

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 03:34 PM EDT

PDB ID	:	7L0K
Title	:	Crystal structure of Plasmodium falciparum dihydroorotate dehydrogenase
		bound with Inhibitor DSM784 (3-(1-(3-methyl-4-((6-(trifluoromethyl)py
		ridin-3-yl) methyl)-1 H-pyrrole-2-carboxamido) ethyl)-1 H-pyrazole-5-carboxamido) ethyl H-pyrazole-5-carboxamid
		de)
Authors	:	Deng, X.; Phillips, M.; Tomchick, D.
Deposited on		
Resolution	:	1.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) 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 : 2.35.1	
buster-report : $1.1.7$ (2018)	
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2	019)
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) : 2.35.1	

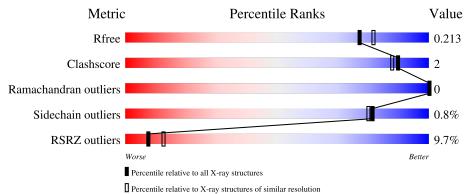


1 Overall quality at a glance (i)

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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 <=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	А	401	9%	5% 5%
1	В	401	9%	• 7%



2 Entry composition (i)

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			Atom	IS			ZeroOcc	AltConf	Trace
1	Δ	381	Total	С	Η	Ν	0	\mathbf{S}	0	2	0
	A	301	6105	1939	3071	507	572	16	0	5	U
1	р	371	Total	С	Η	Ν	0	S	0	2	0
1	D	571	5956	1892	3001	495	553	15	0	3	0

$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	Chain	Residue	Modelled	Actual	Comment	Reference
A-17HIS-expression tagUNP Q08210A-16HIS-expression tagUNP Q08210A-15HIS-expression tagUNP Q08210A-14HIS-expression tagUNP Q08210A-13HIS-expression tagUNP Q08210A-12HIS-expression tagUNP Q08210A-11ALA-expression tagUNP Q08210A-10GLU-expression tagUNP Q08210A-10GLU-expression tagUNP Q08210A-9ASN-expression tagUNP Q08210A-9ASN-expression tagUNP Q08210A-6PHE-expression tagUNP Q08210A-6PHE-expression tagUNP Q08210A-5GLN-expression tagUNP Q08210A-4GLY-expression tagUNP Q08210A-3ALA-expression tagUNP Q08210A-3ALA-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A-1PRO-exp	А	-19	MET	-	initiating methionine	UNP Q08210
A-16HIS-expression tagUNP Q08210A-15HIS-expression tagUNP Q08210A-14HIS-expression tagUNP Q08210A-13HIS-expression tagUNP Q08210A-13HIS-expression tagUNP Q08210A-12HIS-expression tagUNP Q08210A-11ALA-expression tagUNP Q08210A-10GLU-expression tagUNP Q08210A-9ASN-expression tagUNP Q08210A-9ASN-expression tagUNP Q08210A-9ASN-expression tagUNP Q08210A-5GLN-expression tagUNP Q08210A-6PHE-expression tagUNP Q08210A-5GLN-expression tagUNP Q08210A-3ALA-expression tagUNP Q08210A-2ASP-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A-1PRO-expr	А	-18	GLY	-	expression tag	UNP Q08210
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-17	HIS	-	expression tag	UNP Q08210
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-16	HIS	-	expression tag	UNP Q08210
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	A	-15	HIS	-	expression tag	UNP Q08210
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-14	HIS	-	expression tag	UNP Q08210
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-13	HIS	-	expression tag	UNP Q08210
A-10GLU-expression tagUNP Q08210A-9ASN-expression tagUNP Q08210A-8LEU-expression tagUNP Q08210A-7TYR-expression tagUNP Q08210A-6PHE-expression tagUNP Q08210A-6PHE-expression tagUNP Q08210A-5GLN-expression tagUNP Q08210A-3ALA-expression tagUNP Q08210A-3ALA-expression tagUNP Q08210A-2ASP-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A?-SERdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-GLUdeletionUNP Q08210A?-TYRdeletionUNP Q08210	А	-12	HIS	-	expression tag	UNP Q08210
A-9ASN-expression tagUNP Q08210A-8LEU-expression tagUNP Q08210A-7TYR-expression tagUNP Q08210A-6PHE-expression tagUNP Q08210A-5GLN-expression tagUNP Q08210A-5GLN-expression tagUNP Q08210A-4GLY-expression tagUNP Q08210A-3ALA-expression tagUNP Q08210A-2ASP-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A?-SERdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-GLUdeletionUNP Q08210A?-TYRdeletionUNP Q08210	А	-11	ALA	-	expression tag	UNP Q08210
A-8LEU-expression tagUNP Q08210A-7TYR-expression tagUNP Q08210A-6PHE-expression tagUNP Q08210A-5GLN-expression tagUNP Q08210A-4GLY-expression tagUNP Q08210A-4GLY-expression tagUNP Q08210A-3ALA-expression tagUNP Q08210A-2ASP-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A?-SERdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-GLUdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А	-10	GLU	-	expression tag	UNP Q08210
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-9	ASN	-	expression tag	UNP Q08210
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	-8	LEU	-	expression tag	UNP Q08210
A-5GLN-expression tagUNP Q08210A-4GLY-expression tagUNP Q08210A-3ALA-expression tagUNP Q08210A-2ASP-expression tagUNP Q08210A-2ASP-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A?-SERdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-TYRdeletionUNP Q08210A?-GLUdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А	-7	TYR	-	expression tag	UNP Q08210
A-4GLY-expression tagUNP Q08210A-3ALA-expression tagUNP Q08210A-2ASP-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A?-SERdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-GLUdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А	-6	PHE	-	expression tag	UNP Q08210
A-3ALA-expression tagUNP Q08210A-2ASP-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A?-SERdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-TKRdeletionUNP Q08210A?-GLUdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А	-5	GLN	-	expression tag	UNP Q08210
A-2ASP-expression tagUNP Q08210A-1PRO-expression tagUNP Q08210A?-SERdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-TKRdeletionUNP Q08210A?-GLUdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А	-4	GLY	-	expression tag	UNP Q08210
A-1PRO-expression tagUNP Q08210A?-SERdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-TYRdeletionUNP Q08210A?-TYRdeletionUNP Q08210A?-GLUdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А	-3	ALA	-	expression tag	UNP Q08210
A?-SERdeletionUNP Q08210A?-THRdeletionUNP Q08210A?-TYRdeletionUNP Q08210A?-ASNdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А	-2	ASP	-	expression tag	UNP Q08210
A?-THRdeletionUNP Q08210A?-TYRdeletionUNP Q08210A?-ASNdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А		PRO	-	expression tag	UNP Q08210
A?-TYRdeletionUNP Q08210A?-ASNdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А	?	-	SER	deletion	UNP Q08210
A?-ASNdeletionUNP Q08210A?-GLUdeletionUNP Q08210	А		-	THR	deletion	UNP Q08210
A ? - GLU deletion UNP Q08210	А		-	TYR	deletion	UNP Q08210
	A		-	ASN	deletion	UNP Q08210
A ? - ASP deletion UNP Q08210	А		-	GLU	deletion	UNP Q08210
	А	?	-	ASP	deletion	UNP Q08210

There are 98 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	?	-	ASN	deletion	UNP Q08210
А	?	-	LYS	deletion	UNP Q08210
А	?	-	ILE	deletion	UNP Q08210
А	?	-	VAL	deletion	UNP Q08210
А	?	-	GLU	deletion	UNP Q08210
А	?	-	LYS	deletion	UNP Q08210
А	?	_	LYS	deletion	UNP Q08210
А	?	-	ASN	deletion	UNP Q08210
А	?	-	ASN	deletion	UNP Q08210
А	?	-	PHE	deletion	UNP Q08210
А	?	-	ASN	deletion	UNP Q08210
А	?	-	LYS	deletion	UNP Q08210
А	?	-	ASN	deletion	UNP Q08210
А	?	-	ASN	deletion	UNP Q08210
А	?	-	SER	deletion	UNP Q08210
А	?	-	HIS	deletion	UNP Q08210
А	?	-	MET	deletion	UNP Q08210
А	?	-	MET	deletion	UNP Q08210
А	?	-	LYS	deletion	UNP Q08210
А	?	-	ASP	deletion	UNP Q08210
А	?	-	ALA	deletion	UNP Q08210
А	?	-	LYS	deletion	UNP Q08210
А	?	-	ASP	deletion	UNP Q08210
А	?	-	ASN	deletion	UNP Q08210
В	139	MET	-	initiating methionine	UNP Q08210
В	140	GLY	-	expression tag	UNP Q08210
В	141	HIS	-	expression tag	UNP Q08210
В	142	HIS	-	expression tag	UNP Q08210
В	143	HIS	-	expression tag	UNP Q08210
В	144	HIS	-	expression tag	UNP Q08210
В	145	HIS	-	expression tag	UNP Q08210
В	146	HIS	-	expression tag	UNP Q08210
В	147	ALA	-	expression tag	UNP Q08210
В	148	GLU	-	expression tag	UNP Q08210
В	149	ASN	-	expression tag	UNP Q08210
В	150	LEU	-	expression tag	UNP Q08210
В	151	TYR	-	expression tag	UNP Q08210
В	152	PHE	-	expression tag	UNP Q08210
В	153	GLN	-	expression tag	UNP Q08210
В	154	GLY	-	expression tag	UNP Q08210
В	155	ALA	-	expression tag	UNP Q08210
В	156	ASP	-	expression tag	UNP Q08210

Continued from previous page...

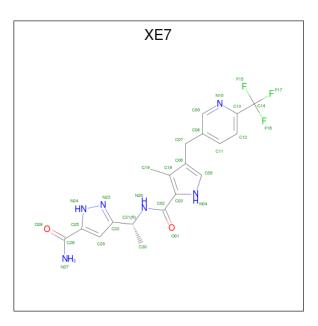


Chain	Residue	Modelled	Actual	Comment	Reference
В	157	PRO	-	expression tag	UNP Q08210
В	?	_	SER	deletion	UNP Q08210
В	?	_	THR	deletion	UNP Q08210
В	?	-	TYR	deletion	UNP Q08210
В	?	-	ASN	deletion	UNP Q08210
В	?	_	GLU	deletion	UNP Q08210
В	?	_	ASP	deletion	UNP Q08210
В	?	-	ASN	deletion	UNP Q08210
В	?	-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

Continued from previous page...

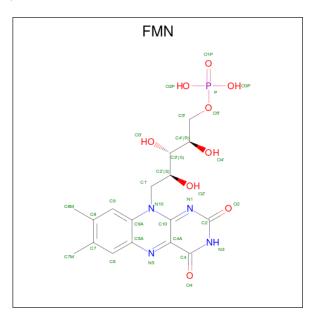
• Molecule 2 is 3-{(1R)-1-[(3-methyl-4-{[6-(trifluoromethyl)pyridin-3-yl]methyl}-1H-pyrrol e-2-carbonyl)amino]ethyl}-1H-pyrazole-5-carboxamide (three-letter code: XE7) (formula: $C_{19}H_{19}F_3N_6O_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		P	Ator	ns			ZeroOcc	AltConf		
2	Λ	1	Total	С	F	Η	Ν	0	0	1		
	A	A	A	1	98	38	6	38	12	4	0	1
0	В	1	Total	С	F	Η	Ν	0	0	1		
	D	1	98	38	6	38	12	4	0	1		

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



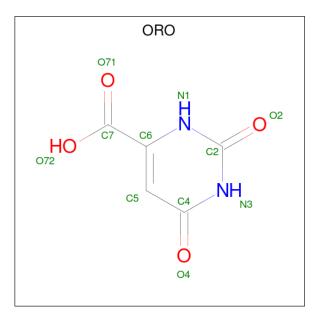
Mol	Chain	Residues		A	tom	IS			ZeroOcc	AltConf
3	А	1	Total 49	C 17	Н 18	N 4	0 9	Р 1	0	0



Continued from previous page...

			1
$\begin{vmatrix} 3 \\ 3 \end{vmatrix} = \begin{vmatrix} B \\ 1 \end{vmatrix} = \begin{vmatrix} Total \\ 49 \\ 17 \\ 18 \\ 4 \end{vmatrix}$	O P 9 1	0	0

• 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		Ate	oms			ZeroOcc	AltConf
4	Λ	1	Total	С	Η	Ν	0	0	0
4	Л	1	14	5	3	2	4	0	0
4	В	1	Total	С	Η	Ν	Ο	0	0
4	D	1	14	5	3	2	4		0

• Molecule 5 is water.

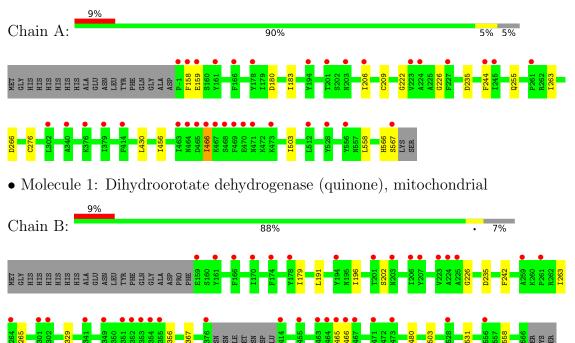
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	161	Total O 161 161	0	0
5	В	155	Total O 155 155	0	0



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: Dihydroorotate dehydrogenase (quinone), mitochondrial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	52.12Å 158.34Å 62.77Å	Depositor
a, b, c, α , β , γ	90.00° 107.28° 90.00°	Depositor
Resolution (Å)	36.21 - 1.96	Depositor
Resolution (A)	36.21 - 1.96	EDS
% Data completeness	85.8 (36.21-1.96)	Depositor
(in resolution range)	85.8 (36.21-1.96)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.46 (at 1.95 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D.	0.179 , 0.213	Depositor
R, R_{free}	0.179 , 0.213	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	$ < L >=0.48, < L^2>=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.

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.



¹Intensities estimated from amplitudes.

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.36	0/3098	0.59	0/4172	
1	В	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	А	3034	3071	3061	12	0
1	В	2955	3001	2989	10	0
2	А	60	38	0	0	0
2	В	60	38	0	0	0
3	А	31	18	19	1	0
3	В	31	18	19	1	0
4	А	11	3	3	0	0
4	В	11	3	3	0	0
5	А	161	0	0	1	0
5	В	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.

The worst 5 of 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

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	А	382/401~(95%)	368~(96%)	14 (4%)	0	100 100
1	В	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 (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	А	341/354~(96%)	339~(99%)	2(1%)	86 85
1	В	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	А	235	ASP
1	А	466	ILE
1	В	202	SER
1	В	235	ASP
1	В	356	GLU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	Turne	Chain	Res	Link	Bo	ond leng	ths	B	Bond angles	
10101	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMN	А	1002	-	33,33,33	1.11	2 (6%)	48,50,50	1.25	7 (14%)
2	XE7	А	1001[A]	-	30,32,32	2.04	8 (26%)	30,47,47	4.50	13 (43%)
3	FMN	В	1002	-	33,33,33	1.00	1 (3%)	48,50,50	1.31	6 (12%)
4	ORO	А	1003	-	9,11,11	1.38	1 (11%)	8,15,15	2.03	2 (25%)
2	XE7	А	1001[B]	-	30,32,32	1.84	8 (26%)	30,47,47	2.56	14 (46%)
2	XE7	В	1001[A]	-	30,32,32	1.90	8 (26%)	30,47,47	2.97	11 (36%)
2	XE7	В	1001[B]	-	30,32,32	2.00	9 (30%)	30,47,47	2.56	12 (40%)
4	ORO	В	1003	-	9,11,11	1.37	1 (11%)	8,15,15	2.58	5 (62%)

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

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	А	1001[A]	XE7	C26-N27	6.10	1.44	1.33
2	В	1001[B]	XE7	C26-N27	4.71	1.42	1.33
2	В	1001[A]	XE7	C26-N27	4.70	1.41	1.33
2	А	1001[B]	XE7	C26-N27	4.61	1.41	1.33
3	А	1002	FMN	C4A-N5	4.59	1.39	1.30

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1001[A]	XE7	C25-C26-N27	18.54	134.59	116.25
2	В	1001[A]	XE7	C25-C26-N27	11.41	127.54	116.25
2	А	1001[A]	XE7	O28-C26-C25	-9.61	111.58	119.61



Continued	from	previous	page	

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1001[B]	XE7	C25-C26-N27	8.06	124.23	116.25
2	В	1001[B]	XE7	C25-C26-N27	7.92	124.09	116.25

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	1003	ORO	N1-C6-C7-O71
4	А	1003	ORO	N1-C6-C7-O72
4	А	1003	ORO	C5-C6-C7-O71
4	А	1003	ORO	C5-C6-C7-O72
4	В	1003	ORO	N1-C6-C7-O71

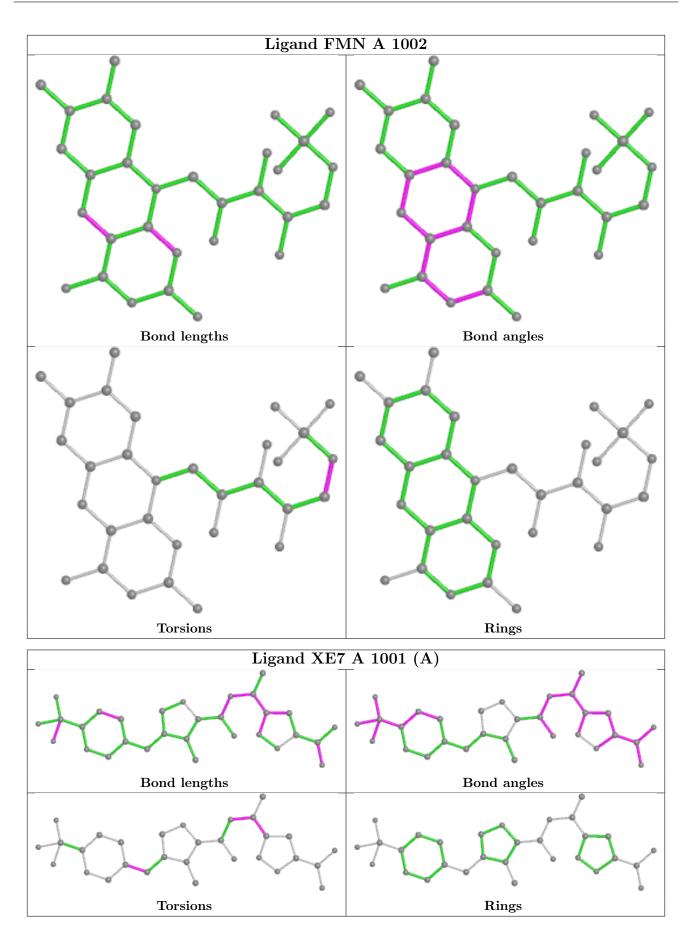
There are no ring outliers.

2 monomers are involved in 2 short contacts:

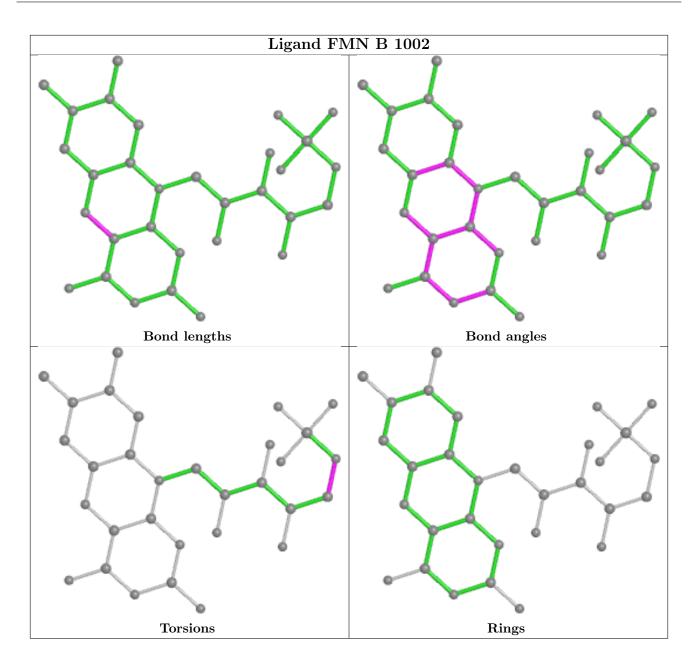
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	1002	FMN	1	0
3	В	1002	FMN	1	0

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 then 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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

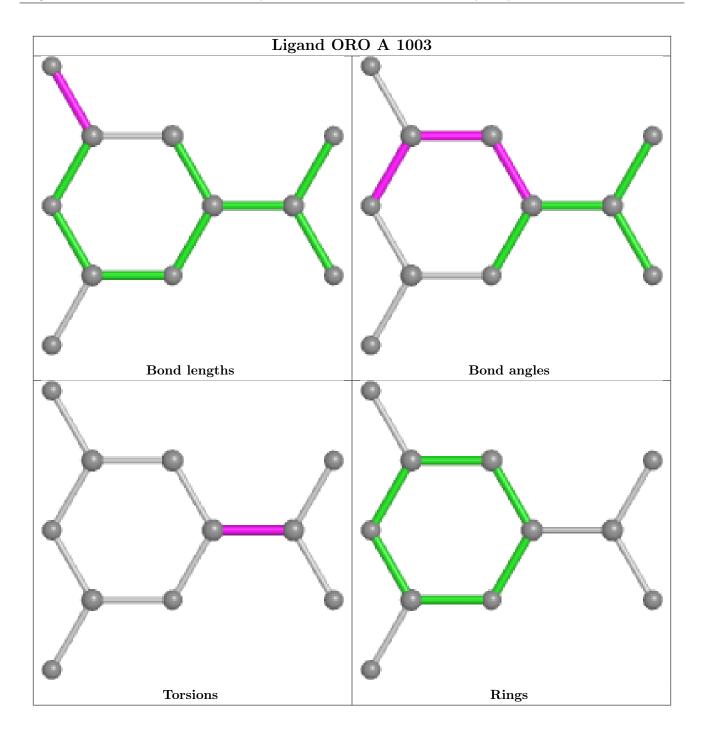






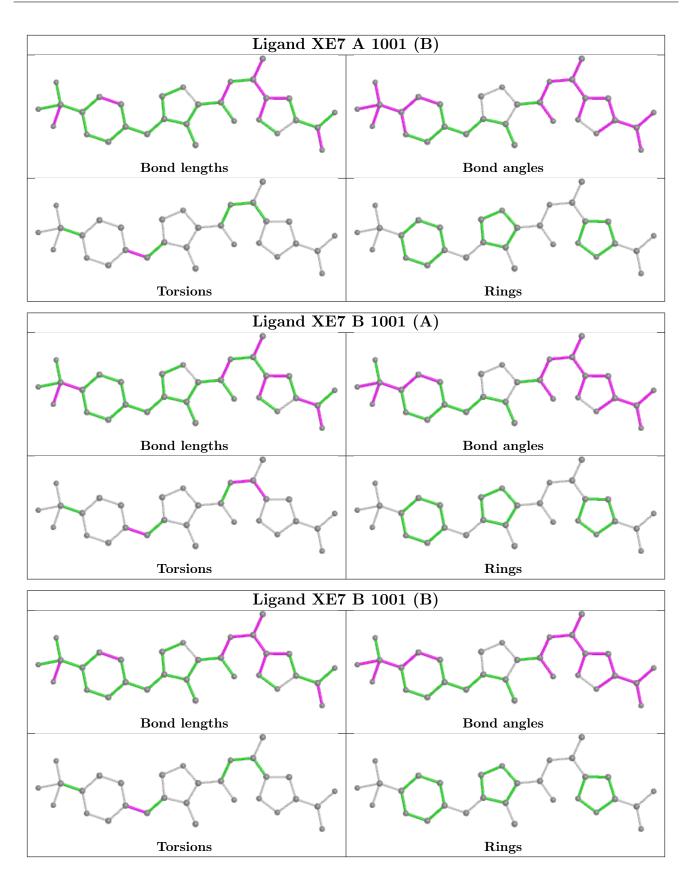




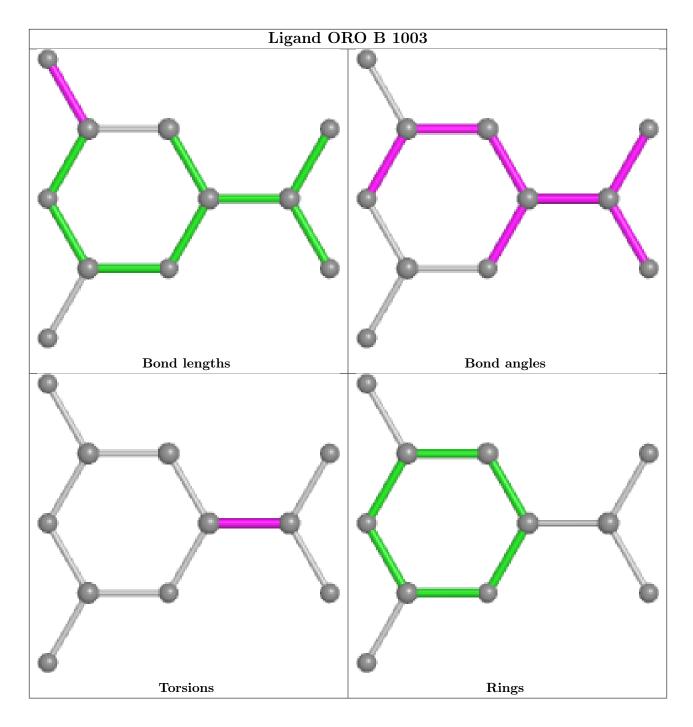












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	381/401~(95%)	0.36	35~(9%) 9	14	13, 30, 58, 91	0
1	В	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

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	201	THR	6.9
1	А	158	PHE	6.4
1	А	464	ASN	5.1
1	А	161	TYR	5.0
1	А	379	ILE	5.0

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.

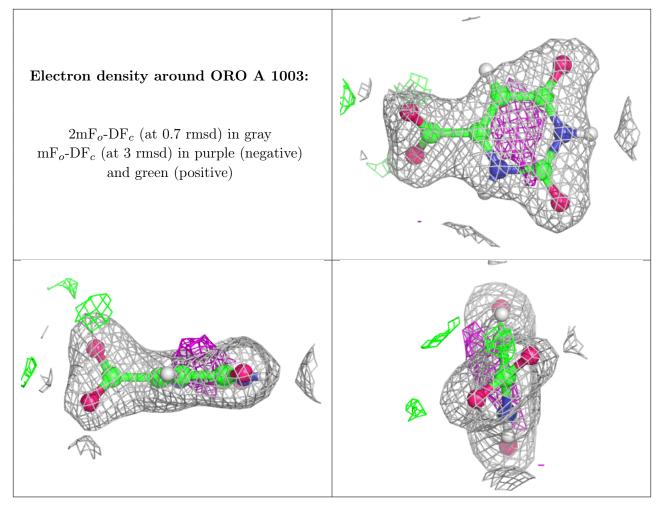
6.4 Ligands (i)

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, 95^{th} 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.

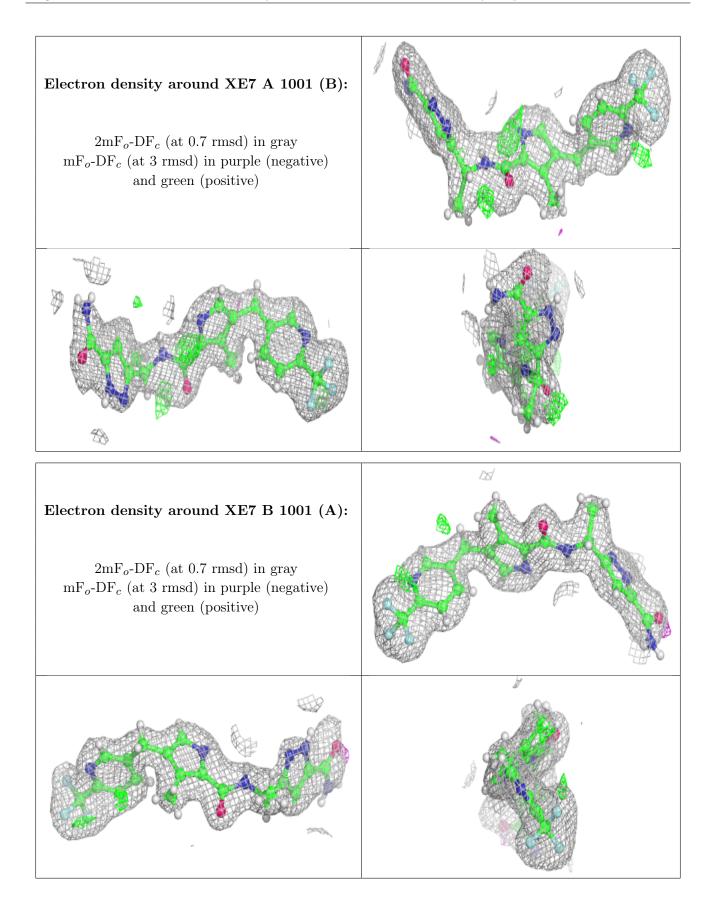


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
4	ORO	А	1003	11/11	0.91	0.10	$28,\!33,\!37,\!39$	0
2	XE7	А	1001[B]	30/30	0.93	0.15	29,35,41,44	49
2	XE7	В	1001[A]	30/30	0.93	0.12	30,37,47,52	49
2	XE7	В	1001[B]	30/30	0.93	0.12	30,37,42,48	49
2	XE7	А	1001[A]	30/30	0.93	0.15	29,36,42,48	49
4	ORO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

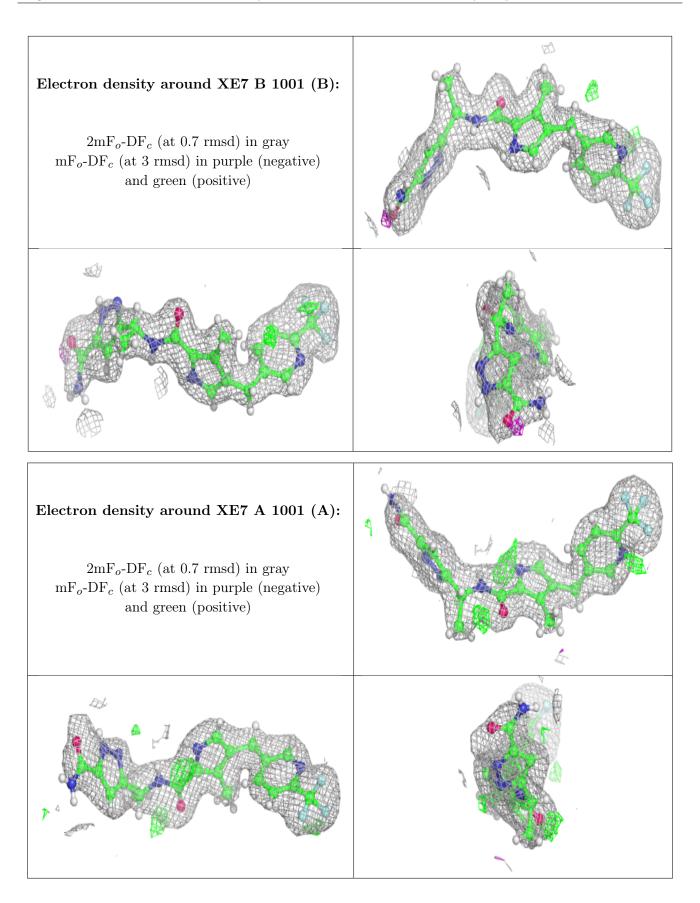
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



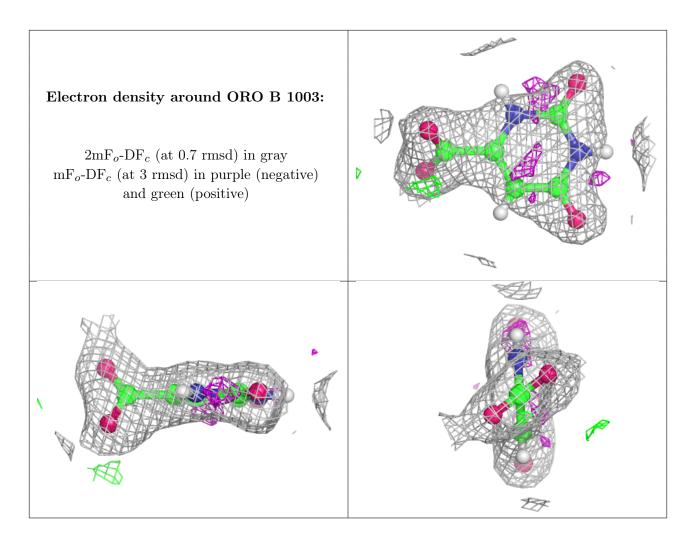




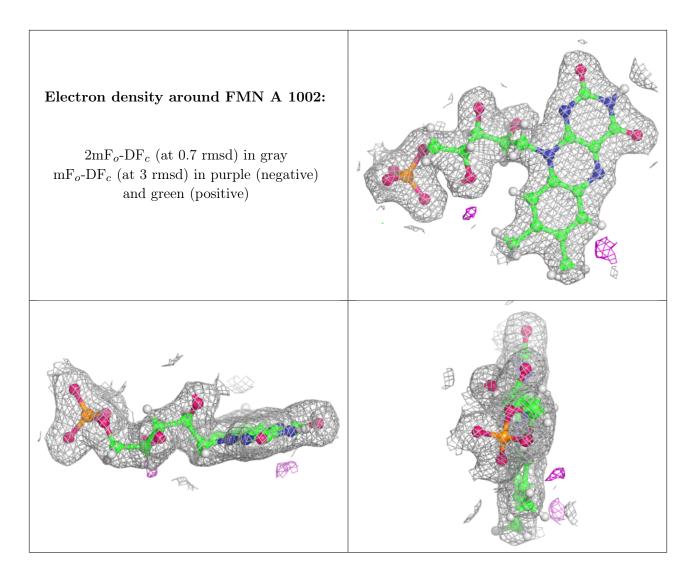




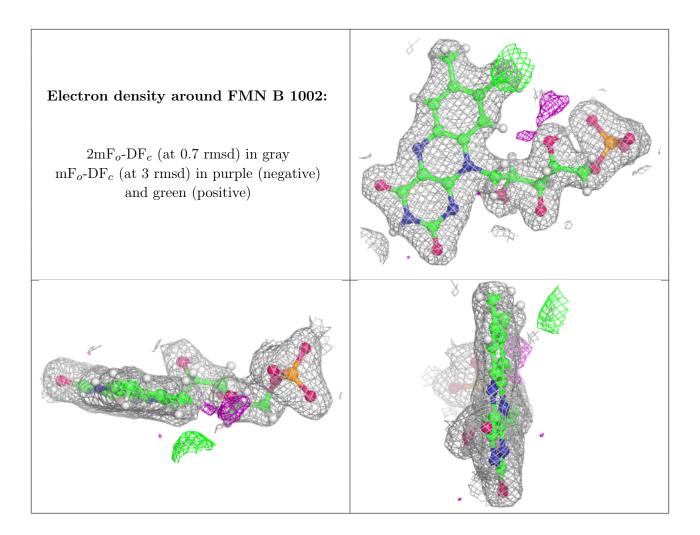












6.5 Other polymers (i)

There are no such residues in this entry.

