



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2021 – 12:04 PM EST

PDB ID : 7L0K
Title : Crystal structure of Plasmodium falciparum dihydroorotate dehydrogenase bound with Inhibitor DSM784 (3-(1-(3-methyl-4-((6-(trifluoromethyl)pyridin-3-yl)methyl)-1H-pyrrole-2-carboxamido)ethyl)-1H-pyrazole-5-carboxamide)
Authors : Deng, X.; Phillips, M.; Tomchick, D.
Deposited on : 2020-12-11
Resolution : 1.96 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

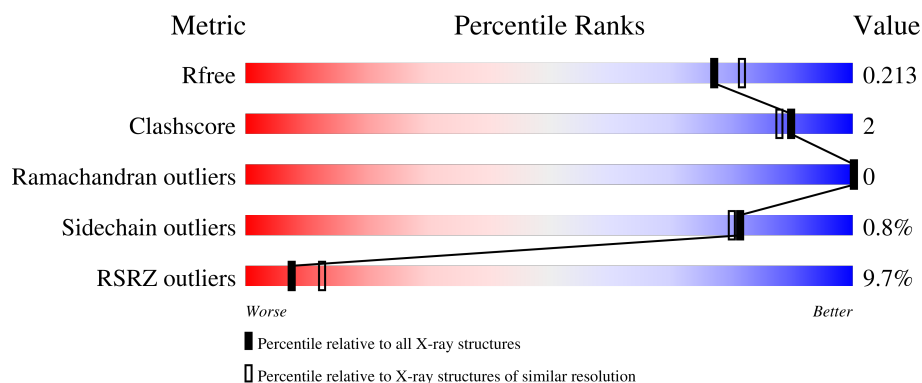
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	401	<div> <div>9%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	B	401	<div> <div>9%</div> <div>88%</div> <div>7%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12699 atoms, of which 6190 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	381	Total	C	H	N	O	S	0	3	0
			6105	1939	3071	507	572	16			
1	B	371	Total	C	H	N	O	S	0	3	0
			5956	1892	3001	495	553	15			

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q08210
A	-18	GLY	-	expression tag	UNP Q08210
A	-17	HIS	-	expression tag	UNP Q08210
A	-16	HIS	-	expression tag	UNP Q08210
A	-15	HIS	-	expression tag	UNP Q08210
A	-14	HIS	-	expression tag	UNP Q08210
A	-13	HIS	-	expression tag	UNP Q08210
A	-12	HIS	-	expression tag	UNP Q08210
A	-11	ALA	-	expression tag	UNP Q08210
A	-10	GLU	-	expression tag	UNP Q08210
A	-9	ASN	-	expression tag	UNP Q08210
A	-8	LEU	-	expression tag	UNP Q08210
A	-7	TYR	-	expression tag	UNP Q08210
A	-6	PHE	-	expression tag	UNP Q08210
A	-5	GLN	-	expression tag	UNP Q08210
A	-4	GLY	-	expression tag	UNP Q08210
A	-3	ALA	-	expression tag	UNP Q08210
A	-2	ASP	-	expression tag	UNP Q08210
A	-1	PRO	-	expression tag	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	THR	deletion	UNP Q08210
A	?	-	TYR	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210

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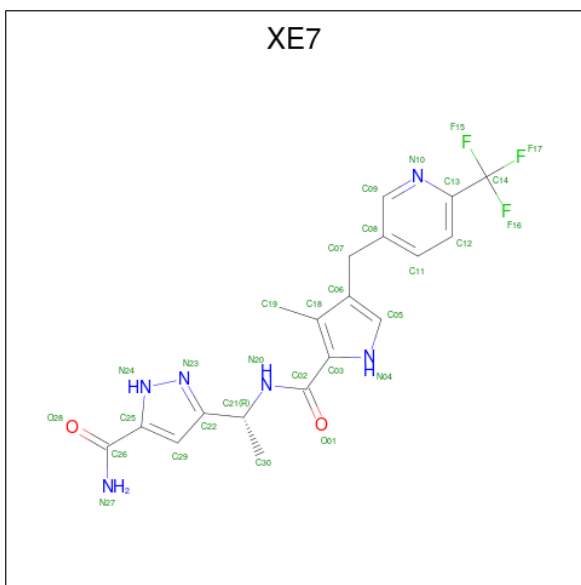
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ILE	deletion	UNP Q08210
A	?	-	VAL	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	PHE	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	HIS	deletion	UNP Q08210
A	?	-	MET	deletion	UNP Q08210
A	?	-	MET	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ALA	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
B	139	MET	-	initiating methionine	UNP Q08210
B	140	GLY	-	expression tag	UNP Q08210
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

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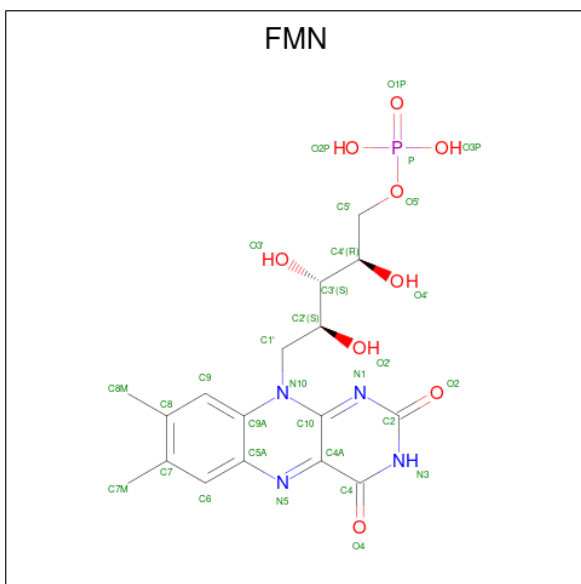
Chain	Residue	Modelled	Actual	Comment	Reference
B	157	PRO	-	expression tag	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	THR	deletion	UNP Q08210
B	?	-	TYR	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ILE	deletion	UNP Q08210
B	?	-	VAL	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	PHE	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	HIS	deletion	UNP Q08210
B	?	-	MET	deletion	UNP Q08210
B	?	-	MET	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ALA	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210

- Molecule 2 is 3-{(1R)-1-[(3-methyl-4-{[6-(trifluoromethyl)pyridin-3-yl]methyl}-1H-pyrrol-2-carbonyl)amino]ethyl}-1H-pyrazole-5-carboxamide (three-letter code: XE7) (formula: C₁₉H₁₉F₃N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	1
			98	38	6	38	12	4		
2	B	1	Total	C	F	H	N	O	0	1
			98	38	6	38	12	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



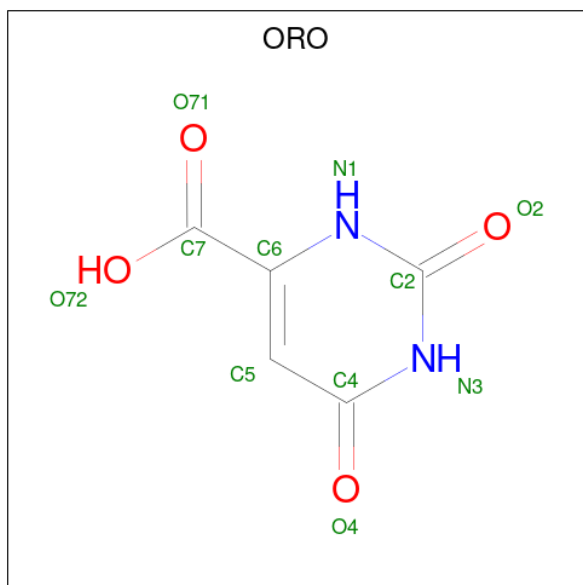
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	P	0	0
			49	17	18	4	9	1		

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

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$) (labeled as "Ligand of Interest" by depositor).



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		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	161	Total	O	0	0
			161	161		
5	B	155	Total	O	0	0
			155	155		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.12Å 158.34Å 62.77Å 90.00° 107.28° 90.00°	Depositor
Resolution (Å)	36.21 – 1.96 36.21 – 1.96	Depositor EDS
% Data completeness (in resolution range)	85.8 (36.21-1.96) 85.8 (36.21-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.179 , 0.213 0.179 , 0.213	Depositor DCC
R_{free} test set	1016 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12699	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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, XE7, ORO

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	0.36	0/3098	0.59	0/4172
1	B	0.36	0/3017	0.60	0/4061
All	All	0.36	0/6115	0.60	0/8233

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3034	3071	3061	12	0
1	B	2955	3001	2989	10	0
2	A	60	38	0	0	0
2	B	60	38	0	0	0
3	A	31	18	19	1	0
3	B	31	18	19	1	0
4	A	11	3	3	0	0
4	B	11	3	3	0	0
5	A	161	0	0	1	0
5	B	155	0	0	0	0
All	All	6509	6190	6094	22	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 (22) 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:263:ILE:HD11	1:A:276:CYS:SG	2.39	0.63
1:B:179:ILE:O	1:B:265:ARG:NH2	2.40	0.53
1:A:558:LEU:C	1:A:558:LEU:HD23	2.30	0.52
1:B:242:PHE:CZ	1:B:531:LEU:HD11	2.45	0.51
1:A:255:GLN:HB2	5:A:1202:HOH:O	2.13	0.49
1:B:466:ILE:HD11	1:B:480:LYS:HG3	1.94	0.48
1:A:206:ILE:HD12	1:A:209[B]:CYS:SG	2.53	0.48
1:B:558:LEU:C	1:B:558:LEU:HD23	2.34	0.48
1:B:503:ILE:HD12	1:B:503:ILE:N	2.30	0.47
1:B:263:ILE:HD12	1:B:263:ILE:O	2.15	0.46
1:A:226:GLY:HA3	3:A:1002:FMN:N5	2.32	0.44
1:A:180:ASP:HB3	1:A:183:ILE:HD12	1.99	0.44
1:A:503:ILE:HD12	1:A:503:ILE:N	2.34	0.43
1:B:191:LEU:HD23	1:B:196:ILE:HD11	2.01	0.42
1:A:158:PHE:O	1:A:159:GLU:HB3	2.20	0.42
1:A:222:GLY:HA3	1:A:244:PHE:CE1	2.55	0.42
1:B:226:GLY:HA3	3:B:1002:FMN:N5	2.35	0.41
1:A:430:LEU:HD12	1:A:456:ILE:HD11	2.03	0.41
1:A:566:HIS:O	1:A:567:SER:HB3	2.22	0.40
1:B:329:ILE:HD11	1:B:367:VAL:HG13	2.03	0.40
1:B:465:ASP:OD1	1:B:465:ASP:N	2.54	0.40
1:A:266:ASP:CB	1:A:466:ILE:HD11	2.51	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	382/401 (95%)	368 (96%)	14 (4%)	0	100	100
1	B	370/401 (92%)	358 (97%)	12 (3%)	0	100	100
All	All	752/802 (94%)	726 (96%)	26 (4%)	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	341/354 (96%)	339 (99%)	2 (1%)	86	85
1	B	331/354 (94%)	328 (99%)	3 (1%)	78	77
All	All	672/708 (95%)	667 (99%)	5 (1%)	81	82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	ASP
1	A	466	ILE
1	B	202	SER
1	B	235	ASP
1	B	356	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	XE7	B	1001[A]	-	30,32,32	1.90	8 (26%)	30,47,47	2.97	11 (36%)
4	ORO	A	1003	-	6,11,11	1.48	1 (16%)	3,15,15	3.12	2 (66%)
4	ORO	B	1003	-	6,11,11	1.43	1 (16%)	3,15,15	3.26	2 (66%)
3	FMN	A	1002	-	31,33,33	1.47	5 (16%)	40,50,50	1.86	7 (17%)
2	XE7	A	1001[B]	-	30,32,32	1.84	8 (26%)	30,47,47	2.56	14 (46%)
3	FMN	B	1002	-	31,33,33	1.35	5 (16%)	40,50,50	1.93	7 (17%)
2	XE7	A	1001[A]	-	30,32,32	2.04	8 (26%)	30,47,47	4.50	13 (43%)
2	XE7	B	1001[B]	-	30,32,32	2.00	9 (30%)	30,47,47	2.56	12 (40%)

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	XE7	B	1001[A]	-	-	5/16/26/26	0/3/3/3
4	ORO	A	1003	-	-	0/0/4/4	0/1/1/1
4	ORO	B	1003	-	-	0/0/4/4	0/1/1/1
3	FMN	A	1002	-	-	1/18/18/18	0/3/3/3
2	XE7	A	1001[B]	-	-	2/16/26/26	0/3/3/3
3	FMN	B	1002	-	-	1/18/18/18	0/3/3/3
2	XE7	A	1001[A]	-	-	5/16/26/26	0/3/3/3
2	XE7	B	1001[B]	-	-	1/16/26/26	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001[A]	XE7	C26-N27	6.10	1.44	1.33
2	B	1001[B]	XE7	C26-N27	4.71	1.42	1.33
2	B	1001[A]	XE7	C26-N27	4.70	1.41	1.33
2	A	1001[B]	XE7	C26-N27	4.61	1.41	1.33
2	A	1001[A]	XE7	C29-C22	4.49	1.48	1.39
3	A	1002	FMN	C4A-N5	4.44	1.39	1.33
2	B	1001[B]	XE7	C22-N23	3.84	1.39	1.34
3	A	1002	FMN	C10-N1	3.72	1.38	1.33
2	B	1001[B]	XE7	C22-C21	3.66	1.56	1.52
2	A	1001[B]	XE7	C22-N23	3.55	1.38	1.34
2	B	1001[B]	XE7	C02-N20	3.53	1.41	1.34
3	B	1002	FMN	C1'-N10	3.51	1.51	1.48
2	B	1001[A]	XE7	C22-N23	3.44	1.38	1.34
2	B	1001[A]	XE7	C14-C13	-3.35	1.45	1.50
3	B	1002	FMN	C4A-N5	3.26	1.38	1.33
2	B	1001[A]	XE7	C29-C22	3.20	1.45	1.39
2	B	1001[A]	XE7	C02-N20	3.18	1.41	1.34
2	A	1001[B]	XE7	C22-C21	3.11	1.55	1.52
2	A	1001[A]	XE7	C22-N23	2.97	1.38	1.34
2	A	1001[B]	XE7	C29-C22	2.95	1.45	1.39
2	A	1001[B]	XE7	C02-N20	2.93	1.40	1.34
3	B	1002	FMN	C10-N1	2.88	1.37	1.33
2	B	1001[B]	XE7	C29-C22	2.84	1.45	1.39
3	A	1002	FMN	C4-N3	2.81	1.37	1.33
2	B	1001[B]	XE7	C21-N20	2.80	1.53	1.47
3	A	1002	FMN	C1'-N10	2.72	1.51	1.48
2	A	1001[B]	XE7	C30-C21	2.70	1.58	1.52
2	A	1001[A]	XE7	C21-N20	2.56	1.52	1.47
3	B	1002	FMN	C4-N3	2.47	1.37	1.33
2	A	1001[A]	XE7	C02-N20	2.38	1.39	1.34
2	B	1001[B]	XE7	C30-C21	2.38	1.57	1.52
3	A	1002	FMN	C5A-N5	2.37	1.39	1.35
2	B	1001[B]	XE7	F16-C14	2.34	1.41	1.32
2	A	1001[B]	XE7	F16-C14	2.30	1.41	1.32
2	B	1001[A]	XE7	F16-C14	2.30	1.41	1.32
4	A	1003	ORO	O4-C4	-2.29	1.18	1.24
2	A	1001[A]	XE7	F16-C14	2.26	1.41	1.32
4	B	1003	ORO	O4-C4	-2.22	1.19	1.24
3	B	1002	FMN	C5A-N5	2.20	1.39	1.35
2	A	1001[A]	XE7	C12-C11	2.19	1.42	1.38
2	B	1001[A]	XE7	C25-C26	-2.15	1.48	1.50
2	A	1001[A]	XE7	C22-C21	2.13	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001[B]	XE7	C12-C11	2.04	1.42	1.38
2	B	1001[A]	XE7	C30-C21	2.01	1.57	1.52
2	B	1001[B]	XE7	C12-C11	2.01	1.42	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001[A]	XE7	C25-C26-N27	18.54	134.59	116.25
2	B	1001[A]	XE7	C25-C26-N27	11.41	127.54	116.25
2	A	1001[A]	XE7	O28-C26-C25	-9.61	111.58	119.61
2	A	1001[B]	XE7	C25-C26-N27	8.06	124.23	116.25
2	B	1001[B]	XE7	C25-C26-N27	7.92	124.09	116.25
2	A	1001[A]	XE7	C30-C21-C22	7.33	119.43	110.95
3	A	1002	FMN	C4-N3-C2	6.90	120.96	115.14
3	B	1002	FMN	C4-N3-C2	6.47	120.61	115.14
2	B	1001[A]	XE7	O28-C26-C25	-6.35	114.30	119.61
2	A	1001[A]	XE7	O28-C26-N27	-6.16	113.83	122.58
3	B	1002	FMN	C1'-N10-C9A	5.64	122.73	118.29
2	B	1001[B]	XE7	C30-C21-C22	5.45	117.25	110.95
2	A	1001[B]	XE7	C30-C21-C22	5.39	117.19	110.95
3	A	1002	FMN	C1'-N10-C9A	4.65	121.95	118.29
4	B	1003	ORO	C4-C5-C6	4.22	119.46	116.73
3	A	1002	FMN	C5A-C9A-N10	4.00	120.61	117.72
3	B	1002	FMN	C5A-C9A-N10	3.91	120.55	117.72
3	B	1002	FMN	C4A-C4-N3	-3.84	118.18	123.43
4	A	1003	ORO	C4-C5-C6	3.82	119.20	116.73
2	B	1001[A]	XE7	C30-C21-C22	3.75	115.28	110.95
2	B	1001[B]	XE7	C21-C22-N23	3.65	126.24	120.30
4	A	1003	ORO	C5-C4-N3	-3.57	119.92	124.08
3	A	1002	FMN	C4A-N5-C5A	3.36	120.13	116.77
2	A	1001[B]	XE7	C21-C22-N23	3.32	125.70	120.30
4	B	1003	ORO	C5-C4-N3	-3.22	120.33	124.08
2	A	1001[B]	XE7	F16-C14-C13	3.13	117.83	112.47
2	B	1001[A]	XE7	O28-C26-N27	-3.11	118.16	122.58
2	A	1001[B]	XE7	O28-C26-C25	-3.00	117.10	119.61
2	B	1001[B]	XE7	O28-C26-C25	-2.99	117.11	119.61
2	B	1001[A]	XE7	C11-C12-C13	-2.97	116.15	118.99
3	B	1002	FMN	C9A-N10-C10	-2.90	118.11	121.91
2	B	1001[A]	XE7	F15-C14-C13	2.85	117.34	112.47
2	B	1001[B]	XE7	C21-N20-C02	2.84	128.71	122.56
2	A	1001[B]	XE7	C29-C25-N24	-2.78	104.92	109.97
3	A	1002	FMN	C4A-C4-N3	-2.77	119.64	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001[B]	XE7	C29-C25-N24	-2.76	104.95	109.97
2	A	1001[A]	XE7	C29-C25-N24	-2.76	104.95	109.97
2	A	1001[B]	XE7	O28-C26-N27	-2.76	118.66	122.58
3	B	1002	FMN	C4A-N5-C5A	2.72	119.49	116.77
2	B	1001[B]	XE7	F15-C14-C13	2.72	117.11	112.47
2	A	1001[A]	XE7	O01-C02-N20	-2.68	117.52	122.45
2	A	1001[A]	XE7	F16-C14-C13	2.67	117.03	112.47
2	B	1001[B]	XE7	O28-C26-N27	-2.66	118.79	122.58
3	A	1002	FMN	C4-C4A-N5	2.64	121.62	118.60
3	B	1002	FMN	C10-C4A-N5	-2.60	119.46	121.26
2	B	1001[B]	XE7	F16-C14-C13	2.60	116.91	112.47
2	A	1001[A]	XE7	C11-C12-C13	-2.58	116.52	118.99
2	B	1001[A]	XE7	C21-N20-C02	2.58	128.16	122.56
2	B	1001[B]	XE7	C29-C22-N23	-2.57	106.84	110.28
2	A	1001[B]	XE7	O01-C02-N20	-2.57	117.73	122.45
2	A	1001[A]	XE7	C29-C22-N23	-2.56	106.85	110.28
2	B	1001[B]	XE7	O01-C02-N20	-2.53	117.80	122.45
2	A	1001[B]	XE7	C29-C22-N23	-2.50	106.94	110.28
2	A	1001[A]	XE7	F17-C14-C13	2.45	116.66	112.47
2	B	1001[A]	XE7	C29-C25-N24	-2.45	105.53	109.97
2	B	1001[A]	XE7	O01-C02-N20	-2.40	118.03	122.45
2	B	1001[B]	XE7	C11-C12-C13	-2.37	116.72	118.99
3	A	1002	FMN	C10-C4A-N5	-2.33	119.64	121.26
2	B	1001[A]	XE7	F16-C14-C13	2.33	116.46	112.47
2	A	1001[A]	XE7	F15-C14-C13	2.33	116.45	112.47
2	A	1001[B]	XE7	C11-C12-C13	-2.29	116.80	118.99
2	A	1001[B]	XE7	C14-C13-N10	2.29	117.36	114.61
2	A	1001[A]	XE7	C29-C22-C21	2.27	132.74	129.25
2	A	1001[B]	XE7	F17-C14-C13	2.25	116.32	112.47
2	A	1001[A]	XE7	C21-N20-C02	2.25	127.45	122.56
2	B	1001[A]	XE7	C29-C22-N23	-2.16	107.39	110.28
2	A	1001[B]	XE7	C21-N20-C02	2.12	127.17	122.56
2	A	1001[B]	XE7	F15-C14-C13	2.05	115.97	112.47

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001[A]	XE7	C30-C21-C22-C29
2	A	1001[A]	XE7	C22-C21-N20-C02
2	A	1001[A]	XE7	C30-C21-C22-C29
2	A	1001[A]	XE7	C30-C21-N20-C02

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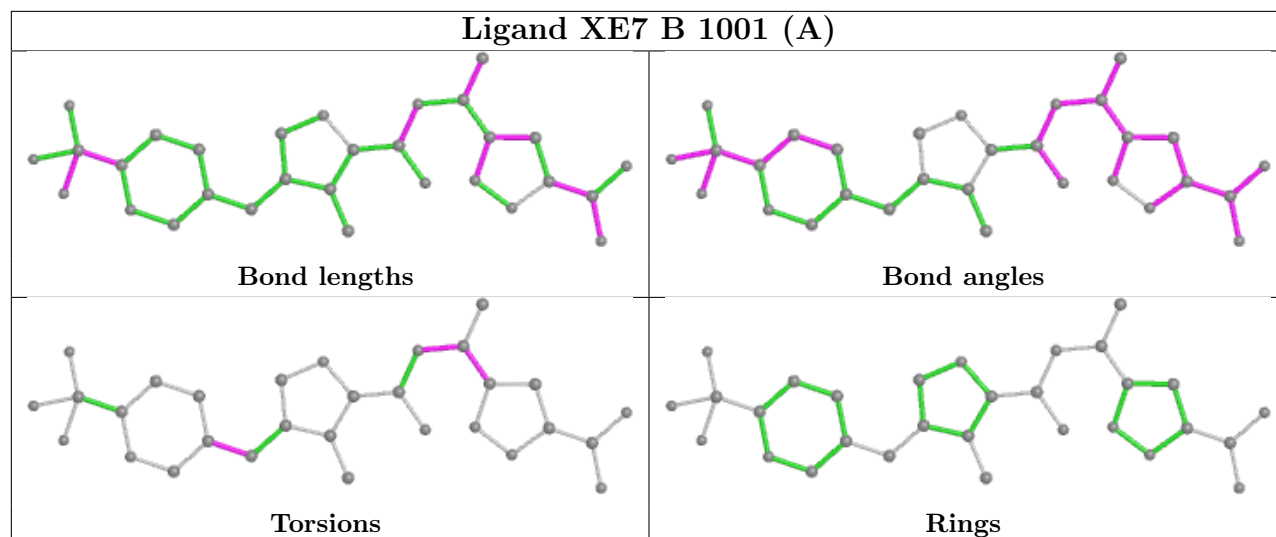
Mol	Chain	Res	Type	Atoms
2	B	1001[A]	XE7	C22-C21-N20-C02
3	B	1002	FMN	C4'-C5'-O5'-P
2	B	1001[A]	XE7	C30-C21-N20-C02
3	A	1002	FMN	C4'-C5'-O5'-P
2	A	1001[B]	XE7	C06-C07-C08-C11
2	A	1001[B]	XE7	C06-C07-C08-C09
2	A	1001[A]	XE7	C06-C07-C08-C11
2	A	1001[A]	XE7	C06-C07-C08-C09
2	B	1001[A]	XE7	C06-C07-C08-C11
2	B	1001[A]	XE7	C06-C07-C08-C09
2	B	1001[B]	XE7	C06-C07-C08-C11

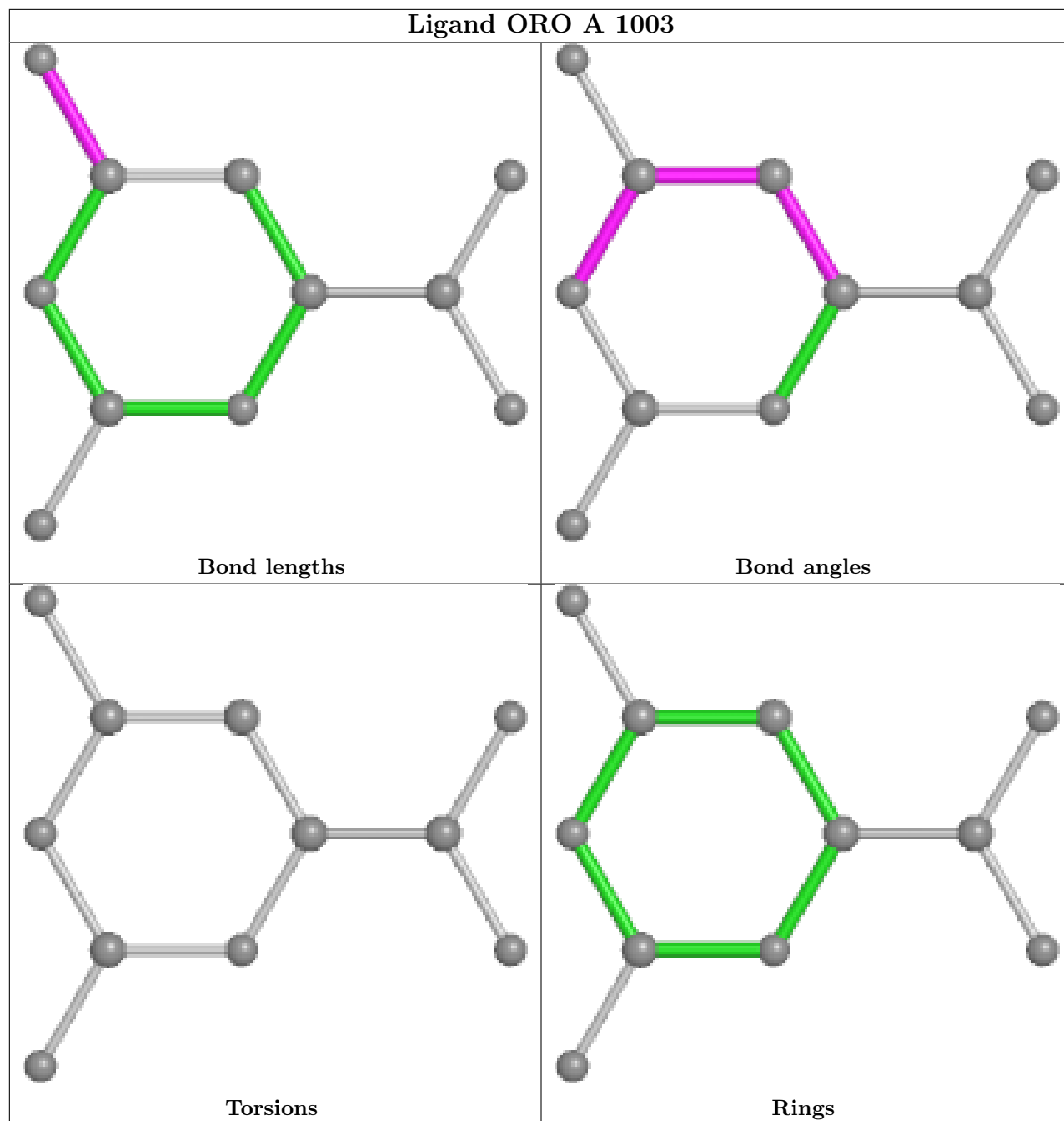
There are no ring outliers.

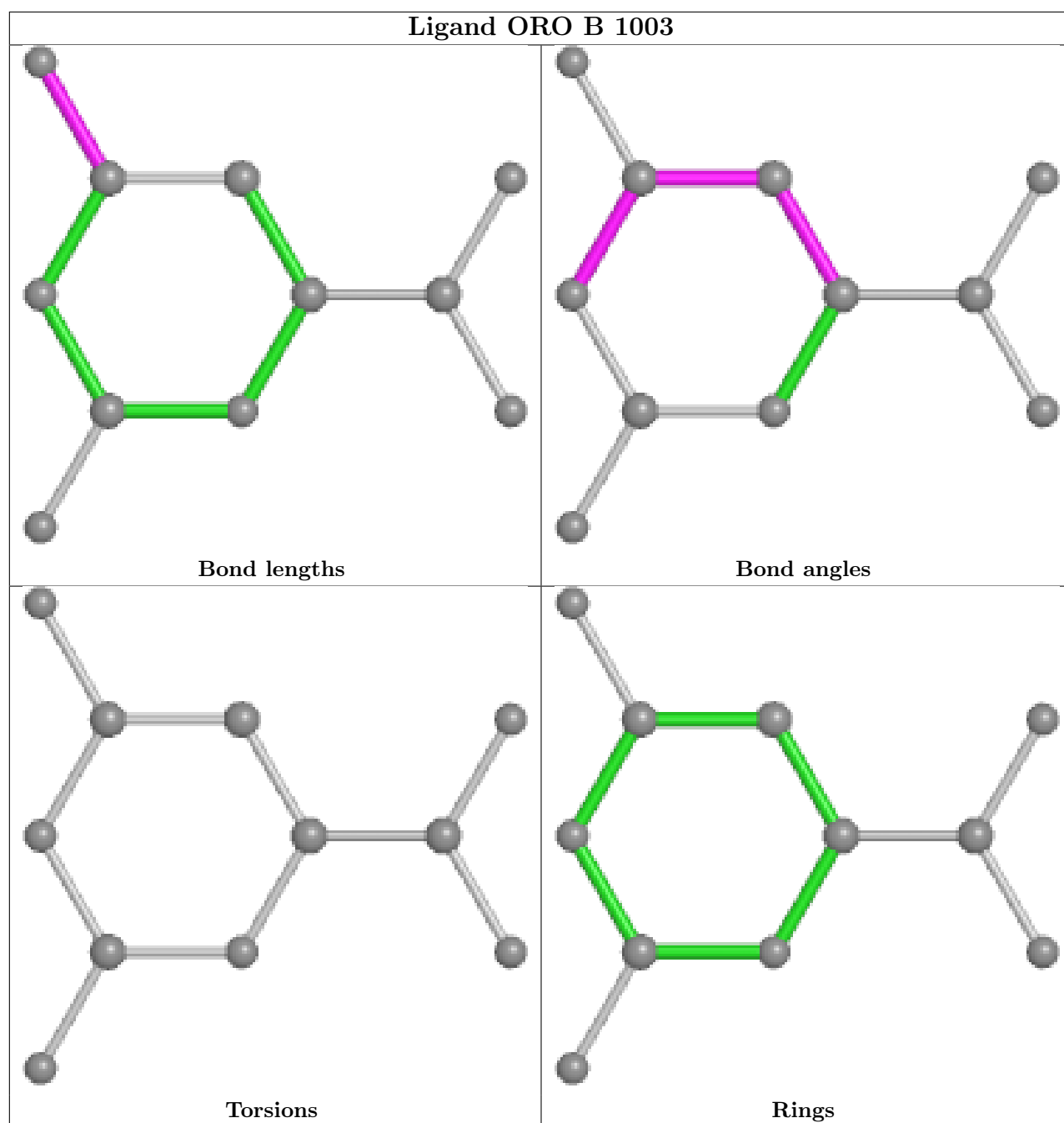
2 monomers are involved in 2 short contacts:

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

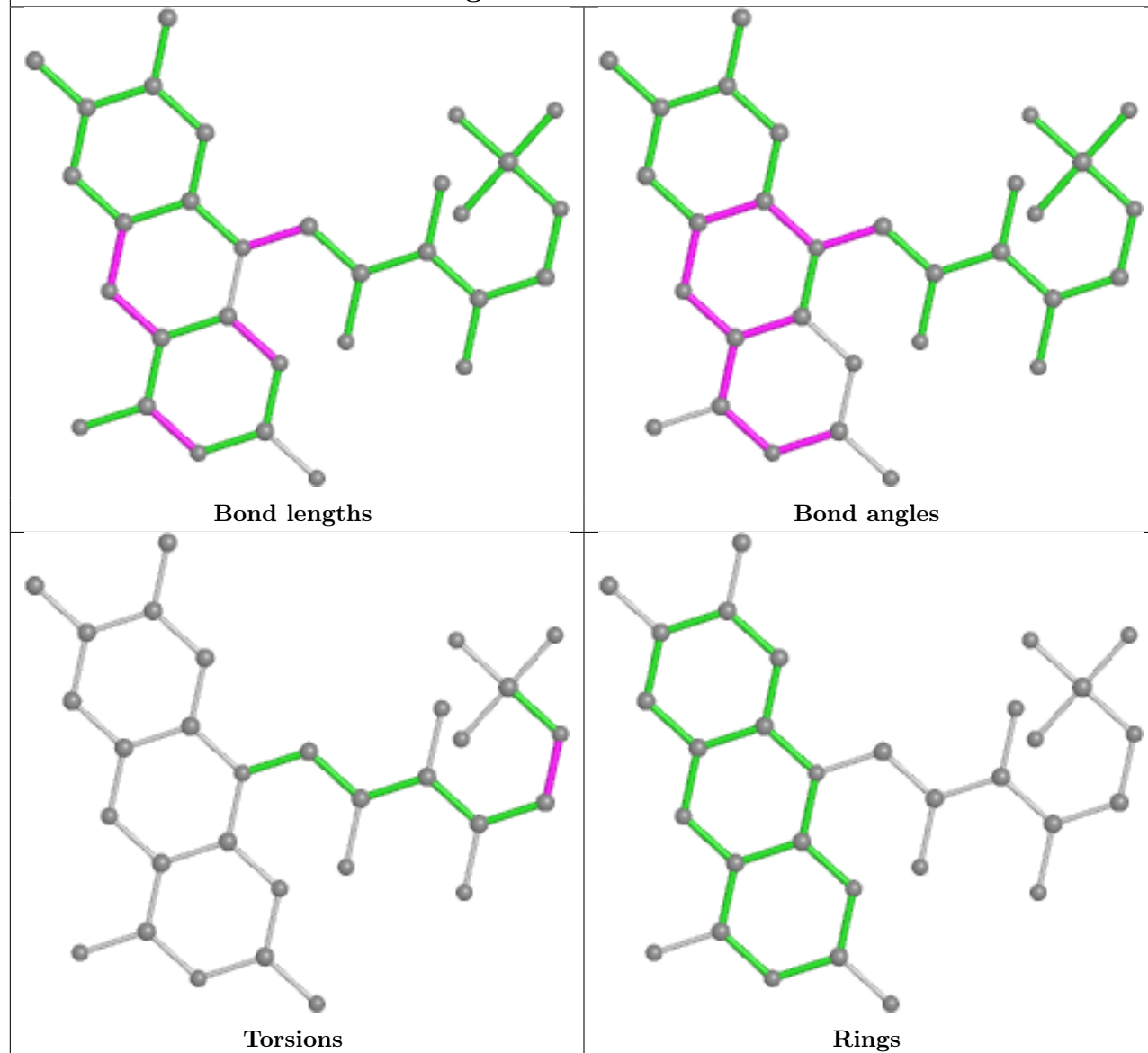
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



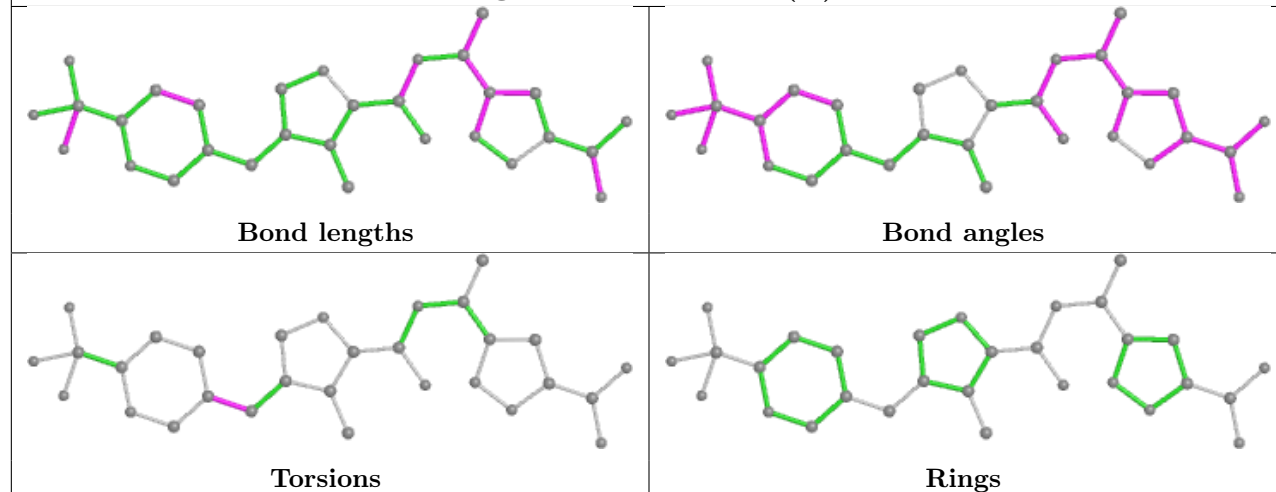




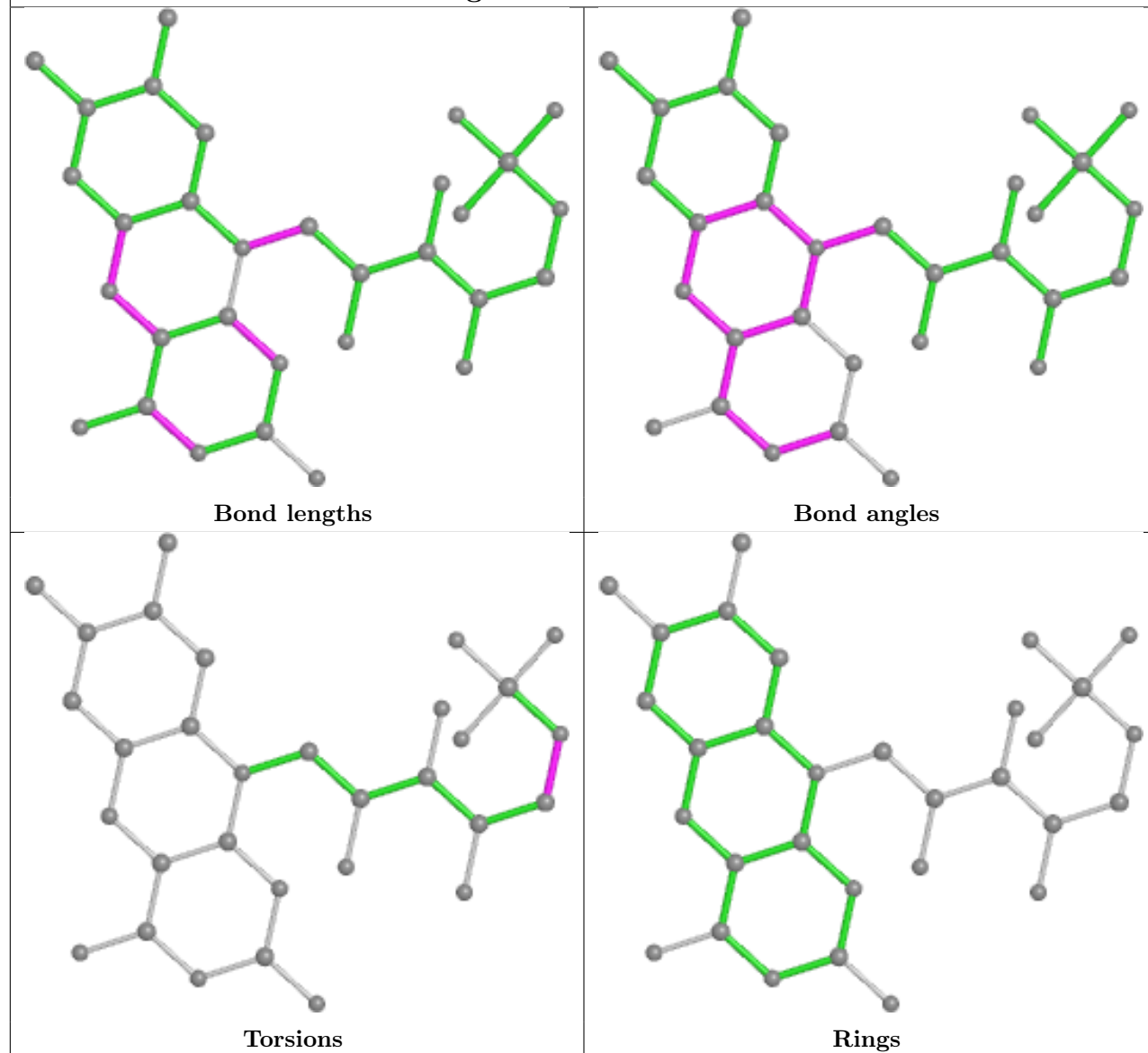
Ligand FMN A 1002



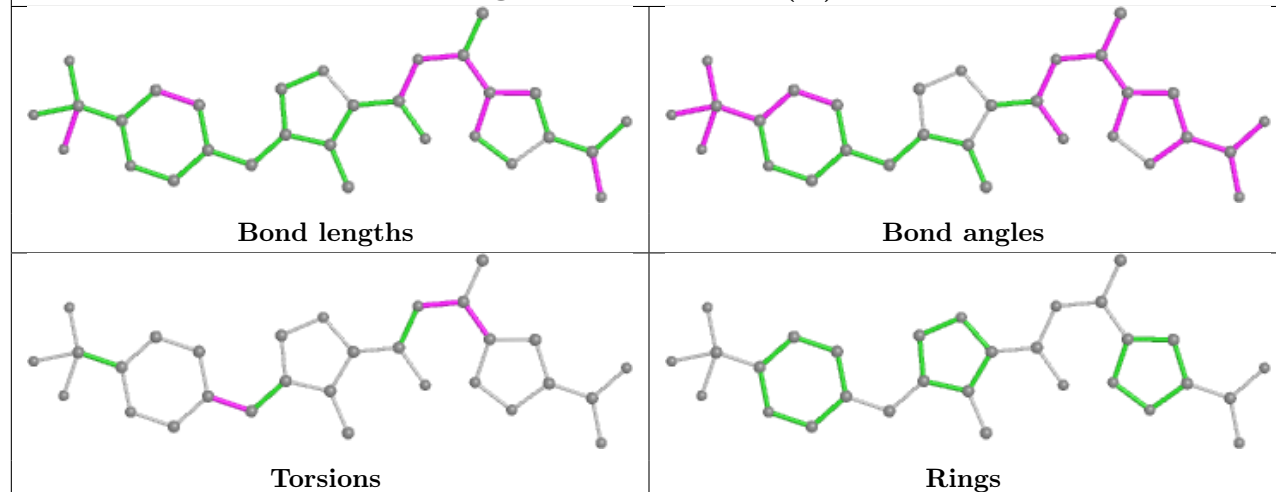
Ligand XE7 A 1001 (B)

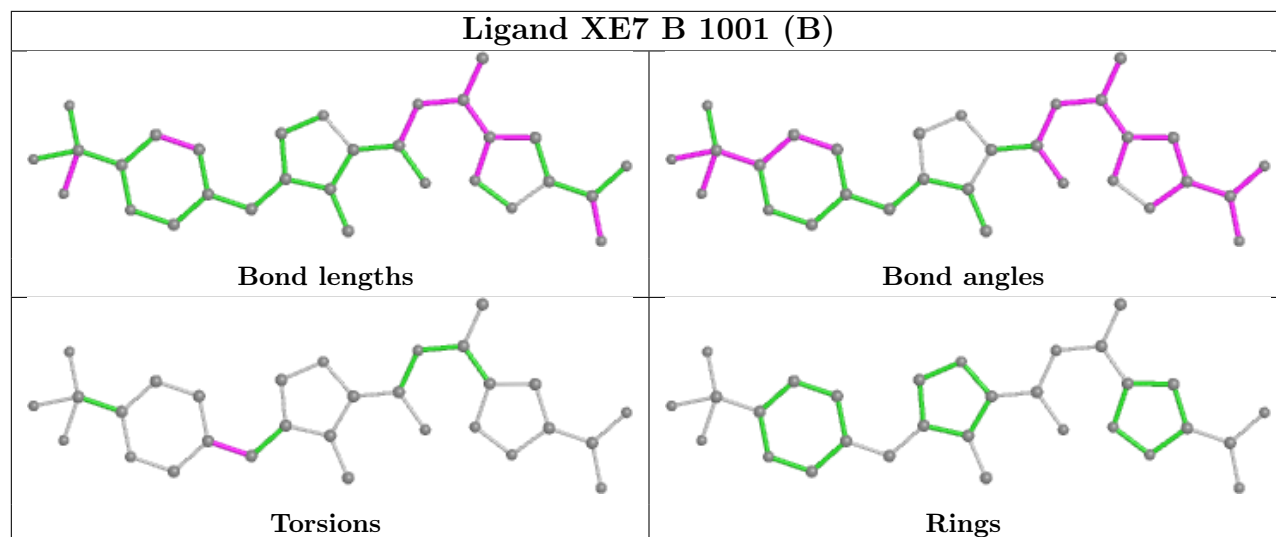


Ligand FMN B 1002



Ligand XE7 A 1001 (A)





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	381/401 (95%)	0.36	35 (9%) 9 14	13, 30, 58, 91	0
1	B	371/401 (92%)	0.42	38 (10%) 6 11	14, 31, 60, 78	0
All	All	752/802 (93%)	0.39	73 (9%) 7 12	13, 30, 59, 91	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	THR	6.9
1	A	158	PHE	6.4
1	A	464	ASN	5.1
1	A	161	TYR	5.0
1	A	379	ILE	5.0
1	B	349	PRO	5.0
1	A	203	ASN	4.3
1	A	201	THR	4.2
1	B	466	ILE	4.1
1	B	161	TYR	4.1
1	B	302	LEU	3.8
1	A	178	TYR	3.8
1	A	194	TYR	3.8
1	A	463	ILE	3.7
1	A	556	TYR	3.5
1	B	376	LYS	3.5
1	B	178	TYR	3.4
1	A	467	LYS	3.4
1	A	471	ASN	3.4
1	B	351	LEU	3.3
1	B	354	ASN	3.3
1	B	463	ILE	3.2
1	B	414	PHE	3.2
1	A	-1	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	194	TYR	3.1
1	B	556	TYR	3.1
1	B	471	ASN	3.0
1	A	473	LYS	3.0
1	B	353	ASP	3.0
1	B	261	PRO	3.0
1	A	159	GLU	2.9
1	B	174	PHE	2.8
1	B	264	PHE	2.8
1	A	206	ILE	2.8
1	B	203	ASN	2.8
1	B	301	LYS	2.8
1	A	223	VAL	2.7
1	B	473	LYS	2.7
1	B	464	ASN	2.7
1	A	567	SER	2.7
1	B	352	ARG	2.6
1	B	166	PHE	2.5
1	A	466	ILE	2.5
1	B	259	ALA	2.5
1	B	465	ASP	2.5
1	A	227	PHE	2.5
1	B	224	ALA	2.4
1	A	470	GLU	2.4
1	A	528	TYR	2.4
1	B	207	TYR	2.4
1	A	469	PHE	2.4
1	B	528	TYR	2.4
1	A	245	ILE	2.4
1	B	206	ILE	2.3
1	A	414	PHE	2.3
1	B	223	VAL	2.3
1	A	261	PRO	2.3
1	B	355	GLN	2.3
1	B	225	ALA	2.2
1	B	170	ILE	2.2
1	B	341	ILE	2.2
1	B	159	GLU	2.2
1	A	224	ALA	2.2
1	A	244	PHE	2.1
1	A	465	ASP	2.1
1	B	467	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	455	ILE	2.1
1	A	302	LEU	2.1
1	A	376	LYS	2.1
1	A	468	SER	2.0
1	A	166	PHE	2.0
1	A	512	LEU	2.0
1	A	340	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

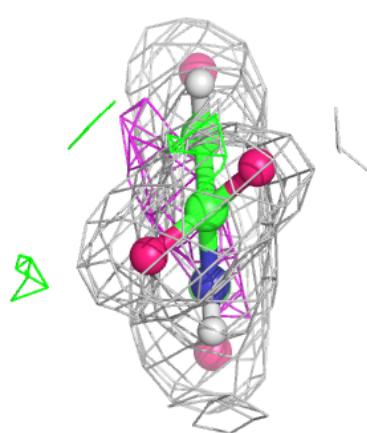
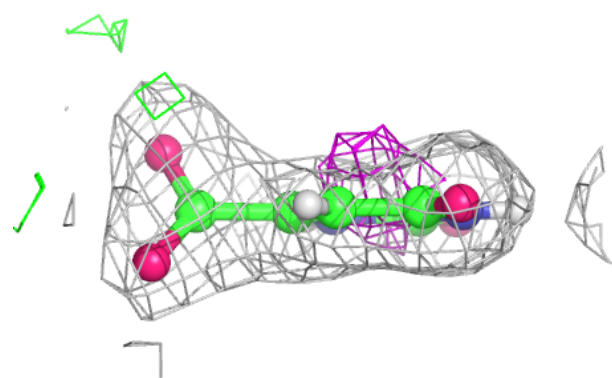
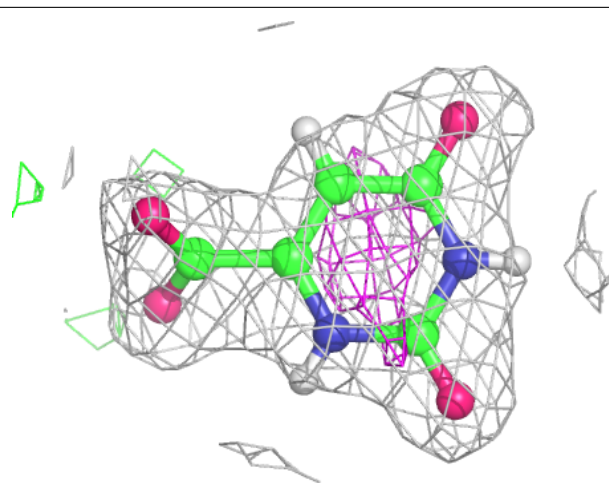
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ORO	A	1003	11/11	0.91	0.10	28,33,37,39	0
2	XE7	A	1001[B]	30/30	0.93	0.15	29,35,41,44	49
2	XE7	B	1001[A]	30/30	0.93	0.12	30,37,47,52	49
2	XE7	B	1001[B]	30/30	0.93	0.12	30,37,42,48	49
2	XE7	A	1001[A]	30/30	0.93	0.15	29,36,42,48	49
4	ORO	B	1003	11/11	0.94	0.10	31,36,42,44	0
3	FMN	A	1002	31/31	0.98	0.17	14,21,31,31	0
3	FMN	B	1002	31/31	0.98	0.17	16,22,31,37	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.

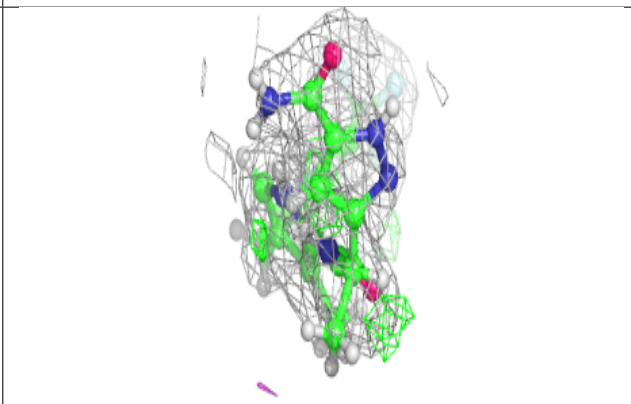
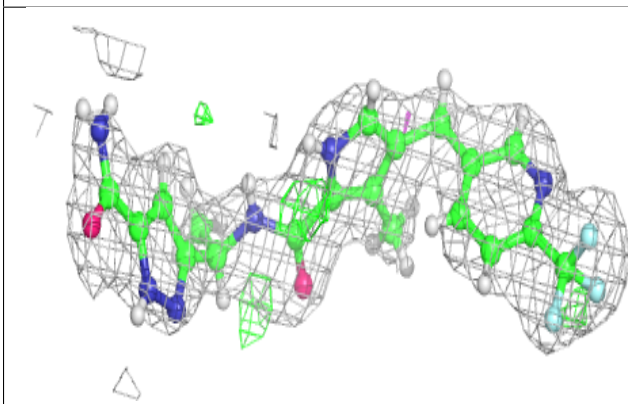
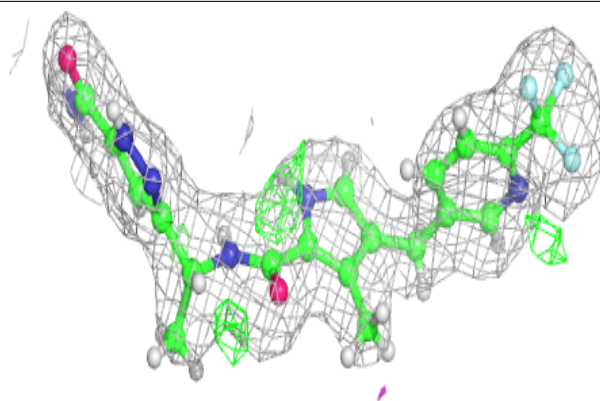
Electron density around ORO A 1003:

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

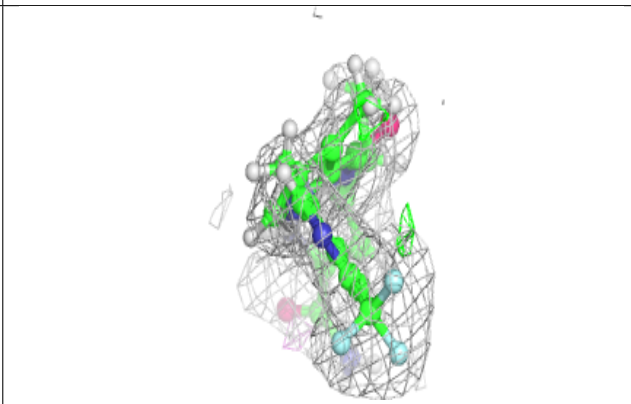
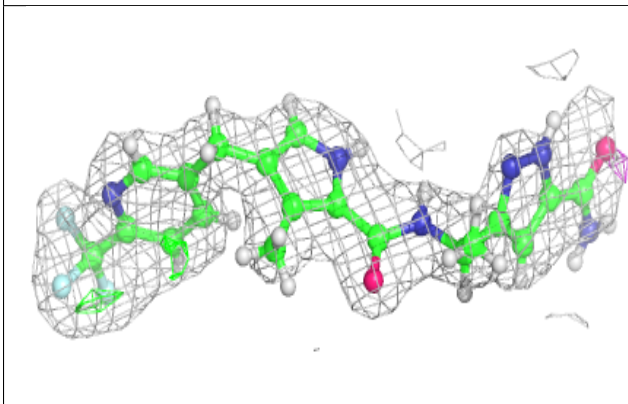
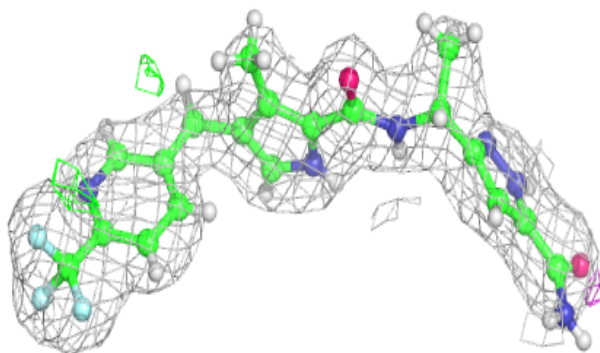


Electron density around XE7 A 1001 (B):

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

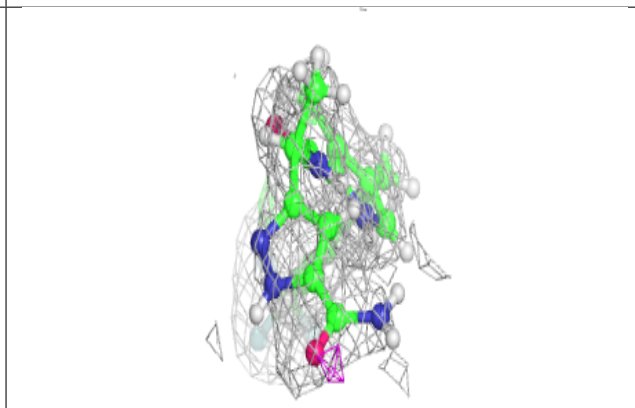
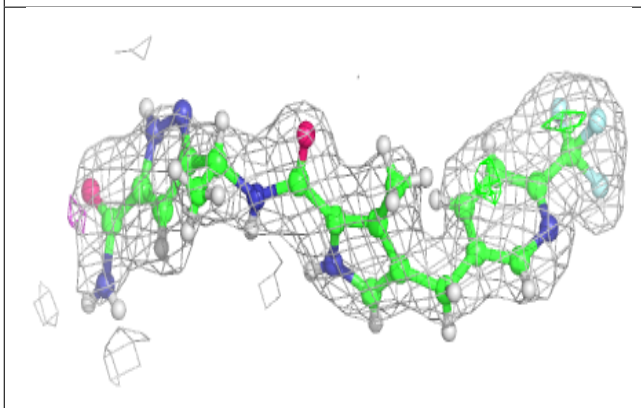
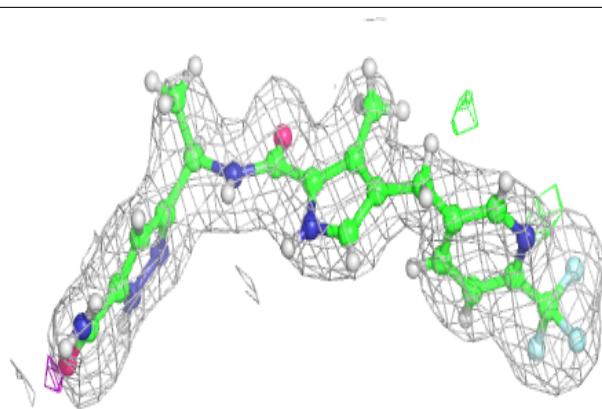
**Electron density around XE7 B 1001 (A):**

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

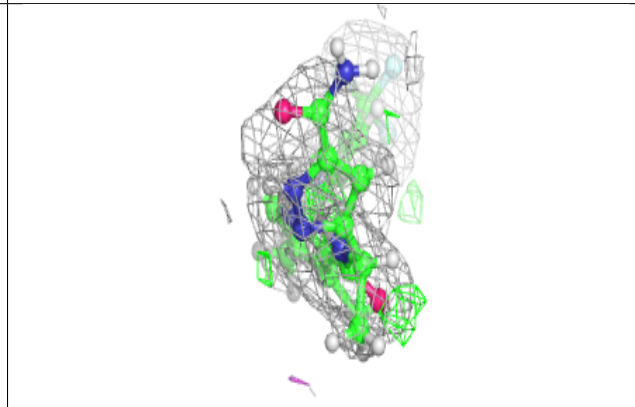
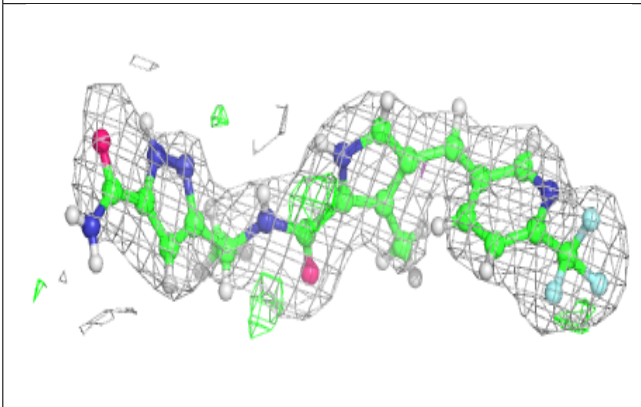
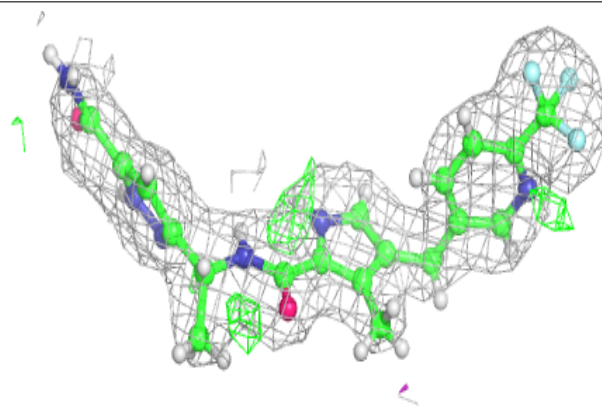


Electron density around XE7 B 1001 (B):

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

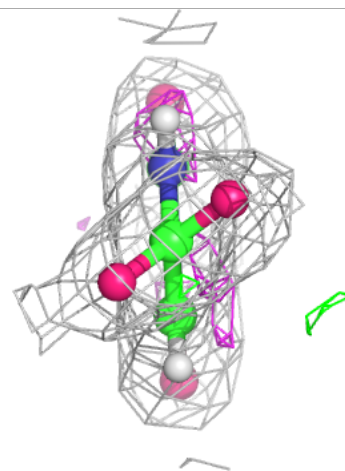
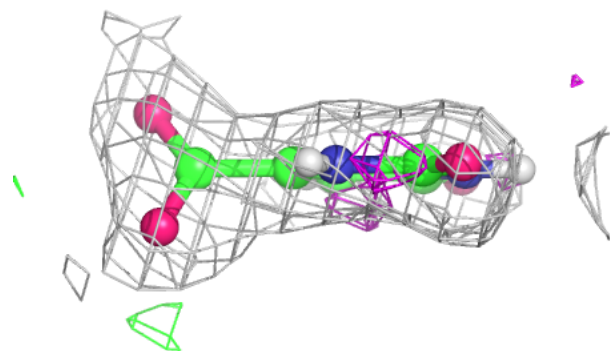
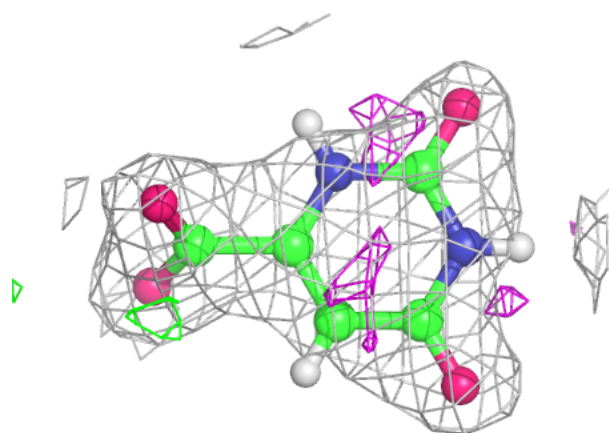
**Electron density around XE7 A 1001 (A):**

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



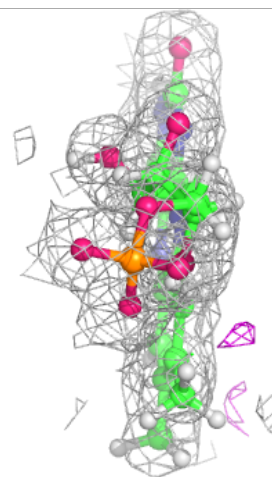
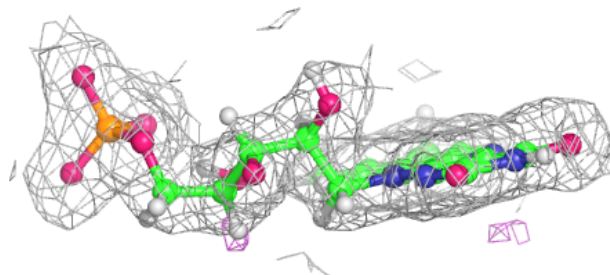
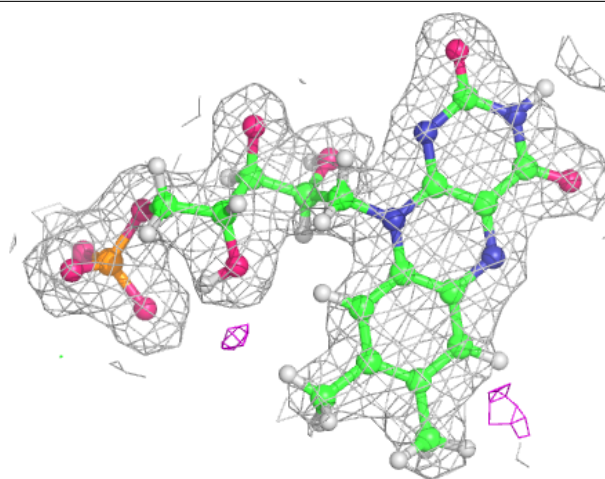
Electron density around ORO B 1003:

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



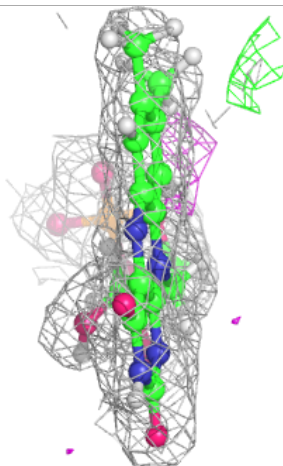
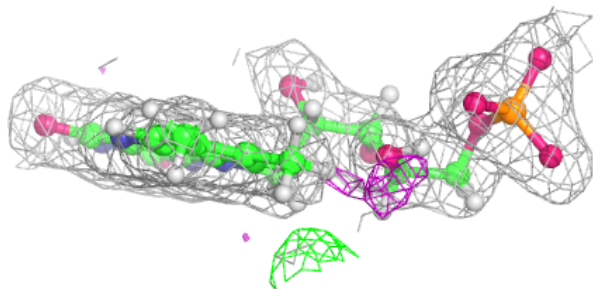
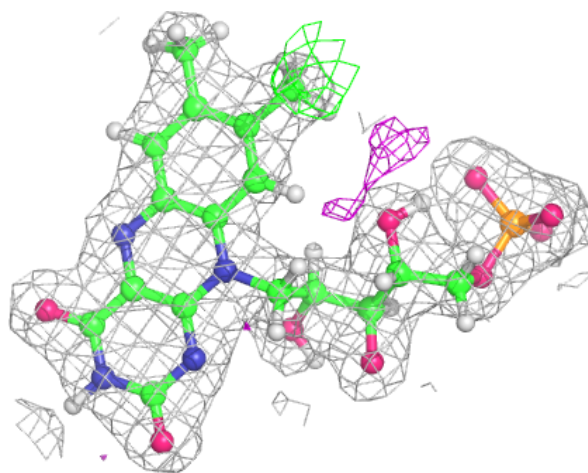
Electron density around FMN A 1002:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.