Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 12:28 PM EDT

PDB ID	:	8UAT
Title	:	Thermus scotoductus SA-01 Ene-reductase Compound 3b Complex
Authors	:	Wilson, L.A.; Guddat, L.W.; Schenk, G.; Scott, C.
Deposited on	:	2023-09-22
Resolution	:	2.76 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 (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 (i)) were used in the production of this report:

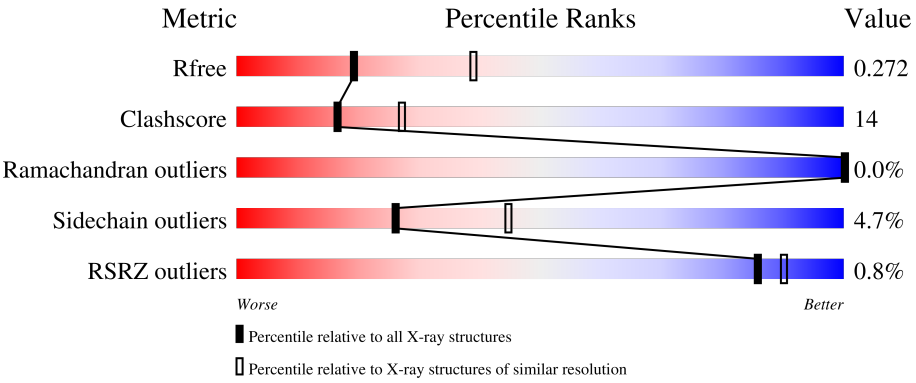
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.76 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 <=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	369	2% 62% 31% • 5%
1	B	369	2% 69% 25% • 5%
1	C	369	% 66% 27% • 5%
1	D	369	65% 28% • 5%
1	E	369	65% 28% • 5%

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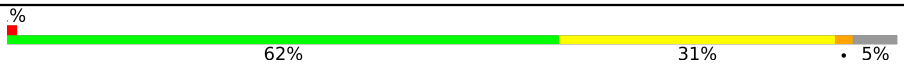
Mol	Chain	Length	Quality of chain
1	F	369	
1	G	369	
1	H	369	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 43906 atoms, of which 21814 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 NADPH dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	349	Total	C	H	N	O	S	0	1	0
			5425	1723	2732	486	476	8			
1	C	349	Total	C	H	N	O	S	0	1	0
			5425	1723	2732	486	476	8			
1	D	349	Total	C	H	N	O	S	0	0	0
			5386	1717	2704	482	475	8			
1	E	349	Total	C	H	N	O	S	0	1	0
			5418	1723	2725	486	476	8			
1	F	351	Total	C	H	N	O	S	0	2	0
			5465	1738	2745	494	480	8			
1	G	349	Total	C	H	N	O	S	0	1	0
			5402	1723	2709	486	476	8			
1	H	349	Total	C	H	N	O	S	0	0	0
			5401	1717	2719	482	475	8			
1	A	349	Total	C	H	N	O	S	0	1	0
			5425	1723	2732	486	476	8			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP E8PRF1
B	-18	GLY	-	expression tag	UNP E8PRF1
B	-17	SER	-	expression tag	UNP E8PRF1
B	-16	SER	-	expression tag	UNP E8PRF1
B	-15	HIS	-	expression tag	UNP E8PRF1
B	-14	HIS	-	expression tag	UNP E8PRF1
B	-13	HIS	-	expression tag	UNP E8PRF1
B	-12	HIS	-	expression tag	UNP E8PRF1
B	-11	HIS	-	expression tag	UNP E8PRF1
B	-10	HIS	-	expression tag	UNP E8PRF1
B	-9	SER	-	expression tag	UNP E8PRF1
B	-8	SER	-	expression tag	UNP E8PRF1
B	-7	GLY	-	expression tag	UNP E8PRF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	LEU	-	expression tag	UNP E8PRF1
B	-5	VAL	-	expression tag	UNP E8PRF1
B	-4	PRO	-	expression tag	UNP E8PRF1
B	-3	ARG	-	expression tag	UNP E8PRF1
B	-2	GLY	-	expression tag	UNP E8PRF1
B	-1	SER	-	expression tag	UNP E8PRF1
B	0	HIS	-	expression tag	UNP E8PRF1
B	1	MET	-	expression tag	UNP E8PRF1
B	2	ALA	-	expression tag	UNP E8PRF1
B	3	LEU	-	expression tag	UNP E8PRF1
C	-19	MET	-	initiating methionine	UNP E8PRF1
C	-18	GLY	-	expression tag	UNP E8PRF1
C	-17	SER	-	expression tag	UNP E8PRF1
C	-16	SER	-	expression tag	UNP E8PRF1
C	-15	HIS	-	expression tag	UNP E8PRF1
C	-14	HIS	-	expression tag	UNP E8PRF1
C	-13	HIS	-	expression tag	UNP E8PRF1
C	-12	HIS	-	expression tag	UNP E8PRF1
C	-11	HIS	-	expression tag	UNP E8PRF1
C	-10	HIS	-	expression tag	UNP E8PRF1
C	-9	SER	-	expression tag	UNP E8PRF1
C	-8	SER	-	expression tag	UNP E8PRF1
C	-7	GLY	-	expression tag	UNP E8PRF1
C	-6	LEU	-	expression tag	UNP E8PRF1
C	-5	VAL	-	expression tag	UNP E8PRF1
C	-4	PRO	-	expression tag	UNP E8PRF1
C	-3	ARG	-	expression tag	UNP E8PRF1
C	-2	GLY	-	expression tag	UNP E8PRF1
C	-1	SER	-	expression tag	UNP E8PRF1
C	0	HIS	-	expression tag	UNP E8PRF1
C	1	MET	-	expression tag	UNP E8PRF1
C	2	ALA	-	expression tag	UNP E8PRF1
C	3	LEU	-	expression tag	UNP E8PRF1
D	-19	MET	-	initiating methionine	UNP E8PRF1
D	-18	GLY	-	expression tag	UNP E8PRF1
D	-17	SER	-	expression tag	UNP E8PRF1
D	-16	SER	-	expression tag	UNP E8PRF1
D	-15	HIS	-	expression tag	UNP E8PRF1
D	-14	HIS	-	expression tag	UNP E8PRF1
D	-13	HIS	-	expression tag	UNP E8PRF1
D	-12	HIS	-	expression tag	UNP E8PRF1
D	-11	HIS	-	expression tag	UNP E8PRF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	HIS	-	expression tag	UNP E8PRF1
D	-9	SER	-	expression tag	UNP E8PRF1
D	-8	SER	-	expression tag	UNP E8PRF1
D	-7	GLY	-	expression tag	UNP E8PRF1
D	-6	LEU	-	expression tag	UNP E8PRF1
D	-5	VAL	-	expression tag	UNP E8PRF1
D	-4	PRO	-	expression tag	UNP E8PRF1
D	-3	ARG	-	expression tag	UNP E8PRF1
D	-2	GLY	-	expression tag	UNP E8PRF1
D	-1	SER	-	expression tag	UNP E8PRF1
D	0	HIS	-	expression tag	UNP E8PRF1
D	1	MET	-	expression tag	UNP E8PRF1
D	2	ALA	-	expression tag	UNP E8PRF1
D	3	LEU	-	expression tag	UNP E8PRF1
E	-19	MET	-	initiating methionine	UNP E8PRF1
E	-18	GLY	-	expression tag	UNP E8PRF1
E	-17	SER	-	expression tag	UNP E8PRF1
E	-16	SER	-	expression tag	UNP E8PRF1
E	-15	HIS	-	expression tag	UNP E8PRF1
E	-14	HIS	-	expression tag	UNP E8PRF1
E	-13	HIS	-	expression tag	UNP E8PRF1
E	-12	HIS	-	expression tag	UNP E8PRF1
E	-11	HIS	-	expression tag	UNP E8PRF1
E	-10	HIS	-	expression tag	UNP E8PRF1
E	-9	SER	-	expression tag	UNP E8PRF1
E	-8	SER	-	expression tag	UNP E8PRF1
E	-7	GLY	-	expression tag	UNP E8PRF1
E	-6	LEU	-	expression tag	UNP E8PRF1
E	-5	VAL	-	expression tag	UNP E8PRF1
E	-4	PRO	-	expression tag	UNP E8PRF1
E	-3	ARG	-	expression tag	UNP E8PRF1
E	-2	GLY	-	expression tag	UNP E8PRF1
E	-1	SER	-	expression tag	UNP E8PRF1
E	0	HIS	-	expression tag	UNP E8PRF1
E	1	MET	-	expression tag	UNP E8PRF1
E	2	ALA	-	expression tag	UNP E8PRF1
E	3	LEU	-	expression tag	UNP E8PRF1
F	-19	MET	-	initiating methionine	UNP E8PRF1
F	-18	GLY	-	expression tag	UNP E8PRF1
F	-17	SER	-	expression tag	UNP E8PRF1
F	-16	SER	-	expression tag	UNP E8PRF1
F	-15	HIS	-	expression tag	UNP E8PRF1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	HIS	-	expression tag	UNP E8PRF1
F	-13	HIS	-	expression tag	UNP E8PRF1
F	-12	HIS	-	expression tag	UNP E8PRF1
F	-11	HIS	-	expression tag	UNP E8PRF1
F	-10	HIS	-	expression tag	UNP E8PRF1
F	-9	SER	-	expression tag	UNP E8PRF1
F	-8	SER	-	expression tag	UNP E8PRF1
F	-7	GLY	-	expression tag	UNP E8PRF1
F	-6	LEU	-	expression tag	UNP E8PRF1
F	-5	VAL	-	expression tag	UNP E8PRF1
F	-4	PRO	-	expression tag	UNP E8PRF1
F	-3	ARG	-	expression tag	UNP E8PRF1
F	-2	GLY	-	expression tag	UNP E8PRF1
F	-1	SER	-	expression tag	UNP E8PRF1
F	0	HIS	-	expression tag	UNP E8PRF1
F	1	MET	-	expression tag	UNP E8PRF1
F	2	ALA	-	expression tag	UNP E8PRF1
F	3	LEU	-	expression tag	UNP E8PRF1
G	-19	MET	-	initiating methionine	UNP E8PRF1
G	-18	GLY	-	expression tag	UNP E8PRF1
G	-17	SER	-	expression tag	UNP E8PRF1
G	-16	SER	-	expression tag	UNP E8PRF1
G	-15	HIS	-	expression tag	UNP E8PRF1
G	-14	HIS	-	expression tag	UNP E8PRF1
G	-13	HIS	-	expression tag	UNP E8PRF1
G	-12	HIS	-	expression tag	UNP E8PRF1
G	-11	HIS	-	expression tag	UNP E8PRF1
G	-10	HIS	-	expression tag	UNP E8PRF1
G	-9	SER	-	expression tag	UNP E8PRF1
G	-8	SER	-	expression tag	UNP E8PRF1
G	-7	GLY	-	expression tag	UNP E8PRF1
G	-6	LEU	-	expression tag	UNP E8PRF1
G	-5	VAL	-	expression tag	UNP E8PRF1
G	-4	PRO	-	expression tag	UNP E8PRF1
G	-3	ARG	-	expression tag	UNP E8PRF1
G	-2	GLY	-	expression tag	UNP E8PRF1
G	-1	SER	-	expression tag	UNP E8PRF1
G	0	HIS	-	expression tag	UNP E8PRF1
G	1	MET	-	expression tag	UNP E8PRF1
G	2	ALA	-	expression tag	UNP E8PRF1
G	3	LEU	-	expression tag	UNP E8PRF1
H	-19	MET	-	initiating methionine	UNP E8PRF1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-18	GLY	-	expression tag	UNP E8PRF1
H	-17	SER	-	expression tag	UNP E8PRF1
H	-16	SER	-	expression tag	UNP E8PRF1
H	-15	HIS	-	expression tag	UNP E8PRF1
H	-14	HIS	-	expression tag	UNP E8PRF1
H	-13	HIS	-	expression tag	UNP E8PRF1
H	-12	HIS	-	expression tag	UNP E8PRF1
H	-11	HIS	-	expression tag	UNP E8PRF1
H	-10	HIS	-	expression tag	UNP E8PRF1
H	-9	SER	-	expression tag	UNP E8PRF1
H	-8	SER	-	expression tag	UNP E8PRF1
H	-7	GLY	-	expression tag	UNP E8PRF1
H	-6	LEU	-	expression tag	UNP E8PRF1
H	-5	VAL	-	expression tag	UNP E8PRF1
H	-4	PRO	-	expression tag	UNP E8PRF1
H	-3	ARG	-	expression tag	UNP E8PRF1
H	-2	GLY	-	expression tag	UNP E8PRF1
H	-1	SER	-	expression tag	UNP E8PRF1
H	0	HIS	-	expression tag	UNP E8PRF1
H	1	MET	-	expression tag	UNP E8PRF1
H	2	ALA	-	expression tag	UNP E8PRF1
H	3	LEU	-	expression tag	UNP E8PRF1
A	-19	MET	-	initiating methionine	UNP E8PRF1
A	-18	GLY	-	expression tag	UNP E8PRF1
A	-17	SER	-	expression tag	UNP E8PRF1
A	-16	SER	-	expression tag	UNP E8PRF1
A	-15	HIS	-	expression tag	UNP E8PRF1
A	-14	HIS	-	expression tag	UNP E8PRF1
A	-13	HIS	-	expression tag	UNP E8PRF1
A	-12	HIS	-	expression tag	UNP E8PRF1
A	-11	HIS	-	expression tag	UNP E8PRF1
A	-10	HIS	-	expression tag	UNP E8PRF1
A	-9	SER	-	expression tag	UNP E8PRF1
A	-8	SER	-	expression tag	UNP E8PRF1
A	-7	GLY	-	expression tag	UNP E8PRF1
A	-6	LEU	-	expression tag	UNP E8PRF1
A	-5	VAL	-	expression tag	UNP E8PRF1
A	-4	PRO	-	expression tag	UNP E8PRF1
A	-3	ARG	-	expression tag	UNP E8PRF1
A	-2	GLY	-	expression tag	UNP E8PRF1
A	-1	SER	-	expression tag	UNP E8PRF1
A	0	HIS	-	expression tag	UNP E8PRF1

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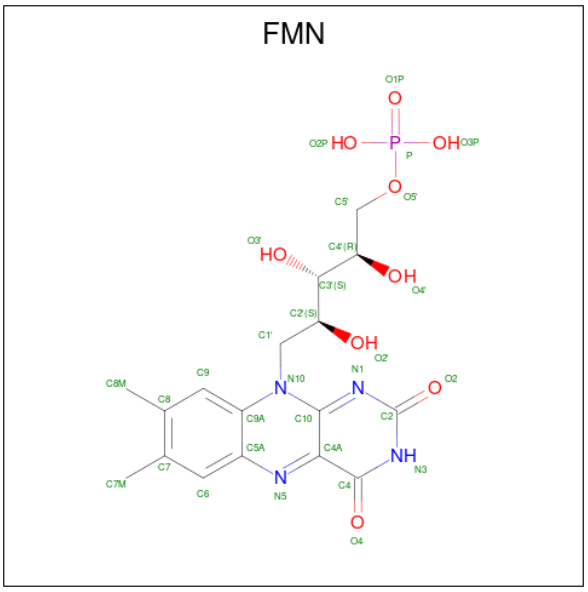
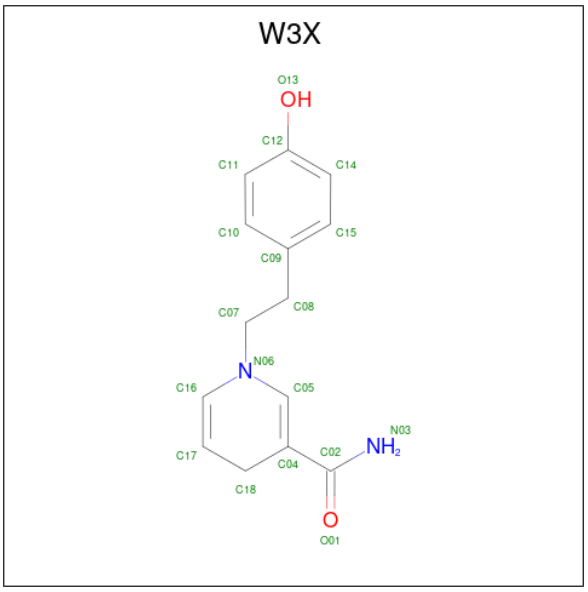
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP E8PRF1
A	2	ALA	-	expression tag	UNP E8PRF1
A	3	LEU	-	expression tag	UNP E8PRF1

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



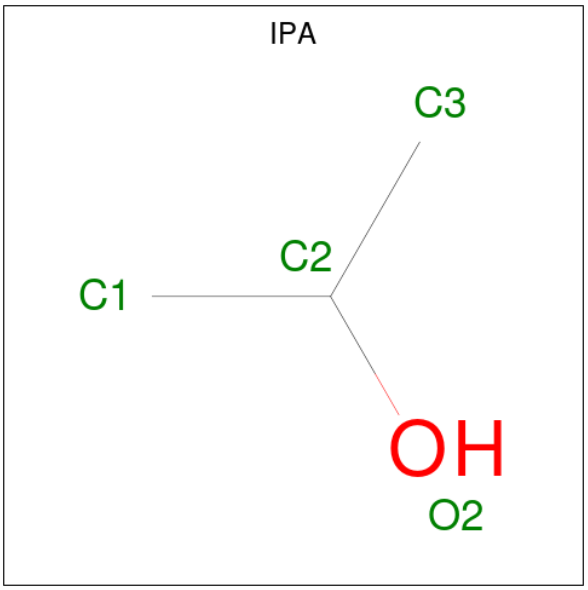
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is 1-[2-(4-hydroxyphenyl)ethyl]-1,4-dihydropyridine-3-carboxamide (three-letter code: W3X) (formula: $C_{14}H_{16}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 18 14 2 2	0	0
3	E	1	Total C N O 9 6 2 1	0	0
3	F	1	Total C N O 9 6 2 1	0	0
3	A	1	Total C N O 18 14 2 2	0	0

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C H O 12 3 8 1	0	0
4	H	1	Total C H O 12 3 8 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total Na 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Cl 1 1	0	0

- Molecule 7 is water.

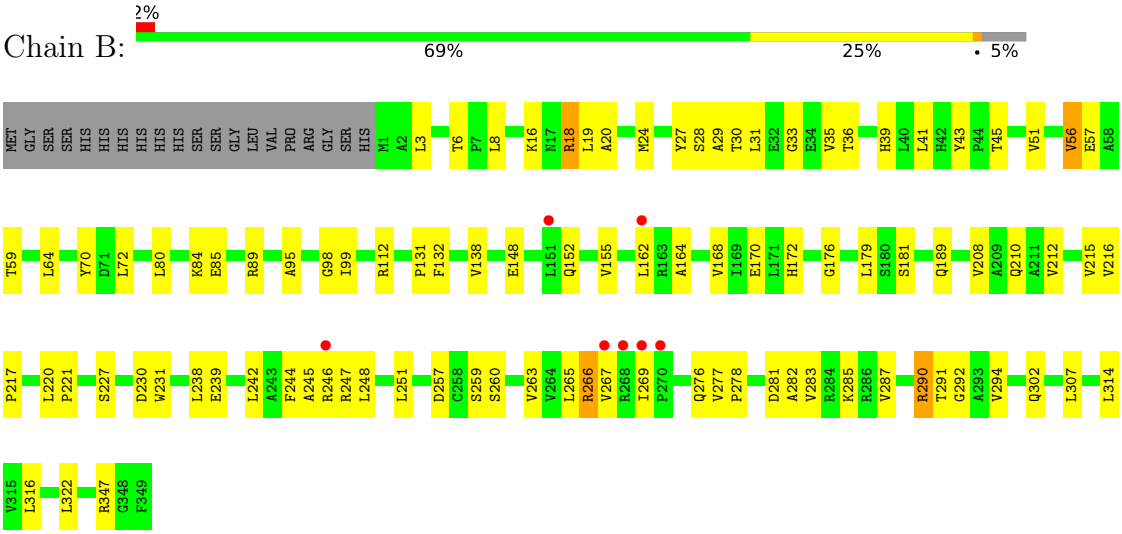
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	28	Total O 28 28	0	0
7	C	31	Total O 31 31	0	0
7	D	18	Total O 18 18	0	0
7	E	25	Total O 25 25	0	0
7	F	37	Total O 37 37	0	0
7	G	30	Total O 30 30	0	0
7	H	28	Total O 28 28	0	0
7	A	34	Total O 34 34	0	0

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.

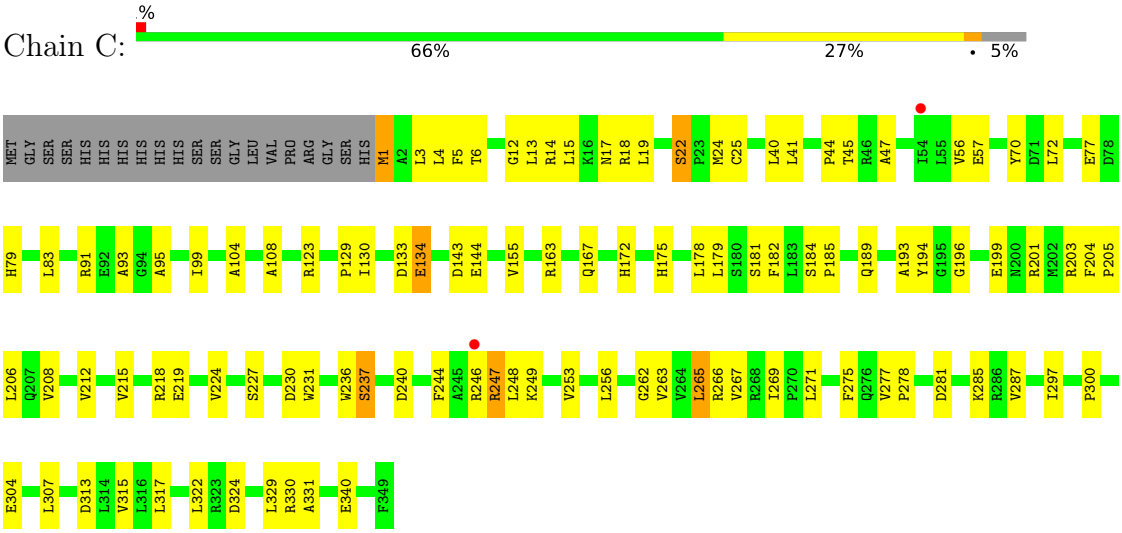
• Molecule 1: NADPH dehydrogenase

Chain B:



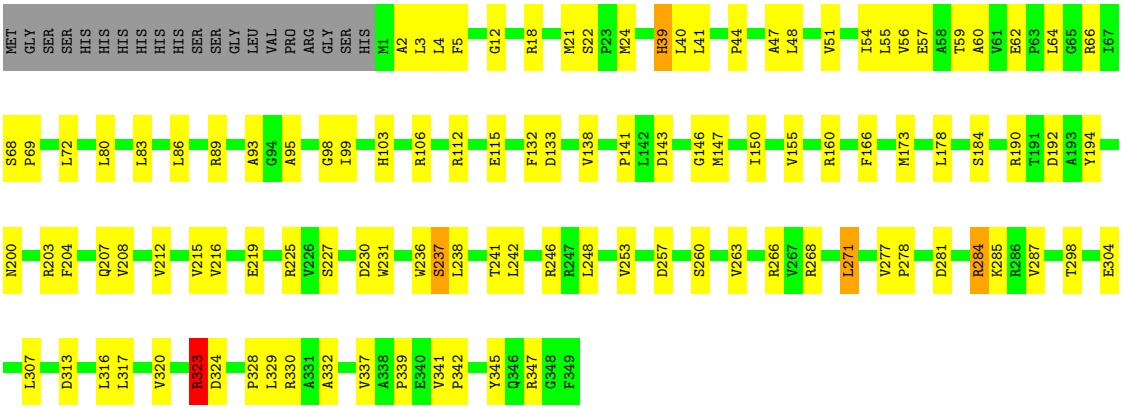
• Molecule 1: NADPH dehydrogenase

Chain C:



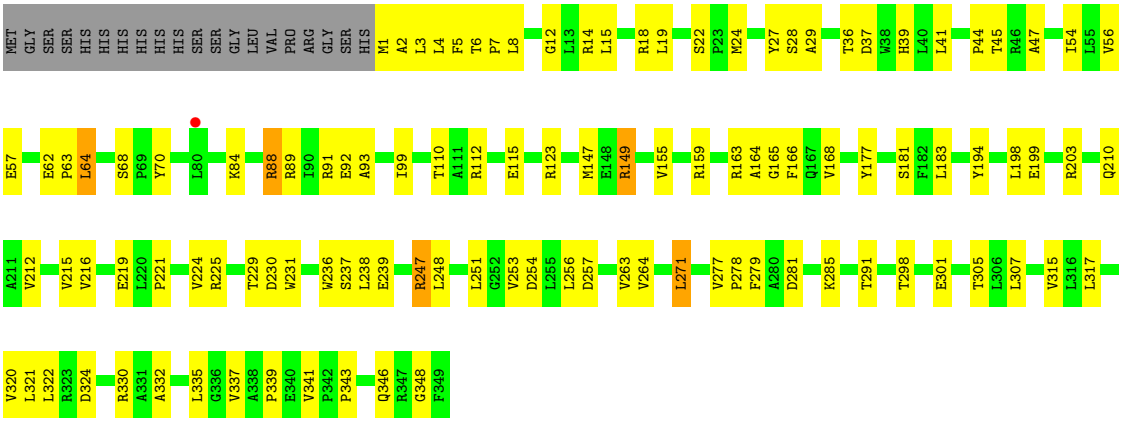
• Molecule 1: NADPH dehydrogenase

Chain D:



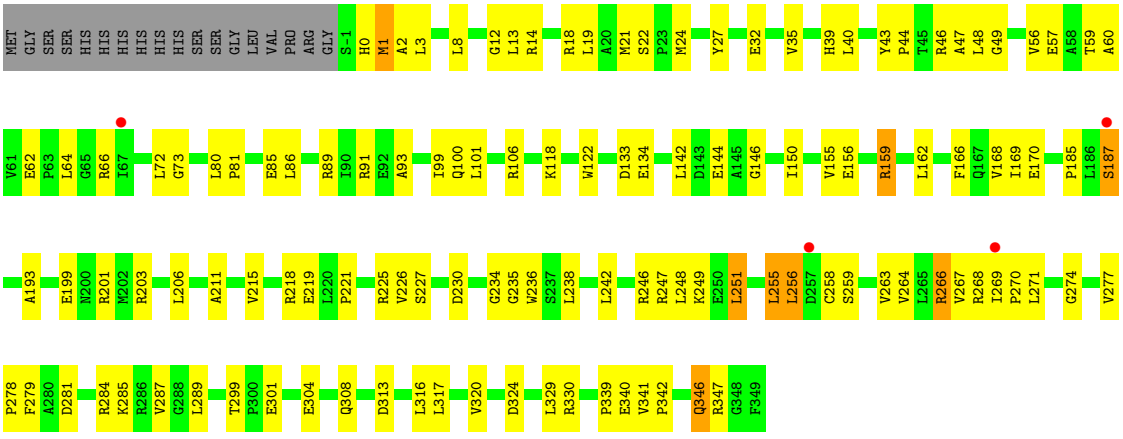
• Molecule 1: NADPH dehydrogenase

Chain E:



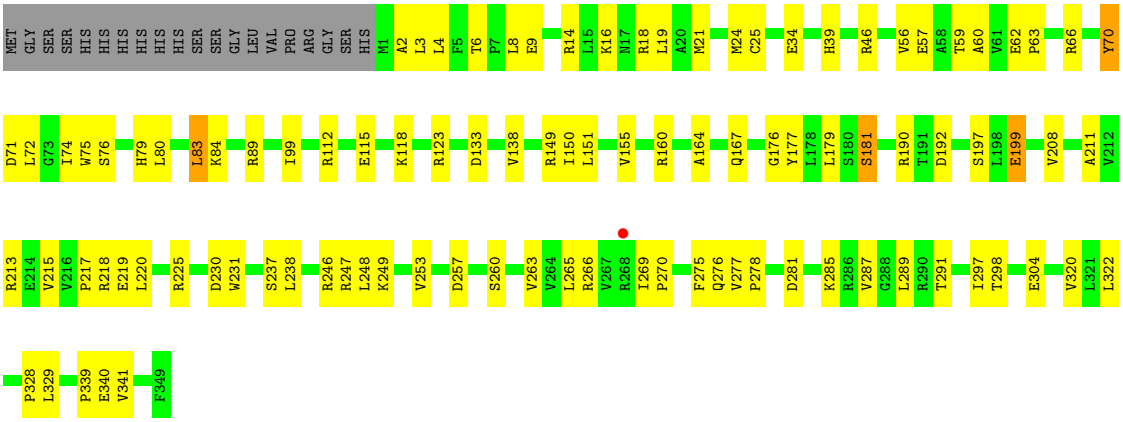
• Molecule 1: NADPH dehydrogenase

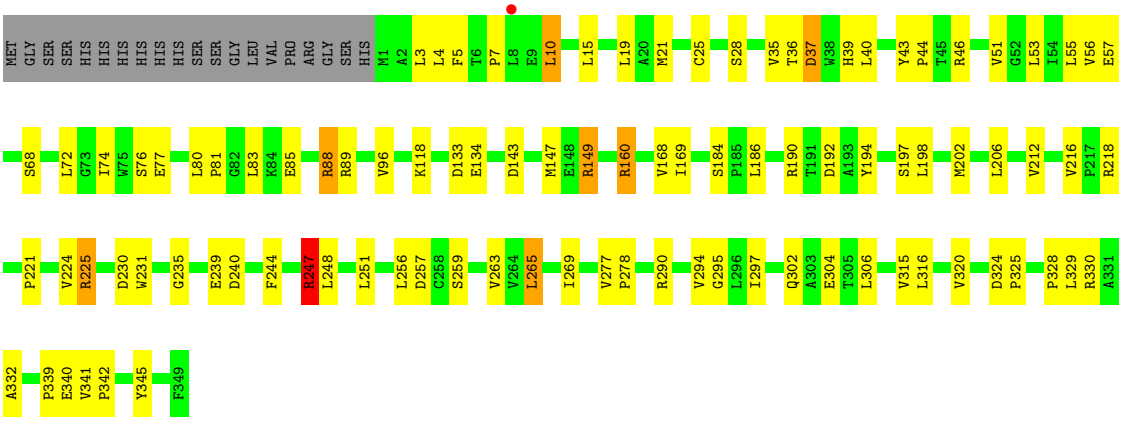
Chain F:



• Molecule 1: NADPH dehydrogenase

Chain G:



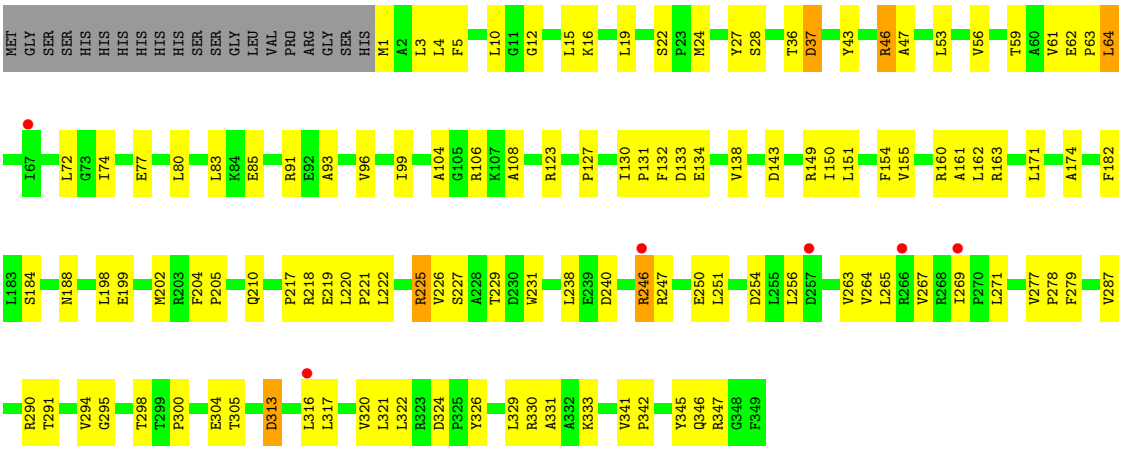


• Molecule 1: NADPH dehydrogenase

Chain H:

• Molecule 1: NADPH dehydrogenase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	97.85Å 100.47Å 100.41Å 89.80° 65.75° 89.92°	Depositor
Resolution (Å)	48.75 – 2.76 48.75 – 2.76	Depositor EDS
% Data completeness (in resolution range)	92.9 (48.75-2.76) 92.1 (48.75-2.76)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.233 , 0.271 0.234 , 0.272	Depositor DCC
R_{free} test set	1926 reflections (2.31%)	wwPDB-VP
Wilson B-factor (Å^2)	50.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 20.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.377 for -h,k,-l 0.016 for l,-k,h 0.023 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	43906	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 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, W3X, IPA, NA, CL

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	0.37	0/2758	0.61	0/3749
1	B	0.40	0/2758	0.61	0/3749
1	C	0.34	1/2758 (0.0%)	0.60	1/3749 (0.0%)
1	D	0.36	0/2747	0.61	0/3735
1	E	0.33	0/2758	0.64	4/3749 (0.1%)
1	F	0.40	0/2786	0.63	2/3786 (0.1%)
1	G	0.46	0/2758	0.68	2/3749 (0.1%)
1	H	0.39	1/2747 (0.0%)	0.63	1/3735 (0.0%)
All	All	0.38	2/22070 (0.0%)	0.63	10/30001 (0.0%)

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	2
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	340	GLU	CD-OE2	5.64	1.31	1.25
1	C	134	GLU	CB-CG	5.04	1.61	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	271	LEU	CA-CB-CG	10.59	139.65	115.30
1	C	134	GLU	CA-CB-CG	-9.45	92.60	113.40
1	E	271	LEU	CB-CG-CD2	-7.16	98.82	111.00
1	F	134	GLU	CG-CD-OE2	-6.97	104.35	118.30
1	F	251	LEU	CA-CB-CG	6.83	131.01	115.30
1	G	3	LEU	CA-CB-CG	6.48	130.20	115.30
1	G	83	LEU	CB-CG-CD1	-6.22	100.42	111.00
1	H	149	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	64	LEU	CA-CB-CG	5.37	127.64	115.30
1	E	247	ARG	CA-CB-CG	5.15	124.74	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	245	ALA	Mainchain
1	D	323	ARG	Sidechain
1	E	247	ARG	Sidechain
1	H	247	ARG	Sidechain

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	2693	2732	2743	91	0
1	B	2693	2732	2743	75	0
1	C	2693	2732	2743	67	2
1	D	2682	2704	2731	80	0
1	E	2693	2725	2743	72	2
1	F	2720	2745	2767	92	1
1	G	2693	2709	2743	81	0
1	H	2682	2719	2731	71	1
2	A	31	0	19	6	0
2	B	31	0	19	3	0
2	C	31	0	19	2	0
2	D	31	0	19	3	0
2	E	31	0	19	3	0
2	F	31	0	19	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	31	0	19	3	0
2	H	31	0	19	3	0
3	A	18	0	0	3	0
3	B	18	0	0	1	0
3	E	9	0	0	2	0
3	F	9	0	0	1	0
4	E	4	8	8	2	0
4	H	4	8	8	0	0
5	F	1	0	0	0	0
6	F	1	0	0	0	0
7	A	34	0	0	3	0
7	B	28	0	0	7	0
7	C	31	0	0	1	0
7	D	18	0	0	2	0
7	E	25	0	0	2	0
7	F	37	0	0	6	0
7	G	30	0	0	4	0
7	H	28	0	0	1	0
All	All	22092	21814	22112	624	3

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 14.

All (624) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ARG:NH1	1:D:313:ASP:OD1	2.01	0.93
1:E:62:GLU:OE2	1:E:149:ARG:NH1	2.06	0.88
1:A:218:ARG:O	7:A:501:HOH:O	1.96	0.83
1:G:24:MET:CE	1:G:322:LEU:HD21	2.09	0.82
1:C:22:SER:OG	2:C:401:FMN:O2'	1.97	0.81
1:H:169:ILE:HD11	1:H:216:VAL:HG21	1.63	0.81
1:H:324:ASP:OD2	1:H:330:ARG:NH2	2.15	0.80
1:D:22:SER:OG	2:D:401:FMN:O2'	2.01	0.79
1:G:74:ILE:HD12	1:G:83:LEU:HD21	1.64	0.79
1:E:281:ASP:OD2	1:E:285:LYS:NZ	2.15	0.78
1:F:56:VAL:HG22	1:F:99:ILE:HG13	1.65	0.78
1:G:24:MET:HE3	1:G:322:LEU:HD21	1.65	0.78
1:A:56:VAL:CG2	1:A:99:ILE:HD12	2.13	0.78
1:G:281:ASP:OD2	1:G:285:LYS:NZ	2.16	0.78
1:B:41:LEU:O	1:B:45:THR:OG1	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:VAL:HG13	1:D:215:VAL:HG11	1.66	0.76
1:D:329:LEU:HD22	1:D:341:VAL:HG12	1.68	0.76
1:D:59:THR:HG21	1:D:99:ILE:HD11	1.68	0.75
1:E:254:ASP:OD2	7:E:501:HOH:O	2.03	0.75
1:B:84:LYS:NZ	7:B:503:HOH:O	2.20	0.74
1:H:133:ASP:HB2	1:H:265:LEU:HD21	1.70	0.73
1:B:56:VAL:HG22	1:B:99:ILE:HD12	1.69	0.72
1:A:132:PHE:CE2	1:A:265:LEU:HD11	2.23	0.72
1:D:56:VAL:HG11	1:D:86:LEU:HD21	1.71	0.72
1:G:56:VAL:CG2	1:G:99:ILE:HD12	2.20	0.71
1:G:74:ILE:HD12	1:G:83:LEU:CD2	2.19	0.71
1:E:248:LEU:HD22	1:E:253:VAL:HG21	1.71	0.71
1:G:249:LYS:NZ	1:G:287:VAL:O	2.23	0.70
1:B:210:GLN:HG3	1:B:251:LEU:CD2	2.22	0.70
1:F:329:LEU:HD23	1:F:341:VAL:HG12	1.73	0.70
1:B:260:SER:OG	1:B:276:GLN:OE1	2.08	0.70
1:F:284:ARG:NH1	1:F:313:ASP:OD1	2.25	0.70
1:H:225:ARG:NH2	2:H:401:FMN:O3'	2.26	0.69
1:A:27:TYR:OH	3:A:402:W3X:N03	2.25	0.69
1:H:190:ARG:NH2	1:H:192:ASP:OD2	2.26	0.69
1:D:150:ILE:HD12	1:D:150:ILE:H	1.57	0.68
1:F:230:ASP:OD2	1:F:236:TRP:N	2.24	0.68
1:B:33:GLY:O	7:B:501:HOH:O	2.10	0.68
1:E:248:LEU:CD2	1:E:253:VAL:HG21	2.24	0.68
1:B:281:ASP:OD2	1:B:285:LYS:NZ	2.26	0.68
2:G:401:FMN:O4'	2:G:401:FMN:O2P	2.12	0.68
1:G:247:ARG:NH2	7:G:502:HOH:O	2.22	0.68
1:B:28:SER:O	1:B:36:THR:HG21	1.93	0.68
1:F:32:GLU:OE1	7:F:501:HOH:O	2.11	0.67
1:F:185:PRO:HG2	1:F:235:GLY:HA2	1.77	0.67
1:E:19:LEU:HD22	1:E:317:LEU:HD11	1.76	0.67
1:F:218:ARG:O	7:F:502:HOH:O	2.12	0.67
2:H:401:FMN:HM82	1:A:347:ARG:NE	2.10	0.67
1:D:347:ARG:NH1	3:E:403:W3X:O01	2.28	0.66
1:D:3:LEU:HD11	1:D:307:LEU:HB3	1.77	0.66
1:G:57:GLU:OE2	7:G:501:HOH:O	2.14	0.66
1:A:162:LEU:HD22	1:A:220:LEU:HD13	1.76	0.66
1:A:199:GLU:OE1	1:A:199:GLU:N	2.24	0.66
1:E:163:ARG:NH1	7:E:503:HOH:O	2.29	0.66
1:F:39:HIS:CD2	1:F:72:LEU:HD21	2.30	0.66
1:B:20:ALA:HB3	1:B:316:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:VAL:HG13	1:G:215:VAL:HG11	1.76	0.65
1:F:281:ASP:OD2	1:F:285:LYS:NZ	2.28	0.65
1:D:56:VAL:HG23	1:D:99:ILE:HG13	1.79	0.65
1:H:57:GLU:HG2	1:H:72:LEU:HD12	1.77	0.65
1:H:28:SER:O	1:H:36:THR:HG21	1.97	0.65
1:A:62:GLU:HG2	1:A:63:PRO:HD2	1.78	0.65
1:F:269:ILE:HG22	1:F:271:LEU:HD12	1.78	0.64
1:A:294:VAL:HG22	1:A:316:LEU:HB2	1.80	0.64
1:H:118:LYS:NZ	7:H:502:HOH:O	2.29	0.64
1:A:28:SER:O	1:A:36:THR:HG21	1.98	0.64
1:B:56:VAL:CG2	1:B:99:ILE:HD12	2.27	0.64
1:G:80:LEU:HD11	1:G:160:ARG:HG3	1.79	0.64
1:A:231:TRP:CE2	1:A:269:ILE:HG23	2.33	0.64
1:G:57:GLU:HG2	1:G:72:LEU:HD12	1.81	0.63
1:F:3:LEU:N	1:F:304:GLU:OE2	2.31	0.63
1:F:59:THR:HG23	1:F:72:LEU:C	2.18	0.63
1:H:224:VAL:HG13	1:H:256:LEU:HD12	1.79	0.63
1:E:64:LEU:HD12	4:E:402:IPA:H31	1.81	0.63
1:F:226:VAL:HG12	1:F:256:LEU:HD11	1.81	0.62
1:B:217:PRO:HD2	1:B:220:LEU:HD12	1.81	0.62
1:C:230:ASP:OD2	1:C:236:TRP:N	2.29	0.62
1:D:200:ASN:OD1	1:D:203:ARG:NH2	2.32	0.62
1:E:183:LEU:HD22	1:E:236:TRP:CH2	2.35	0.62
1:A:24:MET:HE1	1:A:322:LEU:HG	1.80	0.62
1:C:204:PHE:O	1:C:208:VAL:HG23	2.00	0.62
1:D:184:SER:HB3	1:D:263:VAL:HG11	1.82	0.62
1:A:3:LEU:N	1:A:304:GLU:OE2	2.32	0.62
1:A:19:LEU:HD22	1:A:317:LEU:HD11	1.82	0.62
1:B:56:VAL:HG13	1:B:98:GLY:O	1.99	0.61
1:F:62:GLU:OE1	1:F:64:LEU:N	2.32	0.61
1:F:168:VAL:HG22	1:F:221:PRO:HG2	1.81	0.61
1:G:275:PHE:CZ	1:G:276:GLN:HG3	2.35	0.61
1:H:133:ASP:OD1	1:H:134:GLU:N	2.33	0.61
1:H:202:MET:HE3	1:H:206:LEU:HD11	1.83	0.61
1:C:193:ALA:O	1:C:203:ARG:NH2	2.28	0.60
1:D:323:ARG:HD3	1:E:348:GLY:O	2.02	0.60
1:H:21:MET:HE1	1:H:46:ARG:HD3	1.82	0.60
1:E:212:VAL:O	1:E:216:VAL:HG23	2.02	0.60
1:G:24:MET:HE1	1:G:322:LEU:HD21	1.82	0.60
1:F:238:LEU:HD13	1:F:279:PHE:HD1	1.66	0.60
1:G:4:LEU:HD11	1:G:19:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:TRP:CE2	1:B:269:ILE:HG23	2.36	0.60
1:A:346:GLN:OE1	7:A:502:HOH:O	2.16	0.60
1:D:80:LEU:HD11	1:D:160:ARG:HG3	1.81	0.60
1:G:4:LEU:N	1:G:304:GLU:OE1	2.34	0.60
1:A:226:VAL:CG1	1:A:256:LEU:HD21	2.32	0.60
1:E:88[A]:ARG:NH2	1:G:34:GLU:OE2	2.33	0.60
1:G:59:THR:HG23	1:G:72:LEU:HB3	1.83	0.59
1:F:155:VAL:HG13	1:F:215:VAL:HG11	1.84	0.59
1:C:91:ARG:NH1	1:C:167:GLN:OE1	2.36	0.59
1:F:1:MET:HG2	1:F:2:ALA:H	1.66	0.59
1:H:324:ASP:CG	1:H:330:ARG:NH2	2.55	0.59
1:F:39:HIS:NE2	1:F:72:LEU:HD21	2.18	0.59
1:G:9:GLU:OE2	1:G:14:ARG:NH2	2.35	0.59
1:B:212:VAL:O	1:B:216:VAL:HG23	2.03	0.59
2:F:401:FMN:O4'	2:F:401:FMN:O3P	2.19	0.59
1:C:4:LEU:N	1:C:304:GLU:OE1	2.36	0.59
1:B:29:ALA:N	7:B:507:HOH:O	2.36	0.58
2:A:401:FMN:H4'	3:A:402:W3X:C11	2.33	0.58
1:E:324:ASP:OD2	1:E:330:ARG:NH2	2.34	0.58
1:F:19:LEU:HD22	1:F:317:LEU:HD11	1.84	0.58
1:G:179:LEU:HD21	1:G:208:VAL:HG21	1.85	0.58
1:A:59:THR:HG21	1:A:99:ILE:HD11	1.84	0.58
1:C:300:PRO:HB3	1:C:331:ALA:HB1	1.86	0.58
1:G:56:VAL:HG21	1:G:99:ILE:HD12	1.85	0.58
1:E:339:PRO:HB2	1:E:341:VAL:HG23	1.85	0.58
1:A:225:ARG:NH2	2:A:401:FMN:O3'	2.37	0.58
1:D:57:GLU:HG2	1:D:72:LEU:HD12	1.86	0.58
1:F:193:ALA:HB1	1:F:203:ARG:NH1	2.18	0.58
1:C:179:LEU:HD22	1:C:205:PRO:HA	1.86	0.57
1:C:77:GLU:OE2	1:C:163:ARG:NH2	2.36	0.57
1:D:281:ASP:OD2	1:D:285:LYS:NZ	2.25	0.57
1:E:224:VAL:O	1:E:256:LEU:HD12	2.04	0.57
2:F:401:FMN:O3'	7:F:503:HOH:O	2.17	0.57
1:H:212:VAL:O	1:H:216:VAL:HG23	2.04	0.57
1:F:22:SER:OG	1:F:225:ARG:NH2	2.37	0.57
1:B:132:PHE:CE2	1:B:265:LEU:HD21	2.40	0.56
1:F:264:VAL:HG23	1:F:267:VAL:HG11	1.86	0.56
1:A:56:VAL:HG23	1:A:99:ILE:HD12	1.87	0.56
1:G:298:THR:HG22	1:G:320:VAL:HG22	1.88	0.56
1:A:210:GLN:HB2	1:A:251:LEU:HD21	1.87	0.56
1:D:56:VAL:HG22	1:D:98:GLY:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:VAL:CG2	1:F:99:ILE:HG13	2.32	0.56
1:A:1:MET:HE2	1:A:3:LEU:HD12	1.88	0.56
1:D:12:GLY:N	1:D:219:GLU:O	2.38	0.56
1:E:22:SER:OG	1:E:225:ARG:NH2	2.38	0.56
2:B:401:FMN:O2P	2:B:401:FMN:O4'	2.20	0.56
1:E:24:MET:CE	1:E:322:LEU:HD21	2.35	0.56
1:F:150:ILE:HD12	1:F:150:ILE:H	1.71	0.56
1:G:275:PHE:CE2	1:G:276:GLN:HG3	2.40	0.56
1:A:324:ASP:OD2	1:A:330:ARG:NH2	2.38	0.56
1:B:277:VAL:N	1:B:278:PRO:HD2	2.21	0.56
1:G:4:LEU:HD11	1:G:19:LEU:CD2	2.35	0.56
1:G:34:GLU:HA	7:G:512:HOH:O	2.05	0.56
1:G:84:LYS:CG	1:G:164:ALA:HA	2.35	0.56
1:C:277:VAL:N	1:C:278:PRO:HD2	2.21	0.56
1:D:248:LEU:HD22	1:D:253:VAL:HG21	1.88	0.56
1:D:231:TRP:HZ2	1:D:260:SER:HG	1.54	0.55
1:G:84:LYS:HG3	1:G:164:ALA:HA	1.89	0.55
1:H:277:VAL:N	1:H:278:PRO:HD2	2.21	0.55
1:H:247:ARG:CZ	1:H:247:ARG:HA	2.35	0.55
1:A:12:GLY:N	1:A:219:GLU:O	2.39	0.55
1:D:347:ARG:HB3	2:E:401:FMN:HM82	1.88	0.55
1:G:133:ASP:OD2	1:G:265:LEU:HD12	2.06	0.55
1:H:4:LEU:HD11	1:H:19:LEU:HD21	1.87	0.55
1:F:49:GLY:O	1:F:329:LEU:HD12	2.06	0.55
1:A:53:LEU:HD12	1:A:96:VAL:O	2.06	0.55
1:C:13:LEU:HD12	1:C:14:ARG:H	1.72	0.55
1:F:1:MET:HG2	1:F:2:ALA:N	2.21	0.55
1:F:12:GLY:N	1:F:219:GLU:O	2.37	0.55
1:C:155:VAL:HG13	1:C:215:VAL:HG11	1.89	0.55
1:D:112:ARG:NH1	1:D:115:GLU:OE2	2.40	0.55
1:D:324:ASP:OD2	1:D:330:ARG:NH2	2.34	0.55
1:A:320:VAL:O	1:A:324:ASP:N	2.40	0.55
1:E:271:LEU:HD23	1:F:0:HIS:HB2	1.89	0.55
1:H:324:ASP:OD1	1:H:330:ARG:NH2	2.39	0.55
1:F:155:VAL:CG2	1:F:211:ALA:HB1	2.37	0.54
1:H:4:LEU:N	1:H:304:GLU:OE1	2.41	0.54
1:B:231:TRP:HE1	1:B:260:SER:HB2	1.72	0.54
1:E:24:MET:HA	2:E:401:FMN:N5	2.23	0.54
1:F:299:THR:HG22	1:F:301:GLU:H	1.71	0.54
1:A:184:SER:CB	1:A:263:VAL:HG11	2.37	0.54
1:C:12:GLY:N	1:C:219:GLU:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:LYS:NZ	7:F:507:HOH:O	2.40	0.54
1:E:155:VAL:HG13	1:E:215:VAL:HG11	1.90	0.54
1:G:225:ARG:NH2	2:G:401:FMN:O3'	2.41	0.54
1:A:277:VAL:N	1:A:278:PRO:HD2	2.23	0.54
1:D:266:ARG:O	7:D:501:HOH:O	2.18	0.54
1:B:179:LEU:HD21	1:B:208:VAL:HG21	1.89	0.54
1:H:53:LEU:HD12	1:H:96:VAL:O	2.08	0.54
1:E:2:ALA:O	1:E:6:THR:HG23	2.07	0.53
1:F:40:LEU:HD22	1:F:89:ARG:HD3	1.89	0.53
1:F:247:ARG:O	1:F:251:LEU:HD22	2.07	0.53
1:B:3:LEU:HD23	1:B:307:LEU:HB3	1.89	0.53
1:B:131:PRO:N	1:B:138:VAL:HG23	2.22	0.53
1:D:39:HIS:CD2	1:D:72:LEU:HD21	2.44	0.53
1:E:99:ILE:HD12	1:E:166:PHE:CZ	2.42	0.53
1:F:206:LEU:HD23	1:F:248:LEU:CD2	2.39	0.53
1:A:4:LEU:HD23	1:A:5:PHE:CE2	2.44	0.53
1:E:12:GLY:N	1:E:219:GLU:O	2.41	0.53
1:H:329:LEU:HD22	1:H:341:VAL:HG22	1.91	0.53
1:F:146:GLY:O	1:F:150:ILE:HD12	2.08	0.53
1:F:346:GLN:NE2	7:F:506:HOH:O	2.39	0.53
1:A:217:PRO:HG2	1:A:220:LEU:HD12	1.90	0.53
1:C:246[A]:ARG:HG3	1:C:287:VAL:HG22	1.91	0.53
1:H:206:LEU:HD23	1:H:248:LEU:HD23	1.90	0.53
1:E:91:ARG:NH2	1:E:165:GLY:O	2.42	0.53
1:F:27:TYR:OH	3:F:404:W3X:N03	2.41	0.53
1:A:130:ILE:N	1:A:130:ILE:HD12	2.24	0.53
1:B:231:TRP:NE1	1:B:269:ILE:HG23	2.24	0.53
1:D:47:ALA:CA	1:D:54:ILE:HD11	2.39	0.53
1:A:294:VAL:HG12	2:A:401:FMN:H5'1	1.90	0.53
1:B:27:TYR:HB3	1:B:112:ARG:HD2	1.90	0.53
1:H:74:ILE:HG23	1:H:74:ILE:O	2.09	0.53
1:D:22:SER:OG	1:D:225:ARG:NH2	2.42	0.52
1:G:79:HIS:O	1:G:83:LEU:HB2	2.10	0.52
1:D:47:ALA:CB	1:D:93:ALA:HB3	2.40	0.52
1:G:238:LEU:HD12	1:G:238:LEU:O	2.08	0.52
1:G:248:LEU:HD22	1:G:253:VAL:HG21	1.91	0.52
1:C:324:ASP:OD2	1:C:330:ARG:NH2	2.42	0.52
1:A:64:LEU:HD11	1:A:123:ARG:O	2.08	0.52
1:D:47:ALA:HA	1:D:54:ILE:HD11	1.91	0.52
1:D:208:VAL:O	1:D:212:VAL:HG23	2.09	0.52
1:G:230:ASP:O	1:G:231:TRP:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:SER:N	7:B:507:HOH:O	2.34	0.52
1:G:151:LEU:HD21	1:G:211:ALA:CB	2.40	0.52
1:F:24:MET:HA	2:F:401:FMN:N5	2.25	0.52
1:D:212:VAL:O	1:D:216:VAL:HG23	2.10	0.52
1:A:229:THR:HG22	1:A:231:TRP:N	2.25	0.52
1:E:36:THR:OG1	1:E:37:ASP:N	2.43	0.52
1:G:277:VAL:N	1:G:278:PRO:HD2	2.25	0.52
1:A:22:SER:OG	2:A:401:FMN:O2'	2.27	0.52
1:E:343:PRO:O	1:E:346:GLN:HG2	2.10	0.52
1:D:146:GLY:O	1:D:150:ILE:HD12	2.09	0.51
1:F:22:SER:HG	2:F:401:FMN:HO2'	1.58	0.51
1:A:46:ARG:HH12	1:A:322:LEU:HA	1.75	0.51
1:A:341:VAL:HG13	1:A:342:PRO:HD2	1.91	0.51
1:E:36:THR:HG22	1:E:39:HIS:CE1	2.45	0.51
1:G:24:MET:HA	2:G:401:FMN:N5	2.25	0.51
1:G:340:GLU:HA	1:G:340:GLU:OE1	2.09	0.51
1:A:59:THR:HG22	1:A:72:LEU:HB3	1.92	0.51
1:C:4:LEU:HD11	1:C:19:LEU:HD21	1.93	0.51
1:D:147:MET:HA	1:D:150:ILE:HD13	1.93	0.51
1:D:345:TYR:CD1	1:E:322:LEU:HD22	2.45	0.51
1:D:347:ARG:NE	2:E:401:FMN:HM82	2.26	0.51
1:F:22:SER:HA	1:F:316:LEU:HD23	1.92	0.51
1:H:51:VAL:HG13	1:H:328:PRO:HG2	1.92	0.51
1:C:179:LEU:HD21	1:C:208:VAL:HG21	1.93	0.51
1:C:224:VAL:O	1:C:256:LEU:HD12	2.10	0.51
1:H:306:LEU:HD11	1:H:315:VAL:HG22	1.92	0.51
1:B:51:VAL:O	1:B:95:ALA:HB2	2.11	0.51
1:C:19:LEU:HD22	1:C:317:LEU:HD11	1.93	0.51
1:D:40:LEU:O	1:D:44:PRO:HG2	2.11	0.51
1:E:28:SER:O	1:E:36:THR:HG21	2.11	0.51
1:E:168:VAL:HG22	1:E:221:PRO:HG2	1.91	0.51
1:H:147:MET:HE1	1:H:194:TYR:CZ	2.46	0.51
1:C:4:LEU:HD11	1:C:19:LEU:CD2	2.40	0.51
1:A:131:PRO:HG3	1:A:138:VAL:HG22	1.93	0.51
1:A:198:LEU:HD11	1:A:240:ASP:HB3	1.93	0.51
1:C:40:LEU:O	1:C:44:PRO:HG2	2.11	0.51
2:D:401:FMN:O3P	2:D:401:FMN:O4'	2.25	0.51
1:B:138:VAL:CG1	1:B:138:VAL:O	2.58	0.50
1:B:24:MET:HA	2:B:401:FMN:N5	2.26	0.50
1:A:80:LEU:HD21	1:A:163:ARG:HG2	1.94	0.50
1:A:346:GLN:NE2	7:A:506:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:THR:N	1:A:313:ASP:OD1	2.40	0.50
1:A:226:VAL:HG11	1:A:256:LEU:HD21	1.92	0.50
1:A:298:THR:HA	1:A:320:VAL:HG21	1.94	0.50
1:C:15:LEU:N	7:C:501:HOH:O	2.28	0.50
1:D:47:ALA:HB3	1:D:93:ALA:HB3	1.92	0.50
1:G:177:TYR:O	1:G:181:SER:OG	2.29	0.50
1:B:246[B]:ARG:NH2	7:B:510:HOH:O	2.38	0.50
1:D:83:LEU:HD22	1:D:166:PHE:HE2	1.77	0.50
1:E:301:GLU:OE1	1:F:299:THR:OG1	2.29	0.50
1:F:266[B]:ARG:O	1:F:266[B]:ARG:HG2	2.12	0.50
1:B:84:LYS:HG2	1:B:164:ALA:HA	1.94	0.50
1:D:277:VAL:N	1:D:278:PRO:HD2	2.27	0.50
1:F:13:LEU:HG	1:F:14:ARG:N	2.27	0.50
1:F:199:GLU:OE2	1:F:247:ARG:NH1	2.45	0.50
1:B:80:LEU:HG	1:B:84:LYS:HE3	1.93	0.49
1:F:185:PRO:CG	1:F:235:GLY:HA2	2.42	0.49
1:A:10:LEU:HD21	1:A:290:ARG:HD2	1.94	0.49
1:D:2:ALA:HB3	1:D:337:VAL:HG21	1.94	0.49
1:G:339:PRO:O	1:G:341:VAL:HG23	2.12	0.49
1:B:247:ARG:O	1:B:251:LEU:HD12	2.12	0.49
1:E:229:THR:HG22	1:E:231:TRP:H	1.77	0.49
1:F:155:VAL:HG21	1:F:211:ALA:HB1	1.93	0.49
1:C:56:VAL:HB	1:C:99:ILE:HD12	1.93	0.49
1:B:64:LEU:H	1:B:64:LEU:HD22	1.78	0.49
2:B:401:FMN:HO4'	2:B:401:FMN:P	2.35	0.49
1:D:59:THR:HG22	1:D:72:LEU:HB2	1.95	0.49
1:H:4:LEU:HD11	1:H:19:LEU:CD2	2.42	0.49
1:A:246[A]:ARG:HG3	1:A:287:VAL:HG13	1.95	0.49
1:H:147:MET:HE1	1:H:194:TYR:CE1	2.47	0.49
1:B:217:PRO:CD	1:B:220:LEU:HD12	2.43	0.49
1:C:24:MET:HA	2:C:401:FMN:N5	2.27	0.49
1:C:246[B]:ARG:HA	1:C:249:LYS:HG2	1.93	0.49
1:D:237:SER:OG	7:D:502:HOH:O	2.19	0.49
1:G:39:HIS:ND1	1:G:72:LEU:HD21	2.27	0.49
1:A:143:ASP:OD1	1:A:143:ASP:N	2.38	0.49
1:E:194:TYR:CE2	1:E:203:ARG:HD2	2.48	0.49
1:A:226:VAL:HG12	1:A:256:LEU:HD21	1.94	0.49
1:F:59:THR:HG23	1:F:73:GLY:N	2.28	0.49
1:G:16:LYS:NZ	7:G:504:HOH:O	2.36	0.49
1:A:46:ARG:NH1	1:A:321:LEU:O	2.46	0.49
1:G:231:TRP:CZ3	1:G:270:PRO:CD	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:ILE:O	1:H:320:VAL:HG21	2.13	0.49
1:H:345:TYR:CD1	1:A:322:LEU:HD22	2.47	0.49
1:B:257:ASP:OD1	1:B:257:ASP:N	2.42	0.48
1:A:59:THR:HG22	1:A:72:LEU:CB	2.43	0.48
1:D:83:LEU:HD22	1:D:166:PHE:CE2	2.48	0.48
1:E:24:MET:HE1	1:E:322:LEU:HG	1.95	0.48
1:B:16:LYS:O	7:B:502:HOH:O	2.19	0.48
1:D:190:ARG:NH2	1:D:192:ASP:OD2	2.47	0.48
1:G:25:CYS:HA	1:G:57:GLU:HB2	1.95	0.48
1:G:199:GLU:HG2	1:G:247:ARG:NH1	2.28	0.48
1:D:298:THR:HG22	1:D:320:VAL:HB	1.96	0.48
1:E:47:ALA:HB3	1:E:93:ALA:HB3	1.95	0.48
1:C:70:TYR:CD1	1:C:70:TYR:N	2.82	0.48
1:D:4:LEU:N	1:D:304:GLU:OE1	2.45	0.48
1:E:263:VAL:HG22	1:E:264:VAL:HG13	1.96	0.48
1:G:190:ARG:NH2	1:G:192:ASP:OD2	2.45	0.48
1:B:283:VAL:HB	1:B:291:THR:HG21	1.96	0.48
1:G:225:ARG:NH1	1:G:257:ASP:OD2	2.47	0.48
1:A:171:LEU:HD13	1:A:222:LEU:HD11	1.95	0.48
1:A:238:LEU:HD13	1:A:279:PHE:HD1	1.78	0.48
1:C:1:MET:CE	1:C:3:LEU:CD2	2.91	0.48
1:D:320:VAL:HA	1:D:323:ARG:NH1	2.29	0.48
1:E:5:PHE:HE2	1:E:335:LEU:HD12	1.77	0.48
1:E:278:PRO:HG3	1:F:308:GLN:O	2.13	0.48
1:C:24:MET:HE1	1:C:322:LEU:HD13	1.95	0.48
1:D:106:ARG:CZ	1:D:132:PHE:HA	2.44	0.48
1:H:25:CYS:HA	1:H:57:GLU:HB2	1.96	0.48
1:H:35:VAL:HG23	1:H:83:LEU:HD12	1.95	0.48
1:H:85:GLU:HG3	1:H:89:ARG:HD2	1.96	0.48
1:B:138:VAL:O	1:B:138:VAL:HG13	2.13	0.47
1:B:238:LEU:HD21	1:B:282:ALA:HB3	1.95	0.47
1:H:143:ASP:O	1:H:147:MET:N	2.42	0.47
1:H:184:SER:HB3	1:H:263:VAL:HG11	1.96	0.47
1:E:29:ALA:HB3	1:E:70:TYR:O	2.15	0.47
2:A:401:FMN:H1'2	3:A:402:W3X:C10	2.44	0.47
1:A:24:MET:CE	1:A:322:LEU:HG	2.44	0.47
1:A:77:GLU:OE1	1:A:160:ARG:NH1	2.47	0.47
1:C:1:MET:HE2	1:C:3:LEU:HD22	1.97	0.47
1:D:57:GLU:CG	1:D:72:LEU:HD12	2.44	0.47
1:F:150:ILE:HD12	1:F:150:ILE:N	2.29	0.47
1:A:174:ALA:HB2	1:A:226:VAL:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:HB2	1:A:226:VAL:CA	2.44	0.47
1:C:79:HIS:HB3	1:C:83:LEU:HD12	1.96	0.47
1:G:39:HIS:CE1	1:G:72:LEU:HD21	2.50	0.47
1:G:63:PRO:HG3	1:G:75:TRP:CE2	2.50	0.47
1:H:4:LEU:HD23	1:H:5:PHE:CE2	2.49	0.47
1:B:43:TYR:CE1	1:B:56:VAL:HA	2.50	0.47
1:B:148:GLU:O	1:B:152:GLN:HG3	2.14	0.47
1:D:246:ARG:HG3	1:D:287:VAL:HG13	1.97	0.47
1:E:198:LEU:HD11	1:E:236:TRP:CZ3	2.50	0.47
1:E:305:THR:HG23	1:F:274:GLY:HA3	1.96	0.47
1:F:43:TYR:CZ	1:F:56:VAL:HB	2.50	0.47
1:F:60:ALA:HB3	1:F:66:ARG:HG2	1.96	0.47
1:F:277:VAL:N	1:F:278:PRO:HD2	2.30	0.47
1:G:260:SER:N	1:G:276:GLN:OE1	2.47	0.47
1:H:186:LEU:HD12	1:H:230:ASP:OD2	2.15	0.47
1:A:184:SER:HB3	1:A:263:VAL:HG11	1.96	0.47
1:B:231:TRP:CD1	1:B:269:ILE:HG12	2.49	0.47
1:D:48:LEU:HD22	1:D:342:PRO:CG	2.44	0.47
1:E:27:TYR:OH	3:E:403:W3X:N03	2.47	0.47
1:F:47:ALA:HB3	1:F:93:ALA:HB3	1.97	0.47
1:G:329:LEU:HD23	1:G:341:VAL:HG13	1.97	0.47
1:H:324:ASP:CG	1:H:330:ARG:HH21	2.15	0.47
1:C:25:CYS:HA	1:C:57:GLU:HB2	1.96	0.47
1:D:103:HIS:ND1	1:D:178:LEU:HD22	2.30	0.47
1:H:332:ALA:HB3	1:H:339:PRO:HB3	1.97	0.47
1:B:230:ASP:O	1:B:231:TRP:HB2	2.14	0.47
1:C:307:LEU:HD21	1:C:315:VAL:HG23	1.97	0.47
1:E:62:GLU:HG2	1:E:63:PRO:HD2	1.96	0.47
1:E:230:ASP:O	1:E:231:TRP:HB2	2.15	0.47
1:F:266[B]:ARG:O	1:F:266[B]:ARG:CG	2.61	0.46
1:H:225:ARG:NE	2:H:401:FMN:O2	2.48	0.46
1:H:55:LEU:HD12	1:H:316:LEU:HD21	1.96	0.46
1:B:64:LEU:HD22	1:B:64:LEU:N	2.30	0.46
1:A:229:THR:HG22	1:A:231:TRP:H	1.80	0.46
1:C:57:GLU:HG2	1:C:72:LEU:HD12	1.97	0.46
1:D:271:LEU:HG	1:D:271:LEU:O	2.16	0.46
1:F:256:LEU:HD12	1:F:258:CYS:SG	2.56	0.46
1:F:256:LEU:HD23	1:F:289:LEU:HD21	1.97	0.46
1:F:57:GLU:OE2	7:F:504:HOH:O	2.20	0.46
1:F:64:LEU:HD13	1:F:122:TRP:CE3	2.51	0.46
1:C:133:ASP:OD2	1:C:265:LEU:HD21	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:LEU:O	1:E:291:THR:HA	2.16	0.46
1:G:2:ALA:O	1:G:6:THR:HG23	2.14	0.46
1:D:39:HIS:HD2	1:D:72:LEU:HD11	1.81	0.46
1:D:204:PHE:HA	1:D:207:GLN:HG3	1.98	0.46
1:E:41:LEU:O	1:E:45:THR:OG1	2.28	0.46
1:H:184:SER:CB	1:H:263:VAL:HG11	2.46	0.46
1:E:277:VAL:N	1:E:278:PRO:CD	2.79	0.46
1:A:1:MET:CE	1:A:3:LEU:CD1	2.93	0.46
1:A:74:ILE:HD12	1:A:83:LEU:HD13	1.98	0.46
1:B:30:THR:HG22	1:B:31:LEU:H	1.81	0.46
1:B:162:LEU:HD22	1:B:220:LEU:HD13	1.98	0.46
1:D:257:ASP:OD2	1:D:316:LEU:HD22	2.15	0.46
1:A:133:ASP:CG	1:A:134:GLU:H	2.18	0.46
1:C:175:HIS:N	1:C:227:SER:OG	2.43	0.46
1:C:246[A]:ARG:HA	1:C:249:LYS:HG2	1.96	0.46
1:F:206:LEU:HD23	1:F:248:LEU:HD21	1.97	0.46
1:A:250:GLU:O	1:A:250:GLU:HG3	2.15	0.46
1:D:48:LEU:HD22	1:D:342:PRO:HG2	1.98	0.45
1:H:77:GLU:O	1:H:77:GLU:HG3	2.15	0.45
1:A:99:ILE:HG21	1:A:161:ALA:CB	2.47	0.45
1:F:48:LEU:HD22	1:F:342:PRO:CG	2.46	0.45
1:F:156:GLU:OE2	1:F:159:ARG:HD2	2.17	0.45
1:A:106:ARG:CZ	1:A:132:PHE:HA	2.46	0.45
1:C:237:SER:OG	1:C:240:ASP:OD1	2.34	0.45
1:F:86:LEU:HD23	1:F:166:PHE:HZ	1.80	0.45
1:E:317:LEU:HB2	1:E:321:LEU:HD11	1.97	0.45
1:C:1:MET:HE1	1:C:3:LEU:CD2	2.47	0.45
1:F:226:VAL:CG1	1:F:256:LEU:HD11	2.45	0.45
1:G:289:LEU:O	1:G:291:THR:HG23	2.16	0.45
1:B:27:TYR:OH	3:B:402:W3X:N03	2.50	0.45
1:B:29:ALA:HA	1:B:36:THR:HG23	1.99	0.45
1:C:194:TYR:CE1	1:C:203:ARG:HD2	2.51	0.45
1:D:143:ASP:OD1	1:D:143:ASP:N	2.45	0.45
1:F:80:LEU:N	1:F:81:PRO:HD2	2.32	0.45
1:F:85:GLU:OE2	1:F:89:ARG:HD2	2.17	0.45
1:G:176:GLY:HA3	1:G:263:VAL:HA	1.99	0.45
1:A:229:THR:CG2	1:A:231:TRP:H	2.29	0.45
1:A:300:PRO:HB3	1:A:331:ALA:HB1	1.99	0.45
1:E:238:LEU:HD13	1:E:279:PHE:HD1	1.82	0.45
1:F:100:GLN:HA	1:F:170:GLU:O	2.17	0.45
1:G:75:TRP:O	1:G:160:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246[B]:ARG:HD3	1:G:287:VAL:HG13	1.98	0.45
1:A:36:THR:OG1	1:A:37:ASP:N	2.50	0.45
1:H:265:LEU:HD23	1:H:265:LEU:H	1.82	0.45
1:B:246[A]:ARG:HG3	1:B:287:VAL:HG22	1.99	0.45
1:B:276:GLN:HG3	1:B:294:VAL:O	2.16	0.45
1:B:290:ARG:HG2	1:B:290:ARG:HH11	1.82	0.45
1:D:238:LEU:O	1:D:242:LEU:HD23	2.16	0.45
1:A:269:ILE:O	1:A:271:LEU:N	2.50	0.45
1:C:184:SER:HB2	1:C:263:VAL:HG21	1.99	0.45
1:A:47:ALA:HB3	1:A:93:ALA:HB3	1.98	0.45
1:D:41:LEU:HD11	1:E:44:PRO:HB2	1.98	0.44
1:H:40:LEU:O	1:H:44:PRO:HG2	2.17	0.44
1:A:133:ASP:HB2	1:A:265:LEU:CD1	2.47	0.44
1:E:159:ARG:O	1:E:163:ARG:HG3	2.18	0.44
1:F:162:LEU:HD23	1:F:169:ILE:HD11	1.99	0.44
1:H:43:TYR:OH	1:H:57:GLU:HB3	2.17	0.44
1:C:6:THR:O	1:C:18:ARG:NH1	2.50	0.44
1:H:341:VAL:HG12	1:H:345:TYR:HB2	2.00	0.44
1:E:4:LEU:HD23	1:E:5:PHE:CE2	2.53	0.44
1:G:70:TYR:N	1:G:70:TYR:CD1	2.85	0.44
1:G:155:VAL:HG21	1:G:211:ALA:HB1	1.99	0.44
1:H:294:VAL:HG22	1:H:295:GLY:N	2.32	0.44
1:C:206:LEU:HD13	1:C:247:ARG:HD3	1.99	0.44
1:H:133:ASP:OD2	1:H:265:LEU:HD11	2.18	0.44
1:A:99:ILE:HG21	1:A:161:ALA:HB1	2.00	0.44
1:G:199:GLU:HG2	1:G:247:ARG:HH12	1.83	0.44
1:H:5:PHE:CE2	1:H:332:ALA:HA	2.53	0.44
1:B:39:HIS:CE1	1:B:72:LEU:HD21	2.53	0.44
1:B:57:GLU:CG	1:B:72:LEU:HD12	2.48	0.44
1:B:131:PRO:CA	1:B:138:VAL:HG23	2.48	0.44
1:B:238:LEU:HD21	1:B:282:ALA:CB	2.47	0.44
1:C:218:ARG:HG3	1:C:219:GLU:N	2.33	0.44
1:D:51:VAL:HG13	1:D:328:PRO:HG2	2.00	0.44
1:D:184:SER:CB	1:D:263:VAL:HG11	2.47	0.44
1:F:106:ARG:NH2	1:F:263:VAL:O	2.51	0.44
1:E:7:PRO:HA	1:E:15:LEU:O	2.18	0.43
1:E:56:VAL:HG12	1:E:57:GLU:N	2.33	0.43
1:H:80:LEU:CD1	1:H:160:ARG:HG3	2.48	0.43
1:C:5:PHE:HA	1:C:17:ASN:HB2	1.99	0.43
1:C:271:LEU:HD23	1:C:275:PHE:CE2	2.54	0.43
1:D:21:MET:O	1:D:55:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:MET:HE1	1:D:194:TYR:CD2	2.53	0.43
1:F:48:LEU:HD22	1:F:342:PRO:HG3	2.00	0.43
1:G:19:LEU:HD12	1:G:328:PRO:HB3	1.99	0.43
1:A:149:ARG:NH2	1:A:150:ILE:HD11	2.33	0.43
1:B:231:TRP:NE1	1:B:260:SER:HB2	2.34	0.43
1:D:66:ARG:NH1	1:D:69:PRO:O	2.52	0.43
1:D:242:LEU:HD12	1:D:287:VAL:HG23	2.00	0.43
1:F:249:LYS:HB2	1:F:289:LEU:HB2	2.01	0.43
1:G:138:VAL:O	1:G:138:VAL:HG13	2.18	0.43
1:G:167:GLN:O	1:G:220:LEU:HD22	2.19	0.43
1:H:39:HIS:CE1	1:H:72:LEU:HD21	2.52	0.43
1:B:302:GLN:OE1	1:A:305:THR:OG1	2.32	0.43
1:E:147:MET:SD	1:E:194:TYR:CE2	3.12	0.43
1:F:59:THR:OG1	1:F:99:ILE:HD11	2.19	0.43
1:B:57:GLU:HG2	1:B:72:LEU:HD12	2.00	0.43
1:C:91:ARG:HA	1:C:95:ALA:O	2.19	0.43
1:C:178:LEU:O	1:C:181:SER:OG	2.29	0.43
1:G:80:LEU:HD11	1:G:160:ARG:CG	2.46	0.43
1:G:149:ARG:HH21	1:G:150:ILE:HD11	1.84	0.43
1:A:264:VAL:HG22	1:A:265:LEU:N	2.33	0.43
1:C:212:VAL:O	1:C:215:VAL:HG22	2.18	0.43
1:H:36:THR:OG1	1:H:37:ASP:N	2.52	0.43
1:H:325:PRO:HD3	1:A:326:TYR:CD2	2.54	0.43
1:B:8:LEU:HD23	1:B:314:LEU:HD13	2.00	0.43
1:C:56:VAL:HG12	1:C:57:GLU:N	2.34	0.43
1:E:1:MET:CE	1:E:3:LEU:HD22	2.49	0.43
1:F:47:ALA:CB	1:F:93:ALA:HB3	2.49	0.43
1:D:22:SER:HA	1:D:316:LEU:HD23	2.01	0.43
1:D:236:TRP:NE1	1:D:241:THR:OG1	2.51	0.43
1:E:307:LEU:HD21	1:E:315:VAL:HG23	2.01	0.43
1:G:8:LEU:HB2	1:G:18:ARG:CD	2.49	0.43
1:B:155:VAL:HG13	1:B:215:VAL:HG11	2.00	0.43
1:D:146:GLY:O	1:D:150:ILE:CD1	2.66	0.43
1:H:56:VAL:HG12	1:H:57:GLU:N	2.33	0.43
1:C:196:GLY:O	1:C:201:ARG:NH1	2.52	0.42
1:D:332:ALA:HB3	1:D:339:PRO:HB3	2.01	0.42
1:E:112:ARG:NH2	1:E:115:GLU:OE2	2.52	0.42
1:H:7:PRO:HA	1:H:15:LEU:O	2.19	0.42
1:H:168:VAL:HG22	1:H:221:PRO:HG2	1.99	0.42
1:C:231:TRP:CE2	1:C:269:ILE:HG23	2.54	0.42
1:D:24:MET:HA	2:D:401:FMN:N5	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:VAL:O	1:D:138:VAL:CG1	2.67	0.42
1:F:185:PRO:HG2	1:F:234:GLY:O	2.19	0.42
1:G:24:MET:HE1	1:G:322:LEU:CD2	2.46	0.42
1:A:221:PRO:HA	1:A:254:ASP:OD2	2.20	0.42
1:B:168:VAL:HG22	1:B:221:PRO:HD2	2.02	0.42
1:C:281:ASP:OD2	1:C:285:LYS:NZ	2.47	0.42
1:F:317:LEU:HB3	1:F:320:VAL:HG12	2.00	0.42
1:G:217:PRO:HD2	1:G:220:LEU:HD12	2.01	0.42
1:G:218:ARG:HG2	1:G:219:GLU:N	2.34	0.42
1:H:206:LEU:HD23	1:H:251:LEU:HD11	2.01	0.42
1:H:231:TRP:CE2	1:H:269:ILE:HG23	2.54	0.42
1:B:246[A]:ARG:NE	1:B:287:VAL:HG22	2.35	0.42
1:B:265:LEU:HB2	1:B:266:ARG:HD3	2.01	0.42
1:D:5:PHE:CE2	1:D:332:ALA:HA	2.54	0.42
1:D:60:ALA:HB3	1:D:66:ARG:HG2	2.01	0.42
1:A:151:LEU:O	1:A:155:VAL:HG23	2.19	0.42
1:B:347:ARG:NH2	7:B:509:HOH:O	2.36	0.42
1:C:236:TRP:CZ3	1:C:240:ASP:HB3	2.55	0.42
1:F:101:LEU:HD13	1:F:169:ILE:CG2	2.50	0.42
1:F:339:PRO:O	1:F:341:VAL:HG13	2.19	0.42
1:G:297:ILE:O	1:G:320:VAL:HG21	2.20	0.42
1:A:341:VAL:CG1	1:A:345:TYR:HB2	2.49	0.42
1:A:341:VAL:HG12	1:A:342:PRO:O	2.19	0.42
1:C:104:ALA:HB3	1:C:108:ALA:HB2	2.02	0.42
1:C:129:PRO:O	1:C:130:ILE:HD13	2.20	0.42
1:C:182:PHE:O	1:C:201:ARG:HB3	2.20	0.42
1:E:8:LEU:HD13	1:E:18:ARG:HH11	1.85	0.42
1:F:206:LEU:HD23	1:F:248:LEU:HD23	2.01	0.42
1:F:269:ILE:HG23	1:F:270:PRO:HD2	2.02	0.42
1:E:89:ARG:HA	1:E:92:GLU:HB2	2.02	0.42
1:F:48:LEU:O	1:F:329:LEU:HD11	2.20	0.42
1:B:24:MET:CE	1:B:322:LEU:HD21	2.50	0.42
1:B:227:SER:HA	1:B:259:SER:O	2.20	0.42
1:B:244:PHE:CZ	1:B:248:LEU:HD11	2.55	0.42
1:C:248:LEU:HD22	1:C:253:VAL:HG21	2.01	0.42
1:D:54:ILE:HG13	1:D:95:ALA:CB	2.50	0.42
1:E:22:SER:O	1:E:24:MET:HG3	2.19	0.42
1:E:64:LEU:HA	4:E:402:IPA:H32	2.02	0.42
1:F:101:LEU:HD13	1:F:169:ILE:HG23	2.02	0.42
1:G:84:LYS:HG2	1:G:164:ALA:HA	2.01	0.42
1:C:1:MET:HE2	1:C:3:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:LEU:HB3	1:D:320:VAL:CG1	2.50	0.41
1:E:210:GLN:HG3	1:E:251:LEU:HD22	2.01	0.41
1:F:22:SER:OG	2:F:401:FMN:O2'	2.34	0.41
1:G:60:ALA:CB	1:G:66:ARG:HG2	2.50	0.41
1:G:84:LYS:HA	1:G:164:ALA:HB1	2.01	0.41
1:G:151:LEU:C	1:G:151:LEU:HD23	2.40	0.41
1:B:59:THR:HG23	1:B:72:LEU:HB3	2.00	0.41
1:C:175:HIS:HA	1:C:262:GLY:HA3	2.02	0.41
1:E:177:TYR:O	1:E:181:SER:OG	2.36	0.41
1:F:255:LEU:HD23	1:F:256:LEU:O	2.20	0.41
1:G:39:HIS:CD2	1:G:39:HIS:N	2.88	0.41
1:H:10:LEU:HD21	1:H:290:ARG:HD2	2.01	0.41
1:H:244:PHE:CZ	1:H:248:LEU:HD11	2.55	0.41
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.94	0.41
1:C:199:GLU:CD	1:C:199:GLU:H	2.24	0.41
1:F:35:VAL:HG22	1:F:72:LEU:HD22	2.02	0.41
1:H:39:HIS:CD2	1:H:39:HIS:N	2.88	0.41
1:A:43:TYR:CE1	1:A:56:VAL:HA	2.55	0.41
1:A:294:VAL:HG12	1:A:295:GLY:N	2.36	0.41
1:B:170:GLU:OE1	1:B:257:ASP:OD2	2.39	0.41
1:C:175:HIS:H	1:C:227:SER:HG	1.66	0.41
1:E:298:THR:HG22	1:E:320:VAL:HG22	2.01	0.41
1:B:176:GLY:HA3	1:B:263:VAL:HA	2.02	0.41
1:D:62:GLU:OE1	1:D:64:LEU:N	2.54	0.41
1:H:198:LEU:HD11	1:H:240:ASP:HB3	2.02	0.41
1:A:24:MET:HA	2:A:401:FMN:N5	2.36	0.41
1:E:84:LYS:HG3	1:E:164:ALA:HA	2.02	0.41
1:F:8:LEU:HB2	1:F:18:ARG:HD3	2.02	0.41
1:H:39:HIS:ND1	1:H:72:LEU:HD21	2.36	0.41
1:H:341:VAL:HG13	1:H:342:PRO:HD2	2.03	0.41
1:C:297:ILE:HD13	1:C:315:VAL:HG13	2.03	0.41
1:A:104:ALA:HB3	1:A:108:ALA:HB2	2.02	0.41
1:A:204:PHE:HB3	1:A:205:PRO:HD3	2.03	0.41
1:B:6:THR:O	1:B:18:ARG:HD2	2.19	0.41
1:B:35:VAL:HG13	1:B:39:HIS:HB2	2.03	0.41
1:E:332:ALA:HB1	1:E:337:VAL:HB	2.03	0.41
1:F:324:ASP:OD2	1:F:330:ARG:NH2	2.53	0.41
1:G:83:LEU:HA	1:G:83:LEU:HD12	1.83	0.41
1:B:29:ALA:HB3	1:B:70:TYR:O	2.21	0.41
1:D:230:ASP:O	1:D:231:TRP:HB2	2.21	0.41
1:E:47:ALA:CB	1:E:93:ALA:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:VAL:O	1:E:215:VAL:HG22	2.21	0.41
1:E:225:ARG:NE	1:E:257:ASP:OD2	2.52	0.41
1:F:43:TYR:HB2	1:F:44:PRO:HD3	2.03	0.41
1:F:106:ARG:CZ	1:F:187:SER:HB3	2.51	0.41
1:F:246[A]:ARG:HG3	1:F:287:VAL:HG13	2.03	0.41
1:G:112:ARG:HB2	1:G:115:GLU:HG3	2.03	0.41
1:G:230:ASP:O	1:G:231:TRP:CB	2.68	0.41
1:H:88:ARG:HG3	1:H:89:ARG:N	2.36	0.41
1:A:182:PHE:HA	1:A:188:ASN:HD22	1.86	0.41
1:G:231:TRP:CE2	1:G:269:ILE:HG23	2.56	0.41
1:A:15:LEU:HD22	1:A:53:LEU:HB2	2.03	0.41
1:A:61:VAL:HG11	1:A:154:PHE:HA	2.02	0.41
1:A:202:MET:CE	1:A:247:ARG:CZ	2.99	0.41
1:C:244:PHE:CE2	1:C:248:LEU:HD11	2.55	0.40
1:F:21:MET:HE3	1:F:46:ARG:HG2	2.03	0.40
1:H:80:LEU:HB3	1:H:81:PRO:HD3	2.03	0.40
1:B:292:GLY:HA2	1:B:314:LEU:O	2.21	0.40
1:G:21:MET:HE2	1:G:46:ARG:HD3	2.03	0.40
1:B:85:GLU:HG3	1:B:89:ARG:HD2	2.03	0.40
1:C:41:LEU:O	1:C:45:THR:OG1	2.32	0.40
1:C:47:ALA:HB3	1:C:93:ALA:HB3	2.03	0.40
1:C:300:PRO:HB3	1:C:331:ALA:CB	2.50	0.40
1:D:150:ILE:HD12	1:D:150:ILE:N	2.29	0.40
1:G:60:ALA:HB3	1:G:66:ARG:HG2	2.03	0.40
1:G:213:ARG:NH2	1:G:217:PRO:O	2.55	0.40
1:H:297:ILE:HA	1:H:302:GLN:NE2	2.37	0.40
1:A:163:ARG:HG3	1:A:163:ARG:HH11	1.87	0.40
1:C:329:LEU:N	1:C:329:LEU:HD23	2.36	0.40
1:H:80:LEU:HB3	1:H:81:PRO:CD	2.52	0.40
1:H:230:ASP:OD2	1:H:235:GLY:HA3	2.21	0.40
1:H:239:GLU:O	1:H:239:GLU:HG3	2.20	0.40
1:D:345:TYR:HA	1:E:322:LEU:HD13	2.04	0.40
1:E:14:ARG:CZ	1:G:123:ARG:HG3	2.52	0.40
1:F:238:LEU:O	1:F:242:LEU:HD12	2.21	0.40
1:A:329:LEU:HD22	1:A:341:VAL:HG22	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ARG:NH1	1:E:199:GLU:OE2[1_456]	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ARG:HH12	1:E:199:GLU:OE2[1_456]	1.14	0.46
1:F:218:ARG:HH12	1:H:143:ASP:OD2[1_554]	1.45	0.15

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	348/369 (94%)	326 (94%)	21 (6%)	1 (0%)	41	60
1	B	348/369 (94%)	333 (96%)	15 (4%)	0	100	100
1	C	348/369 (94%)	332 (95%)	16 (5%)	0	100	100
1	D	347/369 (94%)	328 (94%)	19 (6%)	0	100	100
1	E	348/369 (94%)	331 (95%)	17 (5%)	0	100	100
1	F	351/369 (95%)	330 (94%)	21 (6%)	0	100	100
1	G	348/369 (94%)	332 (95%)	16 (5%)	0	100	100
1	H	347/369 (94%)	329 (95%)	18 (5%)	0	100	100
All	All	2785/2952 (94%)	2641 (95%)	143 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/292 (94%)	263 (95%)	13 (5%)	26	45
1	B	276/292 (94%)	266 (96%)	10 (4%)	35	55
1	C	276/292 (94%)	260 (94%)	16 (6%)	20	35
1	D	275/292 (94%)	262 (95%)	13 (5%)	26	45
1	E	276/292 (94%)	267 (97%)	9 (3%)	38	58
1	F	279/292 (96%)	260 (93%)	19 (7%)	16	28
1	G	276/292 (94%)	265 (96%)	11 (4%)	31	51
1	H	275/292 (94%)	260 (94%)	15 (6%)	21	37
All	All	2209/2336 (95%)	2103 (95%)	106 (5%)	26	44

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	ARG
1	B	56	VAL
1	B	172	HIS
1	B	181	SER
1	B	189	GLN
1	B	239	GLU
1	B	242	LEU
1	B	266	ARG
1	B	267	VAL
1	B	290	ARG
1	C	1	MET
1	C	22	SER
1	C	123	ARG
1	C	134	GLU
1	C	143	ASP
1	C	144	GLU
1	C	172	HIS
1	C	185	PRO
1	C	189	GLN
1	C	237	SER
1	C	247	ARG
1	C	265	LEU
1	C	266	ARG
1	C	267	VAL
1	C	313	ASP
1	C	340	GLU
1	D	18	ARG

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Mol	Chain	Res	Type
1	D	39	HIS
1	D	68	SER
1	D	89	ARG
1	D	133	ASP
1	D	141	PRO
1	D	173	MET
1	D	227	SER
1	D	237	SER
1	D	268	ARG
1	D	271	LEU
1	D	284	ARG
1	D	323	ARG
1	E	54	ILE
1	E	68	SER
1	E	88[A]	ARG
1	E	88[B]	ARG
1	E	110	THR
1	E	123	ARG
1	E	149	ARG
1	E	237	SER
1	E	239	GLU
1	F	1	MET
1	F	91	ARG
1	F	118	LYS
1	F	133	ASP
1	F	142	LEU
1	F	144	GLU
1	F	159	ARG
1	F	187	SER
1	F	201	ARG
1	F	227	SER
1	F	255	LEU
1	F	256	LEU
1	F	259	SER
1	F	266[A]	ARG
1	F	266[B]	ARG
1	F	268	ARG
1	F	340	GLU
1	F	346	GLN
1	F	347	ARG
1	G	62	GLU
1	G	70	TYR

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Mol	Chain	Res	Type
1	G	71	ASP
1	G	76	SER
1	G	89	ARG
1	G	118	LYS
1	G	181	SER
1	G	197	SER
1	G	199	GLU
1	G	237	SER
1	G	266	ARG
1	H	3	LEU
1	H	10	LEU
1	H	37	ASP
1	H	68	SER
1	H	76	SER
1	H	88	ARG
1	H	149	ARG
1	H	160	ARG
1	H	197	SER
1	H	218	ARG
1	H	225	ARG
1	H	247	ARG
1	H	257	ASP
1	H	259	SER
1	H	265	LEU
1	A	16	LYS
1	A	37	ASP
1	A	46	ARG
1	A	64	LEU
1	A	85	GLU
1	A	91	ARG
1	A	225	ARG
1	A	227	SER
1	A	246[A]	ARG
1	A	246[B]	ARG
1	A	267	VAL
1	A	313	ASP
1	A	333	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	HIS

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Mol	Chain	Res	Type
1	B	189	GLN
1	D	152	GLN
1	F	100	GLN
1	F	172	HIS
1	F	210	GLN
1	G	39	HIS
1	G	152	GLN
1	H	39	HIS
1	A	308	GLN

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)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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	$\#\|Z\| > 2$
4	IPA	H	402	-	3,3,3	0.51	0	3,3,3	0.47	0
2	FMN	B	401	-	33,33,33	2.79	10 (30%)	48,50,50	2.01	14 (29%)
2	FMN	D	401	-	33,33,33	2.74	10 (30%)	48,50,50	2.02	12 (25%)
3	W3X	F	404	-	9,9,19	6.74	7 (77%)	6,11,25	1.66	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	W3X	A	402	-	19,19,19	3.53	8 (42%)	18,25,25	1.06	1 (5%)
2	FMN	H	401	-	33,33,33	2.79	10 (30%)	48,50,50	1.98	12 (25%)
3	W3X	B	402	-	19,19,19	3.51	7 (36%)	18,25,25	1.32	1 (5%)
2	FMN	G	401	-	33,33,33	2.78	10 (30%)	48,50,50	1.97	11 (22%)
2	FMN	E	401	-	33,33,33	2.78	10 (30%)	48,50,50	2.03	13 (27%)
4	IPA	E	402	-	3,3,3	0.50	0	3,3,3	0.47	0
2	FMN	C	401	-	33,33,33	2.75	10 (30%)	48,50,50	2.03	14 (29%)
2	FMN	F	401	-	33,33,33	2.77	11 (33%)	48,50,50	2.01	13 (27%)
2	FMN	A	401	-	33,33,33	2.76	10 (30%)	48,50,50	2.00	13 (27%)
3	W3X	E	403	-	9,9,19	6.77	7 (77%)	6,11,25	1.28	1 (16%)

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	FMN	B	401	-	-	1/18/18/18	0/3/3/3
2	FMN	D	401	-	-	1/18/18/18	0/3/3/3
3	W3X	F	404	-	-	1/3/12/19	0/1/1/2
3	W3X	A	402	-	-	5/8/19/19	0/2/2/2
2	FMN	H	401	-	-	4/18/18/18	0/3/3/3
3	W3X	B	402	-	-	4/8/19/19	0/2/2/2
2	FMN	G	401	-	-	1/18/18/18	0/3/3/3
2	FMN	E	401	-	-	8/18/18/18	0/3/3/3
2	FMN	C	401	-	-	5/18/18/18	0/3/3/3
2	FMN	F	401	-	-	1/18/18/18	0/3/3/3
2	FMN	A	401	-	-	8/18/18/18	0/3/3/3
3	W3X	E	403	-	-	0/3/12/19	0/1/1/2

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	403	W3X	C05-C04	13.01	1.53	1.36
3	F	404	W3X	C05-C04	12.93	1.53	1.36
3	E	403	W3X	C16-C17	10.96	1.52	1.33
3	A	402	W3X	C16-C17	10.95	1.52	1.33
3	F	404	W3X	C16-C17	10.89	1.52	1.33
3	B	402	W3X	C16-C17	10.81	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	404	W3X	C05-N06	8.70	1.45	1.35
3	E	403	W3X	C05-N06	8.69	1.45	1.35
2	H	401	FMN	C4A-N5	7.59	1.45	1.30
2	F	401	FMN	C4A-N5	7.53	1.45	1.30
2	G	401	FMN	C4A-N5	7.50	1.45	1.30
2	B	401	FMN	C4A-N5	7.49	1.45	1.30
2	E	401	FMN	C4A-N5	7.33	1.45	1.30
2	A	401	FMN	C4A-N5	7.27	1.44	1.30
2	C	401	FMN	C4A-N5	7.26	1.44	1.30
2	D	401	FMN	C4A-N5	7.12	1.44	1.30
2	E	401	FMN	C10-N1	6.71	1.47	1.33
2	B	401	FMN	C10-N1	6.67	1.46	1.33
2	H	401	FMN	C10-N1	6.63	1.46	1.33
2	G	401	FMN	C10-N1	6.60	1.46	1.33
2	D	401	FMN	C10-N1	6.59	1.46	1.33
2	F	401	FMN	C10-N1	6.57	1.46	1.33
3	B	402	W3X	C05-C04	6.57	1.53	1.34
2	A	401	FMN	C10-N1	6.54	1.46	1.33
2	C	401	FMN	C10-N1	6.52	1.46	1.33
3	A	402	W3X	C05-C04	6.43	1.52	1.34
2	H	401	FMN	C5A-N5	5.25	1.49	1.39
2	B	401	FMN	C5A-N5	5.22	1.49	1.39
2	F	401	FMN	C5A-N5	5.21	1.49	1.39
2	A	401	FMN	C5A-N5	5.16	1.49	1.39
2	G	401	FMN	C5A-N5	5.14	1.49	1.39
2	E	401	FMN	C5A-N5	5.09	1.49	1.39
2	B	401	FMN	C2-N1	5.05	1.48	1.36
2	C	401	FMN	C5A-N5	5.04	1.49	1.39
2	E	401	FMN	C2-N1	5.03	1.48	1.36
2	D	401	FMN	C2-N1	5.02	1.48	1.36
2	G	401	FMN	C2-N1	4.95	1.48	1.36
2	A	401	FMN	C2-N1	4.95	1.48	1.36
2	F	401	FMN	C2-N1	4.94	1.48	1.36
2	H	401	FMN	C2-N1	4.93	1.48	1.36
2	E	401	FMN	C9A-N10	4.92	1.49	1.41
2	D	401	FMN	C5A-N5	4.92	1.49	1.39
2	C	401	FMN	C2-N1	4.92	1.48	1.36
2	C	401	FMN	C9A-N10	4.81	1.49	1.41
2	D	401	FMN	C9A-N10	4.80	1.49	1.41
2	G	401	FMN	C9A-N10	4.75	1.49	1.41
2	F	401	FMN	C9A-N10	4.71	1.49	1.41
2	H	401	FMN	C9A-N10	4.64	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	403	W3X	C02-N03	4.62	1.45	1.33
3	F	404	W3X	C02-N03	4.59	1.45	1.33
3	A	402	W3X	C02-N03	4.59	1.45	1.33
2	B	401	FMN	C9A-N10	4.58	1.49	1.41
3	B	402	W3X	C02-N03	4.57	1.45	1.33
2	A	401	FMN	C9A-N10	4.54	1.49	1.41
2	G	401	FMN	C2-N3	4.40	1.49	1.39
2	A	401	FMN	C2-N3	4.31	1.49	1.39
2	B	401	FMN	C2-N3	4.27	1.48	1.39
2	H	401	FMN	C2-N3	4.26	1.48	1.39
2	E	401	FMN	C2-N3	4.21	1.48	1.39
3	B	402	W3X	C05-N06	4.19	1.45	1.37
2	D	401	FMN	C2-N3	4.14	1.48	1.39
3	A	402	W3X	C05-N06	4.11	1.44	1.37
2	C	401	FMN	C2-N3	4.11	1.48	1.39
2	F	401	FMN	C2-N3	4.04	1.48	1.39
3	A	402	W3X	C16-N06	3.98	1.45	1.36
2	D	401	FMN	C10-N10	3.97	1.46	1.37
2	G	401	FMN	C4-N3	3.90	1.46	1.38
2	A	401	FMN	C4-N3	3.90	1.46	1.38
3	B	402	W3X	C16-N06	3.88	1.44	1.36
2	H	401	FMN	C4-N3	3.88	1.46	1.38
2	B	401	FMN	C4-N3	3.81	1.45	1.38
2	B	401	FMN	C10-N10	3.78	1.45	1.37
2	F	401	FMN	C10-N10	3.76	1.45	1.37
2	E	401	FMN	C10-N10	3.76	1.45	1.37
2	E	401	FMN	C4-N3	3.75	1.45	1.38
2	C	401	FMN	C10-N10	3.73	1.45	1.37
2	H	401	FMN	C10-N10	3.72	1.45	1.37
2	A	401	FMN	C10-N10	3.69	1.45	1.37
2	G	401	FMN	C10-N10	3.62	1.45	1.37
2	D	401	FMN	C4-N3	3.58	1.45	1.38
2	C	401	FMN	C4-N3	3.56	1.45	1.38
2	F	401	FMN	C4-N3	3.54	1.45	1.38
2	C	401	FMN	O2-C2	-3.41	1.18	1.24
2	D	401	FMN	O2-C2	-3.30	1.18	1.24
2	F	401	FMN	O2-C2	-3.27	1.18	1.24
3	E	403	W3X	C16-N06	3.14	1.45	1.35
3	F	404	W3X	C16-N06	3.14	1.45	1.35
2	B	401	FMN	O2-C2	-3.09	1.18	1.24
2	E	401	FMN	O2-C2	-3.06	1.18	1.24
2	H	401	FMN	O2-C2	-3.03	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	O2-C2	-2.99	1.18	1.24
2	G	401	FMN	O2-C2	-2.99	1.18	1.24
2	F	401	FMN	O4-C4	-2.72	1.18	1.23
2	C	401	FMN	O4-C4	-2.70	1.18	1.23
2	E	401	FMN	O4-C4	-2.69	1.18	1.23
2	H	401	FMN	O4-C4	-2.62	1.18	1.23
2	B	401	FMN	O4-C4	-2.61	1.18	1.23
2	A	401	FMN	O4-C4	-2.56	1.18	1.23
2	G	401	FMN	O4-C4	-2.54	1.18	1.23
2	D	401	FMN	O4-C4	-2.48	1.18	1.23
3	F	404	W3X	O01-C02	-2.38	1.18	1.24
3	E	403	W3X	O01-C02	-2.32	1.19	1.24
3	B	402	W3X	O01-C02	-2.30	1.19	1.24
3	A	402	W3X	O01-C02	-2.29	1.19	1.24
3	E	403	W3X	C02-C04	2.19	1.53	1.48
3	F	404	W3X	C02-C04	2.18	1.53	1.48
3	B	402	W3X	C18-C04	2.15	1.54	1.49
3	A	402	W3X	C02-C04	2.14	1.53	1.48
3	A	402	W3X	C18-C04	2.13	1.54	1.49
2	F	401	FMN	C4A-C4	2.04	1.52	1.44

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	FMN	C7M-C7-C6	-7.53	105.57	119.49
2	E	401	FMN	C7M-C7-C6	-7.50	105.63	119.49
2	B	401	FMN	C7M-C7-C6	-7.47	105.69	119.49
2	A	401	FMN	C7M-C7-C6	-7.46	105.69	119.49
2	D	401	FMN	C7M-C7-C6	-7.45	105.72	119.49
2	G	401	FMN	C7M-C7-C6	-7.37	105.87	119.49
2	F	401	FMN	C7M-C7-C6	-7.32	105.96	119.49
2	H	401	FMN	C7M-C7-C6	-7.30	105.99	119.49
2	E	401	FMN	C7M-C7-C8	6.76	134.59	120.74
2	C	401	FMN	C7M-C7-C8	6.65	134.37	120.74
2	D	401	FMN	C7M-C7-C8	6.62	134.30	120.74
2	B	401	FMN	C7M-C7-C8	6.61	134.28	120.74
2	A	401	FMN	C7M-C7-C8	6.59	134.25	120.74
2	F	401	FMN	C7M-C7-C8	6.57	134.19	120.74
2	G	401	FMN	C7M-C7-C8	6.55	134.16	120.74
2	H	401	FMN	C7M-C7-C8	6.50	134.06	120.74
3	B	402	W3X	C08-C07-N06	-4.63	106.89	112.35
2	C	401	FMN	C4-N3-C2	-3.59	119.02	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	401	FMN	C4-N3-C2	-3.58	119.03	125.64
2	D	401	FMN	C4-N3-C2	-3.57	119.05	125.64
2	B	401	FMN	C4-N3-C2	-3.46	119.25	125.64
2	H	401	FMN	C4-N3-C2	-3.40	119.36	125.64
2	A	401	FMN	C4-N3-C2	-3.36	119.43	125.64
2	E	401	FMN	C4-N3-C2	-3.31	119.53	125.64
2	G	401	FMN	C4-N3-C2	-3.30	119.55	125.64
3	A	402	W3X	C08-C07-N06	-3.15	108.62	112.35
3	F	404	W3X	C16-N06-C05	-3.01	119.20	121.14
2	E	401	FMN	C4'-C3'-C2'	-2.96	107.21	113.36
2	D	401	FMN	C8M-C8-C7	-2.89	114.81	120.74
2	D	401	FMN	C8M-C8-C9	2.82	124.69	119.49
2	F	401	FMN	C4A-C4-N3	2.80	120.31	113.19
2	H	401	FMN	C4A-C4-N3	2.74	120.15	113.19
2	B	401	FMN	C4'-C3'-C2'	-2.73	107.68	113.36
2	E	401	FMN	C4A-C4-N3	2.72	120.10	113.19
2	B	401	FMN	C4A-C4-N3	2.71	120.08	113.19
2	C	401	FMN	C4A-C4-N3	2.71	120.06	113.19
2	E	401	FMN	O4-C4-C4A	-2.68	119.48	126.60
2	F	401	FMN	C4A-C10-N10	2.67	120.39	116.48
2	C	401	FMN	C4'-C3'-C2'	-2.67	107.81	113.36
2	E	401	FMN	C8M-C8-C7	-2.64	115.32	120.74
2	A	401	FMN	C9A-C5A-N5	-2.63	119.58	122.43
2	D	401	FMN	C4-C4A-C10	2.62	121.19	116.79
2	G	401	FMN	C4A-C4-N3	2.61	119.82	113.19
2	A	401	FMN	C8M-C8-C9	2.61	124.31	119.49
2	A	401	FMN	O4-C4-C4A	-2.59	119.72	126.60
2	E	401	FMN	C8M-C8-C9	2.59	124.28	119.49
2	A	401	FMN	C4A-C4-N3	2.58	119.75	113.19
2	H	401	FMN	C9A-C5A-N5	-2.58	119.63	122.43
2	C	401	FMN	C8M-C8-C7	-2.55	115.51	120.74
2	H	401	FMN	O4-C4-C4A	-2.55	119.84	126.60
2	G	401	FMN	C9A-C5A-N5	-2.54	119.67	122.43
2	C	401	FMN	C8M-C8-C9	2.53	124.17	119.49
2	E	401	FMN	C9A-C5A-N5	-2.52	119.70	122.43
2	D	401	FMN	C4A-C4-N3	2.51	119.57	113.19
2	D	401	FMN	C4A-C10-N10	2.51	120.15	116.48
2	A	401	FMN	C4'-C3'-C2'	-2.51	108.14	113.36
2	B	401	FMN	C9A-C5A-N5	-2.49	119.72	122.43
2	F	401	FMN	C10-C4A-N5	-2.48	119.60	124.86
2	C	401	FMN	C10-C4A-N5	-2.47	119.61	124.86
2	C	401	FMN	C4A-C10-N10	2.46	120.08	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	FMN	C10-C4A-N5	-2.44	119.68	124.86
2	G	401	FMN	O4-C4-C4A	-2.43	120.14	126.60
2	D	401	FMN	C10-C4A-N5	-2.43	119.69	124.86
2	F	401	FMN	C9A-C5A-N5	-2.43	119.79	122.43
3	E	403	W3X	C16-N06-C05	-2.41	119.59	121.14
2	C	401	FMN	C5'-C4'-C3'	-2.40	107.56	112.20
2	G	401	FMN	C10-C4A-N5	-2.40	119.76	124.86
2	G	401	FMN	C8M-C8-C7	-2.40	115.82	120.74
2	C	401	FMN	C9A-C5A-N5	-2.38	119.85	122.43
2	A	401	FMN	C8M-C8-C7	-2.38	115.86	120.74
2	D	401	FMN	C4A-C10-N1	-2.38	119.22	124.73
2	H	401	FMN	C5A-C9A-N10	2.37	120.40	117.95
2	A	401	FMN	C10-C4A-N5	-2.37	119.83	124.86
2	G	401	FMN	C8M-C8-C9	2.37	123.87	119.49
2	B	401	FMN	C8M-C8-C7	-2.36	115.89	120.74
2	B	401	FMN	O4-C4-C4A	-2.36	120.35	126.60
2	G	401	FMN	C4A-C10-N10	2.35	119.92	116.48
2	B	401	FMN	C8M-C8-C9	2.35	123.83	119.49
2	H	401	FMN	C8M-C8-C7	-2.35	115.92	120.74
2	F	401	FMN	C8M-C8-C7	-2.34	115.94	120.74
2	F	401	FMN	C5A-C9A-N10	2.34	120.37	117.95
2	H	401	FMN	C8M-C8-C9	2.31	123.77	119.49
2	D	401	FMN	O4-C4-C4A	-2.30	120.49	126.60
2	H	401	FMN	C5'-C4'-C3'	-2.30	107.76	112.20
2	E	401	FMN	C10-C4A-N5	-2.27	120.04	124.86
2	C	401	FMN	O4-C4-C4A	-2.27	120.59	126.60
2	B	401	FMN	C4A-C10-N10	2.24	119.76	116.48
2	H	401	FMN	C10-C4A-N5	-2.22	120.15	124.86
2	F	401	FMN	C8M-C8-C9	2.20	123.55	119.49
2	H	401	FMN	C4A-C10-N10	2.17	119.66	116.48
2	A	401	FMN	C4-C4A-C10	2.17	120.44	116.79
2	C	401	FMN	C4A-C10-N1	-2.15	119.75	124.73
2	C	401	FMN	C4-C4A-C10	2.13	120.38	116.79
2	E	401	FMN	C5'-C4'-C3'	-2.10	108.14	112.20
2	F	401	FMN	C4A-C10-N1	-2.10	119.85	124.73
2	F	401	FMN	C4'-C3'-C2'	-2.09	109.02	113.36
2	G	401	FMN	C5A-C9A-N10	2.07	120.09	117.95
2	F	401	FMN	O4-C4-C4A	-2.05	121.16	126.60
2	A	401	FMN	C4A-C10-N1	-2.05	119.98	124.73
2	E	401	FMN	C4A-C10-N10	2.03	119.45	116.48
2	A	401	FMN	C4A-C10-N10	2.03	119.45	116.48
2	D	401	FMN	C9A-C5A-N5	-2.03	120.22	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	FMN	C4A-C10-N1	-2.03	120.03	124.73
2	B	401	FMN	C5A-C9A-N10	2.02	120.04	117.95
2	E	401	FMN	C4A-C10-N1	-2.01	120.06	124.73
2	B	401	FMN	C4-C4A-C10	2.00	120.15	116.79

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	FMN	C5'-O5'-P-O2P
2	E	401	FMN	C5'-O5'-P-O3P
2	H	401	FMN	C5'-O5'-P-O3P
2	A	401	FMN	C5'-O5'-P-O2P
2	A	401	FMN	C5'-O5'-P-O3P
3	B	402	W3X	N03-C02-C04-C05
2	F	401	FMN	C4'-C5'-O5'-P
2	E	401	FMN	O3'-C3'-C4'-C5'
2	A	401	FMN	O3'-C3'-C4'-C5'
3	B	402	W3X	N06-C07-C08-C09
2	A	401	FMN	O3'-C3'-C4'-O4'
2	A	401	FMN	C2'-C3'-C4'-C5'
2	A	401	FMN	C2'-C3'-C4'-O4'
2	C	401	FMN	O3'-C3'-C4'-C5'
2	E	401	FMN	C2'-C3'-C4'-O4'
3	A	402	W3X	N06-C07-C08-C09
2	B	401	FMN	C4'-C5'-O5'-P
2	G	401	FMN	C4'-C5'-O5'-P
2	E	401	FMN	C5'-O5'-P-O1P
2	H	401	FMN	C5'-O5'-P-O1P
2	A	401	FMN	C5'-O5'-P-O1P
2	D	401	FMN	C4'-C5'-O5'-P
2	E	401	FMN	C2'-C3'-C4'-C5'
2	E	401	FMN	O3'-C3'-C4'-O4'
2	H	401	FMN	C5'-O5'-P-O2P
2	A	401	FMN	C4'-C5'-O5'-P
3	B	402	W3X	C08-C07-N06-C16
2	C	401	FMN	C4'-C5'-O5'-P
2	H	401	FMN	C4'-C5'-O5'-P
3	A	402	W3X	N03-C02-C04-C05
3	B	402	W3X	O01-C02-C04-C05
3	A	402	W3X	O01-C02-C04-C05
2	C	401	FMN	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
3	A	402	W3X	C07-C08-C09-C15
2	C	401	FMN	C2'-C3'-C4'-C5'
2	C	401	FMN	O3'-C3'-C4'-O4'
3	A	402	W3X	C07-C08-C09-C10
2	E	401	FMN	C4'-C5'-O5'-P
3	F	404	W3X	N03-C02-C04-C05

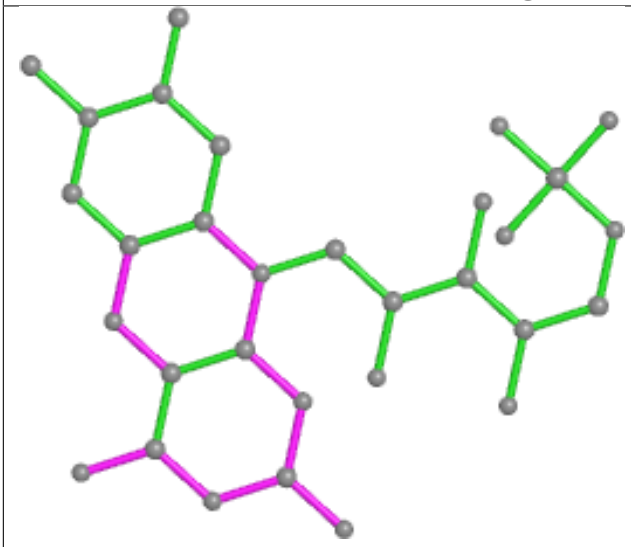
There are no ring outliers.

13 monomers are involved in 35 short contacts:

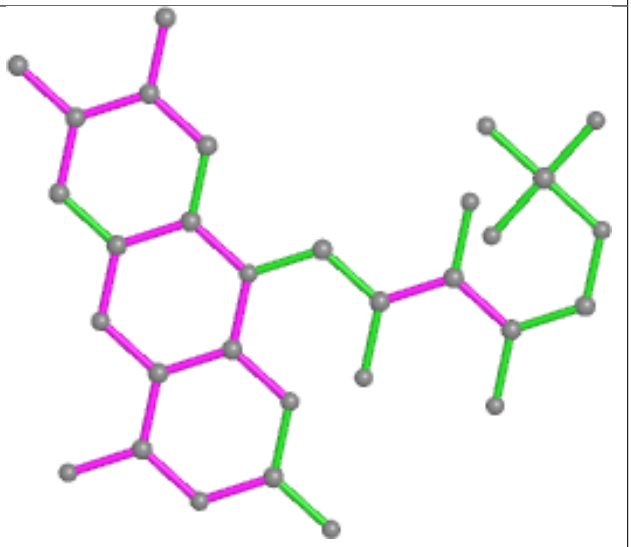
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	FMN	3	0
2	D	401	FMN	3	0
3	F	404	W3X	1	0
3	A	402	W3X	3	0
2	H	401	FMN	3	0
3	B	402	W3X	1	0
2	G	401	FMN	3	0
2	E	401	FMN	3	0
4	E	402	IPA	2	0
2	C	401	FMN	2	0
2	F	401	FMN	5	0
2	A	401	FMN	6	0
3	E	403	W3X	2	0

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 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.

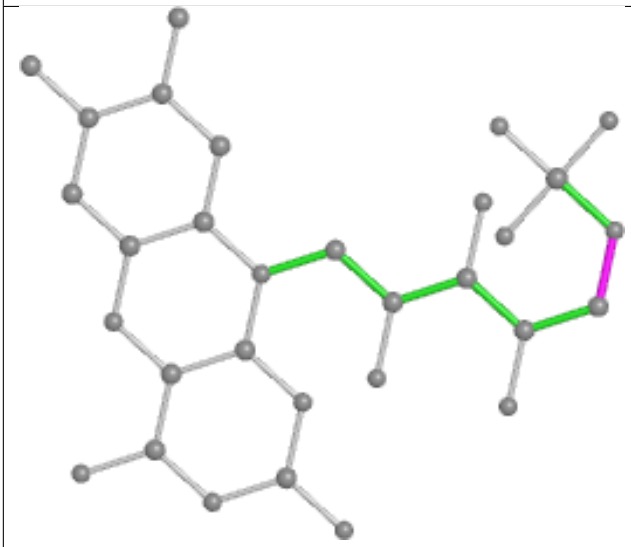
Ligand FMN B 401



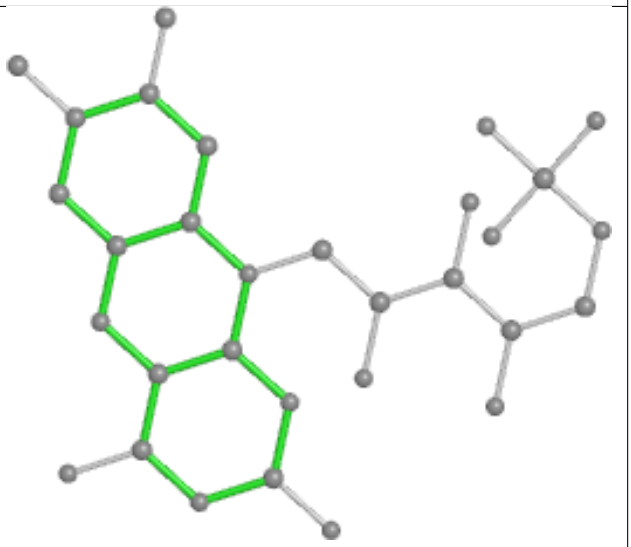
Bond lengths



Bond angles

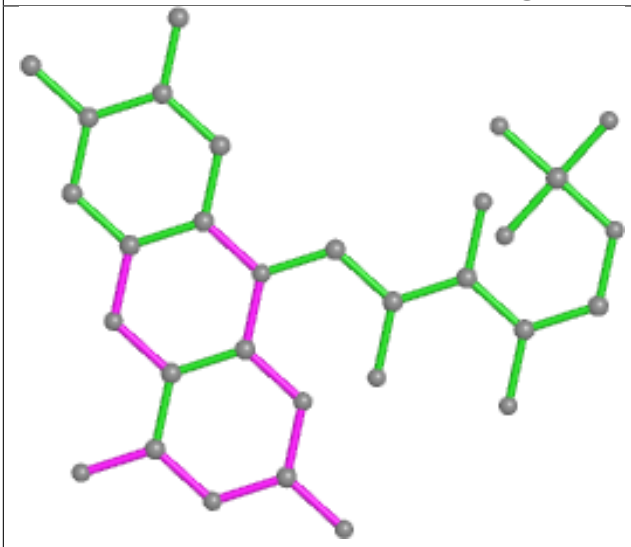


Torsions

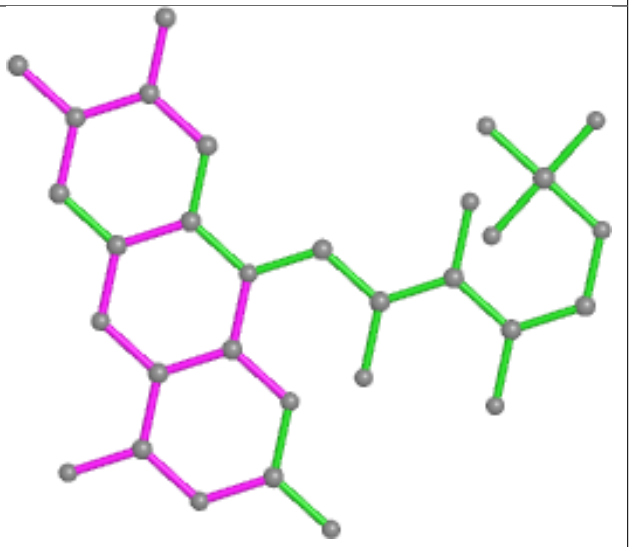


Rings

Ligand FMN D 401



Bond lengths



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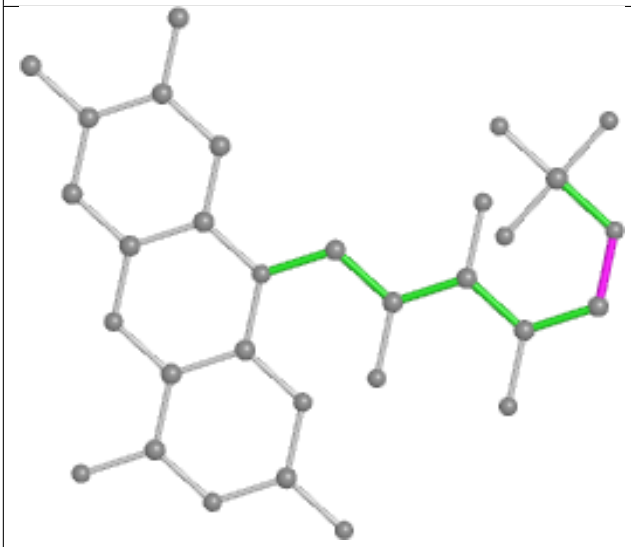

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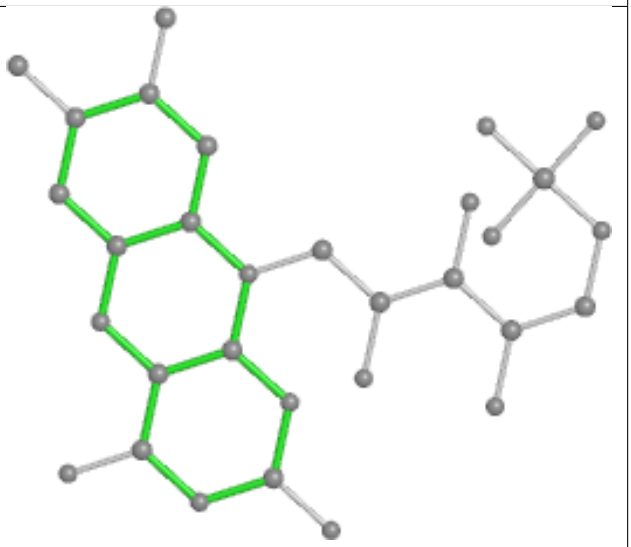
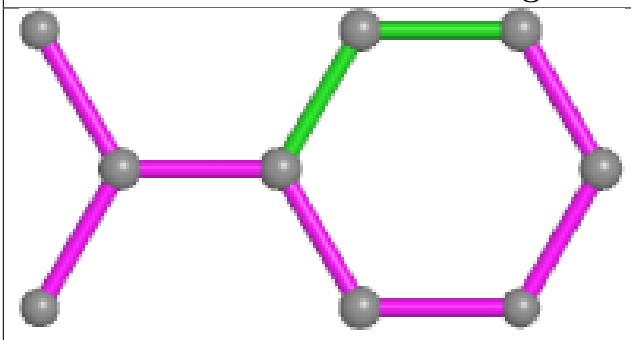


Rings

Ligand W3X F 404



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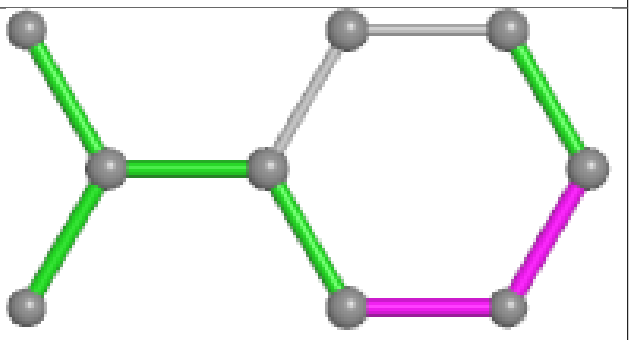
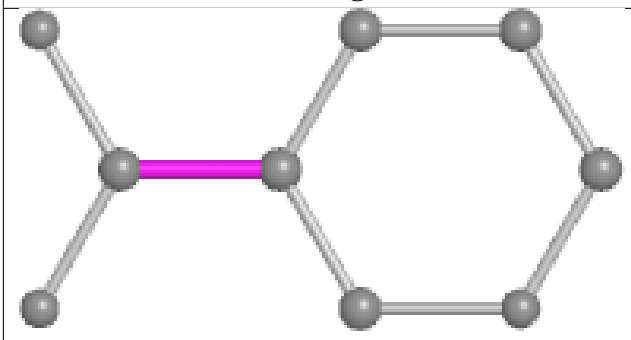


Bond angles



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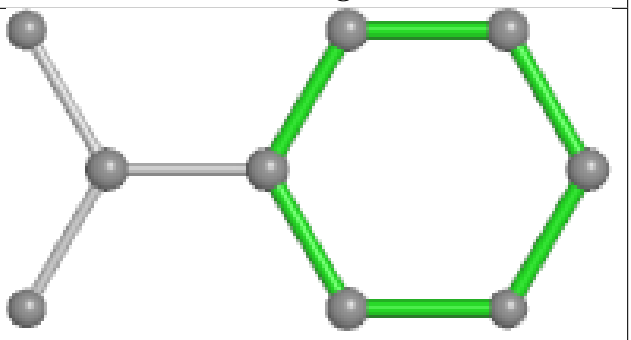
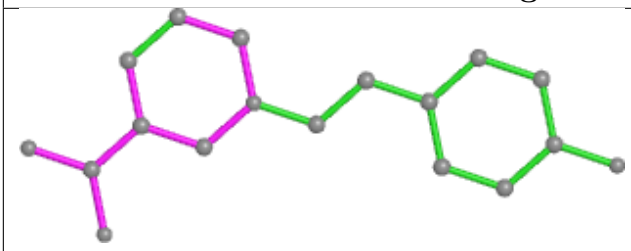


Rings

Ligand W3X A 402



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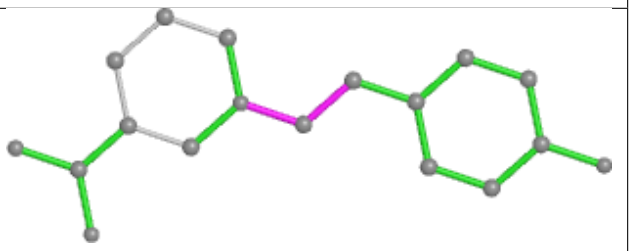

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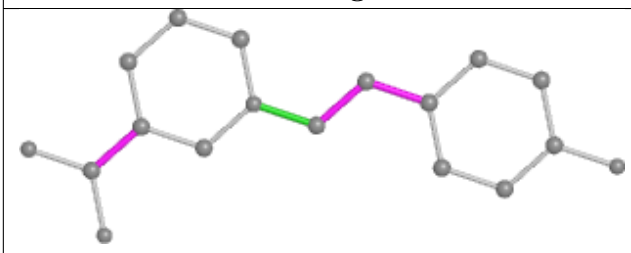
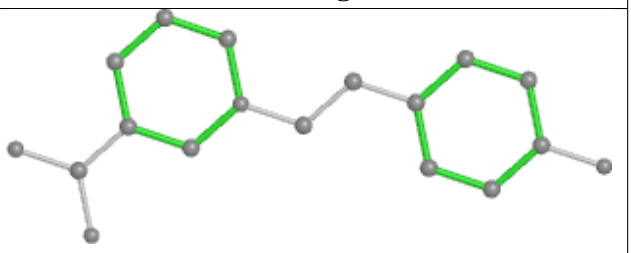
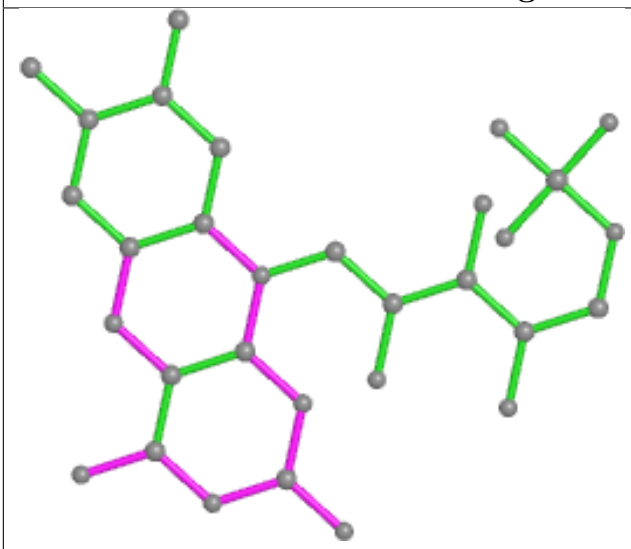


Torsions

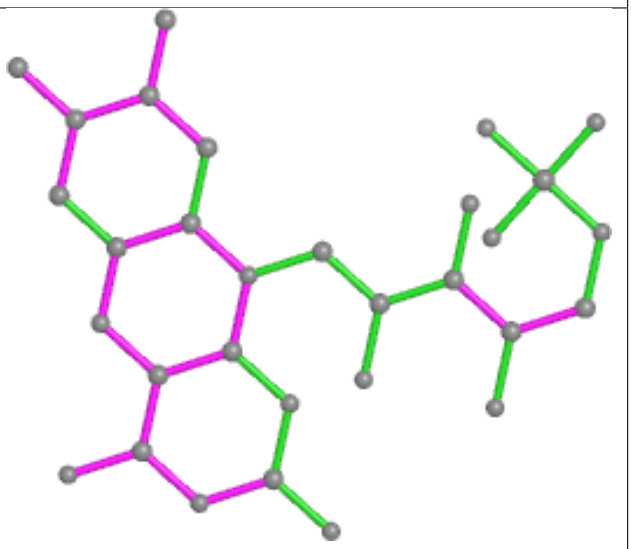


Rings

Ligand FMN H 401



Bond lengths



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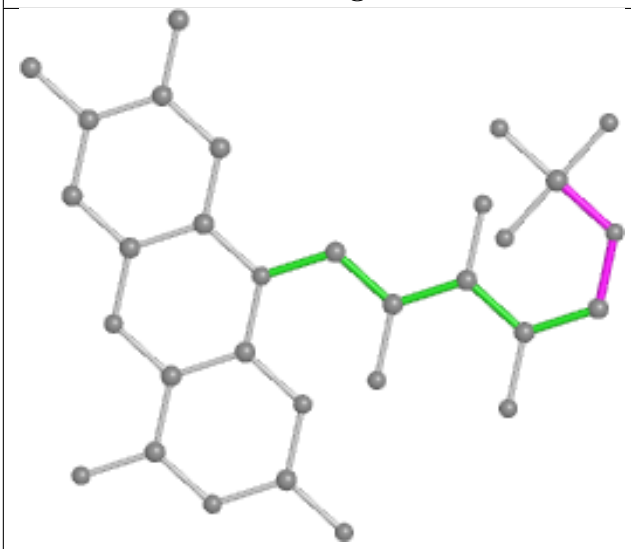

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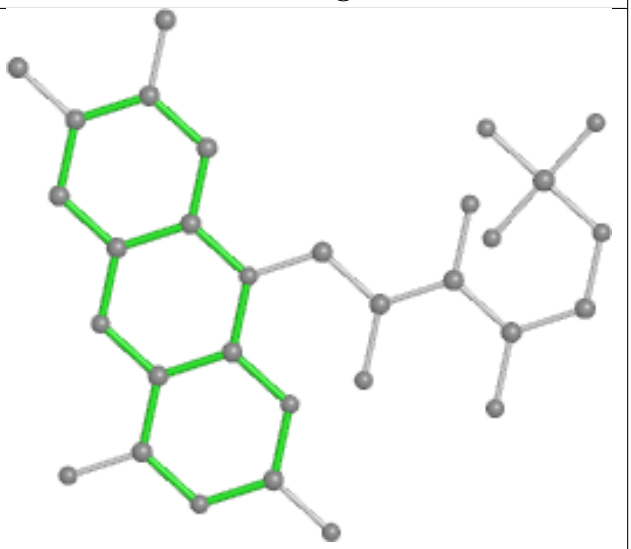
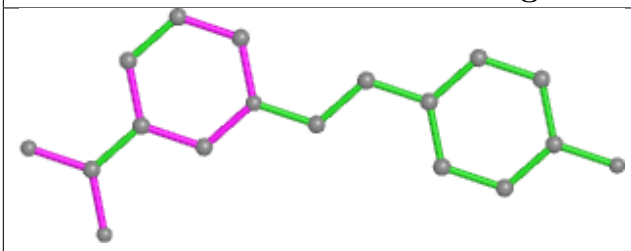


Rings

Ligand W3X B 402



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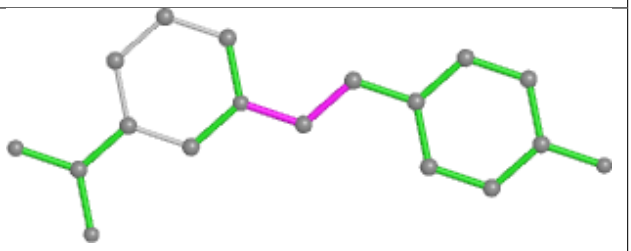
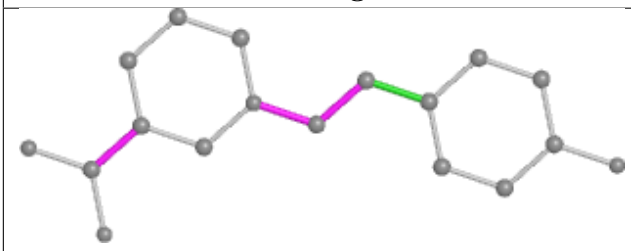


Bond angles



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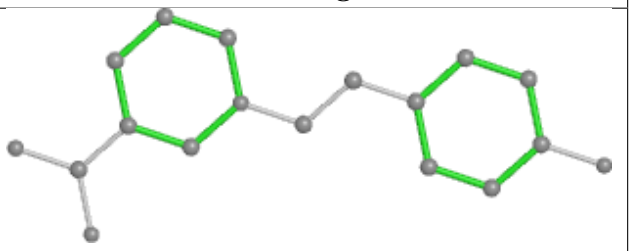
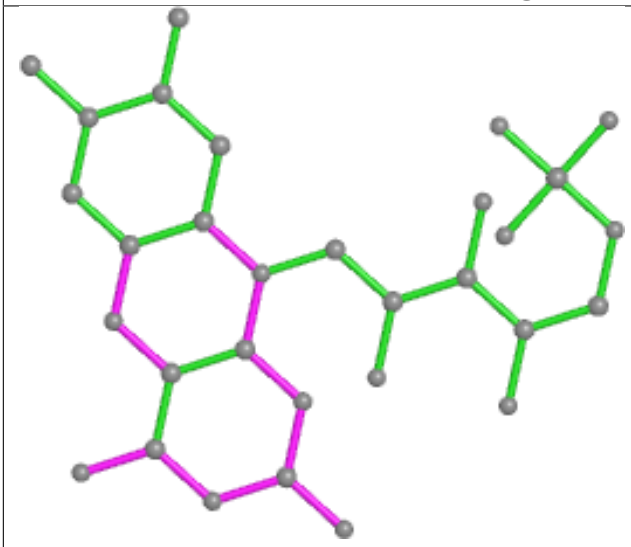


Rings

Ligand FMN G 401



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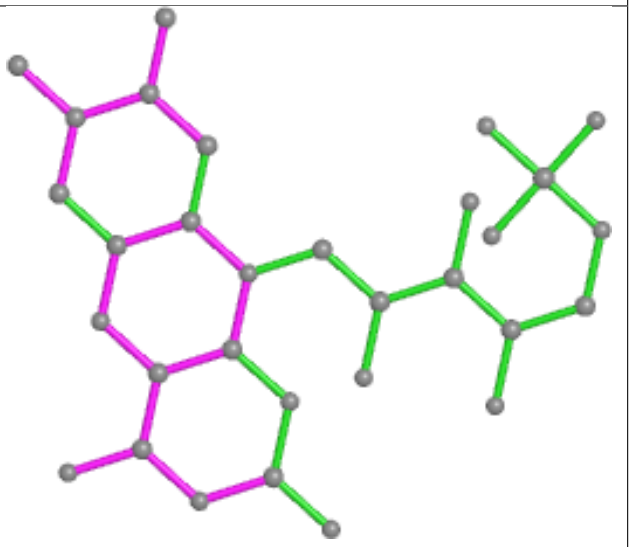

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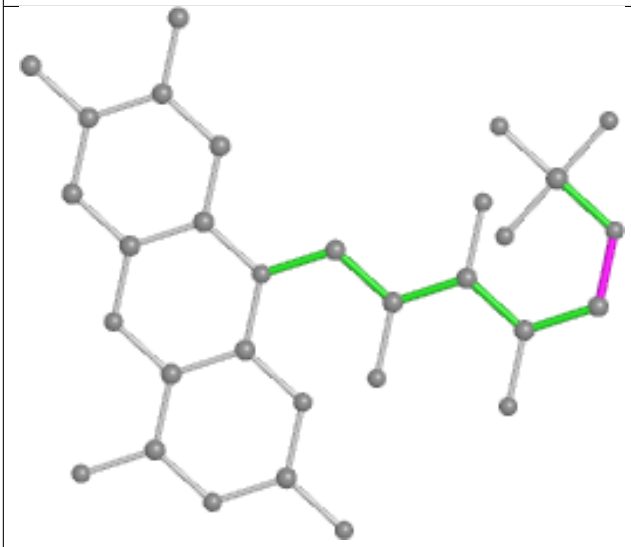

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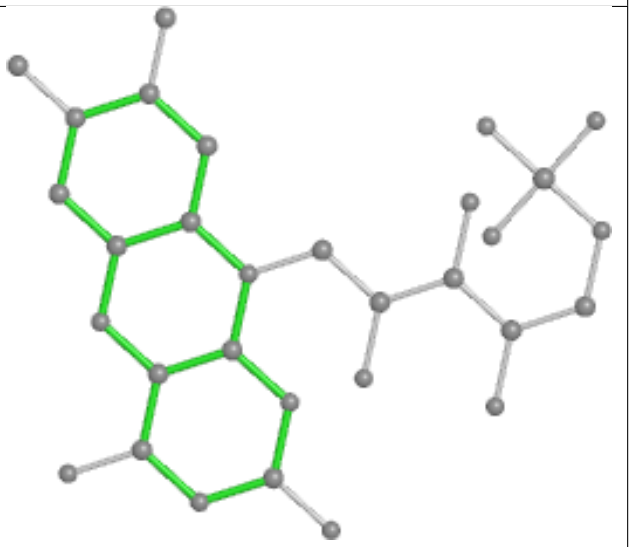
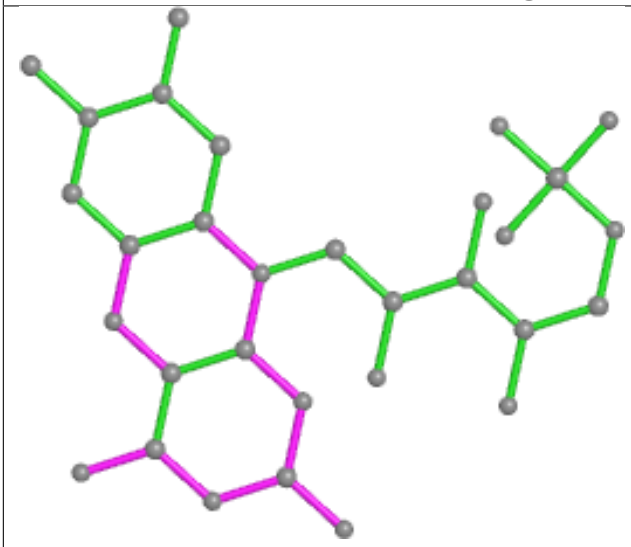


Rings

Ligand FMN E 401



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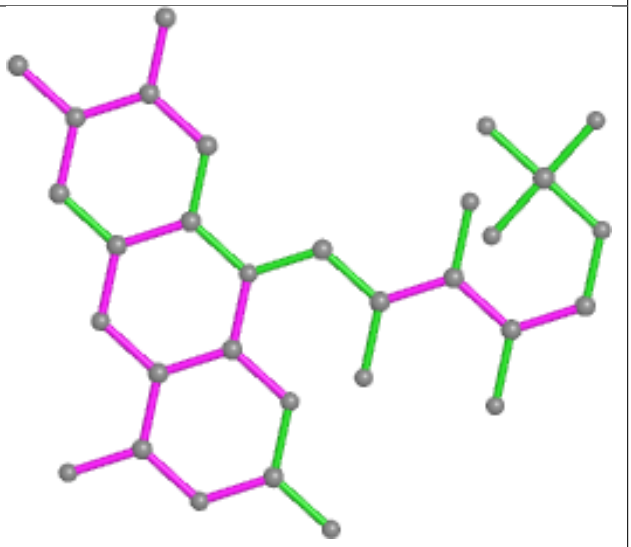

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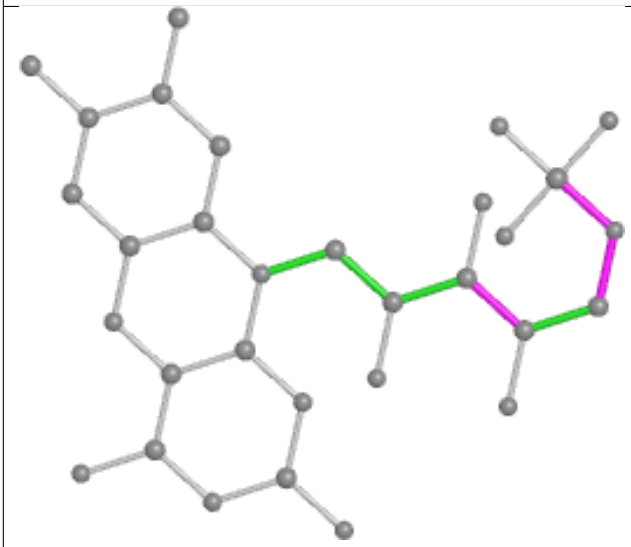

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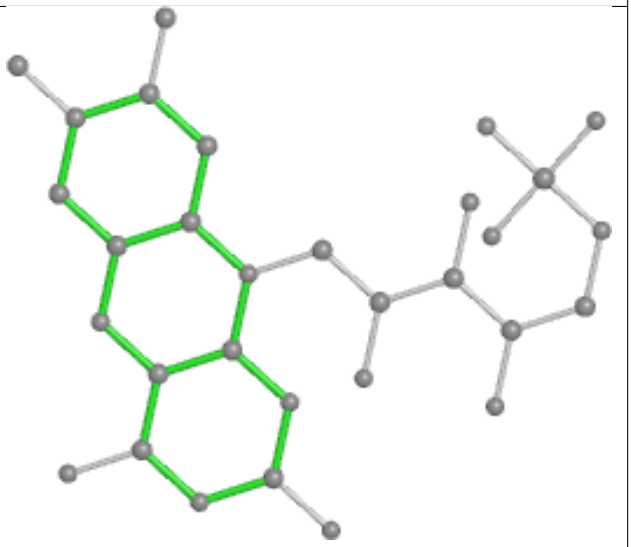
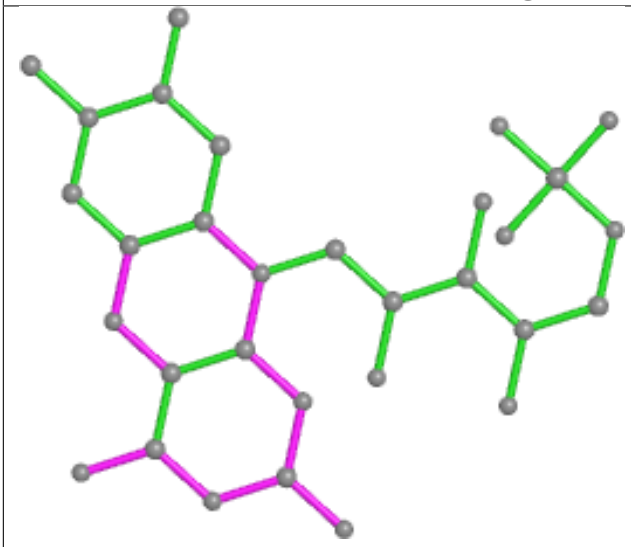


Rings

Ligand FMN C 401



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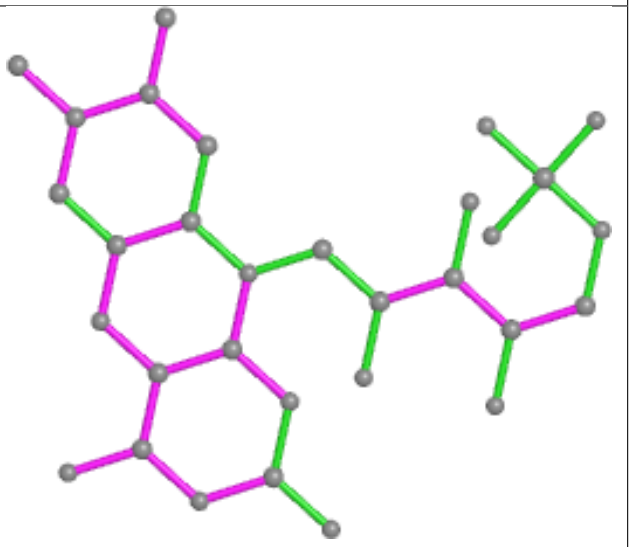
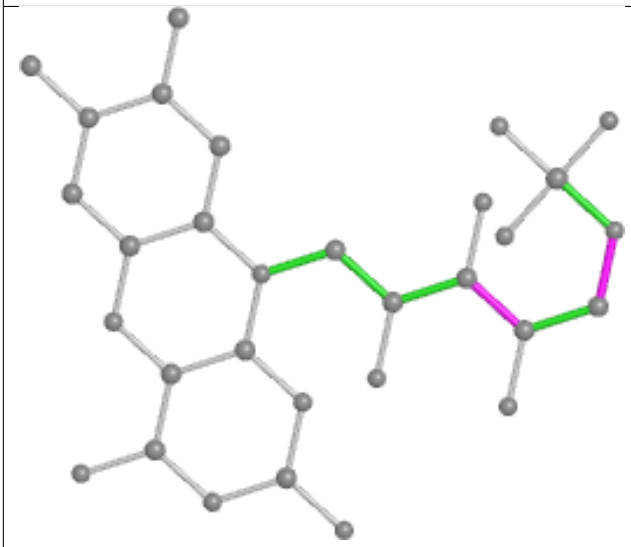


Bond angles



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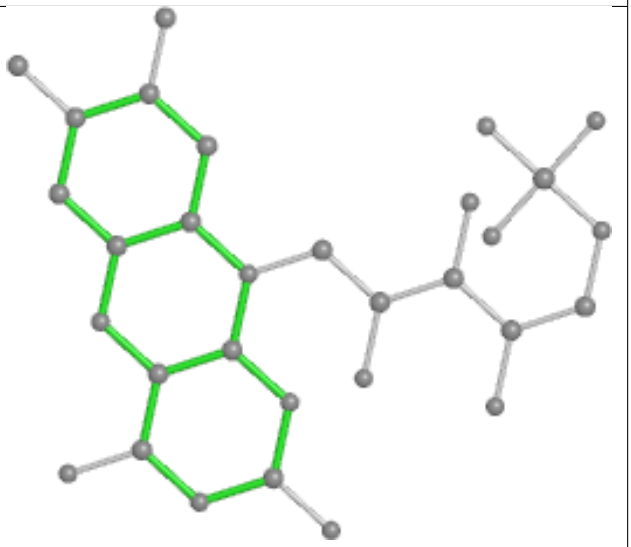
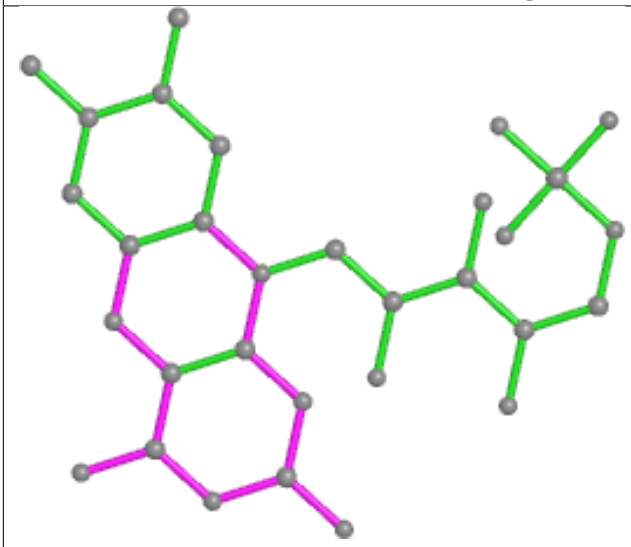


Rings

Ligand FMN F 401



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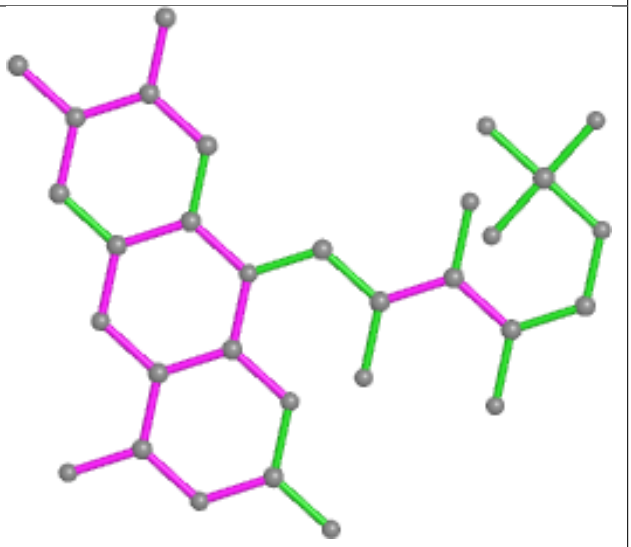
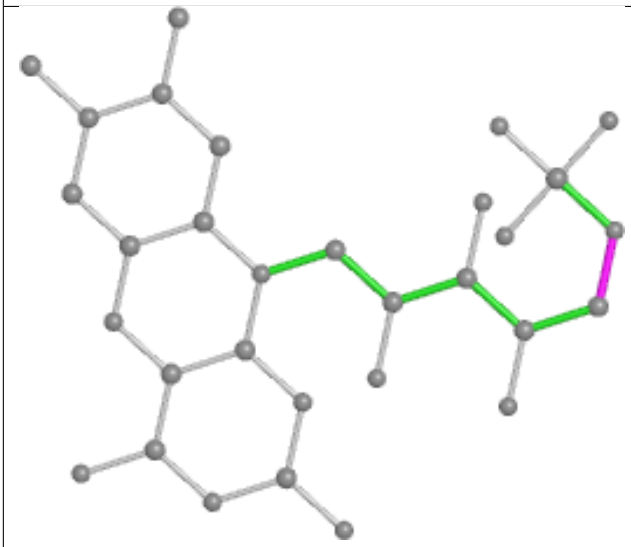
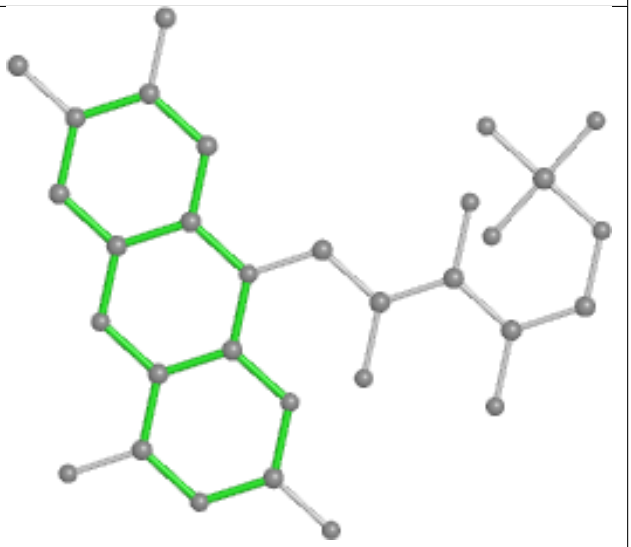


Bond angles

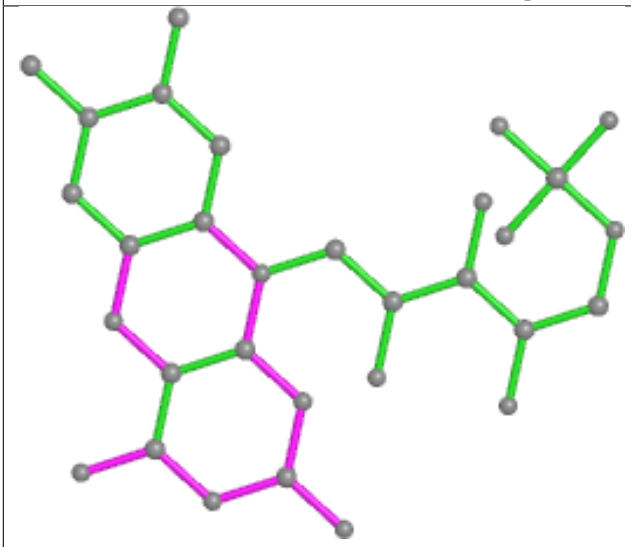


Torsions

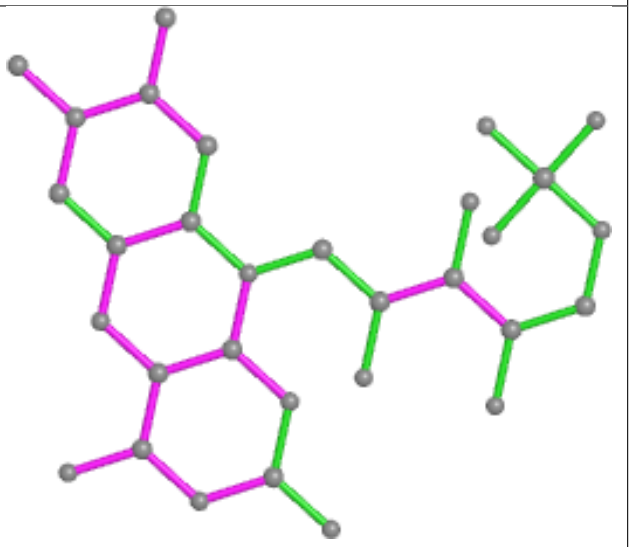


Rings

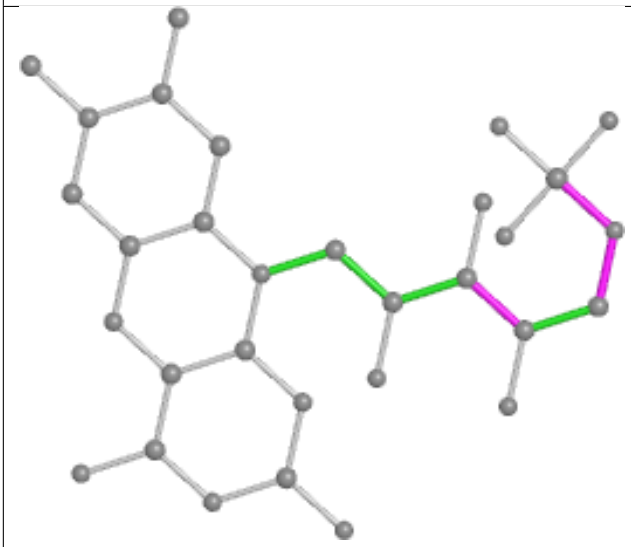
Ligand FMN A 401



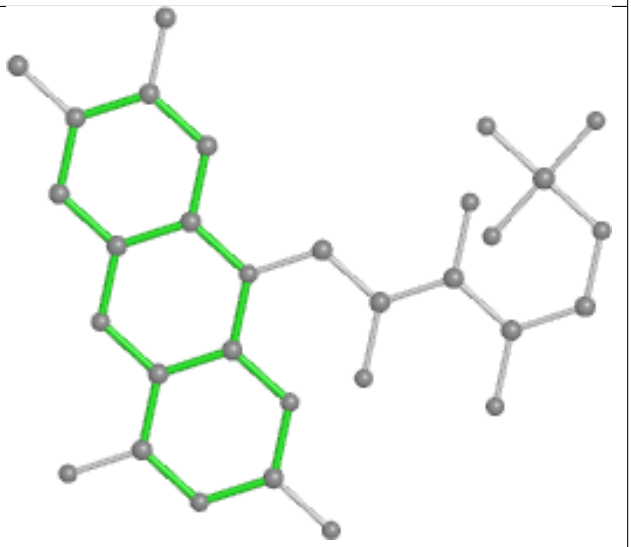
Bond lengths



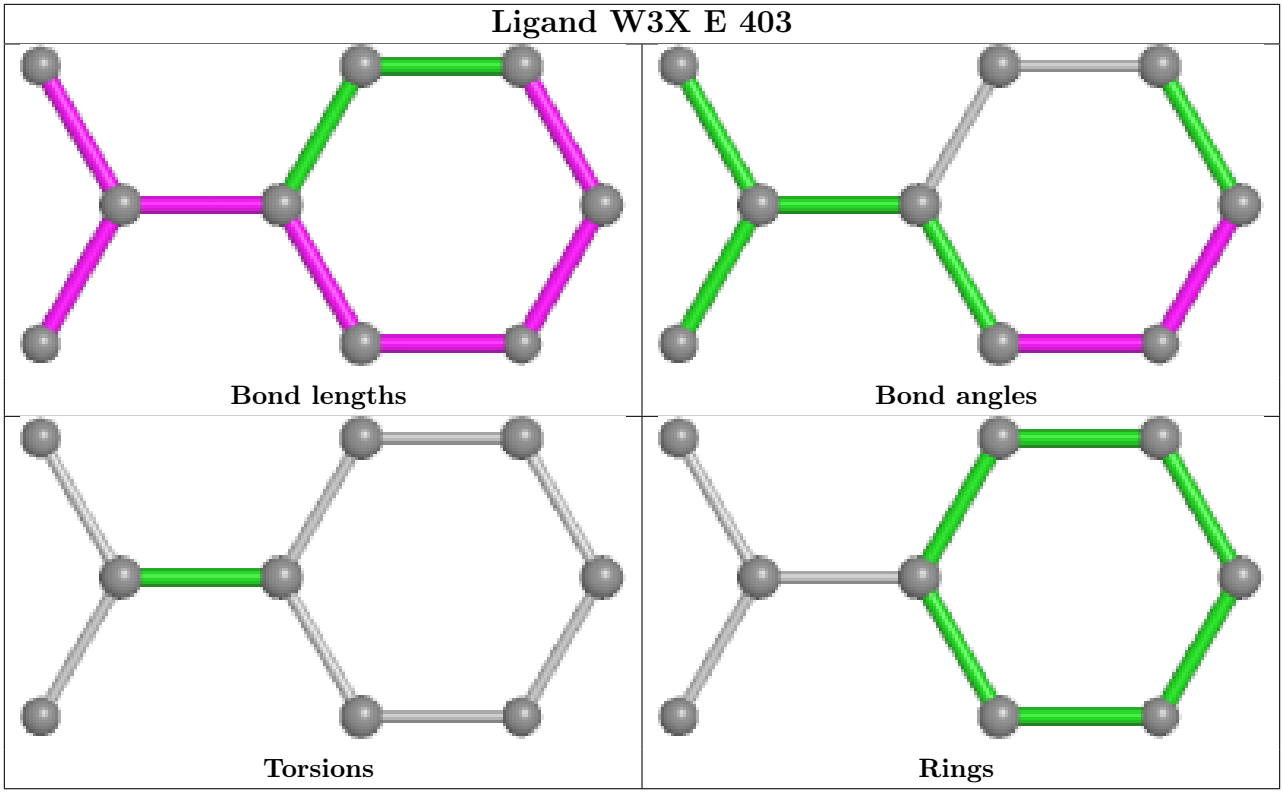
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	349/369 (94%)	0.08	6 (1%) 70 78	39, 48, 61, 82	0
1	B	349/369 (94%)	0.09	7 (2%) 65 73	38, 50, 66, 90	0
1	C	349/369 (94%)	0.07	2 (0%) 89 92	35, 47, 60, 83	0
1	D	349/369 (94%)	0.10	0 100 100	36, 49, 64, 91	0
1	E	349/369 (94%)	0.01	1 (0%) 94 96	32, 47, 59, 79	0
1	F	351/369 (95%)	0.11	4 (1%) 80 86	38, 50, 66, 96	0
1	G	349/369 (94%)	0.07	1 (0%) 94 96	38, 50, 65, 81	0
1	H	349/369 (94%)	0.08	1 (0%) 94 96	38, 48, 60, 76	0
All	All	2794/2952 (94%)	0.08	22 (0%) 86 90	32, 48, 63, 96	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	VAL	4.2
1	B	268	ARG	3.7
1	A	269	ILE	3.7
1	B	269	ILE	3.4
1	H	8	LEU	2.8
1	F	257	ASP	2.8
1	A	266	ARG	2.7
1	C	246[A]	ARG	2.7
1	B	270	PRO	2.6
1	A	316	LEU	2.4
1	F	269	ILE	2.3
1	B	162	LEU	2.3
1	B	246[A]	ARG	2.3
1	B	151	LEU	2.3
1	C	54	ILE	2.3
1	A	246[A]	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	67	ILE	2.1
1	E	80	LEU	2.1
1	G	268	ARG	2.1
1	F	187	SER	2.1
1	A	257	ASP	2.1
1	F	67	ILE	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)

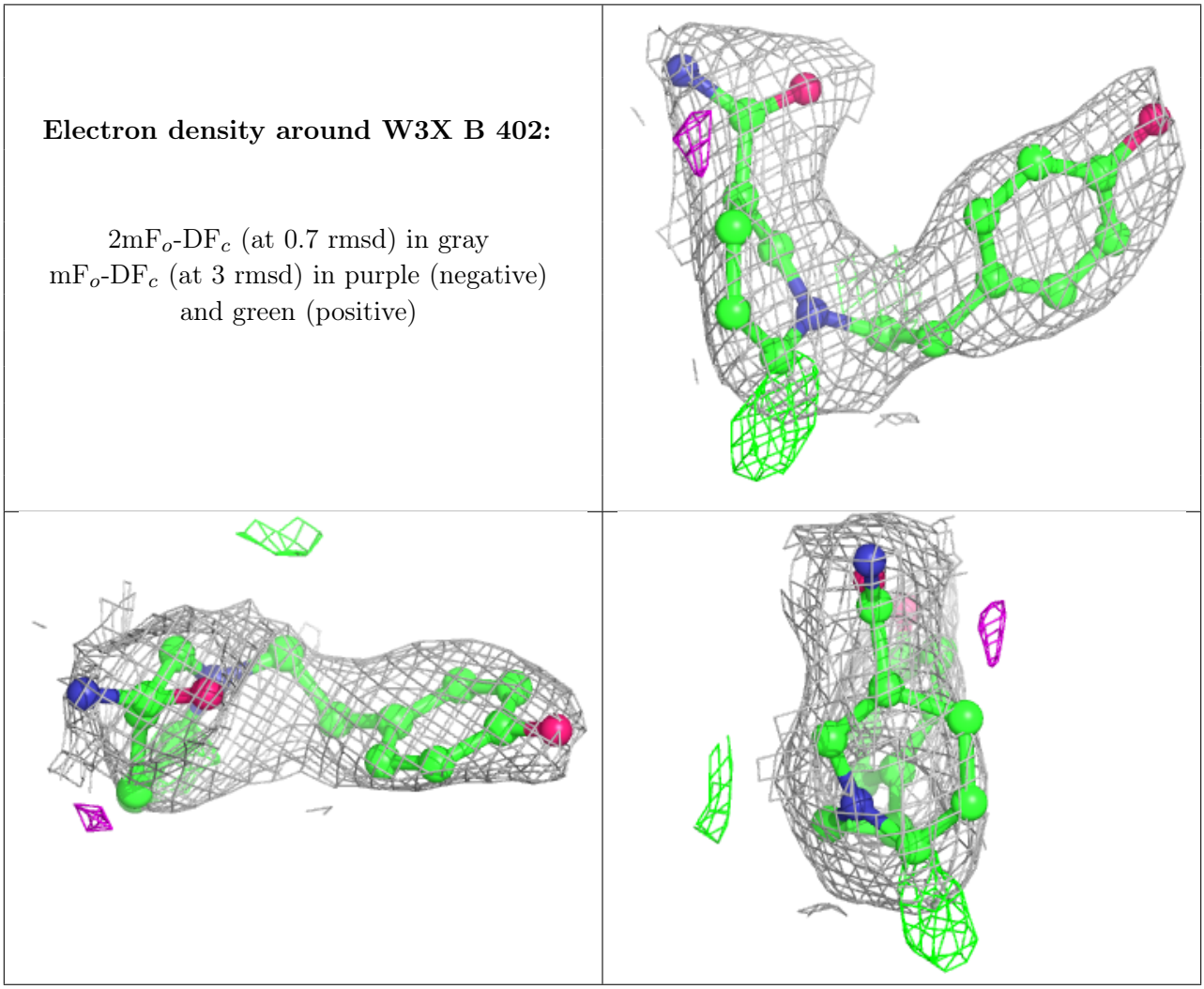
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	W3X	B	402	18/18	0.90	0.25	53,64,73,73	0
3	W3X	A	402	18/18	0.92	0.18	48,55,60,63	0
3	W3X	F	404	9/18	0.93	0.20	50,52,55,57	0
2	FMN	E	401	31/31	0.93	0.17	42,45,48,49	0
5	NA	F	402	1/1	0.93	0.28	49,49,49,49	0
2	FMN	F	401	31/31	0.94	0.19	39,47,50,54	0
2	FMN	A	401	31/31	0.94	0.20	41,46,51,54	0
2	FMN	B	401	31/31	0.95	0.18	41,47,49,52	0
3	W3X	E	403	9/18	0.95	0.22	51,51,57,59	0
2	FMN	C	401	31/31	0.95	0.20	37,41,49,49	0
2	FMN	G	401	31/31	0.95	0.19	39,45,53,60	0
2	FMN	D	401	31/31	0.95	0.19	38,40,44,49	0
4	IPA	H	402	4/4	0.96	0.22	43,52,59,59	0
2	FMN	H	401	31/31	0.96	0.17	43,46,52,53	0
6	CL	F	403	1/1	0.96	0.12	56,56,56,56	0
4	IPA	E	402	4/4	0.97	0.28	44,53,60,60	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.

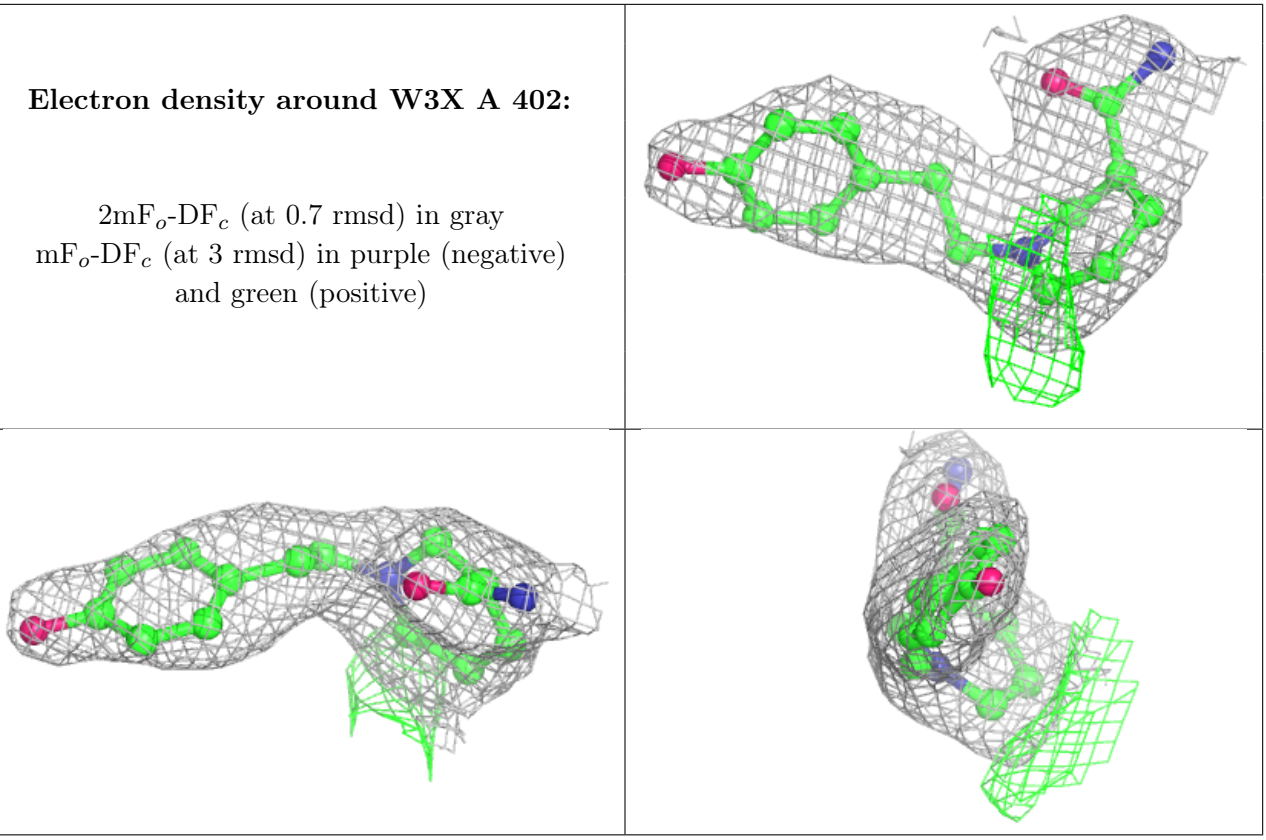
Electron density around W3X B 402:

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



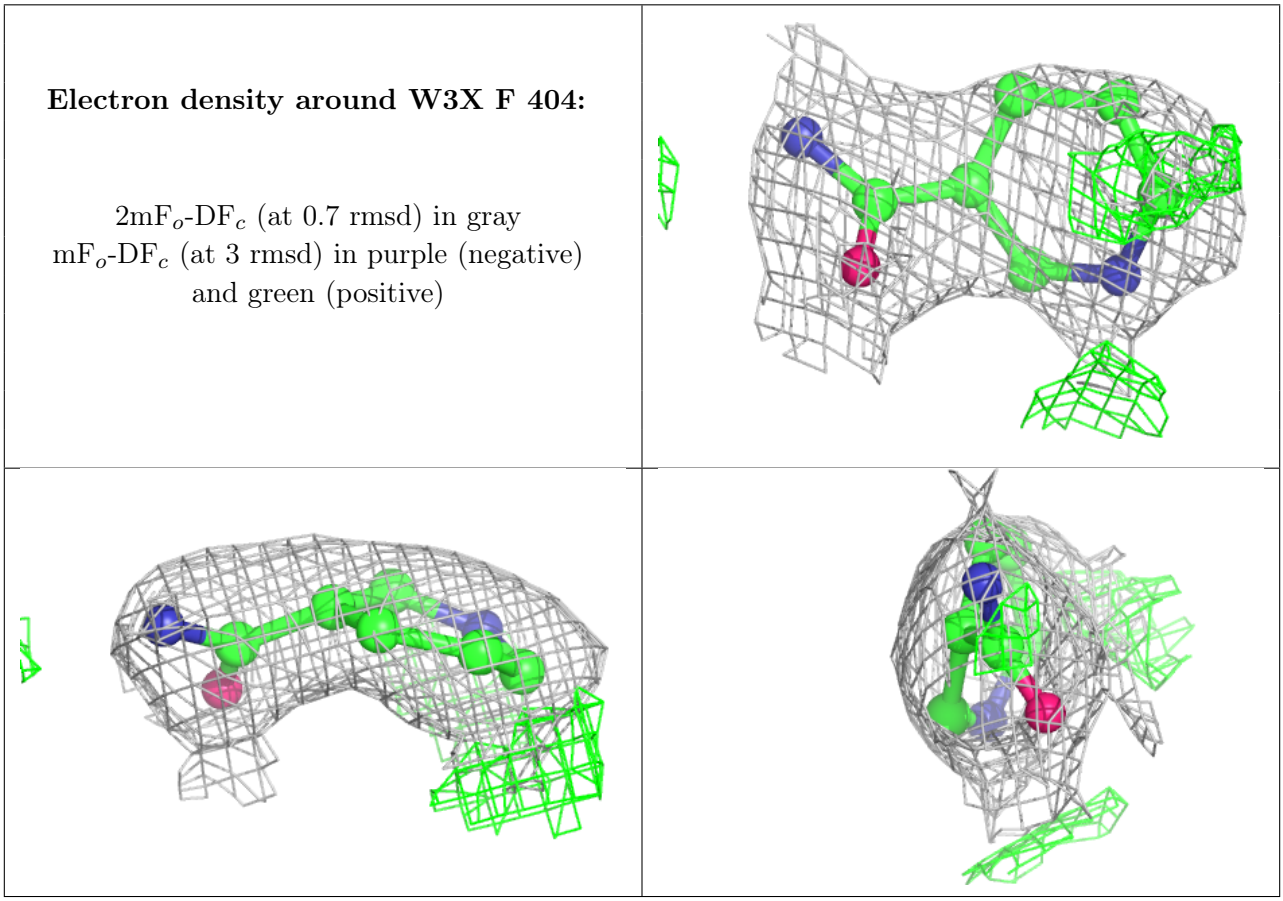
Electron density around W3X A 402:

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



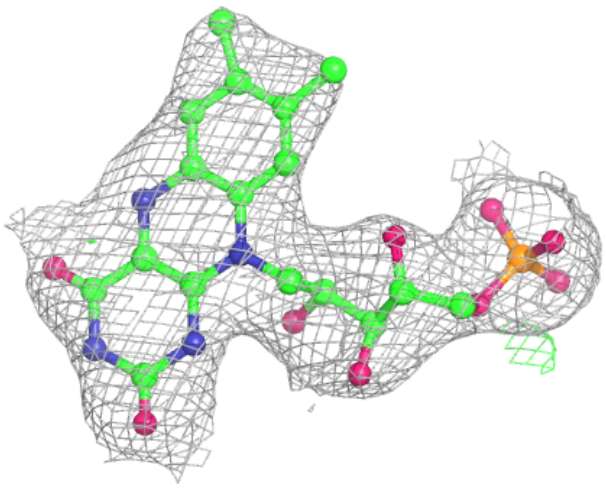
Electron density around W3X F 404:

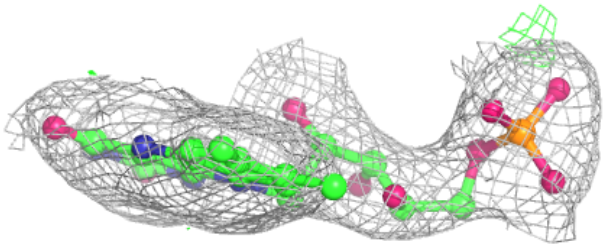
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

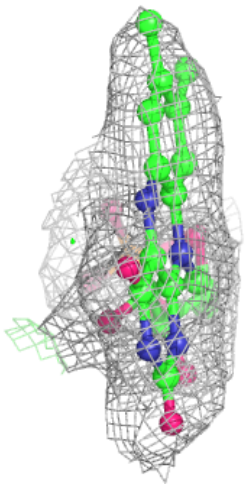


Electron density around FMN E 401:

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

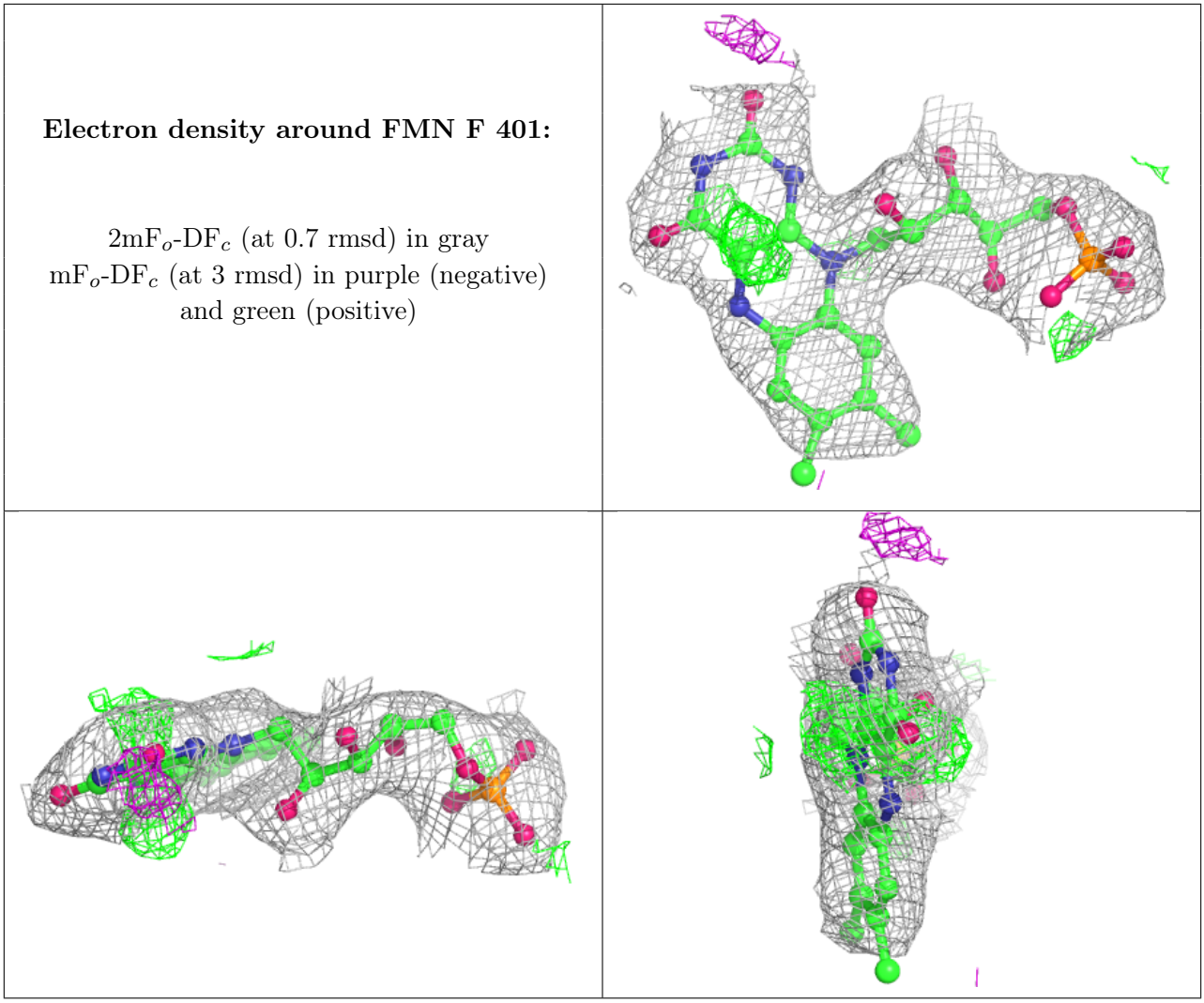






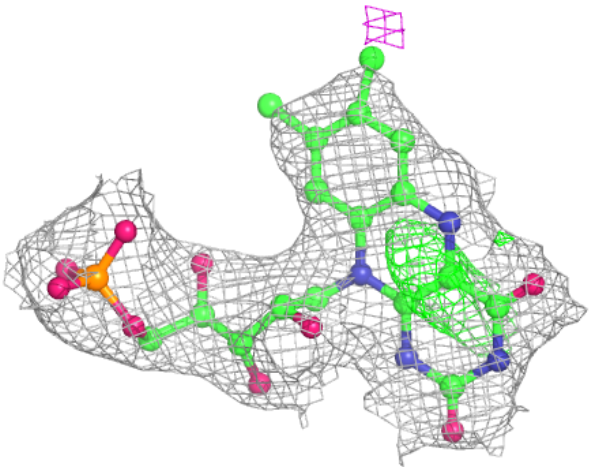
Electron density around FMN F 401:

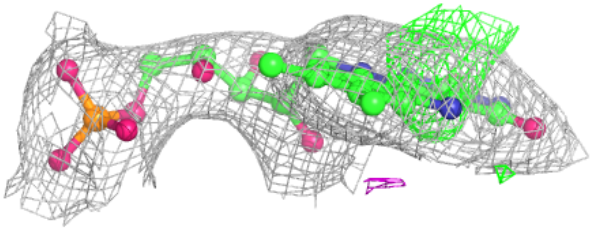
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

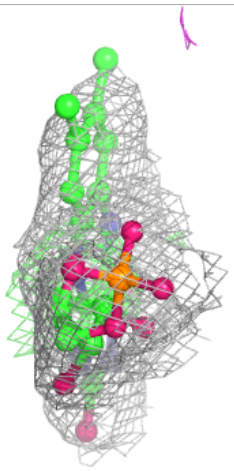


Electron density around FMN A 401:

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

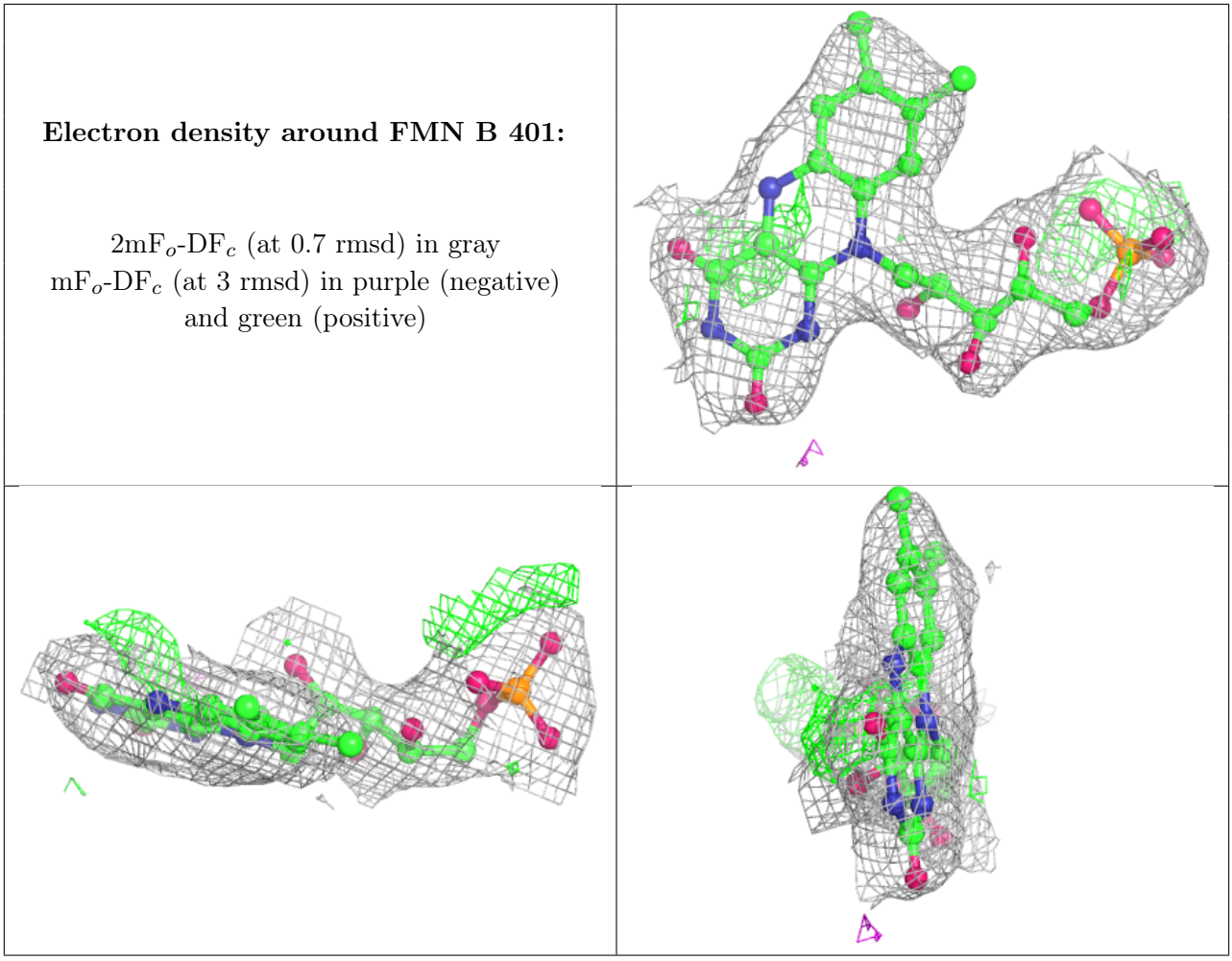






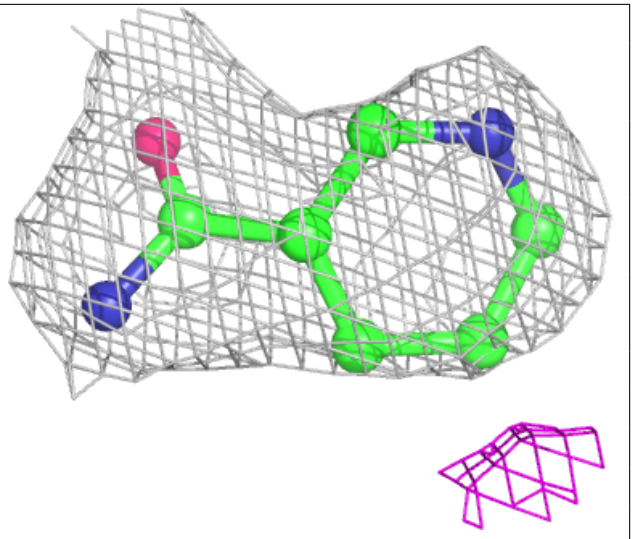
Electron density around FMN B 401:

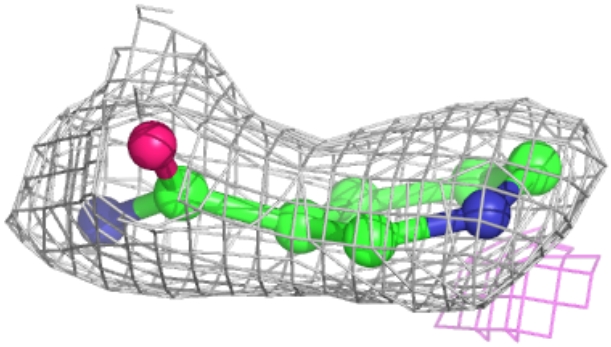
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

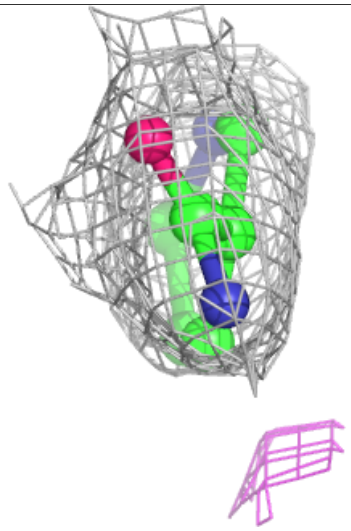


Electron density around W3X E 403:

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

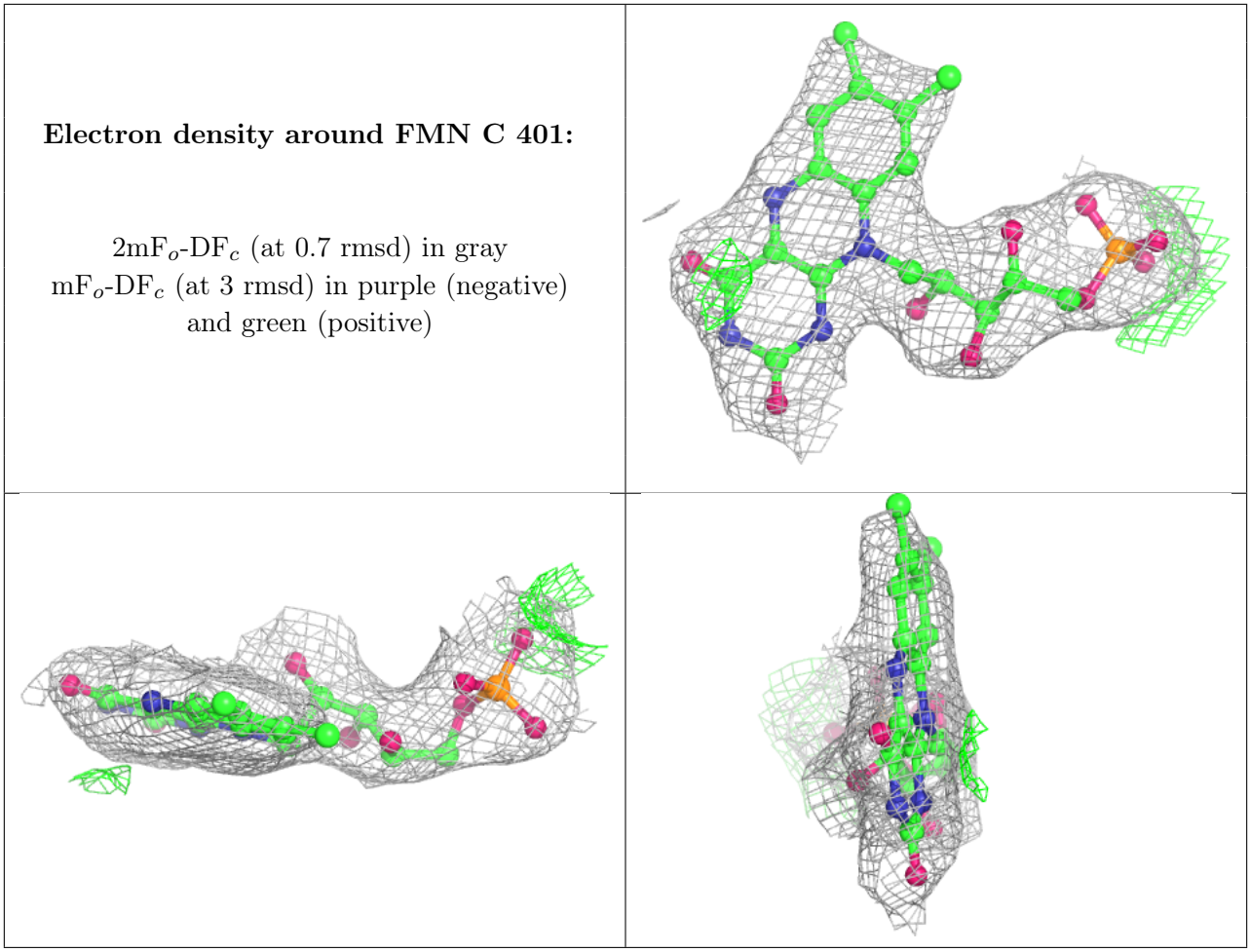






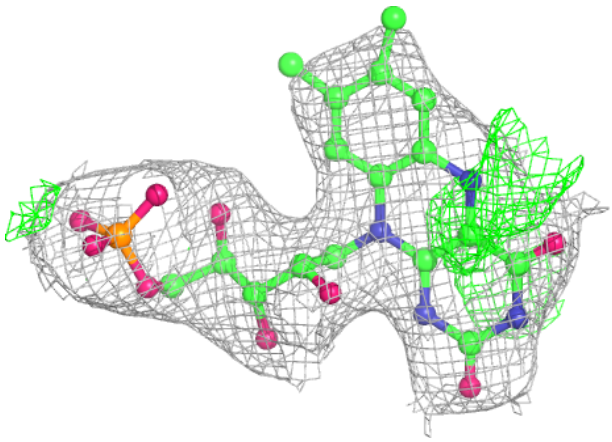
Electron density around FMN C 401:

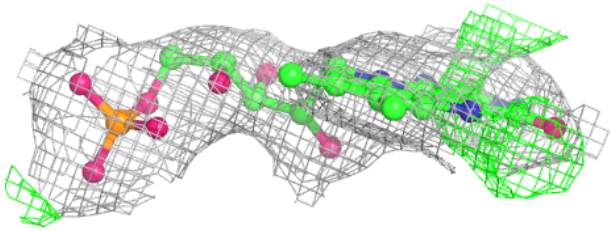
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

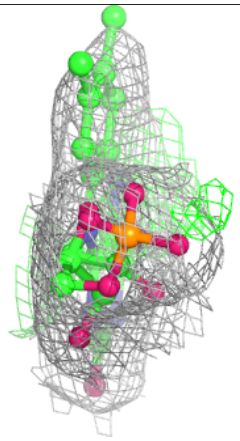


Electron density around FMN G 401:

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

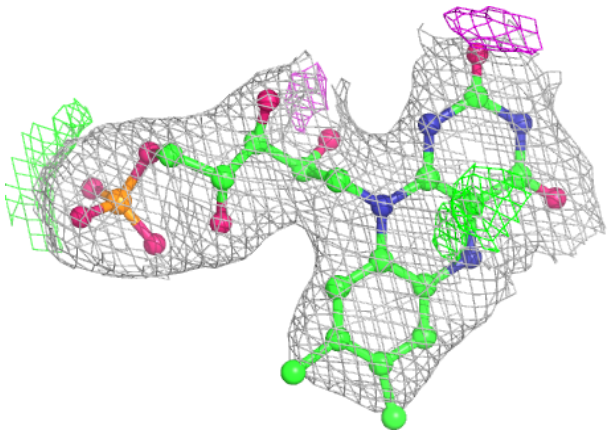


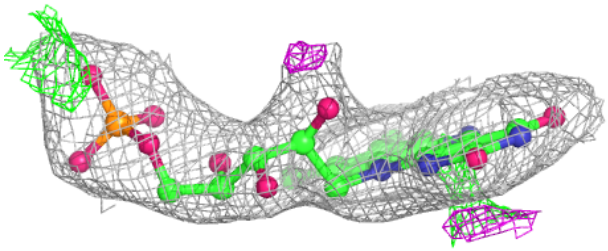


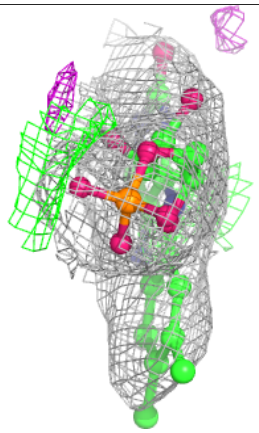


Electron density around FMN D 401:

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

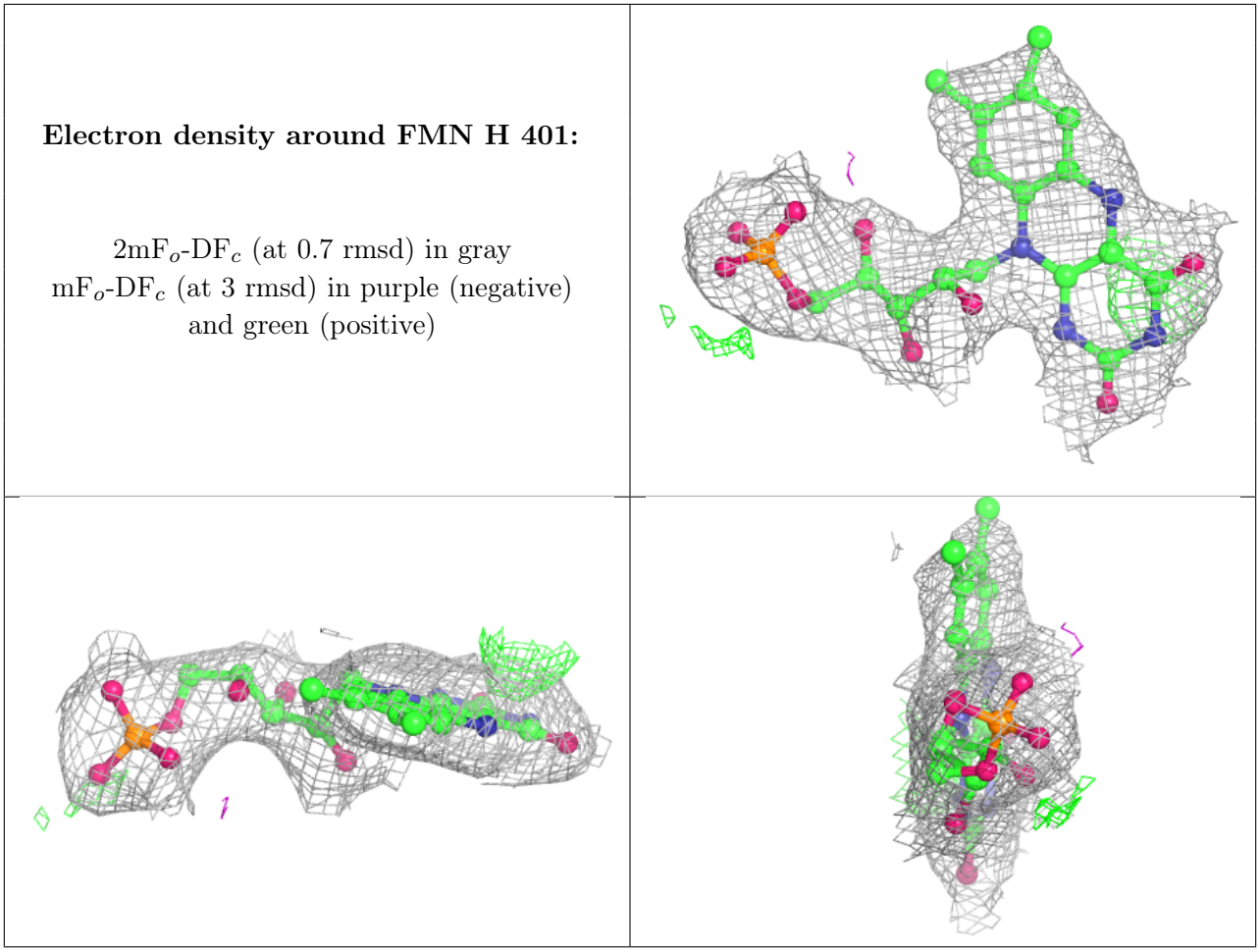






Electron density around FMN H 401:

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



6.5 Other polymers

There are no such residues in this entry.