	FMN	C7M-C7	2.09	1.54	1.51
2	D	1001	RLA	C9-C12	2.06	1.44	1.38
4	D	1003	ORO	C5-C4	-2.03	1.38	1.42
2	B	1001	RLA	C10-C9	2.03	1.42	1.38
4	B	1003	ORO	C6-N1	-2.01	1.34	1.38
2	C	1001	RLA	C7-C1	2.01	1.53	1.49
3	A	1002	FMN	C6-C5A	-2.00	1.36	1.40

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	ORO	C4-N3-C2	-6.56	119.19	125.55
2	C	1001	RLA	C5-C4-C3	5.27	126.07	118.23
4	D	1003	ORO	O72-C7-C6	4.96	124.97	114.27
2	C	1001	RLA	C12-C11-N1	4.84	113.23	107.70
4	A	1003	ORO	C6-N1-C2	-4.76	117.56	122.65
2	C	1001	RLA	C11-N1-C10	-4.74	106.52	110.46
2	C	1001	RLA	C8-C4-C3	-4.62	114.09	120.89
4	D	1003	ORO	C4-N3-C2	-4.62	121.07	125.55
2	A	1001	RLA	O2-C15-C11	-4.61	105.78	112.39
2	D	1001	RLA	C11-N1-C10	-4.47	106.74	110.46
3	D	1002	FMN	C5A-C9A-N10	4.39	121.94	117.97
4	D	1003	ORO	O4-C4-C5	-4.36	119.44	125.46
4	D	1003	ORO	O71-C7-C6	-4.10	112.69	121.01
2	C	1001	RLA	C2-C3-C4	-4.10	115.61	121.00
2	A	1001	RLA	C16-O2-C15	-3.92	109.71	116.49
2	C	1001	RLA	C6-C1-C2	3.87	123.80	118.03
2	C	1001	RLA	C11-C12-C9	-3.80	103.10	107.24
2	D	1001	RLA	C12-C11-N1	3.75	111.99	107.70
2	B	1001	RLA	C11-C12-C9	-3.74	103.16	107.24
2	B	1001	RLA	C12-C11-N1	3.73	111.97	107.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	RLA	C6-C5-C4	-3.68	116.16	121.00
2	A	1001	RLA	C11-C12-C9	-3.64	103.28	107.24
4	D	1003	ORO	C5-C4-N3	3.56	119.67	115.24
3	B	1002	FMN	C5A-C9A-N10	3.51	121.14	117.97
2	D	1001	RLA	C9-C10-N1	3.47	110.59	108.13
2	D	1001	RLA	C11-C12-C9	-3.44	103.50	107.24
4	B	1003	ORO	C5-C4-N3	3.40	119.46	115.24
2	D	1001	RLA	C14-C10-C9	-3.38	125.49	131.20
2	C	1001	RLA	O2-C15-O1	3.36	129.40	123.37
3	D	1002	FMN	C9A-C5A-N5	-3.35	118.90	122.45
2	B	1001	RLA	C16-O2-C15	-3.30	110.79	116.49
4	A	1003	ORO	O2-C2-N1	-3.28	116.04	121.86
3	B	1002	FMN	O3P-P-O2P	3.24	119.97	107.80
4	B	1003	ORO	O4-C4-C5	-3.21	121.03	125.46
2	D	1001	RLA	C15-C11-C12	-3.20	125.98	133.06
3	C	1002	FMN	C5'-C4'-C3'	-3.20	106.19	112.22
3	B	1002	FMN	C4A-C10-N10	3.19	121.04	116.48
4	A	1003	ORO	N3-C2-N1	3.09	120.59	115.74
4	C	1003	ORO	C6-N1-C2	-3.07	119.37	122.65
2	A	1001	RLA	C8-C4-C3	-2.98	116.50	120.89
2	A	1001	RLA	C11-N1-C10	-2.94	108.01	110.46
3	D	1002	FMN	C5'-C4'-C3'	-2.93	106.70	112.22
4	B	1003	ORO	N3-C2-N1	2.91	120.31	115.74
2	A	1001	RLA	C14-C10-C9	-2.91	126.30	131.20
2	B	1001	RLA	C5-C4-C3	2.86	122.49	118.23
2	B	1001	RLA	F2-C7-C1	-2.86	106.78	112.90
3	A	1002	FMN	O3P-P-O2P	2.85	118.49	107.80
2	B	1001	RLA	C15-C11-C12	-2.83	126.79	133.06
2	C	1001	RLA	O2-C15-C11	-2.82	108.35	112.39
4	C	1003	ORO	C5-C6-N1	2.81	124.17	120.87
2	C	1001	RLA	C9-C10-N1	2.81	110.12	108.13
2	A	1001	RLA	C5-C6-C1	-2.79	117.32	121.17
2	D	1001	RLA	C13-C12-C11	2.78	131.28	127.33
2	A	1001	RLA	O1-C15-C11	2.78	129.21	123.89
2	C	1001	RLA	C15-C11-C12	-2.73	127.03	133.06
3	A	1002	FMN	C4A-C4-N3	2.66	120.02	113.25
2	A	1001	RLA	C12-C11-N1	2.65	110.72	107.70
2	A	1001	RLA	C5-C4-C3	2.64	122.15	118.23
3	D	1002	FMN	C4A-C10-N10	2.61	120.22	116.48
3	A	1002	FMN	O4-C4-N3	-2.59	115.25	120.11
2	A	1001	RLA	C9-C10-N1	2.58	109.96	108.13
2	A	1001	RLA	C15-C11-C12	-2.56	127.39	133.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	ORO	C5-C6-N1	2.55	123.86	120.87
4	C	1003	ORO	O72-C7-O71	-2.54	117.84	123.90
2	D	1001	RLA	C5-C4-C3	2.50	121.96	118.23
3	D	1002	FMN	C9-C9A-N10	-2.49	118.51	121.85
2	D	1001	RLA	C8-C4-C3	-2.48	117.24	120.89
4	A	1003	ORO	O72-C7-O71	-2.48	118.00	123.90
2	A	1001	RLA	C6-C1-C2	2.47	121.72	118.03
3	A	1002	FMN	C4-N3-C2	-2.45	121.28	125.64
2	B	1001	RLA	F1-C7-C1	-2.45	107.65	112.90
4	B	1003	ORO	C7-C6-N1	2.45	119.94	115.47
2	C	1001	RLA	F2-C7-C1	-2.44	107.67	112.90
2	C	1001	RLA	C16-O2-C15	-2.44	112.28	116.49
2	B	1001	RLA	C2-C3-C4	-2.43	117.80	121.00
2	D	1001	RLA	F2-C7-C1	-2.42	107.72	112.90
2	B	1001	RLA	F2-C7-F1	2.39	114.39	105.77
2	B	1001	RLA	C8-C4-C3	-2.37	117.40	120.89
2	C	1001	RLA	C13-C12-C11	2.35	130.67	127.33
3	C	1002	FMN	C4A-C10-N10	2.33	119.82	116.48
2	A	1001	RLA	F2-C7-C1	-2.32	107.92	112.90
3	B	1002	FMN	C9-C9A-N10	-2.30	118.76	121.85
2	A	1001	RLA	C8-C9-C12	-2.26	123.34	126.60
3	C	1002	FMN	O3P-P-O1P	2.23	119.52	110.83
4	A	1003	ORO	C4-N3-C2	-2.21	123.40	125.55
3	C	1002	FMN	C6-C5A-C9A	-2.20	116.03	119.05
2	A	1001	RLA	F1-C7-C1	-2.18	108.23	112.90
3	D	1002	FMN	C4A-C4-N3	2.18	118.79	113.25
3	C	1002	FMN	C6-C5A-N5	2.17	122.05	118.44
4	D	1003	ORO	C6-N1-C2	-2.16	120.33	122.65
2	C	1001	RLA	C10-C9-C12	-2.15	106.67	107.61
3	B	1002	FMN	O2-C2-N3	2.13	122.67	118.58
2	B	1001	RLA	C11-N1-C10	-2.13	108.69	110.46
3	D	1002	FMN	C9A-N10-C10	-2.12	117.52	120.75
4	C	1003	ORO	O71-C7-C6	2.11	125.30	121.01
3	C	1002	FMN	O4'-C4'-C3'	2.11	114.18	109.25
2	D	1001	RLA	O2-C15-O1	2.07	127.09	123.37
3	B	1002	FMN	C9A-N10-C10	-2.04	117.65	120.75
3	D	1002	FMN	C4-N3-C2	-2.04	122.03	125.64
4	B	1003	ORO	O2-C2-N1	-2.03	118.25	121.86
4	C	1003	ORO	C5-C4-N3	2.03	117.76	115.24
3	C	1002	FMN	C9A-C9-C8	2.03	123.29	119.22
3	B	1002	FMN	O3'-C3'-C4'	2.02	113.52	108.93
3	A	1002	FMN	C5A-C6-C7	2.00	124.54	120.83

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	ORO	N1-C6-C7-O72
4	A	1003	ORO	C5-C6-C7-O72
4	B	1003	ORO	N1-C6-C7-O71
4	B	1003	ORO	N1-C6-C7-O72
4	C	1003	ORO	N1-C6-C7-O72
4	C	1003	ORO	C5-C6-C7-O72
4	D	1003	ORO	N1-C6-C7-O71
4	B	1003	ORO	C5-C6-C7-O72
3	A	1002	FMN	C4'-C5'-O5'-P
3	C	1002	FMN	C4'-C5'-O5'-P
3	D	1002	FMN	C4'-C5'-O5'-P
4	B	1003	ORO	C5-C6-C7-O71
3	B	1002	FMN	C4'-C5'-O5'-P
2	D	1001	RLA	C11-C15-O2-C16
4	C	1003	ORO	C5-C6-C7-O71
2	A	1001	RLA	C3-C4-C8-C9
2	C	1001	RLA	C3-C4-C8-C9
4	D	1003	ORO	N1-C6-C7-O72
2	B	1001	RLA	C5-C4-C8-C9
2	C	1001	RLA	C5-C4-C8-C9
2	D	1001	RLA	C3-C4-C8-C9
2	D	1001	RLA	C5-C4-C8-C9
2	A	1001	RLA	C5-C4-C8-C9

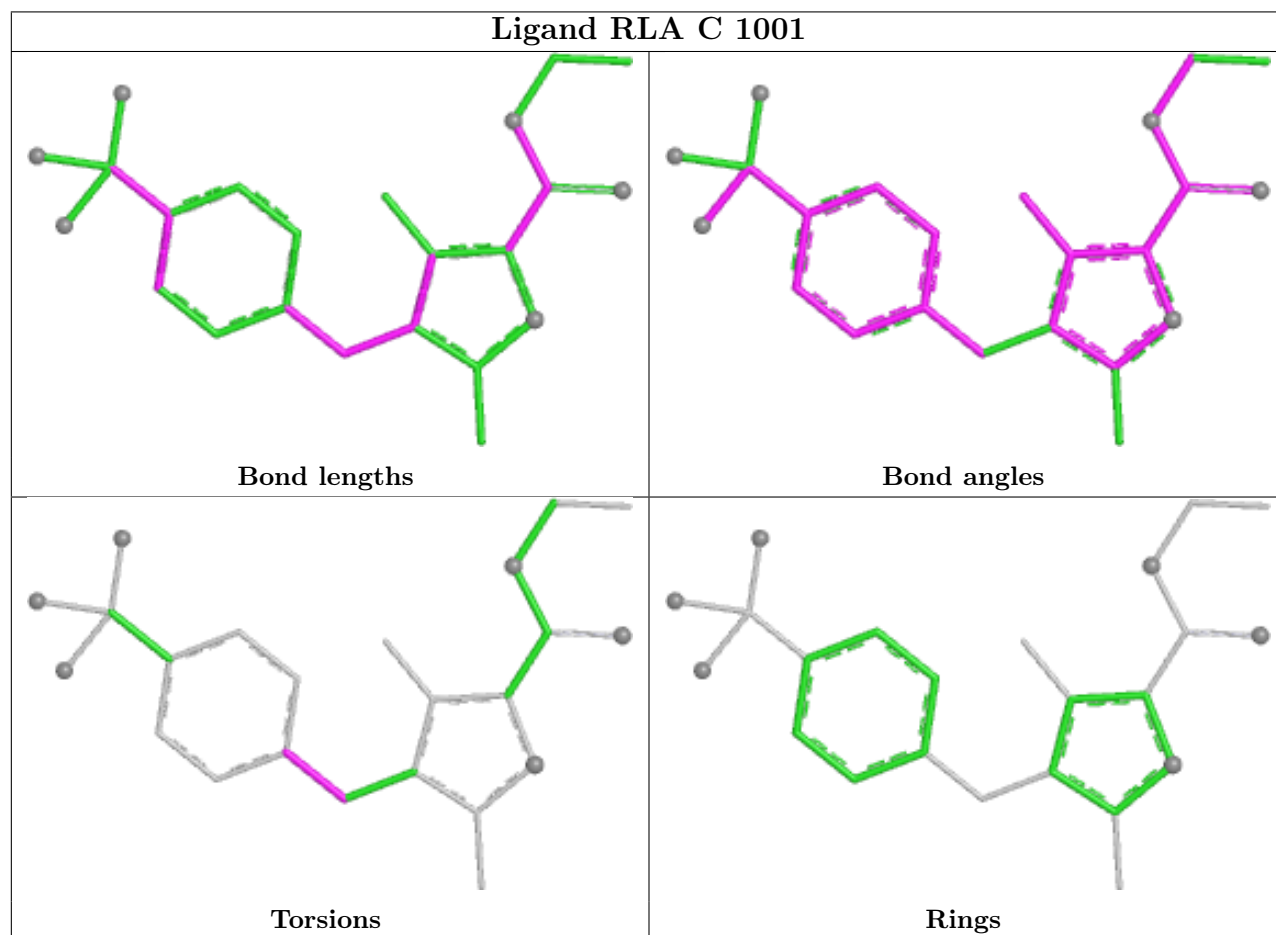
There are no ring outliers.

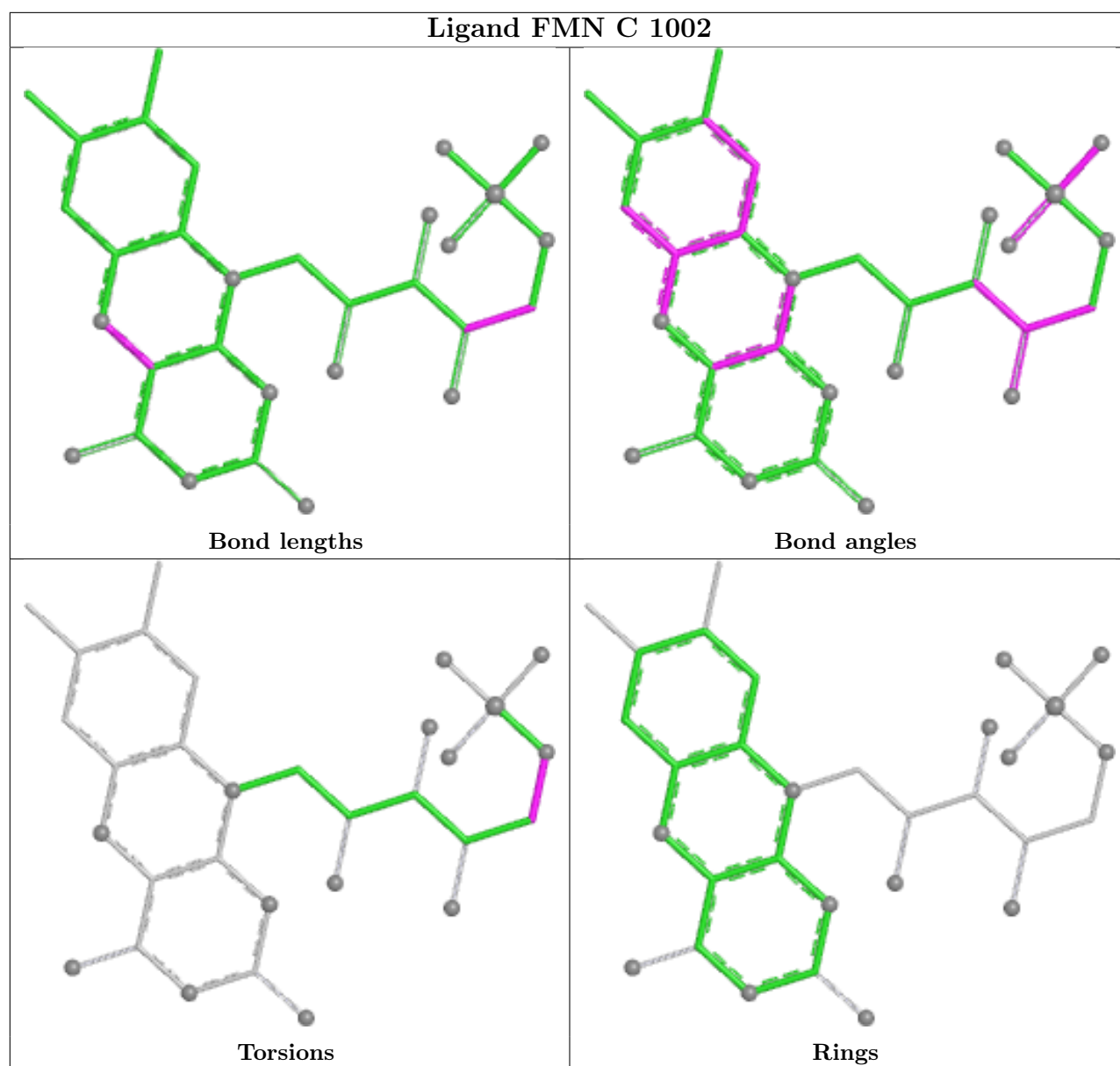
3 monomers are involved in 3 short contacts:

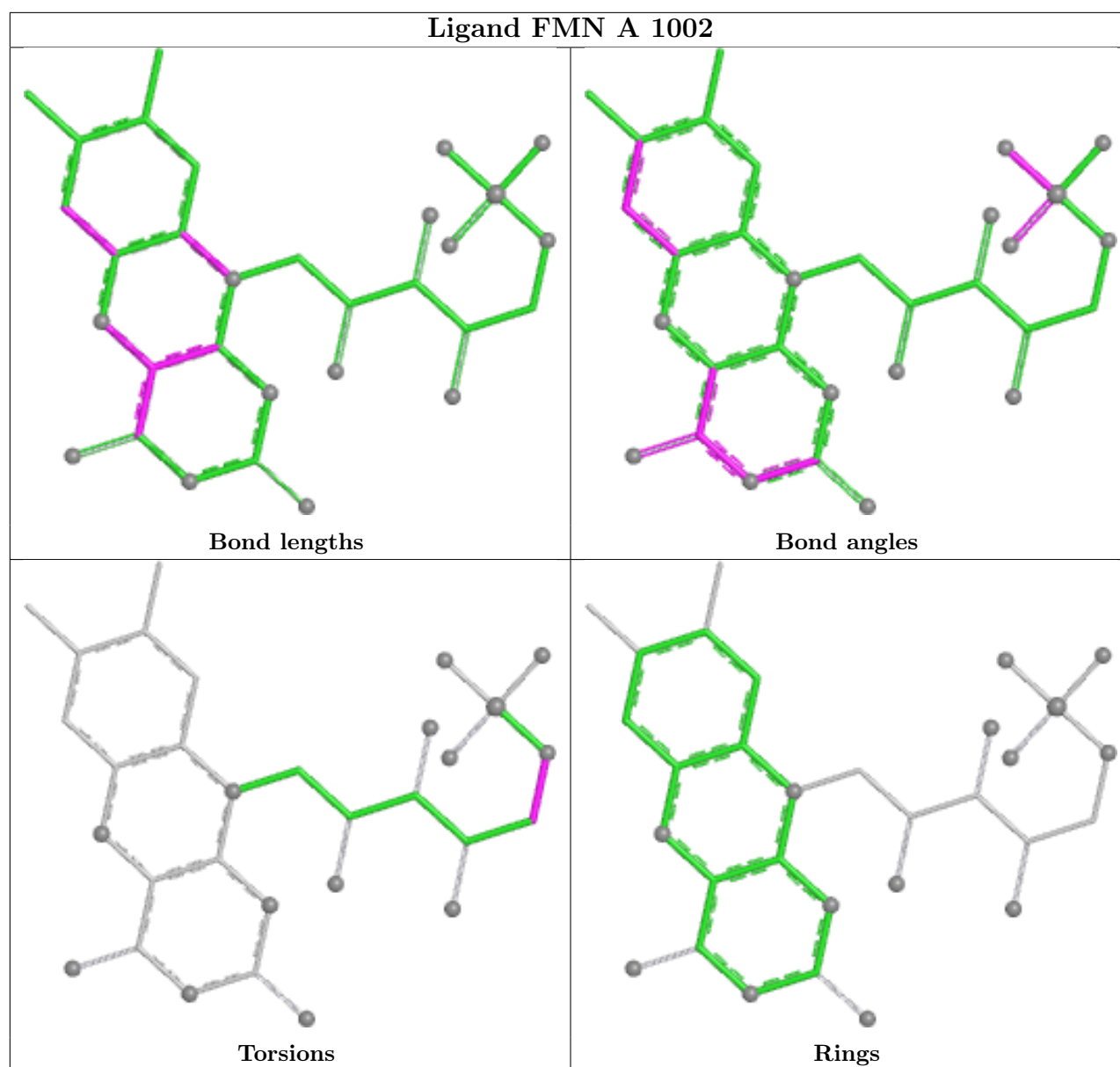
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	FMN	1	0
3	A	1002	FMN	1	0
3	B	1002	FMN	1	0

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

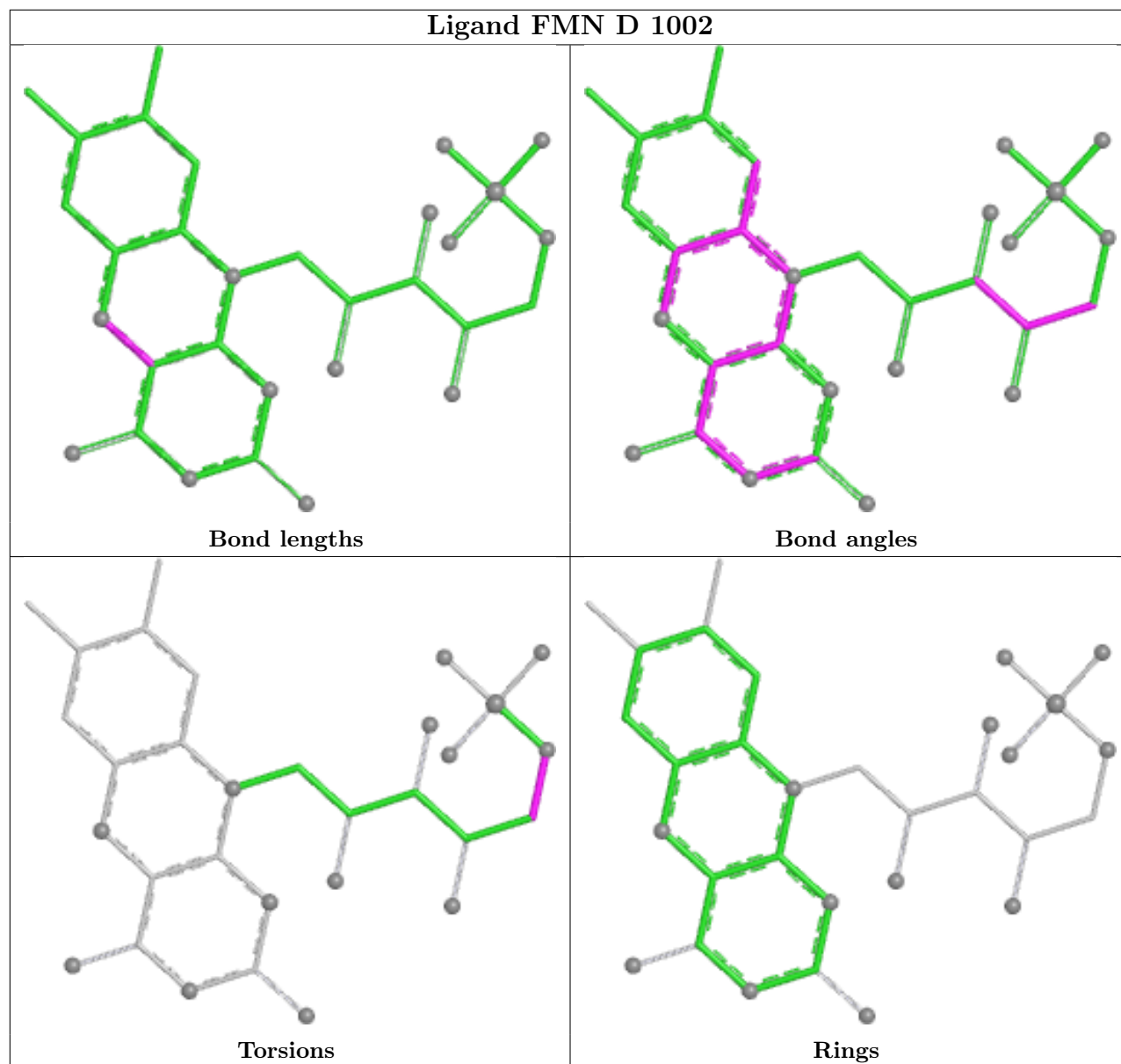
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

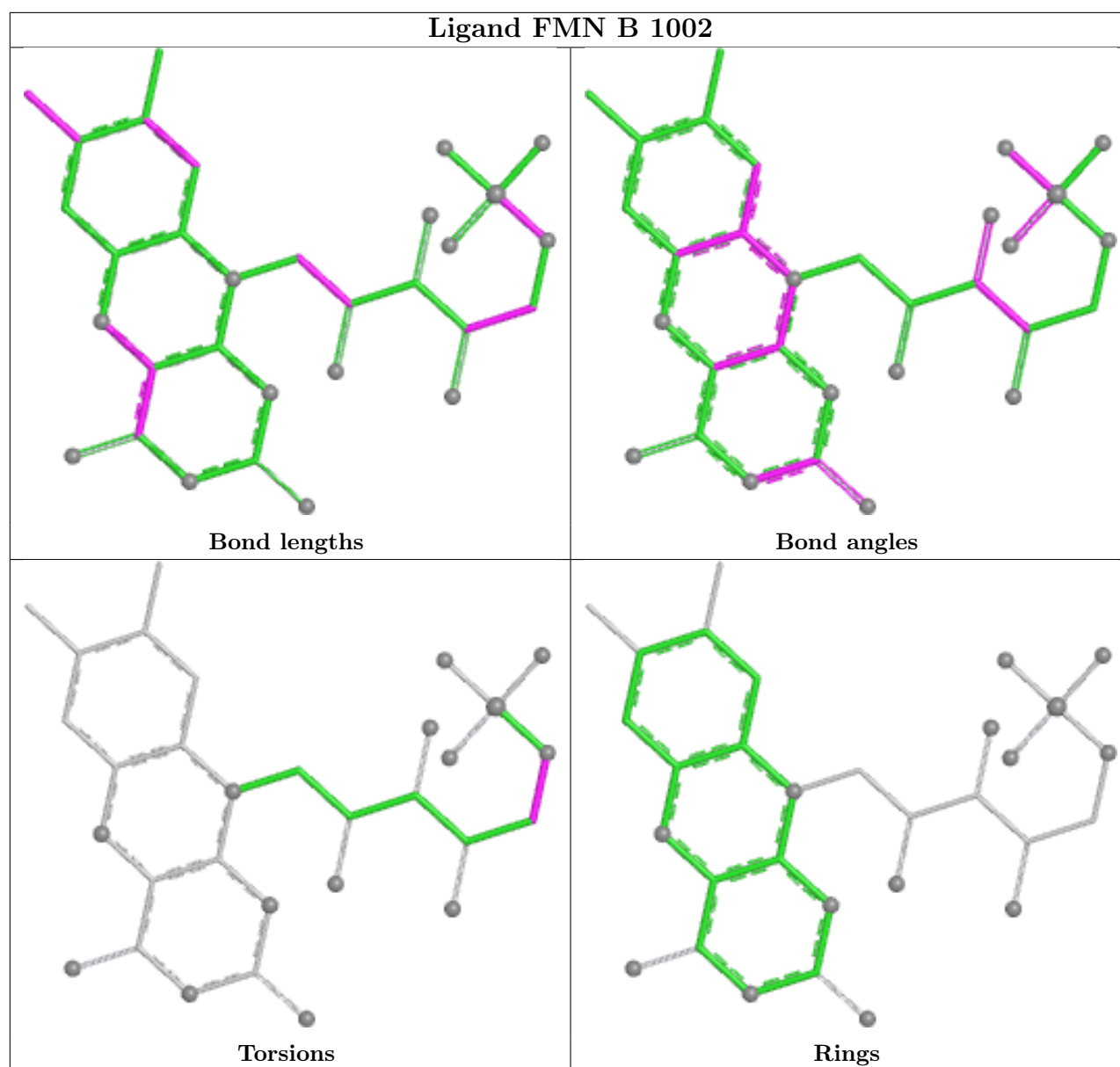


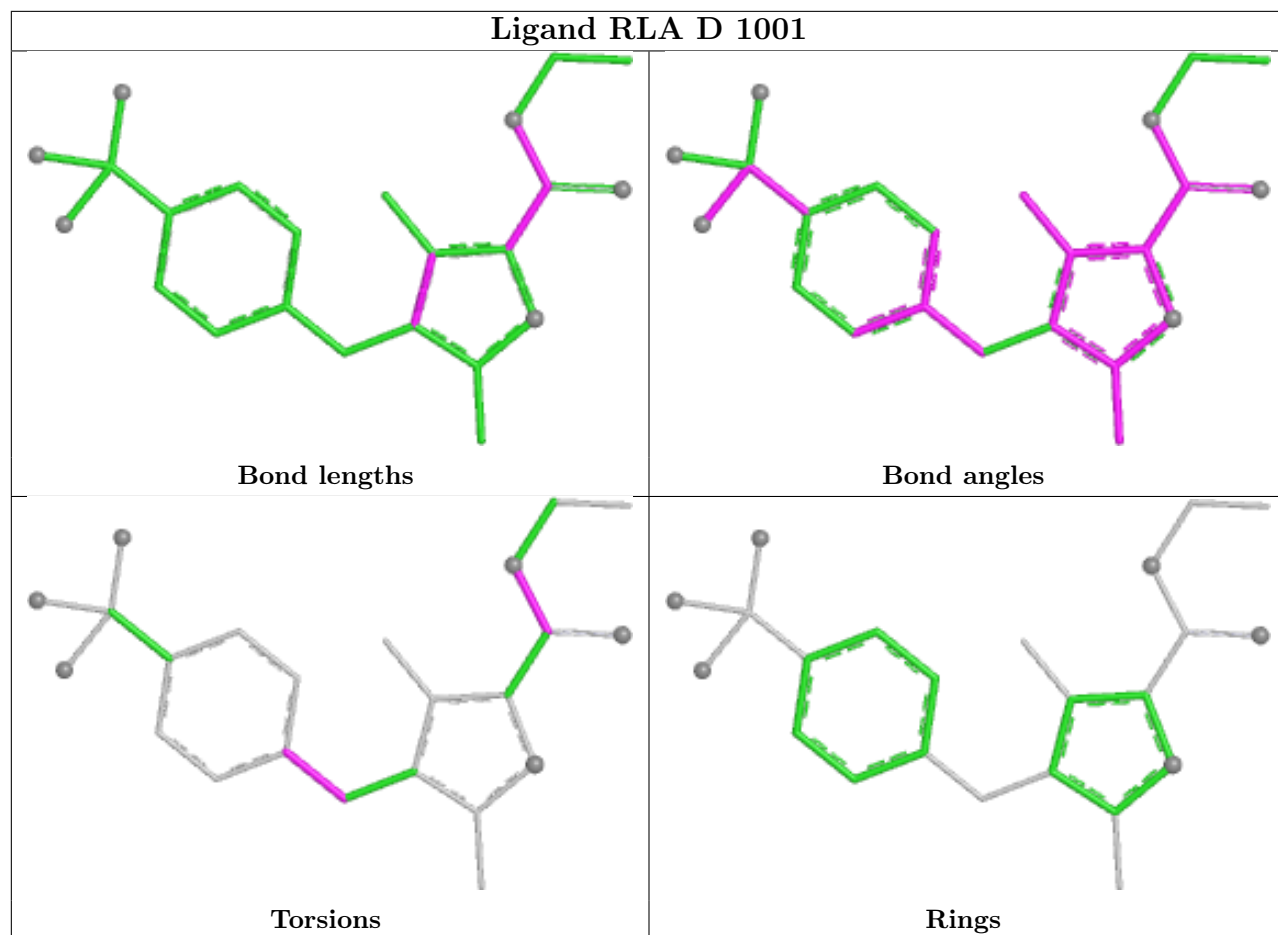


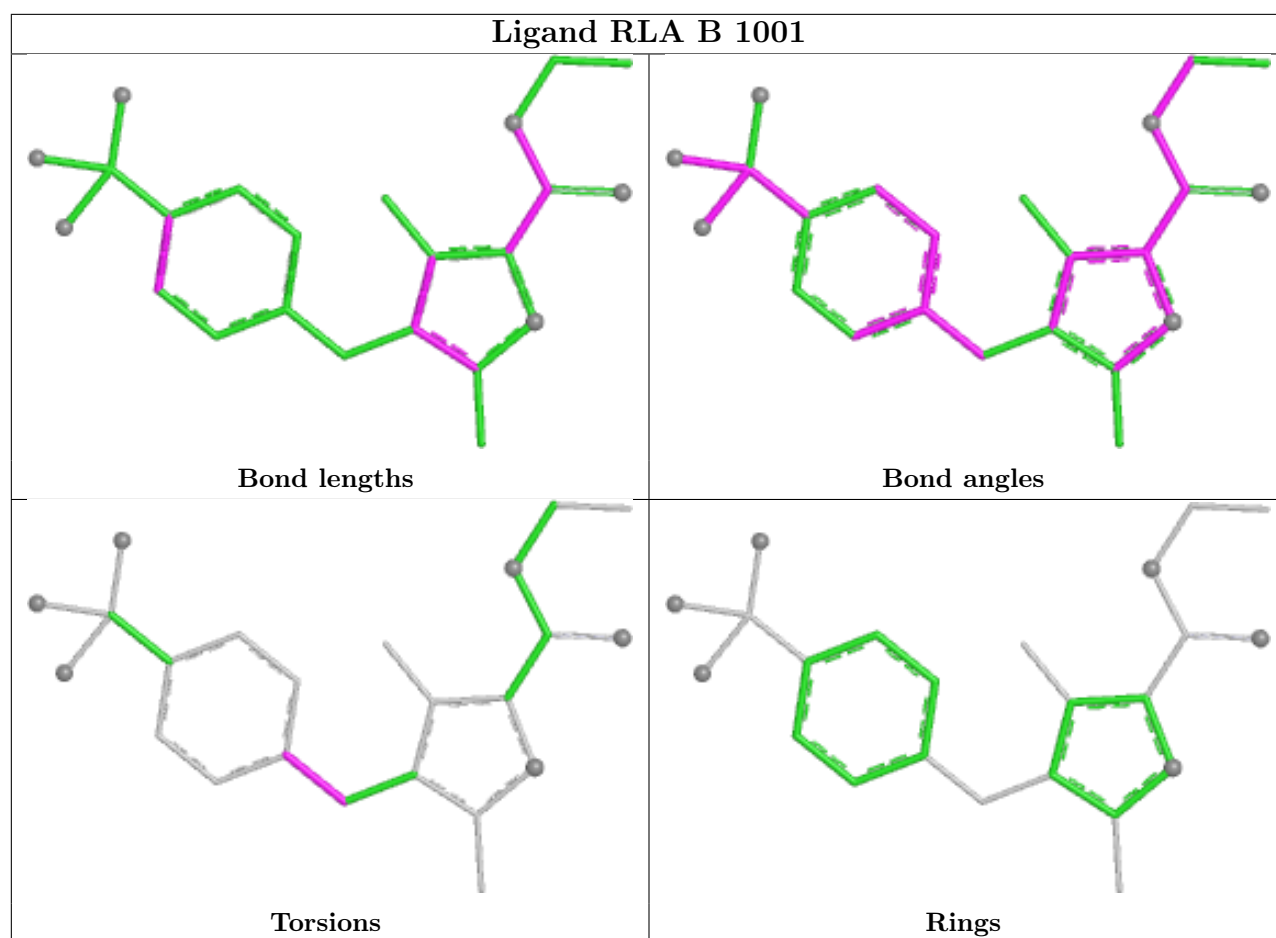


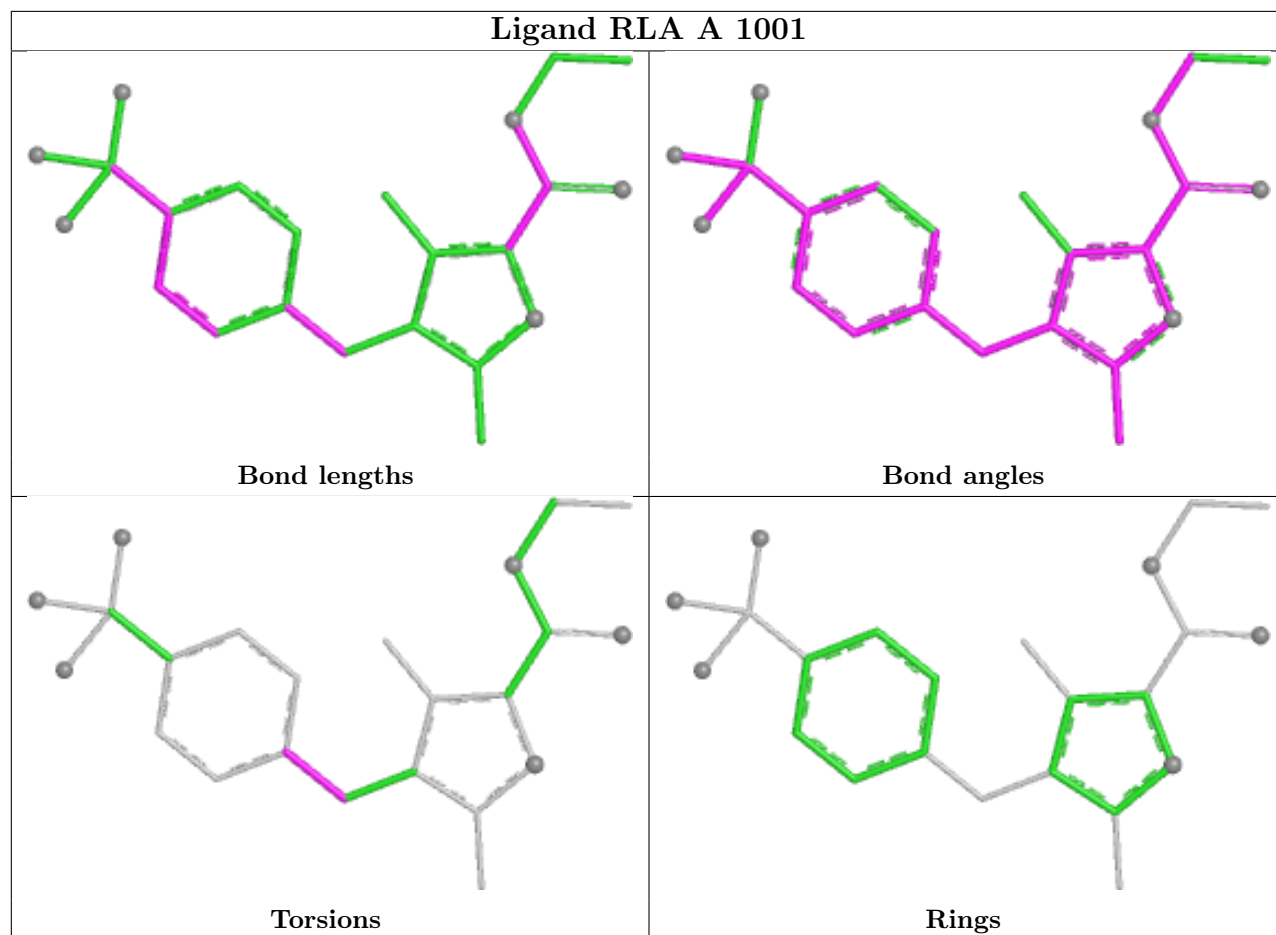
Ligand FMN D 1002











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	377/431 (87%)	-0.46	7 (1%) 66 74	11, 24, 54, 80	1 (0%)
1	B	372/431 (86%)	-0.13	9 (2%) 59 68	15, 34, 64, 91	2 (0%)
1	C	366/431 (84%)	-0.48	11 (3%) 52 60	10, 22, 52, 94	7 (1%)
1	D	368/431 (85%)	-0.08	14 (3%) 44 50	13, 35, 64, 90	3 (0%)
All	All	1483/1724 (86%)	-0.29	41 (2%) 55 62	10, 28, 60, 94	13 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	PHE	10.2
1	A	414	PHE	6.1
1	D	414	PHE	5.3
1	B	414	PHE	5.0
1	D	163	PRO	4.6
1	D	165	PHE	3.9
1	A	155	ALA	3.6
1	C	378	ASN	3.6
1	B	471	ASN	3.5
1	C	556	TYR	3.3
1	D	166	PHE	3.2
1	C	174	PHE	3.2
1	B	161	TYR	3.2
1	C	414	PHE	3.0
1	B	378	ASN	2.9
1	D	167	LEU	2.8
1	A	378	ASN	2.8
1	C	171	PHE	2.7
1	B	160	SER	2.6
1	D	376	LYS	2.6
1	C	167	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	199	TYR	2.5
1	D	377	ASN	2.5
1	C	168	TYR	2.5
1	B	206	ILE	2.5
1	D	462	GLN	2.4
1	D	465	ASP	2.3
1	A	299	GLU	2.3
1	C	170	ILE	2.3
1	A	199	TYR	2.3
1	D	178	TYR	2.3
1	D	174	PHE	2.2
1	A	464	ASN	2.2
1	B	162	ASN	2.2
1	D	164	GLU	2.2
1	D	566	HIS	2.1
1	A	194	TYR	2.1
1	D	353	ASP	2.0
1	C	177	LYS	2.0
1	B	165	PHE	2.0
1	B	473	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($\text{\AA}^2$)	Q<0.9
2	RLA	B	1001	23/23	0.95	0.07	19,31,40,40	0
2	RLA	D	1001	23/23	0.95	0.07	24,32,50,50	0
2	RLA	C	1001	23/23	0.96	0.06	16,27,46,46	0

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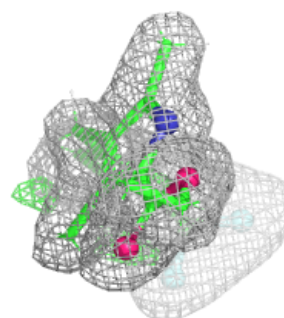
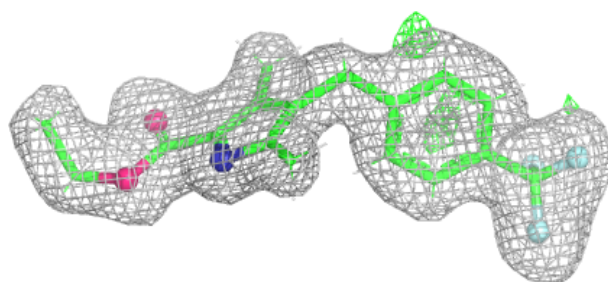
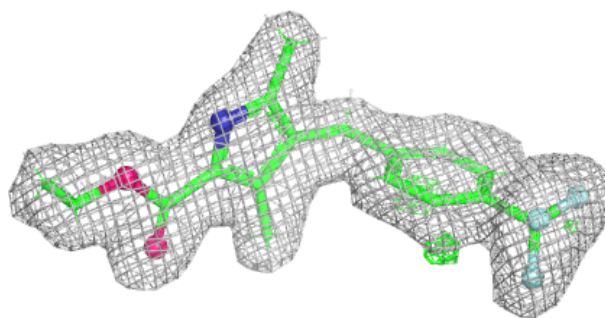
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RLA	A	1001	23/23	0.96	0.06	12,20,28,31	0
4	ORO	B	1003	11/11	0.96	0.05	19,25,27,31	0
4	ORO	D	1003	11/11	0.96	0.06	21,29,36,38	0
3	FMN	D	1002	31/31	0.97	0.06	14,23,31,36	0
3	FMN	B	1002	31/31	0.98	0.05	11,19,30,32	0
4	ORO	A	1003	11/11	0.99	0.03	9,13,17,19	0
3	FMN	C	1002	31/31	0.99	0.04	8,12,18,18	0
4	ORO	C	1003	11/11	0.99	0.03	10,14,18,22	0
3	FMN	A	1002	31/31	0.99	0.04	6,11,18,22	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.

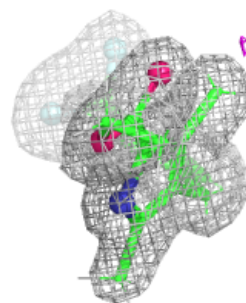
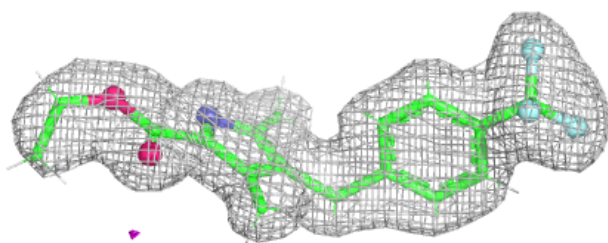
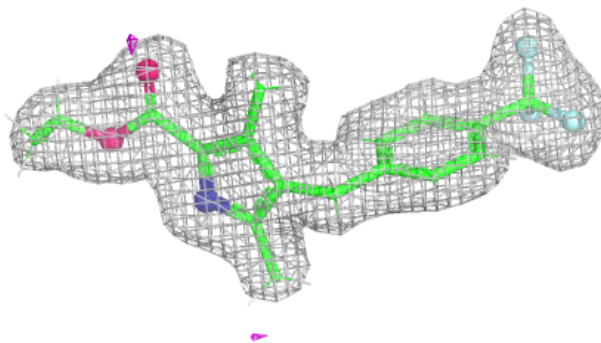
Electron density around RLA B 1001:

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

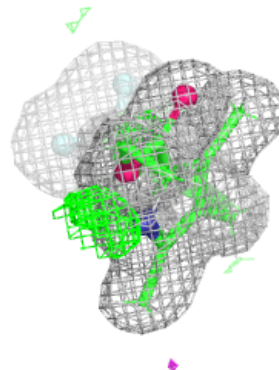
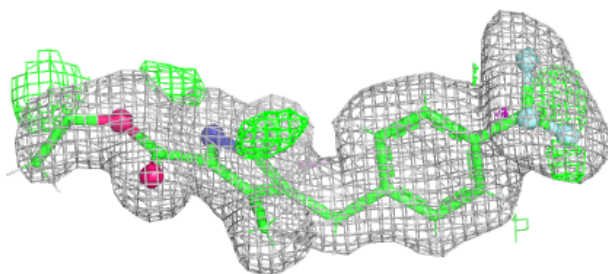
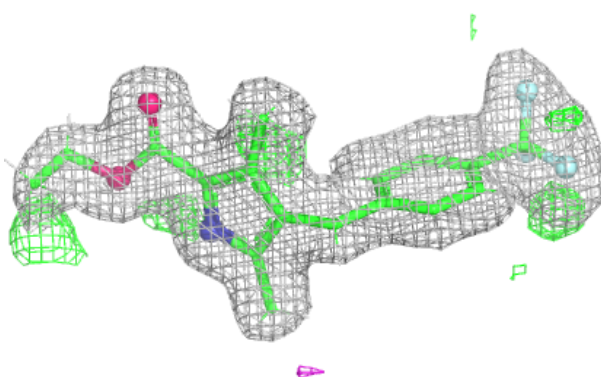


Electron density around RLA D 1001:

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

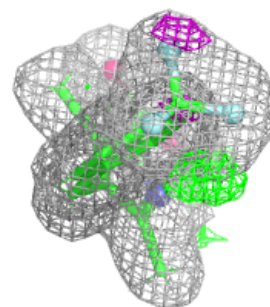
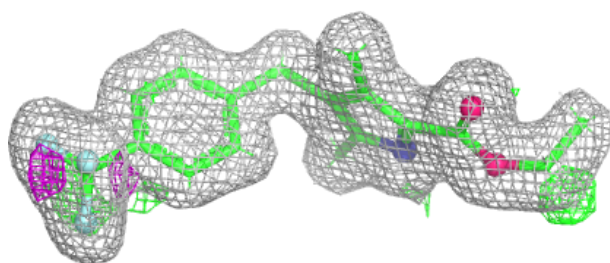
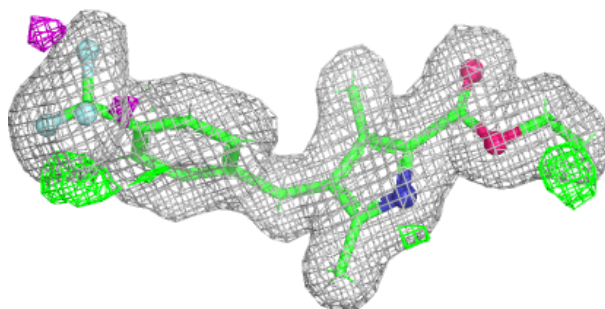
**Electron density around RLA C 1001:**

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



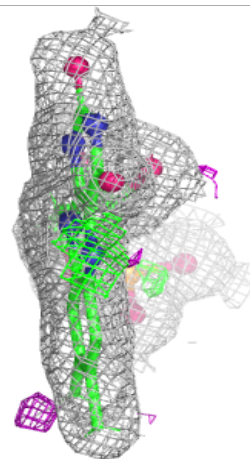
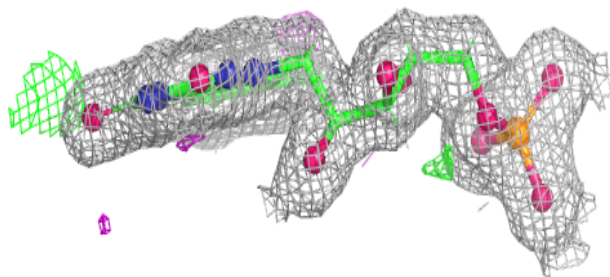
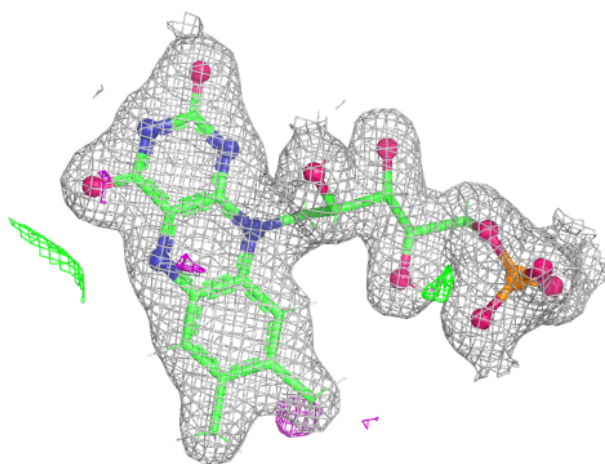
Electron density around RLA A 1001:

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



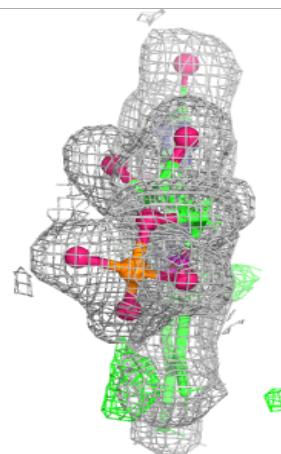
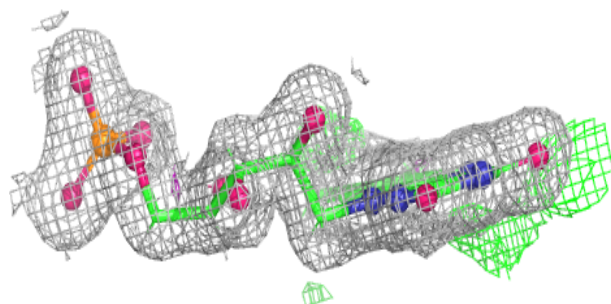
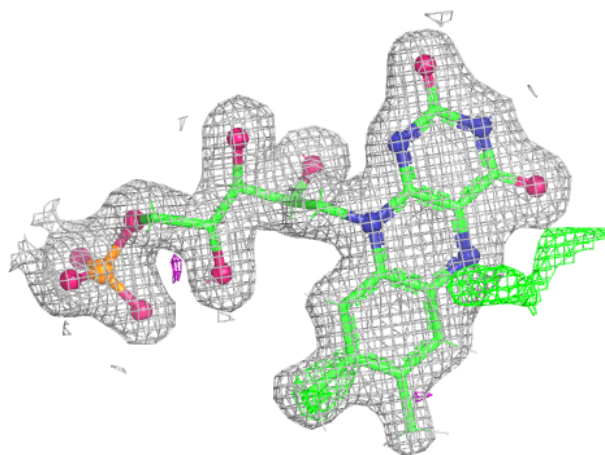
Electron density around FMN D 1002:

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



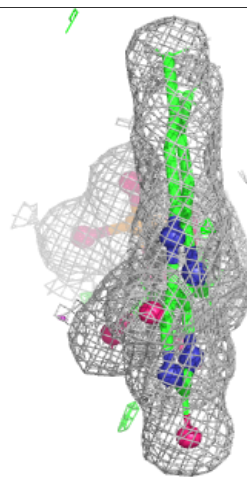
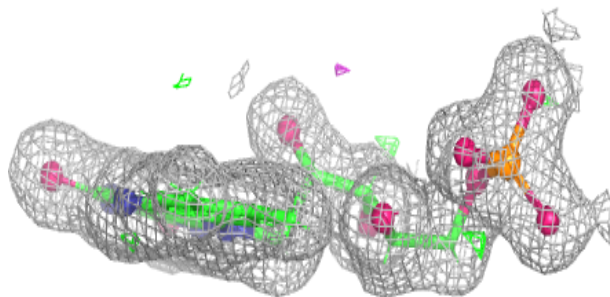
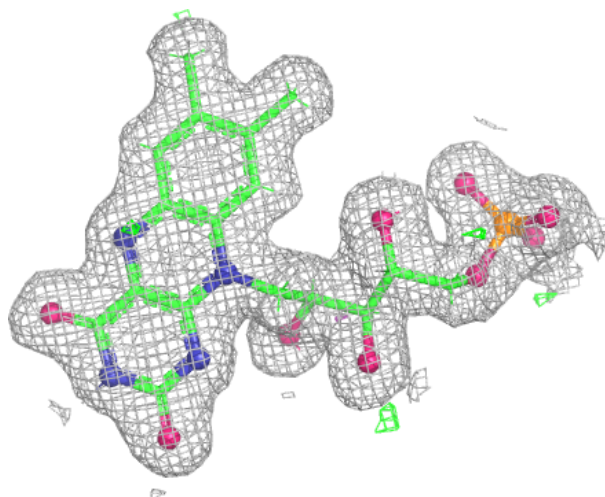
Electron density around FMN B 1002:

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



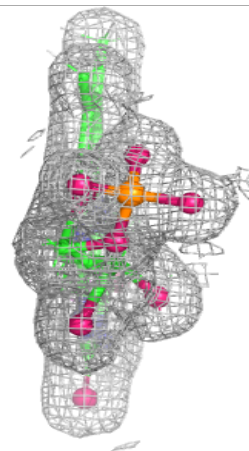
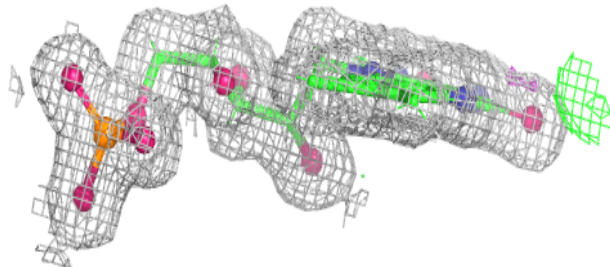
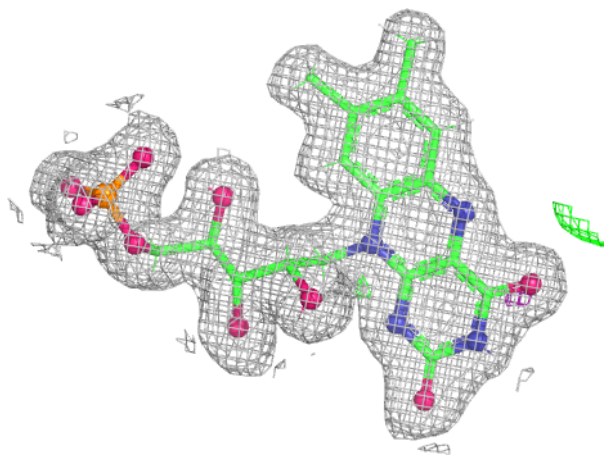
Electron density around FMN C 1002:

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



Electron density around FMN A 1002:

$2mF_o-DF_c$ (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.