



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2021 – 06:12 PM EDT

PDB ID : 7S87
Title : Crystal Structure of Dihydroorotate dehydrogenase from Plasmodium falciparum in complex with Orotate, FMN, and inhibitor NCGC00600348-01
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-09-17
Resolution : 2.75 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 : 2.23.1
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) : 2.23.1

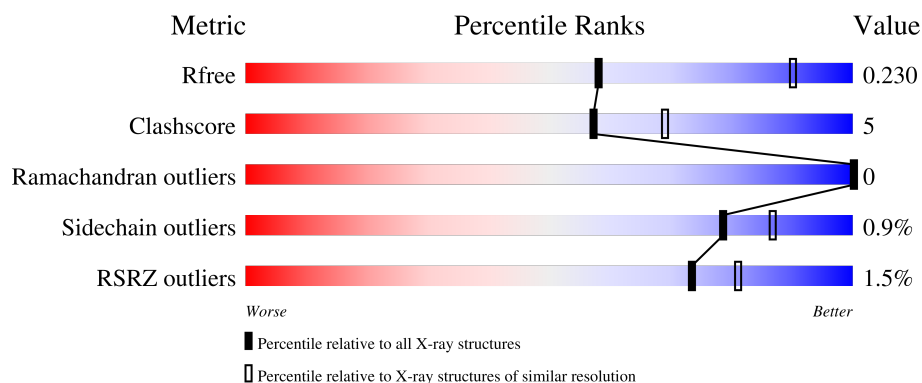
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	 86% 9% 5%
1	B	401	 2% 79% 14% 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5964 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2941	1884	492	551	14			
1	B	373	Total	C	N	O	S	0	1	0
			2740	1758	453	515	14			

There are 98 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
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

Continued on next page...

Continued from previous page...

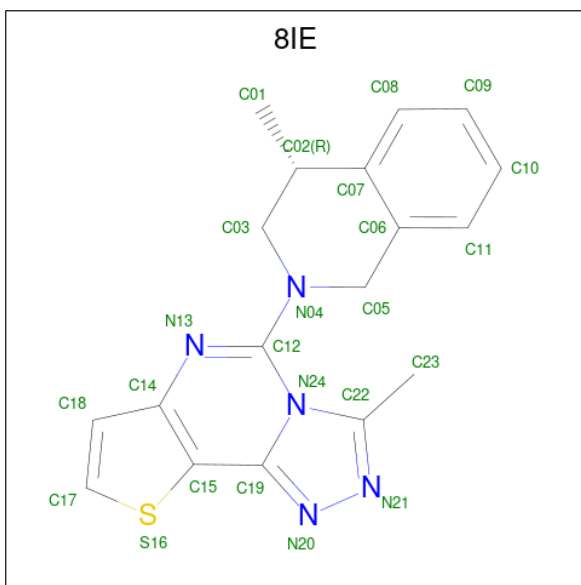
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ILE	deletion	UNP Q08210
A	?	-	VAL	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	ASN	deletion	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

Continued on next page...

Continued from previous page...

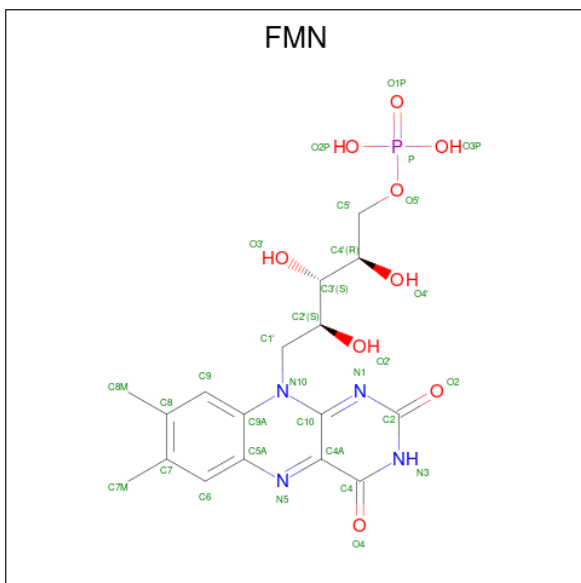
Chain	Residue	Modelled	Actual	Comment	Reference
B	157	PRO	-	expression tag	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	THR	deletion	UNP Q08210
B	?	-	TYR	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	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 (4R)-3-methyl-5-[(4R)-4-methyl-3,4-dihydroisoquinolin-2(1H)-yl]thieno[2,3-e][1,2,4]triazolo[4,3-c]pyrimidine (three-letter code: 8IE) (formula: C₁₈H₁₇N₅S) (labeled as "Ligand of Interest" by depositor).



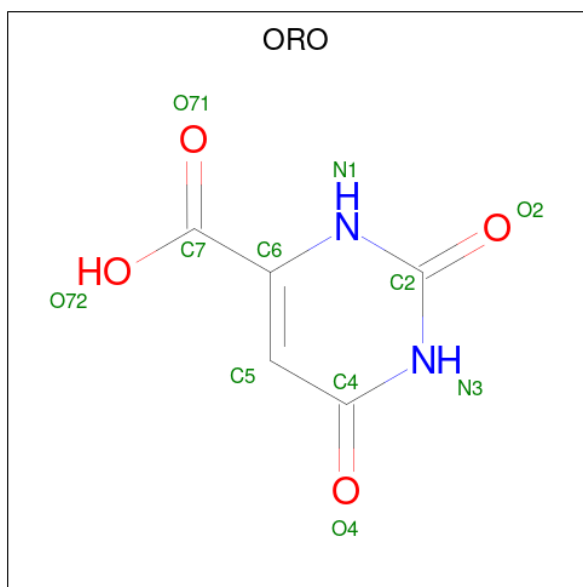
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			24	18	5	1		
2	A	1	Total	C	N	S	0	0
			24	18	5	1		
2	B	1	Total	C	N	S	0	0
			24	18	5	1		
2	B	1	Total	C	N	S	0	0
			24	18	5	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



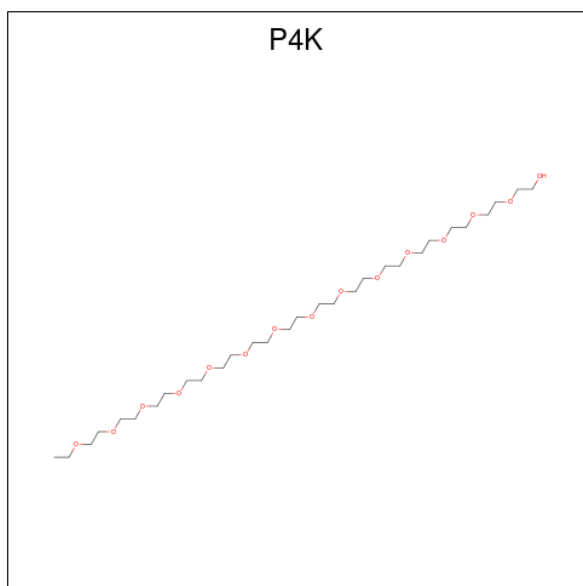
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	5	2	4		
4	B	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



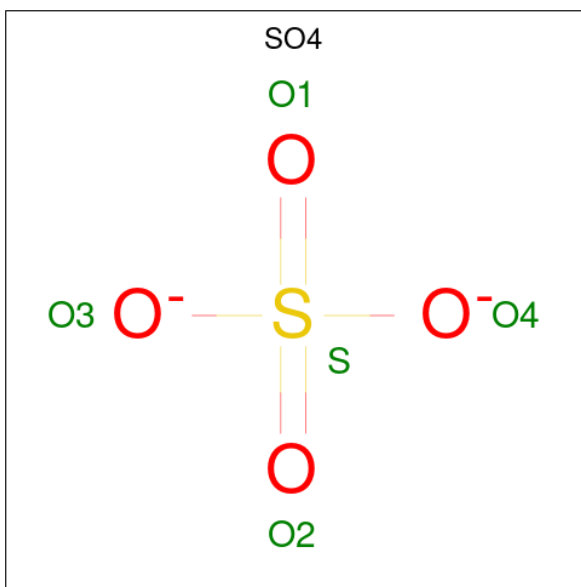
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is polyethylene glycol (three-letter code: P4K) (formula: C₃₀H₆₂O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	7	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		


- Molecule 8 is water.

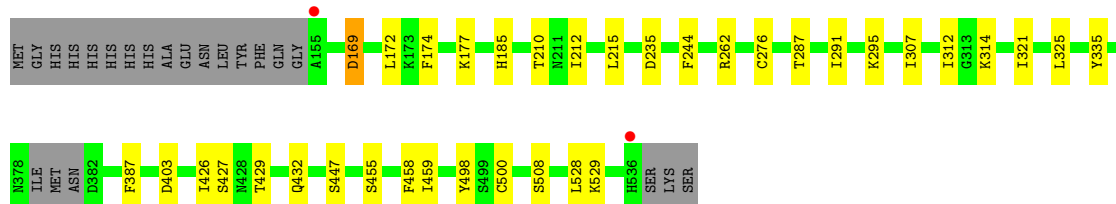
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	60	Total	O	0	0
			60	60		
8	B	19	Total	O	0	0
			19	19		

3 Residue-property plots


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.

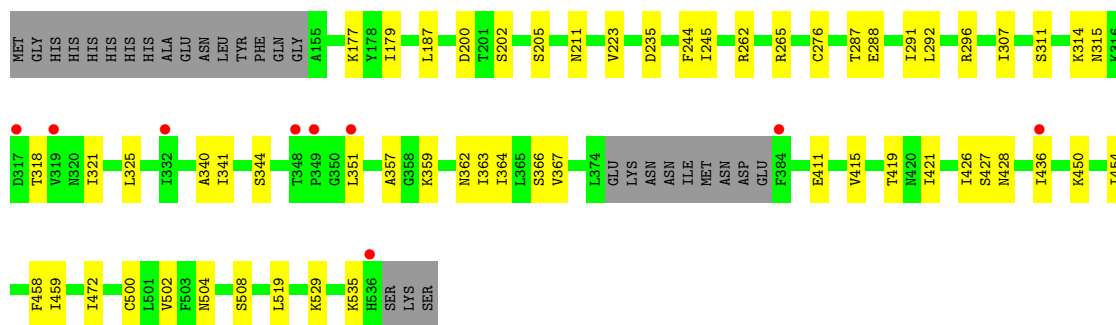
- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial

Chain A: 



- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.73Å 161.09Å 92.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.50 – 2.75 67.49 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.0 (67.50-2.75) 98.0 (67.49-2.75)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.170 , 0.230 0.170 , 0.230	Depositor DCC
R_{free} test set	1251 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5964	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: 8IE, FMN, P4K, SO4, ORO, ACT

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	0.35	0/2993	0.50	0/4042
1	B	0.32	0/2792	0.51	0/3794
All	All	0.34	0/5785	0.51	0/7836

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	535	LYS	Peptide

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	2941	0	2919	21	0
1	B	2740	0	2571	36	0
2	A	48	0	0	1	0
2	B	48	0	0	1	0
3	A	31	0	19	1	0
3	B	31	0	19	0	0
4	A	11	0	3	0	0
4	B	11	0	3	0	0
5	A	4	0	3	0	0
6	A	10	0	0	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	60	0	0	0	0
8	B	19	0	0	0	0
All	All	5964	0	5537	56	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 5.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:SER:HB2	1:B:428:ASN:HB2	1.72	0.72
1:B:292:LEU:O	1:B:296:ARG:HG3	1.99	0.63
1:B:287:THR:O	1:B:291:ILE:HG13	1.99	0.63
1:B:454:ILE:H	1:B:454:ILE:HD12	1.64	0.62
1:B:344:SER:HB2	1:B:428:ASN:CB	2.30	0.61
1:B:288:GLU:O	1:B:292:LEU:HG	2.01	0.59
1:B:436:ILE:HD11	1:B:450:LYS:HD2	1.85	0.59
1:A:498:TYR:HB3	3:A:602:FMN:O2P	2.04	0.56
1:B:341:ILE:HD11	1:B:367:VAL:HG11	1.87	0.56
1:B:362:ASN:O	1:B:366:SER:OG	2.22	0.55
1:A:314:LYS:HB3	1:A:321:ILE:HG13	1.91	0.53
1:A:210:THR:HA	1:A:529:LYS:HE3	1.90	0.53
1:B:357:ALA:HB2	1:B:411:GLU:HG2	1.89	0.53
1:B:364:ILE:HD13	1:B:421:ILE:HD13	1.91	0.52
1:A:291:ILE:O	1:A:295:LYS:HG3	2.11	0.51
1:B:262:ARG:HD2	1:B:276:CYS:HA	1.92	0.51
1:B:223:VAL:HB	1:B:245:ILE:HG13	1.93	0.50
1:B:321:ILE:O	1:B:325:LEU:HG	2.11	0.50
1:B:244:PHE:HB3	1:B:307:ILE:HB	1.93	0.50
1:B:436:ILE:HD11	1:B:450:LYS:CD	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TYR:CD1	1:A:387:PHE:HB3	2.49	0.47
1:B:519:LEU:HD12	1:B:519:LEU:HA	1.68	0.47
1:B:200:ASP:OD1	1:B:202:SER:HB3	2.14	0.47
1:A:312:ILE:HG13	1:A:325:LEU:HD22	1.95	0.47
1:B:426:ILE:HG23	1:B:458:PHE:CD2	2.50	0.46
1:B:459:ILE:HG23	1:B:472:ILE:HD13	1.96	0.46
1:A:403:ASP:OD1	1:A:432:GLN:HG2	2.15	0.46
1:A:210:THR:HB	1:A:528:LEU:HD22	1.97	0.46
1:A:262:ARG:HD2	1:A:276:CYS:HA	1.98	0.45
1:B:179:ILE:O	1:B:265:ARG:NH2	2.44	0.44
1:B:359:LYS:O	1:B:363:ILE:HG13	2.18	0.44
1:A:429:THR:HG22	1:A:447:SER:HB3	1.99	0.44
1:B:500:CYS:SG	1:B:508:SER:HB3	2.57	0.44
1:A:244:PHE:HB3	1:A:307:ILE:HB	1.99	0.44
1:B:177:LYS:HB2	1:B:177:LYS:HE2	1.72	0.44
1:A:426:ILE:HG23	1:A:458:PHE:CD2	2.53	0.43
1:A:174:PHE:CE1	1:B:187:LEU:HD13	2.54	0.43
1:B:211:ASN:OD1	1:B:529:LYS:HE2	2.18	0.43
1:B:187:LEU:HD12	1:B:187:LEU:HA	1.74	0.43
1:A:287:THR:O	1:A:291:ILE:HG13	2.18	0.43
1:A:426:ILE:HA	1:A:427:SER:HA	1.78	0.43
1:B:314:LYS:NZ	1:B:315:ASN:O	2.40	0.43
1:A:500:CYS:SG	1:A:508:SER:HB3	2.59	0.43
1:B:415:VAL:O	1:B:419:THR:OG1	2.31	0.43
1:B:344:SER:HB2	1:B:428:ASN:ND2	2.33	0.43
1:A:177:LYS:HD2	1:A:177:LYS:O	2.18	0.42
1:B:500:CYS:O	1:B:504:ASN:HB2	2.20	0.42
1:A:212:ILE:O	1:A:215:LEU:HB2	2.19	0.42
1:B:311:SER:HA	1:B:340:ALA:HB3	2.02	0.42
1:A:455:SER:O	1:A:459:ILE:HG12	2.20	0.41
1:B:502:VAL:HG22	2:B:602:8IE:C15	2.50	0.41
1:B:321:ILE:HD12	1:B:321:ILE:H	1.86	0.41
1:B:314:LYS:HE2	1:B:318:THR:HB	2.03	0.40
1:A:169:ASP:HA	1:A:172:LEU:HB3	2.03	0.40
1:A:185:HIS:CD2	2:A:601:8IE:C18	3.04	0.40
1:B:426:ILE:HA	1:B:427:SER:HA	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	375/401 (94%)	356 (95%)	19 (5%)	0	100	100
1	B	370/401 (92%)	355 (96%)	15 (4%)	0	100	100
All	All	745/802 (93%)	711 (95%)	34 (5%)	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	318/354 (90%)	316 (99%)	2 (1%)	86	90
1	B	271/354 (77%)	268 (99%)	3 (1%)	73	84
All	All	589/708 (83%)	584 (99%)	5 (1%)	78	88

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

Mol	Chain	Res	Type
1	A	169	ASP
1	A	235	ASP
1	B	205	SER
1	B	235	ASP
1	B	351	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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$
6	P4K	A	605	-	9,9,44	0.53	0	8,8,43	0.38	0
4	ORO	A	603	-	6,11,11	1.43	1 (16%)	3,15,15	3.97	2 (66%)
2	8IE	B	602	-	24,28,28	1.65	6 (25%)	20,42,42	2.46	8 (40%)
2	8IE	A	607	-	24,28,28	1.58	6 (25%)	20,42,42	2.77	8 (40%)
2	8IE	A	601	-	24,28,28	1.73	6 (25%)	20,42,42	2.52	7 (35%)
3	FMN	B	603	-	31,33,33	1.39	5 (16%)	40,50,50	1.48	5 (12%)
7	SO4	B	605	-	4,4,4	0.14	0	6,6,6	0.08	0
5	ACT	A	604	-	1,3,3	6.66	1 (100%)	0,3,3	0.00	-
7	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.10	0
4	ORO	B	604	-	6,11,11	1.53	1 (16%)	3,15,15	3.53	3 (100%)
2	8IE	B	601	-	24,28,28	1.52	5 (20%)	20,42,42	2.61	8 (40%)
3	FMN	A	602	-	31,33,33	1.40	5 (16%)	40,50,50	1.51	7 (17%)

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
6	P4K	A	605	-	-	6/7/7/42	-
4	ORO	A	603	-	-	0/0/4/4	0/1/1/1
2	8IE	B	602	-	-	4/4/22/22	0/5/5/5
2	8IE	A	607	-	-	4/4/22/22	0/5/5/5
2	8IE	A	601	-	-	4/4/22/22	0/5/5/5
3	FMN	B	603	-	-	1/18/18/18	0/3/3/3
4	ORO	B	604	-	-	0/0/4/4	0/1/1/1
2	8IE	B	601	-	-	4/4/22/22	0/5/5/5
3	FMN	A	602	-	-	1/18/18/18	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	ACT	CH3-C	6.66	1.57	1.48
2	A	601	8IE	C12-N04	4.35	1.41	1.35
2	B	602	8IE	C12-N04	4.06	1.41	1.35
3	B	603	FMN	C4A-N5	3.88	1.38	1.33
3	A	602	FMN	C4A-N5	3.85	1.38	1.33
2	A	607	8IE	C12-N04	3.72	1.40	1.35
2	A	601	8IE	C19-N20	-3.72	1.29	1.33
2	B	602	8IE	C19-N20	-3.67	1.29	1.33
2	B	601	8IE	C19-N20	-3.65	1.29	1.33
3	B	603	FMN	C10-N1	3.57	1.37	1.33
2	A	607	8IE	C19-N20	-3.57	1.29	1.33
3	A	602	FMN	C10-N1	3.56	1.37	1.33
2	B	601	8IE	C12-N04	3.37	1.40	1.35
3	B	603	FMN	C4-N3	3.04	1.38	1.33
3	A	602	FMN	C4-N3	3.01	1.38	1.33
2	A	607	8IE	C12-N13	-2.85	1.27	1.32
2	A	601	8IE	C14-C15	-2.66	1.33	1.42
2	B	602	8IE	C14-C15	-2.55	1.34	1.42
2	B	601	8IE	C12-N13	-2.55	1.27	1.32
2	A	601	8IE	C12-N13	-2.51	1.27	1.32
2	B	601	8IE	C14-C15	-2.46	1.34	1.42
2	A	607	8IE	C14-C15	-2.42	1.34	1.42
3	B	603	FMN	C1'-N10	2.33	1.50	1.48
3	A	602	FMN	C1'-N10	2.32	1.50	1.48
2	B	601	8IE	N20-N21	2.29	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	8IE	N20-N21	2.26	1.42	1.37
2	A	607	8IE	N20-N21	2.26	1.42	1.37
4	B	604	ORO	O4-C4	-2.25	1.18	1.24
2	A	601	8IE	N20-N21	2.19	1.42	1.37
2	B	602	8IE	C12-N13	-2.18	1.28	1.32
3	A	602	FMN	C5A-N5	2.09	1.38	1.35
2	A	601	8IE	C05-C06	2.07	1.55	1.51
4	A	603	ORO	O4-C4	-2.06	1.19	1.24
2	B	602	8IE	C22-N21	-2.02	1.29	1.33
3	B	603	FMN	C5A-N5	2.00	1.38	1.35
2	A	607	8IE	C22-N21	-2.00	1.29	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	8IE	C05-N04-C12	6.98	133.63	120.29
2	B	602	8IE	C05-N04-C12	6.53	132.78	120.29
2	B	601	8IE	C05-N04-C03	6.26	121.50	112.59
3	B	603	FMN	C4-N3-C2	6.11	120.30	115.14
2	A	607	8IE	C05-N04-C03	5.79	120.84	112.59
2	A	607	8IE	C18-C14-C15	5.65	114.75	110.62
4	A	603	ORO	C4-C5-C6	5.32	120.17	116.73
3	A	602	FMN	C4-N3-C2	5.24	119.56	115.14
2	B	601	8IE	C18-C14-C15	5.03	114.29	110.62
2	A	601	8IE	C03-N04-C12	-4.78	111.79	122.03
4	B	604	ORO	C4-C5-C6	4.71	119.77	116.73
2	B	602	8IE	C03-N04-C12	-4.61	112.16	122.03
2	A	607	8IE	C06-C05-N04	4.37	116.62	112.09
2	B	601	8IE	C06-C05-N04	4.03	116.27	112.09
2	A	607	8IE	C01-C02-C03	-3.97	103.44	112.14
4	A	603	ORO	C5-C4-N3	-3.92	119.50	124.08
2	A	601	8IE	C11-C06-C07	-3.55	114.91	118.76
2	A	607	8IE	C23-C22-N21	-3.45	117.91	124.17
2	A	601	8IE	C08-C07-C06	3.41	122.91	118.74
4	B	604	ORO	C5-C4-N3	-3.33	120.19	124.08
2	B	602	8IE	C11-C06-C07	-3.32	115.16	118.76
2	B	601	8IE	C23-C22-N21	-3.28	118.22	124.17
2	A	607	8IE	C02-C03-N04	3.28	119.57	111.37
2	B	601	8IE	C02-C03-N04	3.19	119.36	111.37
3	A	602	FMN	C4A-N5-C5A	3.18	119.95	116.77
3	B	603	FMN	C5A-C9A-N10	3.17	120.01	117.72
2	B	601	8IE	C01-C02-C03	-3.14	105.26	112.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	8IE	C08-C07-C06	2.90	122.29	118.74
2	B	602	8IE	C23-C22-N21	-2.89	118.92	124.17
3	A	602	FMN	C5A-C9A-N10	2.88	119.80	117.72
3	A	602	FMN	C10-C4A-N5	-2.84	119.29	121.26
2	A	601	8IE	C10-C09-C08	-2.67	116.13	120.19
3	B	603	FMN	C4A-C4-N3	-2.62	119.86	123.43
3	A	602	FMN	C4A-C4-N3	-2.60	119.88	123.43
2	B	602	8IE	C10-C09-C08	-2.55	116.31	120.19
3	A	602	FMN	C1'-N10-C10	2.53	120.68	118.41
2	B	602	8IE	C18-C14-C15	2.51	112.46	110.62
3	B	603	FMN	C4A-N5-C5A	2.50	119.27	116.77
3	B	603	FMN	C1'-N10-C9A	2.49	120.25	118.29
2	A	601	8IE	C18-C14-C15	2.39	112.36	110.62
2	A	601	8IE	C05-C06-C07	2.27	124.77	120.87
2	A	607	8IE	C03-N04-C12	-2.27	117.18	122.03
2	B	601	8IE	C06-C07-C02	2.22	121.82	117.37
3	A	602	FMN	C1'-N10-C9A	2.20	120.02	118.29
2	B	601	8IE	C23-C22-N24	2.14	131.65	126.79
2	A	607	8IE	C23-C22-N24	2.09	131.52	126.79
2	B	602	8IE	C05-C06-C07	2.04	124.38	120.87
4	B	604	ORO	C5-C6-N1	-2.03	119.94	122.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	8IE	N13-C12-N04-C03
2	A	601	8IE	N13-C12-N04-C05
2	A	601	8IE	N24-C12-N04-C03
2	A	601	8IE	N24-C12-N04-C05
2	A	607	8IE	N13-C12-N04-C03
2	B	601	8IE	N13-C12-N04-C03
2	B	602	8IE	N13-C12-N04-C03
2	B	602	8IE	N13-C12-N04-C05
2	B	602	8IE	N24-C12-N04-C03
2	B	602	8IE	N24-C12-N04-C05
2	A	607	8IE	N24-C12-N04-C03
2	A	607	8IE	N13-C12-N04-C05
6	A	605	P4K	O13-C25-C26-O14
2	A	607	8IE	N24-C12-N04-C05
2	B	601	8IE	N24-C12-N04-C03
2	B	601	8IE	N13-C12-N04-C05

Continued on next page...

Continued from previous page...

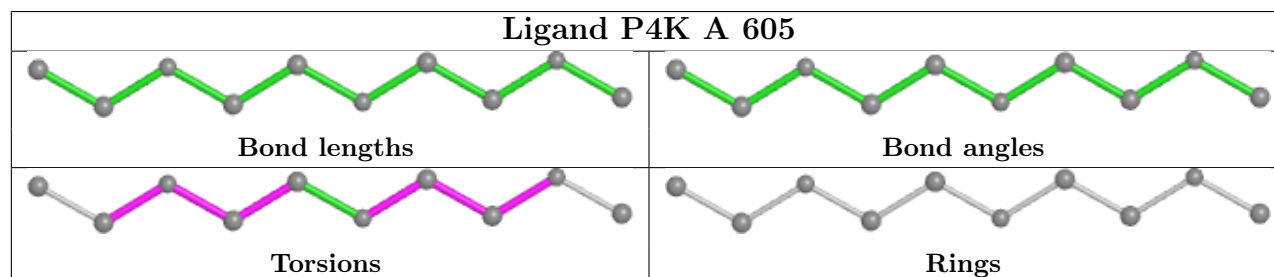
Mol	Chain	Res	Type	Atoms
2	B	601	8IE	N24-C12-N04-C05
6	A	605	P4K	C30-C29-O15-C28
3	A	602	FMN	C4'-C5'-O5'-P
3	B	603	FMN	C4'-C5'-O5'-P
6	A	605	P4K	C25-C26-O14-C27
6	A	605	P4K	C27-C28-O15-C29
6	A	605	P4K	C26-C25-O13-C24
6	A	605	P4K	O14-C27-C28-O15

There are no ring outliers.

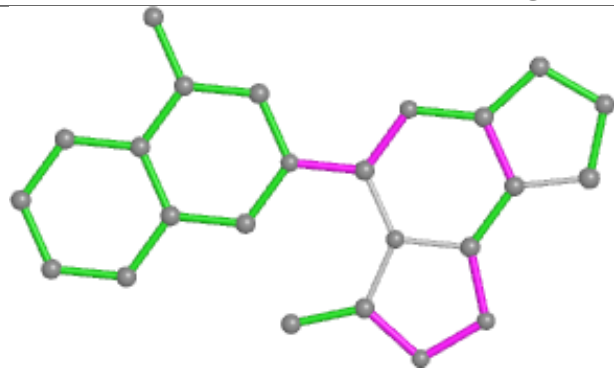
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	8IE	1	0
2	A	601	8IE	1	0
3	A	602	FMN	1	0

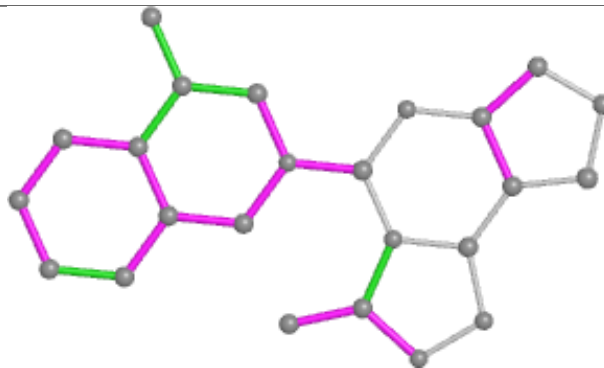
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



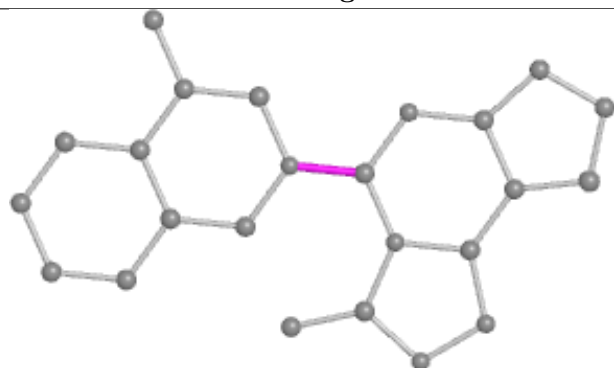
Ligand 8IE B 602



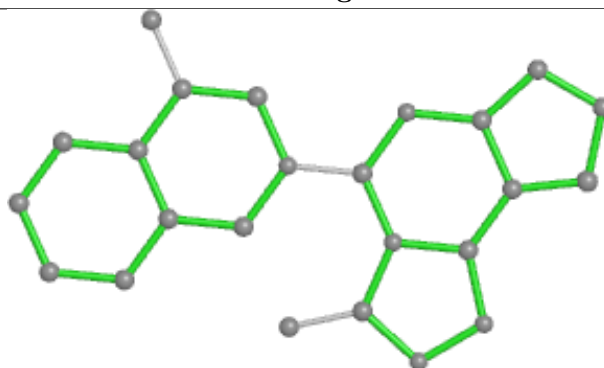
Bond lengths



Bond angles

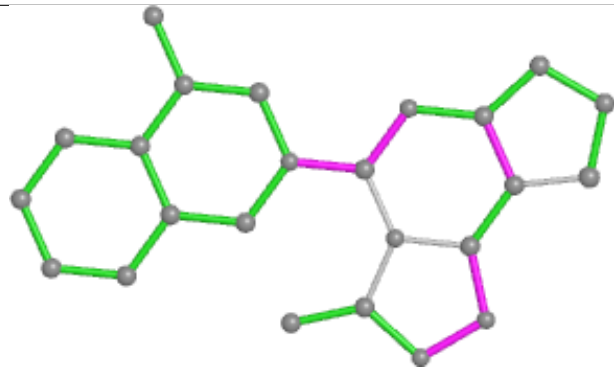


Torsions

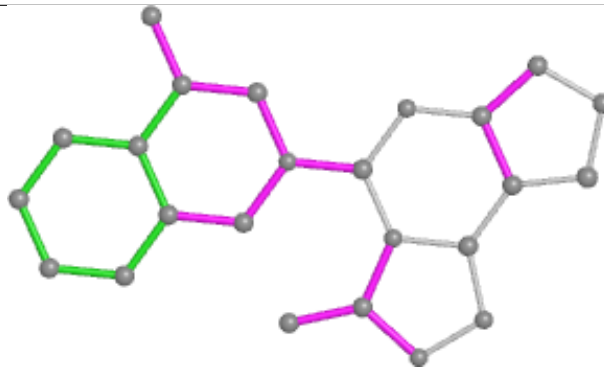


Rings

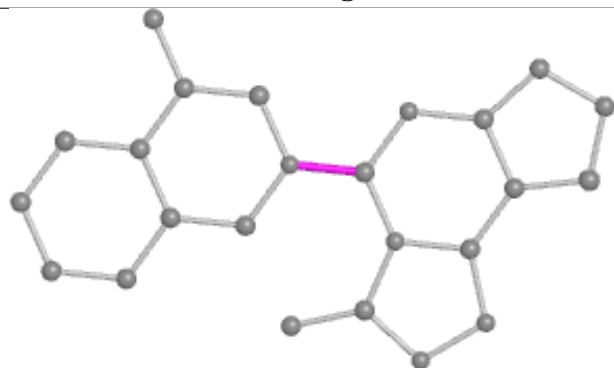
Ligand 8IE A 607



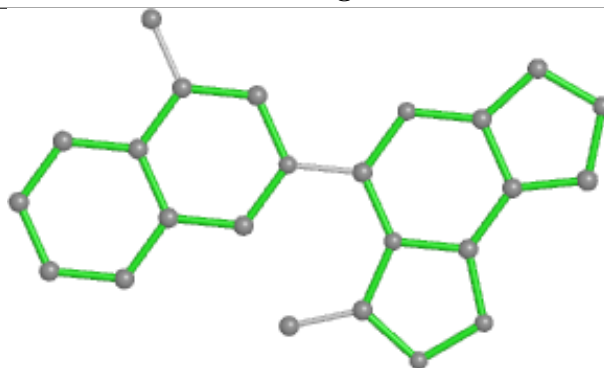
Bond lengths



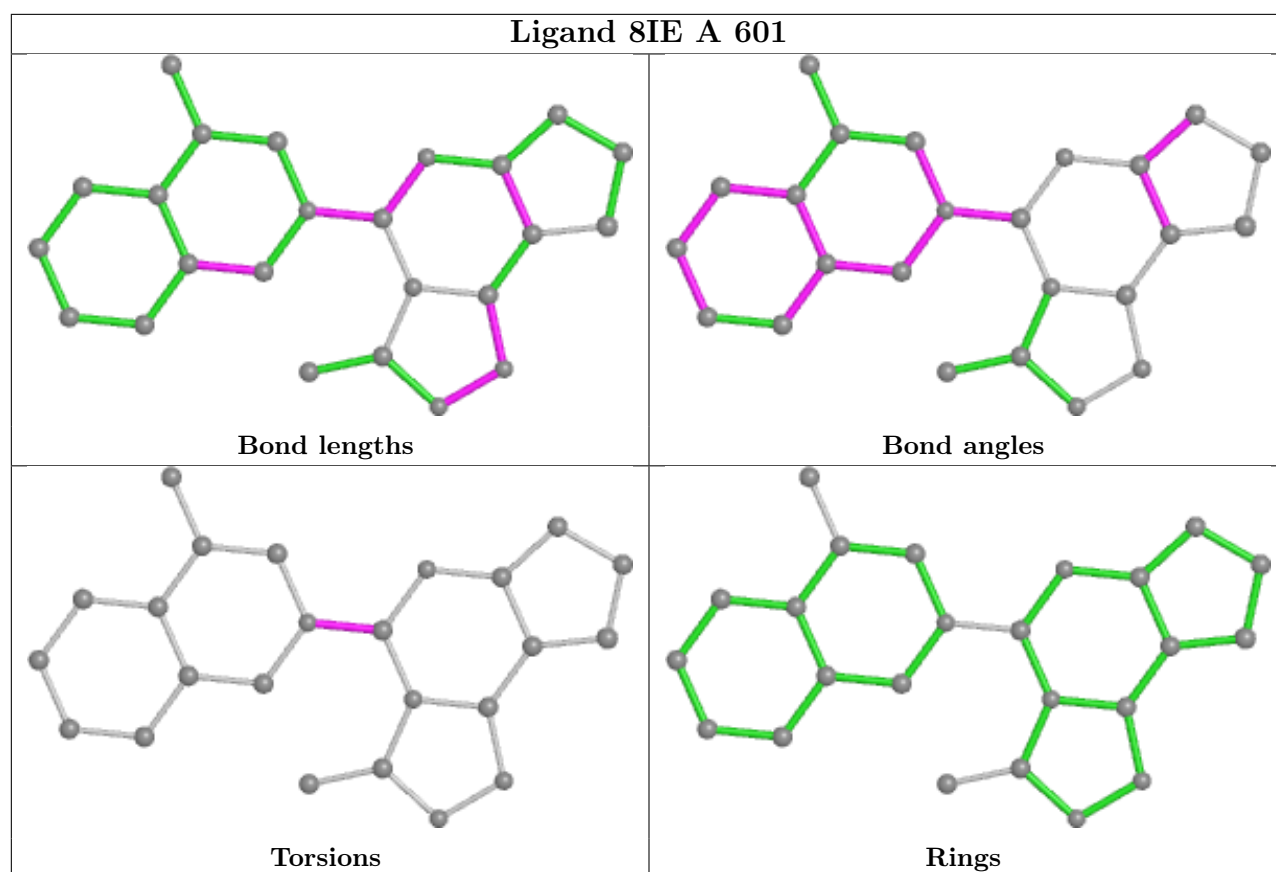
Bond angles

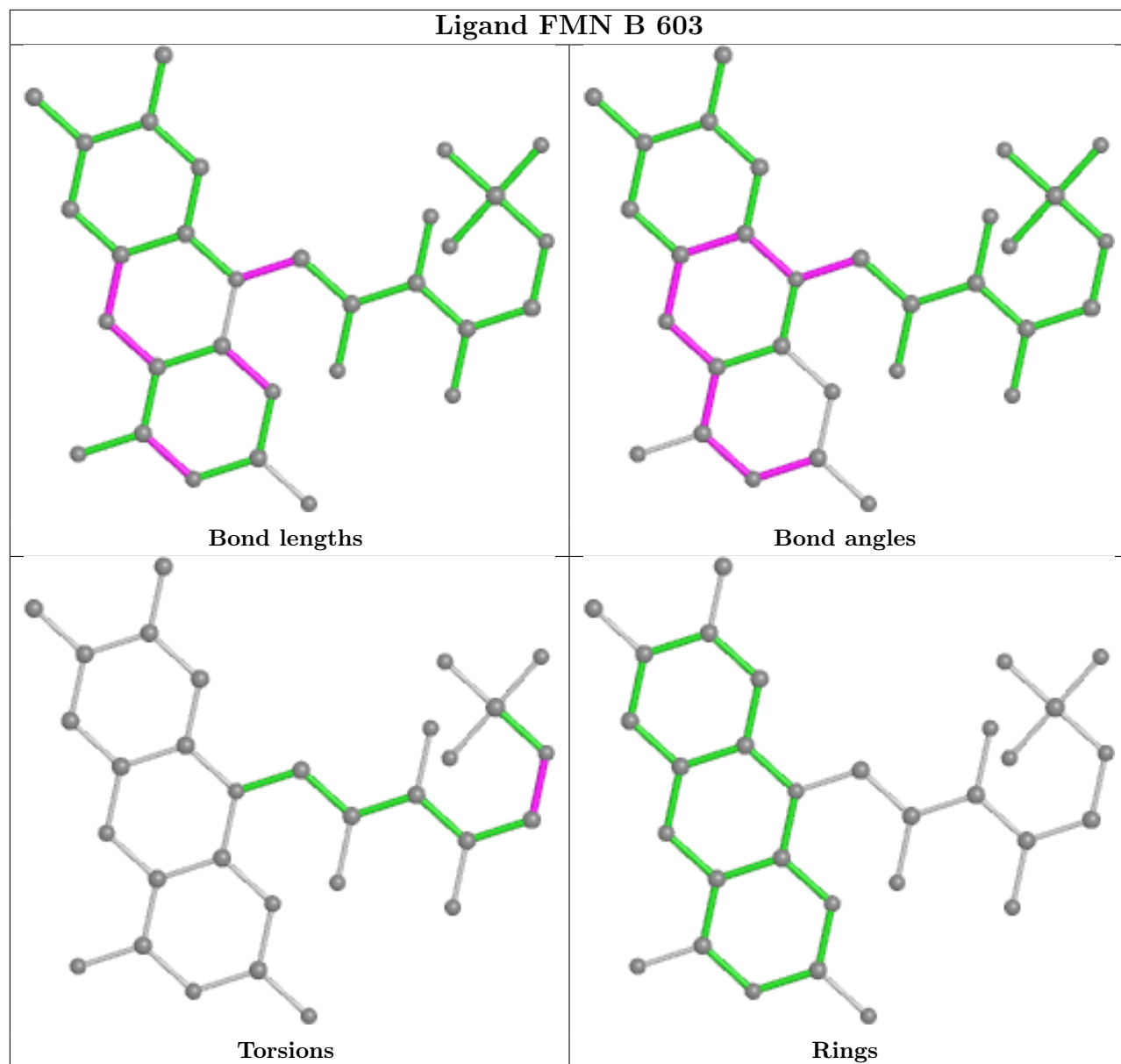


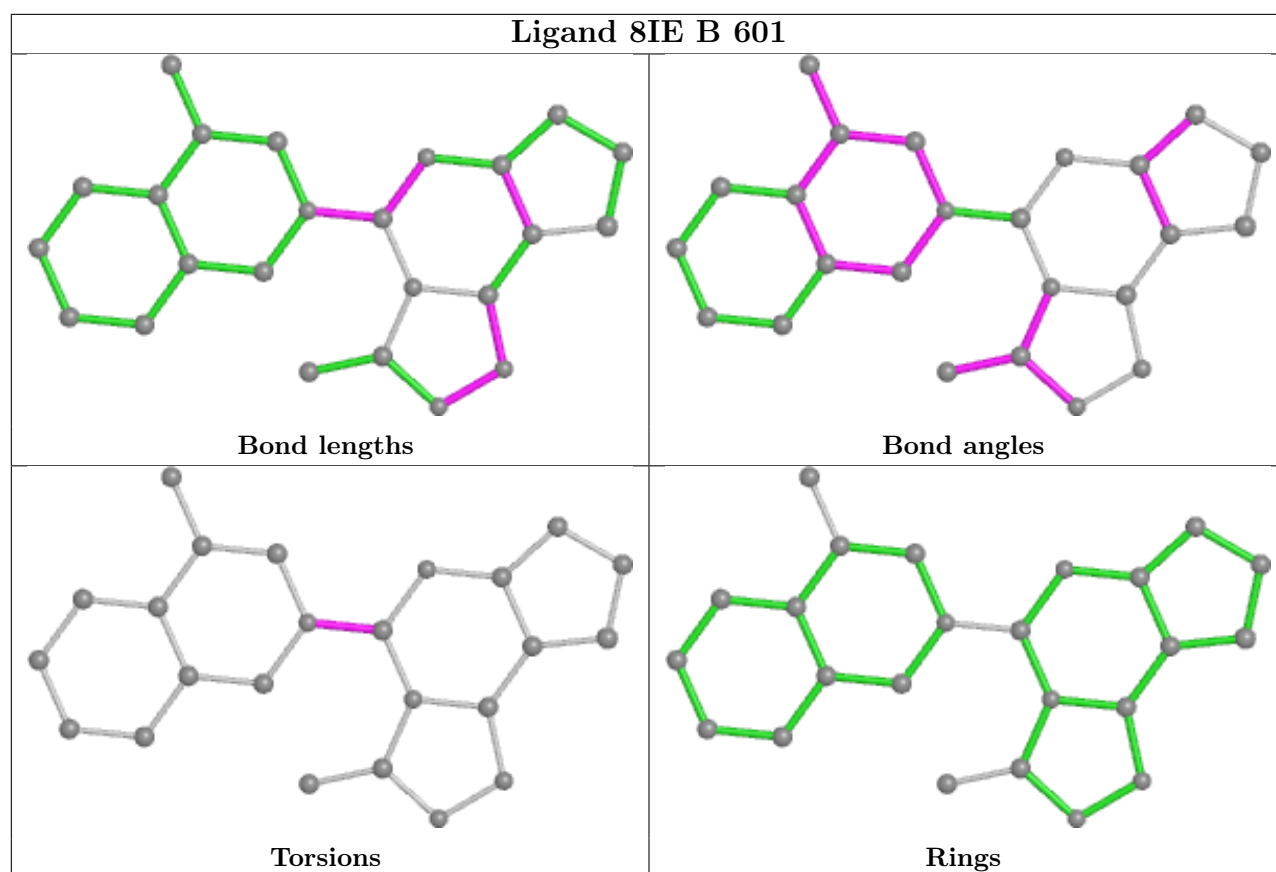
Torsions

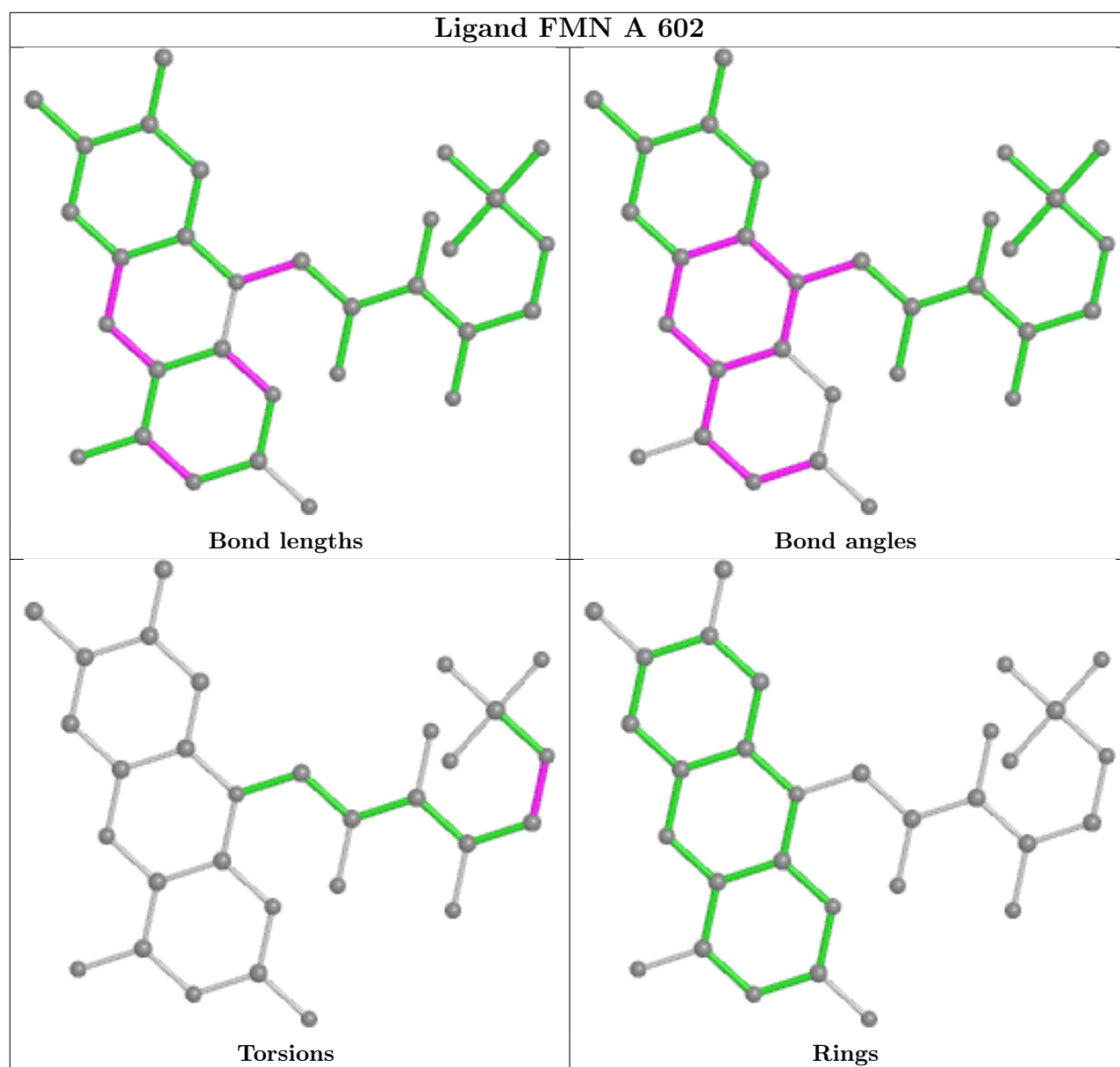


Rings









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, 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	379/401 (94%)	-0.03	2 (0%) 91 94	23, 41, 74, 103	0
1	B	373/401 (93%)	0.20	9 (2%) 59 68	34, 63, 108, 137	0
All	All	752/802 (93%)	0.08	11 (1%) 73 81	23, 51, 97, 137	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	PRO	5.0
1	B	348	THR	4.7
1	A	155	ALA	4.6
1	B	351	LEU	4.1
1	B	332	ILE	3.1
1	B	536	HIS	3.0
1	B	317	ASP	2.6
1	B	436	ILE	2.4
1	A	536	HIS	2.2
1	B	319	VAL	2.1
1	B	384	PHE	2.1

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

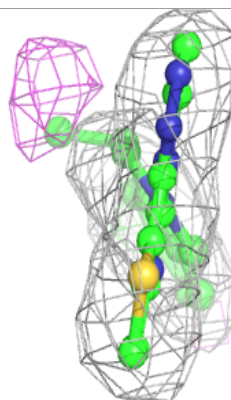
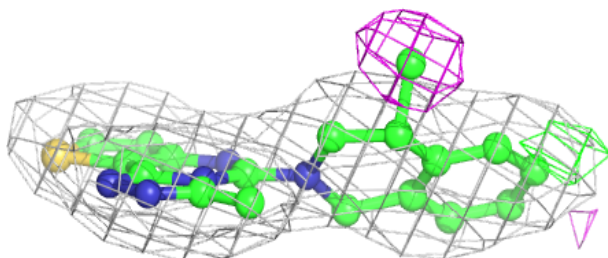
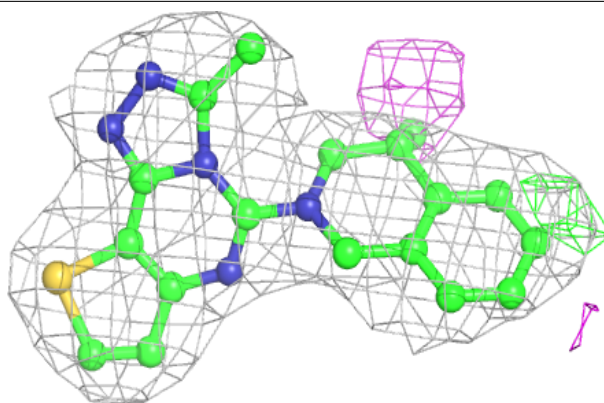
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	B	605	5/5	0.84	0.36	137,138,139,142	0
7	SO4	A	606	5/5	0.91	0.26	91,98,105,118	0
2	8IE	A	607	24/24	0.93	0.23	33,44,54,65	0
5	ACT	A	604	4/4	0.93	0.41	77,81,81,81	4
2	8IE	B	602	24/24	0.94	0.22	28,39,50,56	0
6	P4K	A	605	10/45	0.95	0.21	44,52,58,59	0
4	ORO	B	604	11/11	0.95	0.28	82,83,87,87	0
2	8IE	A	601	24/24	0.95	0.23	20,31,41,53	0
2	8IE	B	601	24/24	0.96	0.22	25,44,50,69	0
3	FMN	B	603	31/31	0.97	0.17	38,50,66,75	0
4	ORO	A	603	11/11	0.98	0.17	35,43,50,53	0
3	FMN	A	602	31/31	0.98	0.18	22,36,42,47	0

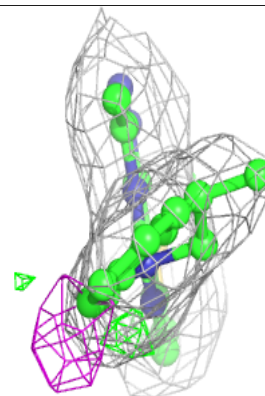
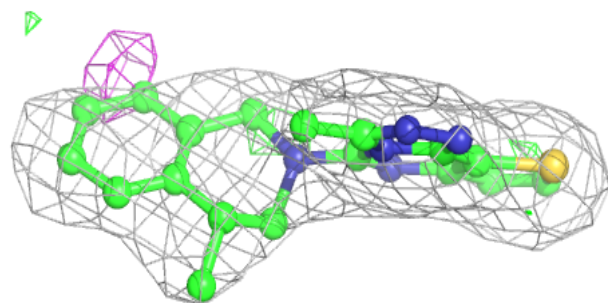
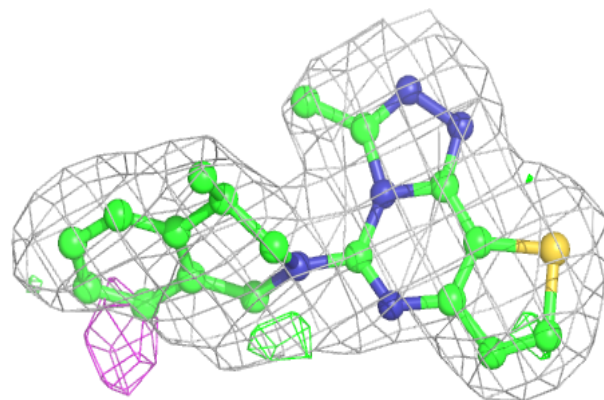
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8IE A 607:

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

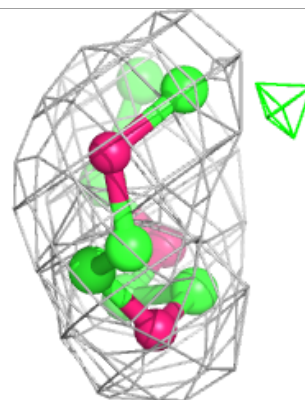
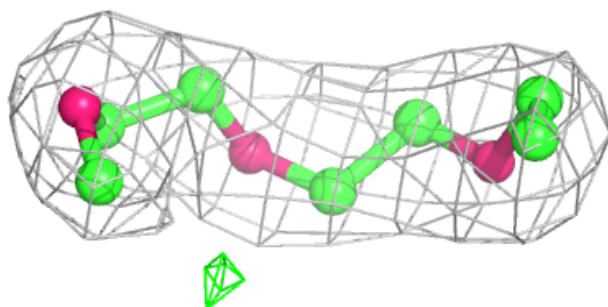
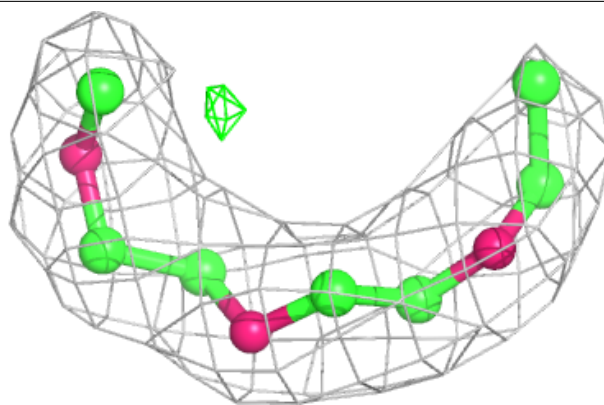
**Electron density around 8IE B 602:**

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

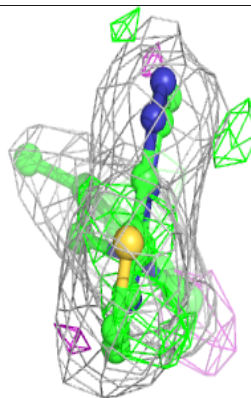
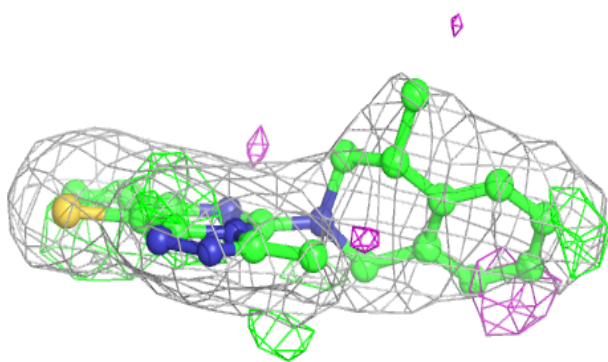
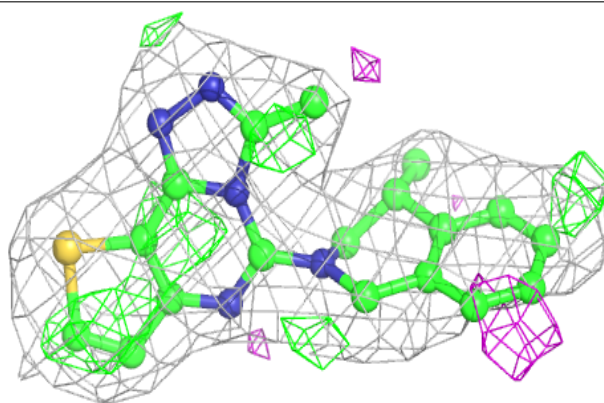


Electron density around P4K A 605:

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

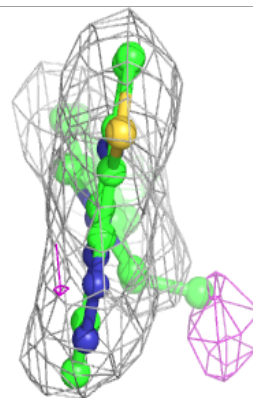
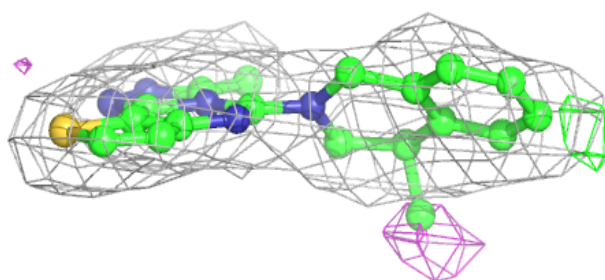
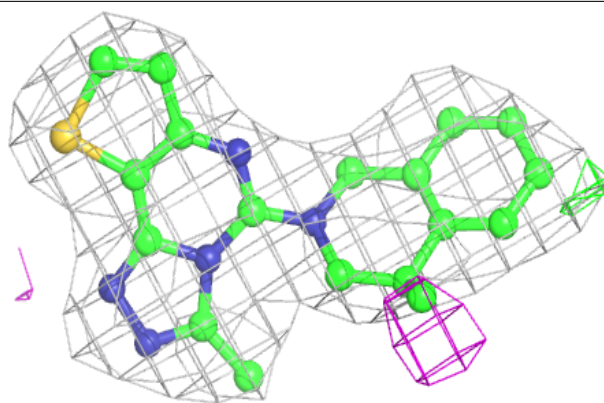
**Electron density around 8IE A 601:**

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



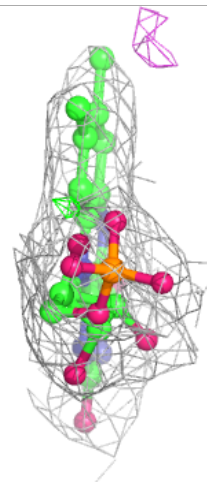
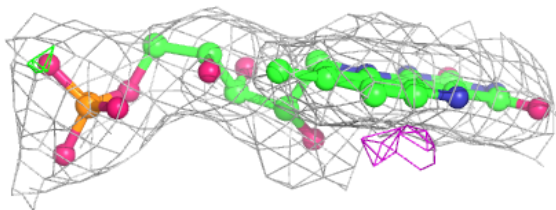
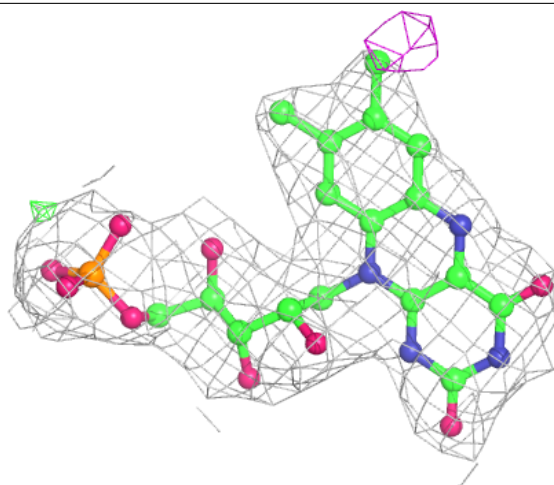
Electron density around 8IE B 601:

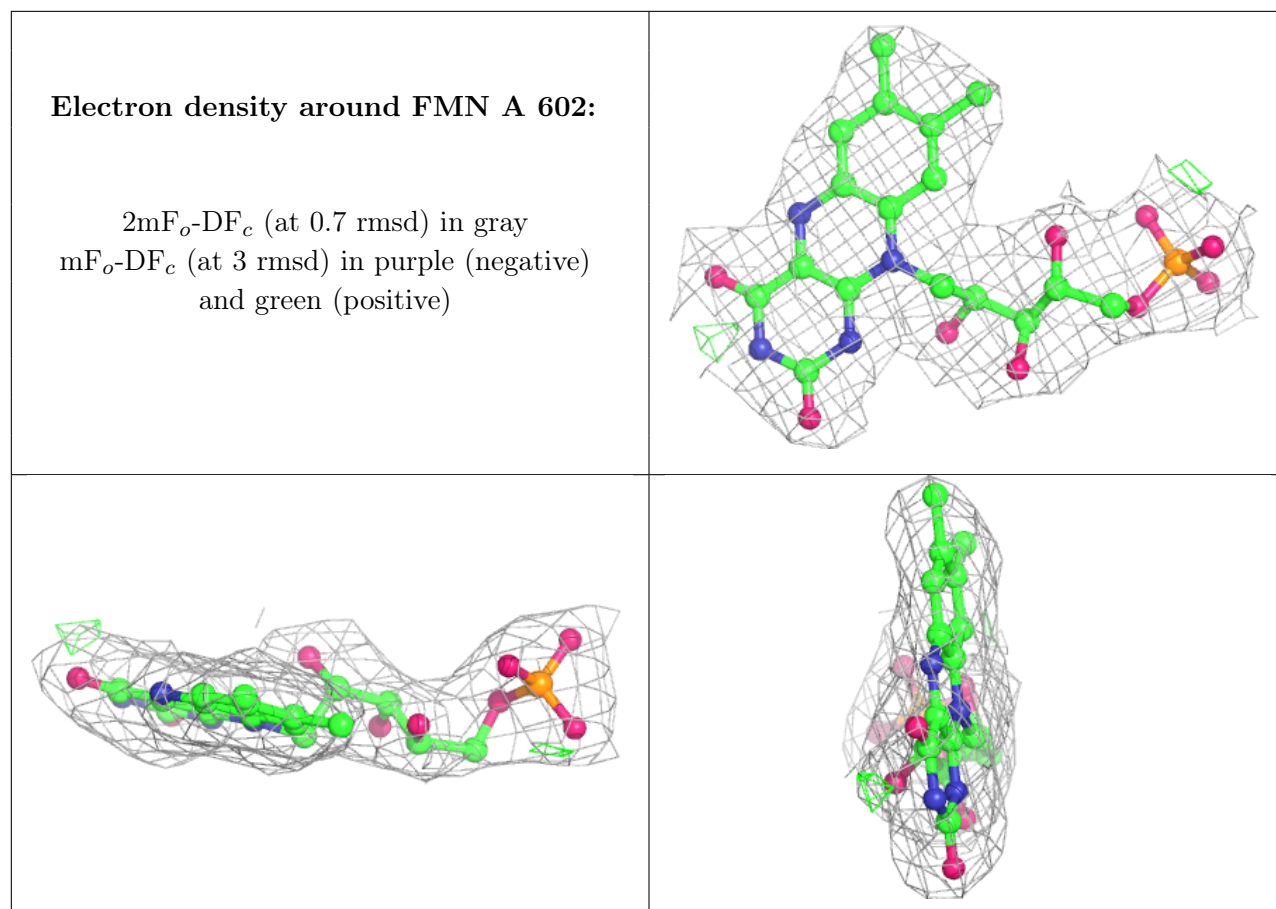
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN B 603:

$2mF_o-DF_c$ (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.