Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 09:35 PM JST

PDB ID	:	7E1S / pdb_00007e1s
Title	:	Crystal structure of dehydrogenase/isomerase FabX from Helicobacter pylori in complex with octanoyl-ACP
Authors	:	Zhou, J.S.; Zhang, L.; Zhang, L.
Deposited on	:	2021-02-03
Resolution	:	2.31 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:

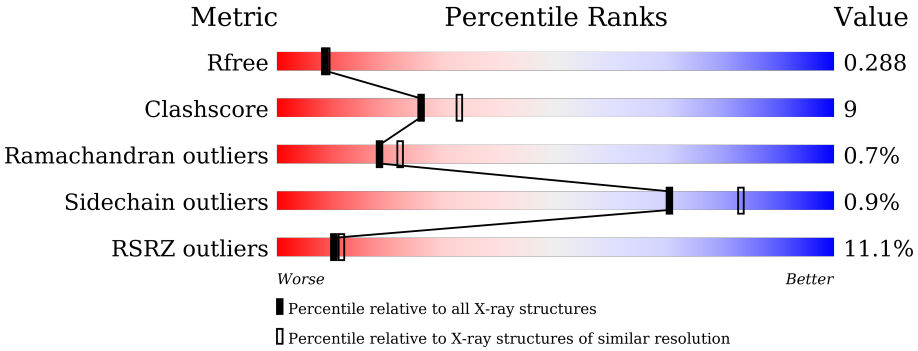
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	372	9%, 78%, 17%, • • •
1	C	372	4%, 80%, 18%, • •
2	B	86	31%, 66%, 16%, •, 16%
2	D	86	17%, 20%, 5%, •, 74%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6695 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 2-nitropropane dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	2819	1803	487	514	15	0	1	0
1	C	366	2818	1802	488	513	15	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP A0A0B2E3F3
A	-7	LYS	-	expression tag	UNP A0A0B2E3F3
A	-6	HIS	-	expression tag	UNP A0A0B2E3F3
A	-5	HIS	-	expression tag	UNP A0A0B2E3F3
A	-4	HIS	-	expression tag	UNP A0A0B2E3F3
A	-3	HIS	-	expression tag	UNP A0A0B2E3F3
A	-2	HIS	-	expression tag	UNP A0A0B2E3F3
A	-1	HIS	-	expression tag	UNP A0A0B2E3F3
A	0	HIS	-	expression tag	UNP A0A0B2E3F3
C	-8	MET	-	initiating methionine	UNP A0A0B2E3F3
C	-7	LYS	-	expression tag	UNP A0A0B2E3F3
C	-6	HIS	-	expression tag	UNP A0A0B2E3F3
C	-5	HIS	-	expression tag	UNP A0A0B2E3F3
C	-4	HIS	-	expression tag	UNP A0A0B2E3F3
C	-3	HIS	-	expression tag	UNP A0A0B2E3F3
C	-2	HIS	-	expression tag	UNP A0A0B2E3F3
C	-1	HIS	-	expression tag	UNP A0A0B2E3F3
C	0	HIS	-	expression tag	UNP A0A0B2E3F3

- Molecule 2 is a protein called Acyl carrier protein,Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	72	553	354	82	115	2	0	0	0

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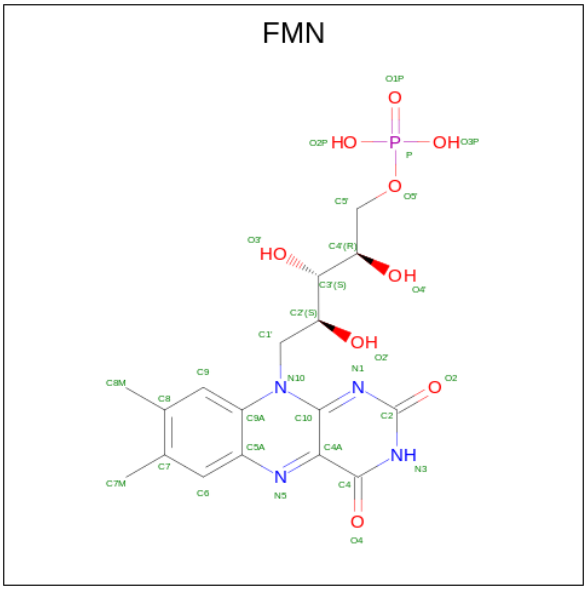
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	22	172	111	23	37	1	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

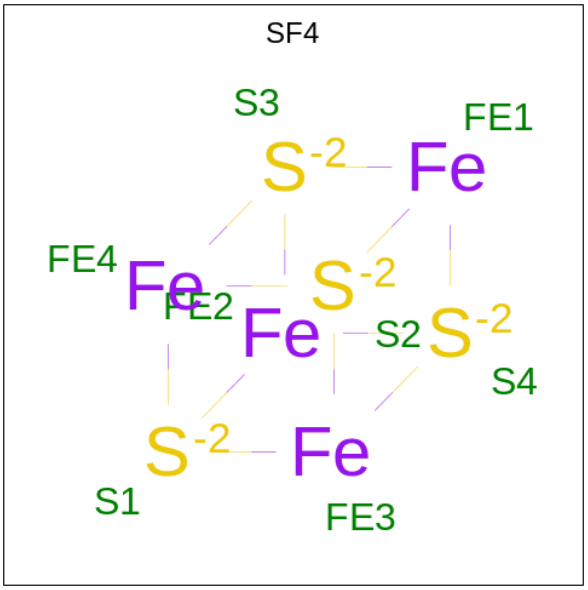
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLY	-	expression tag	UNP A0A2T6RV84
B	-6	THR	-	expression tag	UNP A0A2T6RV84
B	-5	SER	-	expression tag	UNP A0A2T6RV84
B	-4	SER	-	expression tag	UNP A0A2T6RV84
B	-3	MET	-	expression tag	UNP A0A2T6RV84
B	-2	GLY	-	expression tag	UNP A0A2T6RV84
B	-1	TYR	-	expression tag	UNP A0A2T6RV84
B	0	LEU	-	expression tag	UNP A0A2T6RV84
D	-7	GLY	-	expression tag	UNP A0A2T6RV84
D	-6	THR	-	expression tag	UNP A0A2T6RV84
D	-5	SER	-	expression tag	UNP A0A2T6RV84
D	-4	SER	-	expression tag	UNP A0A2T6RV84
D	-3	MET	-	expression tag	UNP A0A2T6RV84
D	-2	GLY	-	expression tag	UNP A0A2T6RV84
D	-1	TYR	-	expression tag	UNP A0A2T6RV84
D	0	LEU	-	expression tag	UNP A0A2T6RV84

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



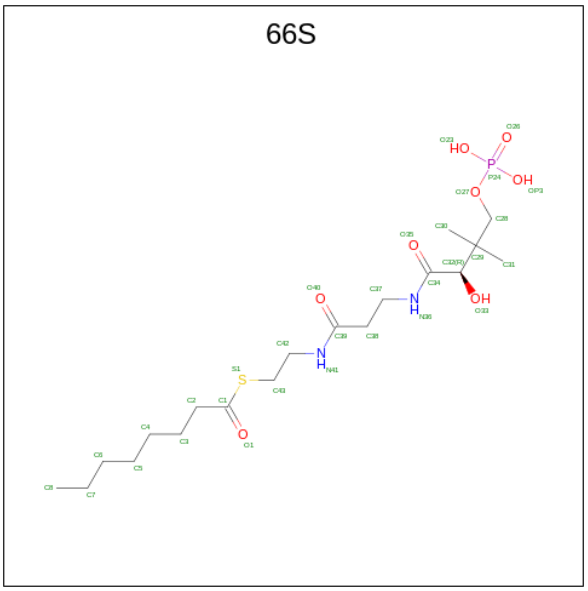
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
3	C	1	31	17	4	9	1	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	8	4	4	0	0
			Total	Fe	S		
4	C	1	8	4	4	0	0

- Molecule 5 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] octanethioate (CCD ID: 66S) (formula: $C_{19}H_{37}N_2O_8PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	B	1	30	19	2	7	1	1	0	0
5	D	1	30	19	2	7	1	1	0	0

- Molecule 6 is water.

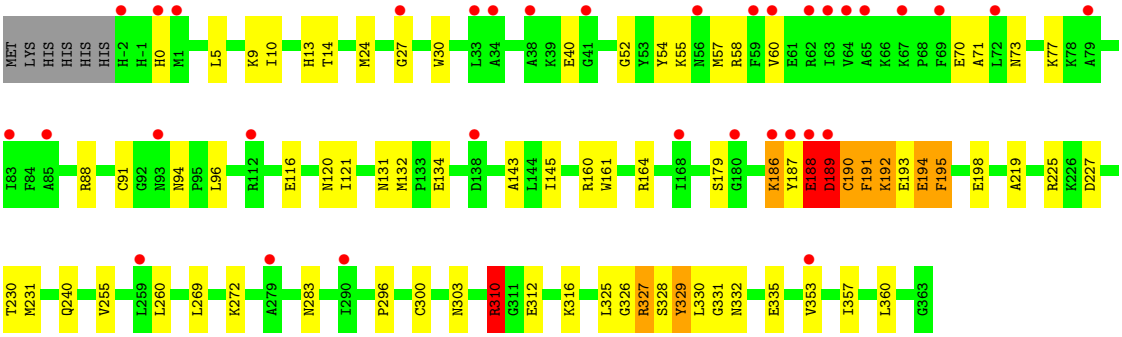
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	69	69	69	0	0
6	B	20	20	20	0	0
6	C	103	103	103	0	0
6	D	3	3	3	0	0

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.

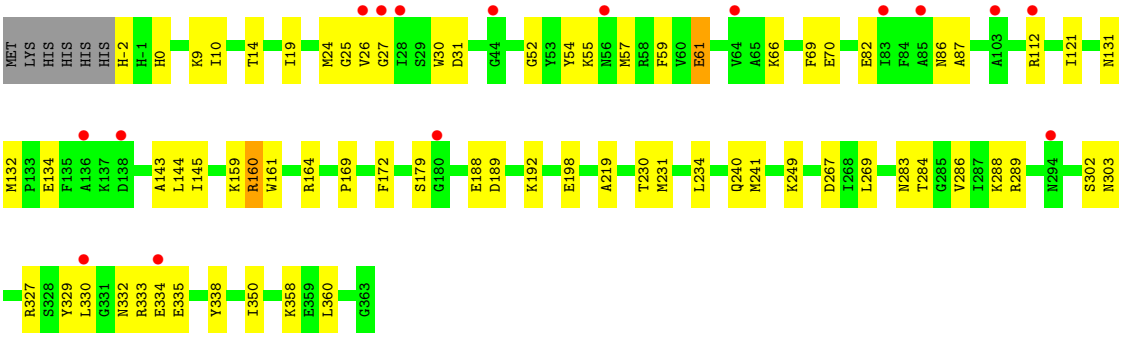
• Molecule 1: 2-nitropropane dioxygenase

Chain A:



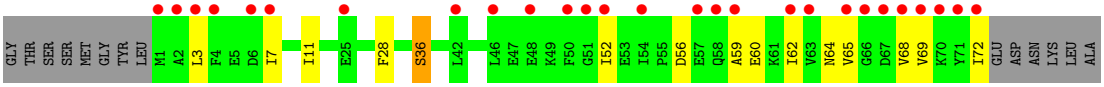
• Molecule 1: 2-nitropropane dioxygenase

Chain C:



• Molecule 2: Acyl carrier protein,Acyl carrier protein

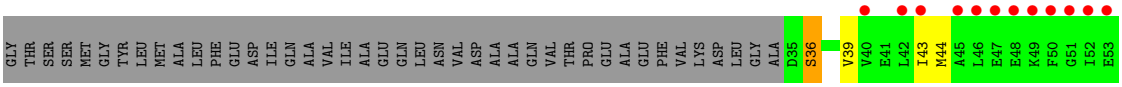
Chain B:

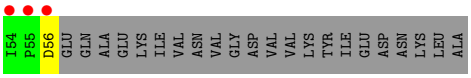


• Molecule 2: Acyl carrier protein,Acyl carrier protein

Chain D:

17%
20%
5%
74%


GLY THR SER SER MET GLY TYR LEU MET ALA LEU PHE GLU ASP ILE GLN ALA VAL ILE ALA GLU GLN LEU ASN VAL ASP ALA ALA GLN VAL THR PRO GLU ALA GLU PHE VAL LYS ASP LEU GLY ALA D35 S36 V39 V40 E41 L42 I43 M44 A45 L46 E47 E48 K49 F50 G51 I52 E53


I54 P55 D56 GLU GLN ALA GLU LYS ILE VAL ASN VAL GLY ASP VAL VAL LYS TYR ILE GLU ASP ASN LYS LEU ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.89Å 100.13Å 105.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.62 – 2.31 72.62 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.62-2.31) 100.0 (72.62-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.233 , 0.286 0.239 , 0.288	Depositor DCC
R_{free} test set	2289 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.986	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6695	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4902e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 66S, SF4, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.71	12/2878 (0.4%)	0.79	7/3881 (0.2%)
1	C	0.45	1/2877 (0.0%)	0.75	5/3880 (0.1%)
2	B	1.18	1/558 (0.2%)	0.68	0/757
2	D	2.03	1/173 (0.6%)	0.81	0/233
All	All	0.74	15/6486 (0.2%)	0.76	12/8751 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	36	SER	CB-OG	-26.17	0.89	1.42
2	D	36	SER	CB-OG	-26.13	0.89	1.42
1	A	325	LEU	C-O	-11.70	1.10	1.24
1	A	190	CYS	C-O	-10.06	1.11	1.24
1	A	326	GLY	C-O	-9.12	1.12	1.23
1	A	329	TYR	C-O	-8.55	1.13	1.24
1	A	328	SER	CA-CB	-8.06	1.40	1.53
1	A	327	ARG	C-O	-8.02	1.14	1.24
1	A	193	GLU	C-O	-7.91	1.14	1.24
1	A	328	SER	C-O	-7.60	1.15	1.24
1	A	191	PHE	C-O	-6.20	1.15	1.23
1	A	195	PHE	C-O	-5.87	1.15	1.23
1	A	192	LYS	C-O	-5.83	1.16	1.23
1	C	61	GLU	C-O	-5.08	1.17	1.23
1	A	310	ARG	C-O	-5.06	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	25	GLY	N-CA-C	7.74	123.05	110.97
1	A	192	LYS	CB-CA-C	-7.39	96.39	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	ASP	CA-CB-CG	-7.20	105.40	112.60
1	C	334	GLU	CB-CG-CD	7.18	124.81	112.60
1	A	189	ASP	CB-CA-C	6.72	123.80	110.42
1	A	188	GLU	CB-CG-CD	6.38	123.45	112.60
1	A	310	ARG	CA-C-O	-6.38	114.44	121.84
1	A	327	ARG	CG-CD-NE	6.17	125.57	112.00
1	C	24	MET	CA-C-N	6.14	126.50	120.98
1	C	24	MET	C-N-CA	6.14	126.50	120.98
1	A	329	TYR	N-CA-C	-5.45	105.50	111.82
1	C	160	ARG	CG-CD-NE	5.01	123.03	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2819	0	2873	57	0
1	C	2818	0	2873	55	0
2	B	553	0	552	12	0
2	D	172	0	169	3	0
3	A	31	0	19	3	0
3	C	31	0	19	2	0
4	A	8	0	0	0	0
4	C	8	0	0	1	0
5	B	30	0	0	0	0
5	D	30	0	0	0	0
6	A	69	0	0	5	0
6	B	20	0	0	0	0
6	C	103	0	0	9	0
6	D	3	0	0	0	0
All	All	6695	0	6505	123	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 9.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:CYS:SG	6:A:1101:HOH:O	2.22	0.97
4:C:1002:SF4:S2	6:C:1101:HOH:O	2.23	0.95
1:C:284:THR:HA	1:C:288:LYS:HD3	1.64	0.80
1:C:179:SER:HB2	3:C:1001:FMN:H4'	1.68	0.76
1:A:303:ASN:N	6:A:1101:HOH:O	2.09	0.75
1:C:241:MET:HE1	1:C:360:LEU:HD13	1.69	0.74
1:A:198:GLU:HG3	1:A:231:MET:HE1	1.69	0.74
1:C:288:LYS:HE2	1:C:289:ARG:HH12	1.53	0.74
1:C:131[A]:ASN:OD1	1:C:164:ARG:NH1	2.20	0.73
1:C:160:ARG:NH1	1:C:164:ARG:HH21	1.87	0.72
1:C:303:ASN:N	6:C:1101:HOH:O	2.06	0.69
1:C:160:ARG:CZ	1:C:164:ARG:HH21	2.06	0.68
1:C:-2:HIS:N	6:C:1107:HOH:O	2.27	0.67
1:C:188:GLU:OE2	6:C:1102:HOH:O	2.15	0.65
1:A:5:LEU:O	6:A:1102:HOH:O	2.13	0.65
1:A:188:GLU:HB2	1:C:234:LEU:HD21	1.79	0.64
1:C:57:MET:HE1	1:C:66:LYS:O	1.97	0.64
1:A:160:ARG:NH2	1:A:164:ARG:HH21	1.96	0.63
1:C:121:ILE:HG12	1:C:143:ALA:HB3	1.80	0.62
1:A:58:ARG:NH1	6:A:1107:HOH:O	2.32	0.61
2:B:62:ILE:HD12	2:B:68:VAL:HG22	1.84	0.60
1:A:188:GLU:CD	1:A:188:GLU:H	2.10	0.59
1:C:332:ASN:OD1	1:C:335:GLU:N	2.34	0.59
1:A:219:ALA:HB2	1:A:240:GLN:HB3	1.83	0.58
1:A:88:ARG:NH2	1:A:94:ASN:O	2.37	0.58
1:C:0:HIS:CE1	1:C:358:LYS:HG2	2.38	0.58
1:C:267:ASP:OD2	6:C:1103:HOH:O	2.17	0.57
1:A:186:LYS:HB2	1:A:189:ASP:HB2	1.86	0.57
1:C:59:PHE:CZ	1:C:82:GLU:HG3	2.39	0.57
2:D:39:VAL:O	2:D:43:ILE:HG12	2.05	0.56
1:A:52:GLY:O	1:A:57:MET:HA	2.05	0.56
1:A:179:SER:HB2	3:A:1001:FMN:H4'	1.88	0.56
1:C:54:TYR:CZ	1:C:55:LYS:HE2	2.41	0.55
2:B:28:PHE:CE1	2:B:65:VAL:HG12	2.42	0.55
2:B:65:VAL:O	2:B:69:VAL:HG23	2.07	0.55
2:B:3:LEU:O	2:B:7:ILE:HG12	2.06	0.55
1:A:255:VAL:HG21	1:A:331:GLY:HA2	1.89	0.54
1:A:60:VAL:HG13	1:A:73:ASN:HB3	1.90	0.54
1:A:312:GLU:O	1:A:316:LYS:HG2	2.07	0.54
1:C:219:ALA:HB2	1:C:240:GLN:HB3	1.90	0.53
1:A:27:GLY:HA2	1:A:30:TRP:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:PRO:HG2	1:C:172:PHE:CZ	2.44	0.52
1:A:296:PRO:HG3	1:A:335:GLU:OE1	2.10	0.52
1:A:310:ARG:HB2	1:A:310:ARG:HH11	1.74	0.52
1:C:160:ARG:HE	1:C:164:ARG:HE	1.58	0.51
1:A:70[B]:GLU:OE1	1:A:71:ALA:N	2.42	0.51
2:B:52:ILE:HD11	2:B:72:ILE:HG12	1.93	0.51
1:C:230:THR:HG22	1:C:231:MET:HE2	1.92	0.51
1:A:164:ARG:NH2	2:B:56:ASP:OD1	2.27	0.51
1:C:27:GLY:HA2	1:C:30:TRP:CE3	2.46	0.51
1:A:269:LEU:HD22	1:A:283:ASN:HB2	1.92	0.51
1:C:9:LYS:HG3	1:C:14:THR:OG1	2.11	0.50
1:C:198:GLU:HG3	1:C:231:MET:HE1	1.93	0.50
1:C:160:ARG:CZ	1:C:164:ARG:NH2	2.74	0.49
1:A:186:LYS:C	1:A:188:GLU:N	2.70	0.49
1:C:329:TYR:CD2	1:C:330:LEU:HD12	2.48	0.49
1:A:24:MET:HG2	3:A:1001:FMN:C6	2.42	0.49
1:C:288:LYS:HE2	1:C:289:ARG:NH1	2.25	0.49
1:C:302:SER:N	6:C:1101:HOH:O	2.46	0.49
1:C:286:VAL:HG22	1:C:335:GLU:O	2.13	0.48
1:C:70:GLU:HG3	6:C:1163:HOH:O	2.13	0.48
1:A:192:LYS:HE3	1:A:194:GLU:HB2	1.95	0.48
2:B:62:ILE:O	2:B:64:ASN:N	2.44	0.48
1:A:10:ILE:HG21	1:A:145:ILE:HD11	1.95	0.48
1:C:132:MET:HE2	1:C:144:LEU:HD22	1.96	0.47
1:A:230:THR:HG22	1:A:231:MET:HE2	1.96	0.47
1:C:52:GLY:O	1:C:57:MET:HA	2.14	0.47
1:C:284:THR:OG1	6:C:1105:HOH:O	2.20	0.47
1:A:160:ARG:HH21	1:A:164:ARG:HE	1.63	0.46
1:A:24:MET:HG2	3:A:1001:FMN:C7	2.45	0.46
1:C:249:LYS:NZ	1:C:350:ILE:O	2.41	0.46
2:B:59:ALA:O	2:B:62:ILE:HG12	2.15	0.46
1:C:284:THR:HA	1:C:288:LYS:CD	2.40	0.45
1:A:189:ASP:OD1	1:C:230:THR:HG23	2.15	0.45
1:C:70:GLU:H	1:C:302:SER:HA	1.81	0.45
1:C:131[A]:ASN:ND2	2:D:56:ASP:OD2	2.50	0.45
1:A:255:VAL:CG2	1:A:331:GLY:HA2	2.46	0.45
1:A:13:HIS:CE1	1:A:120:ASN:HB3	2.52	0.45
1:A:77:LYS:NZ	1:A:116:GLU:OE1	2.42	0.44
1:A:186:LYS:O	1:A:188:GLU:N	2.51	0.44
1:C:27:GLY:HA2	1:C:30:TRP:CD2	2.52	0.44
2:B:11:ILE:HD13	2:B:28:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HG12	1:A:143:ALA:HB3	2.00	0.44
1:C:69:PHE:O	1:C:70:GLU:HB3	2.17	0.43
1:C:189:ASP:HA	1:C:192:LYS:HG3	2.00	0.43
1:A:192:LYS:HE3	1:A:194:GLU:CB	2.48	0.43
1:C:112:ARG:NH1	6:C:1124:HOH:O	2.51	0.43
1:A:327:ARG:HB3	1:A:332:ASN:HB3	1.99	0.43
1:C:132:MET:HB3	1:C:161:TRP:CZ2	2.54	0.43
2:B:7:ILE:CD1	2:B:69:VAL:HG22	2.48	0.43
1:A:54:TYR:CZ	1:A:55:LYS:HE2	2.54	0.43
1:A:131:ASN:O	1:A:134:GLU:HB3	2.19	0.42
1:C:188:GLU:H	1:C:188:GLU:CD	2.27	0.42
1:A:227:ASP:HA	6:A:1121:HOH:O	2.18	0.42
3:C:1001:FMN:HM73	3:C:1001:FMN:HM81	1.79	0.42
1:A:188:GLU:CB	1:C:234:LEU:HD21	2.48	0.42
1:A:225:ARG:HD3	1:A:360:LEU:O	2.19	0.42
1:A:272:LYS:HE3	1:A:272:LYS:HB2	1.80	0.42
1:A:132:MET:HB3	1:A:161:TRP:CZ2	2.54	0.42
1:A:186:LYS:HD2	1:A:195:PHE:CZ	2.53	0.42
1:A:40:GLU:HG3	1:A:353:VAL:HG12	2.00	0.42
1:C:327:ARG:HB3	1:C:332:ASN:HB3	2.02	0.42
1:A:54:TYR:CE1	1:A:55:LYS:HE2	2.55	0.42
1:A:353:VAL:O	1:A:357:ILE:HG12	2.20	0.42
1:C:269:LEU:HD22	1:C:283:ASN:HB2	2.02	0.42
1:C:159:LYS:HD2	2:D:44:MET:HE1	2.02	0.41
1:A:9:LYS:HG3	1:A:14:THR:OG1	2.20	0.41
1:C:19:ILE:HG23	1:C:241:MET:HE2	2.02	0.41
1:C:31:ASP:HA	1:C:87:ALA:HB2	2.02	0.41
1:A:329:TYR:CD2	1:A:330:LEU:HD12	2.55	0.41
1:C:54:TYR:OH	1:C:86:ASN:ND2	2.54	0.41
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.95	0.40
1:A:91:CYS:SG	1:A:96:LEU:HD11	2.61	0.40
1:A:189:ASP:O	1:A:191:PHE:N	2.54	0.40
1:A:195:PHE:HD1	1:A:195:PHE:HA	1.65	0.40
1:A:186:LYS:C	1:A:188:GLU:H	2.30	0.40
1:A:188:GLU:CD	1:A:188:GLU:N	2.78	0.40
2:B:7:ILE:HD11	2:B:69:VAL:HG22	2.02	0.40
1:C:10:ILE:HG21	1:C:145:ILE:HD11	2.03	0.40
1:A:160:ARG:NH2	1:A:164:ARG:NH2	2.66	0.40
2:B:56:ASP:O	2:B:60:GLU:HG3	2.20	0.40
1:C:333:ARG:HA	1:C:338:TYR:OH	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	365/372 (98%)	350 (96%)	10 (3%)	5 (1%)	9 8
1	C	365/372 (98%)	351 (96%)	13 (4%)	1 (0%)	36 45
2	B	70/86 (81%)	63 (90%)	7 (10%)	0	100 100
2	D	20/86 (23%)	20 (100%)	0	0	100 100
All	All	820/916 (90%)	784 (96%)	30 (4%)	6 (1%)	18 22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	TYR
1	A	190	CYS
1	A	186	LYS
1	A	189	ASP
1	A	0	HIS
1	C	26	VAL

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	295/300 (98%)	292 (99%)	3 (1%)	68 81
1	C	295/300 (98%)	294 (100%)	1 (0%)	86 92
2	B	60/71 (84%)	59 (98%)	1 (2%)	53 70
2	D	20/71 (28%)	19 (95%)	1 (5%)	22 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	670/742 (90%)	664 (99%)	6 (1%)	70 83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	GLU
1	A	194	GLU
1	A	310	ARG
2	B	36	SER
1	C	61	GLU
2	D	36	SER

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

Mol	Chain	Res	Type
1	A	86	ASN
2	B	21	GLN
2	B	58	GLN
1	C	0	HIS
1	C	36	ASN
1	C	93	ASN
1	C	99	ASN
1	C	199	ASN
1	C	213	ASN
1	C	240	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
5	66S	D	101	2	23,29,30	2.54	11 (47%)	28,36,39	6.81	15 (53%)
4	SF4	C	1002	6,1	0,12,12	-	-	-		
3	FMN	C	1001	-	33,33,33	1.80	6 (18%)	48,50,50	1.40	11 (22%)
4	SF4	A	1002	1	0,12,12	-	-	-		
5	66S	B	101	2	23,29,30	2.45	11 (47%)	28,36,39	6.54	18 (64%)
3	FMN	A	1001	-	33,33,33	1.89	7 (21%)	48,50,50	1.47	10 (20%)

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
5	66S	D	101	2	-	6/34/36/37	-
4	SF4	C	1002	6,1	-	-	0/6/5/5
3	FMN	C	1001	-	-	5/18/18/18	0/3/3/3
4	SF4	A	1002	1	-	-	0/6/5/5
5	66S	B	101	2	-	11/34/36/37	-
3	FMN	A	1001	-	-	5/18/18/18	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FMN	C8M-C8	-5.65	1.39	1.51
3	C	1001	FMN	C8M-C8	-4.71	1.41	1.51
5	B	101	66S	C42-N41	-4.61	1.35	1.46
5	D	101	66S	C42-N41	-4.57	1.35	1.46
3	A	1001	FMN	C7M-C7	-4.43	1.42	1.51
5	B	101	66S	C34-N36	-4.37	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	101	66S	C34-N36	-4.37	1.24	1.33
3	C	1001	FMN	C10-N1	4.20	1.41	1.33
5	D	101	66S	O40-C39	-4.16	1.14	1.23
5	D	101	66S	O1-C1	-3.99	1.14	1.21
5	B	101	66S	C30-C29	-3.96	1.45	1.53
5	D	101	66S	C30-C29	-3.94	1.45	1.53
3	C	1001	FMN	C7M-C7	-3.83	1.43	1.51
3	A	1001	FMN	C10-N1	3.82	1.41	1.33
5	B	101	66S	O1-C1	-3.81	1.14	1.21
5	B	101	66S	O40-C39	-3.71	1.15	1.23
3	C	1001	FMN	C1'-C2'	3.45	1.57	1.52
5	D	101	66S	O35-C34	-3.32	1.16	1.23
3	A	1001	FMN	C9A-N10	-3.03	1.35	1.41
3	A	1001	FMN	C1'-C2'	2.94	1.56	1.52
5	B	101	66S	O35-C34	-2.82	1.17	1.23
5	B	101	66S	C38-C39	-2.74	1.46	1.51
5	D	101	66S	C38-C39	-2.65	1.46	1.51
5	D	101	66S	C3-C2	-2.63	1.42	1.52
3	C	1001	FMN	C9A-N10	-2.62	1.36	1.41
5	B	101	66S	C39-N41	-2.58	1.27	1.33
5	D	101	66S	C39-N41	-2.47	1.27	1.33
5	B	101	66S	C3-C2	-2.45	1.43	1.52
3	C	1001	FMN	C4A-N5	2.45	1.35	1.30
5	B	101	66S	C2-C1	-2.28	1.48	1.50
5	D	101	66S	C37-N36	-2.28	1.40	1.46
3	A	1001	FMN	C5'-C4'	2.24	1.55	1.51
3	A	1001	FMN	P-O3P	-2.20	1.46	1.54
5	D	101	66S	C2-C1	-2.11	1.48	1.50
5	B	101	66S	C37-N36	-2.04	1.41	1.46

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	101	66S	O1-C1-C2	-19.81	100.60	123.99
5	B	101	66S	O1-C1-C2	-19.30	101.20	123.99
5	D	101	66S	C2-C1-S1	17.33	133.63	113.46
5	B	101	66S	C2-C1-S1	16.41	132.56	113.46
5	D	101	66S	C37-N36-C34	15.21	149.72	122.59
5	B	101	66S	C37-N36-C34	14.48	148.41	122.59
5	D	101	66S	C38-C39-N41	11.38	135.58	116.42
5	B	101	66S	C38-C39-N41	10.12	133.46	116.42
5	D	101	66S	C42-N41-C39	8.26	138.18	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	101	66S	C42-N41-C39	7.72	137.16	122.84
5	D	101	66S	O40-C39-C38	-5.65	111.69	122.02
5	D	101	66S	O40-C39-N41	-5.45	112.73	123.01
5	B	101	66S	C43-C42-N41	-5.44	100.98	112.42
5	B	101	66S	O40-C39-N41	-5.24	113.12	123.01
5	B	101	66S	C30-C29-C28	-4.92	100.21	108.23
5	D	101	66S	C37-C38-C39	-4.73	104.48	112.36
5	B	101	66S	O40-C39-C38	-4.70	113.42	122.02
5	D	101	66S	C30-C29-C28	-4.41	101.04	108.23
5	D	101	66S	C43-C42-N41	-4.17	103.66	112.42
5	D	101	66S	C38-C37-N36	-3.70	104.42	111.90
5	B	101	66S	C38-C37-N36	-3.56	104.70	111.90
5	B	101	66S	C37-C38-C39	-3.35	106.78	112.36
3	A	1001	FMN	C4-N3-C2	-3.17	119.78	125.64
3	A	1001	FMN	C9A-C5A-N5	-3.08	119.08	122.43
3	C	1001	FMN	C4A-C10-N10	3.03	120.91	116.48
3	C	1001	FMN	C5'-C4'-C3'	-2.95	106.51	112.20
3	A	1001	FMN	C4A-C4-N3	2.85	120.43	113.19
3	C	1001	FMN	C4A-C4-N3	2.80	120.30	113.19
5	B	101	66S	C43-S1-C1	-2.79	93.19	101.87
5	B	101	66S	O1-C1-S1	2.79	126.23	122.61
3	A	1001	FMN	C4A-C10-N10	2.74	120.49	116.48
5	B	101	66S	C31-C29-C28	2.71	112.65	108.23
3	A	1001	FMN	O3P-P-O5'	-2.70	99.54	106.73
5	B	101	66S	O33-C32-C29	2.70	116.60	110.25
5	B	101	66S	C4-C3-C2	-2.67	103.58	113.19
3	C	1001	FMN	C10-C4A-N5	-2.64	119.25	124.86
5	D	101	66S	C4-C3-C2	-2.52	104.14	113.19
3	C	1001	FMN	C4-N3-C2	-2.50	121.02	125.64
3	A	1001	FMN	O3P-P-O2P	2.43	116.94	107.64
5	D	101	66S	O1-C1-S1	2.43	125.77	122.61
3	A	1001	FMN	C10-C4A-N5	-2.42	119.73	124.86
3	C	1001	FMN	C4-C4A-N5	2.41	121.66	118.23
5	B	101	66S	C3-C2-C1	2.35	117.55	112.33
3	A	1001	FMN	C5'-C4'-C3'	-2.30	107.76	112.20
3	C	1001	FMN	O3P-P-O2P	2.30	116.42	107.64
3	A	1001	FMN	O4-C4-C4A	-2.27	120.58	126.60
5	D	101	66S	C43-S1-C1	-2.24	94.89	101.87
3	A	1001	FMN	C4A-C10-N1	-2.17	119.70	124.73
3	C	1001	FMN	C10-N1-C2	2.15	121.20	116.90
3	C	1001	FMN	C9A-C5A-N5	-2.14	120.11	122.43
5	B	101	66S	C5-C4-C3	-2.07	103.93	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1001	FMN	O4-C4-C4A	-2.07	121.12	126.60
5	D	101	66S	C5-C4-C3	-2.03	104.14	114.42
3	C	1001	FMN	C4A-C10-N1	-2.02	120.04	124.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	101	66S	O27-C28-C29-C32
5	B	101	66S	O33-C32-C34-N36
5	D	101	66S	O33-C32-C34-N36
5	B	101	66S	C38-C39-N41-C42
5	D	101	66S	C38-C39-N41-C42
3	A	1001	FMN	C2'-C3'-C4'-O4'
5	B	101	66S	O40-C39-N41-C42
5	D	101	66S	O40-C39-N41-C42
3	A	1001	FMN	C2'-C3'-C4'-C5'
3	A	1001	FMN	O3'-C3'-C4'-C5'
3	C	1001	FMN	C2'-C3'-C4'-O4'
3	C	1001	FMN	C2'-C3'-C4'-C5'
3	A	1001	FMN	O3'-C3'-C4'-O4'
5	D	101	66S	O33-C32-C34-O35
3	A	1001	FMN	C4'-C5'-O5'-P
3	C	1001	FMN	C4'-C5'-O5'-P
5	B	101	66S	S1-C1-C2-C3
5	B	101	66S	O1-C1-C2-C3
5	D	101	66S	S1-C1-C2-C3
5	D	101	66S	O1-C1-C2-C3
5	B	101	66S	N36-C37-C38-C39
5	B	101	66S	O27-C28-C29-C30
5	B	101	66S	C42-C43-S1-C1
5	B	101	66S	O1-C1-S1-C43
3	C	1001	FMN	O3'-C3'-C4'-C5'
5	B	101	66S	O33-C32-C34-O35
3	C	1001	FMN	O3'-C3'-C4'-O4'

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1002	SF4	1	0

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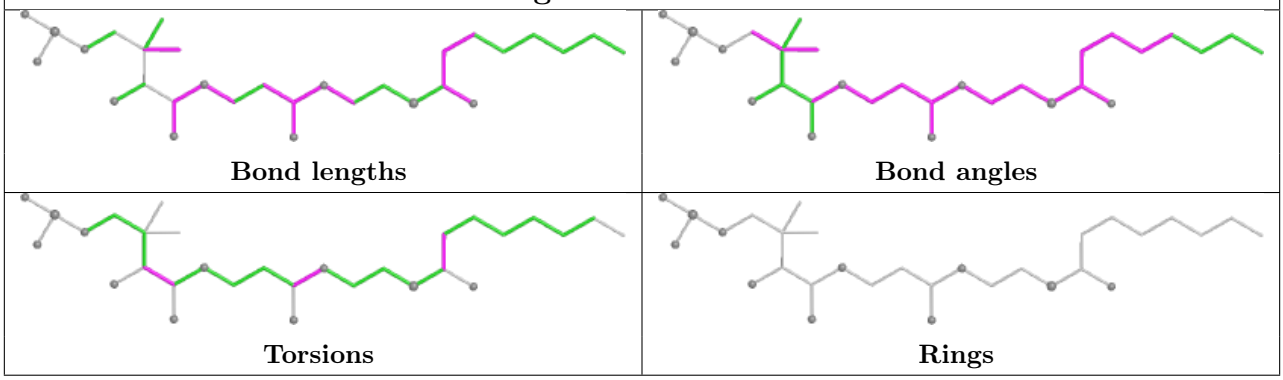
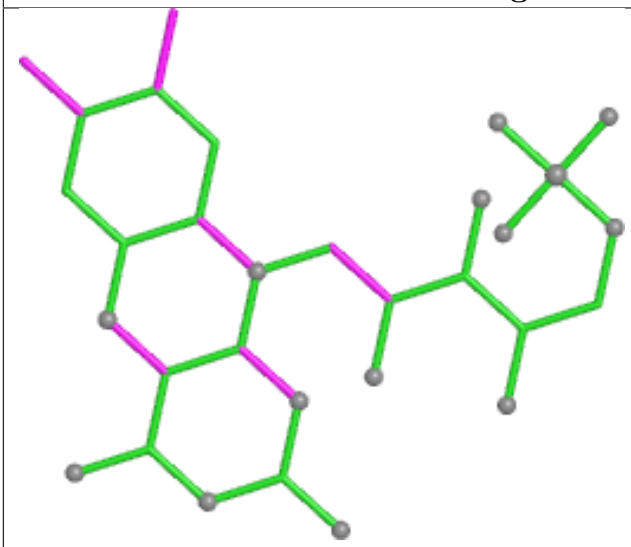
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	FMN	2	0
3	A	1001	FMN	3	0

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.

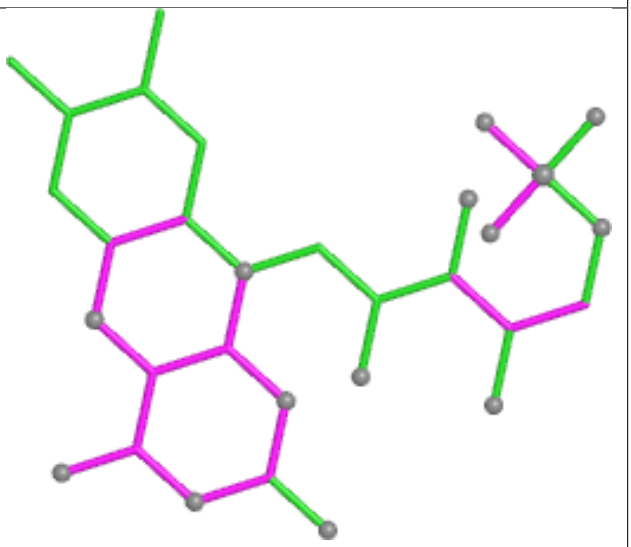
Ligand 66S D 101



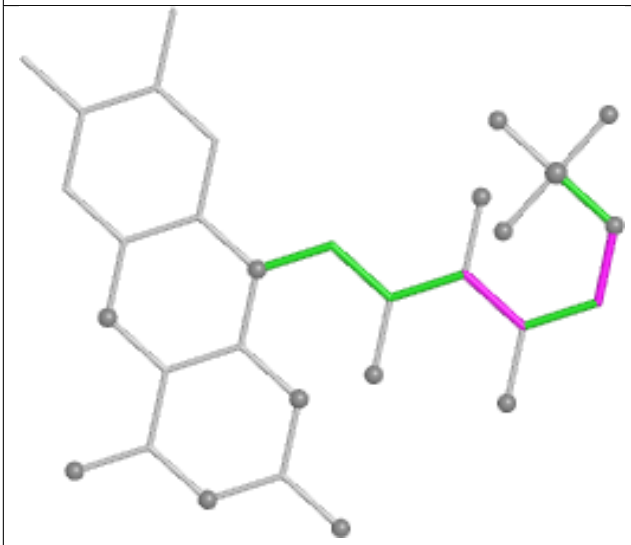
Ligand FMN C 1001



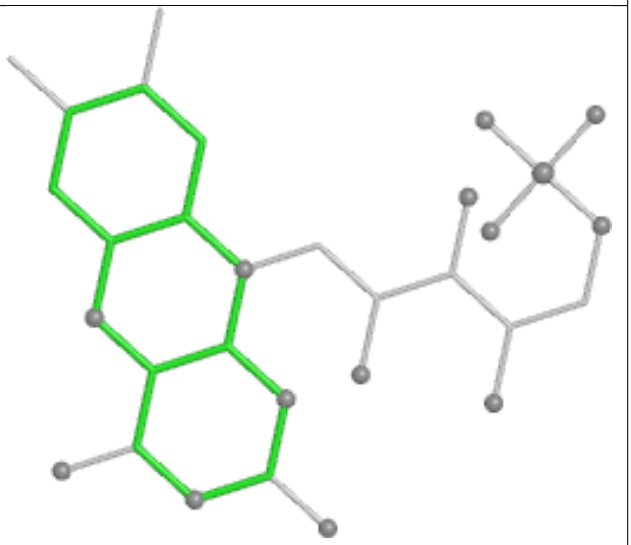
Bond lengths



Bond angles

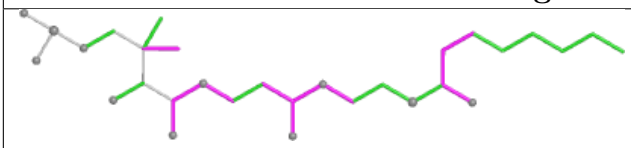


Torsions

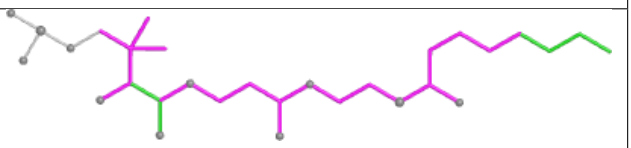


Rings

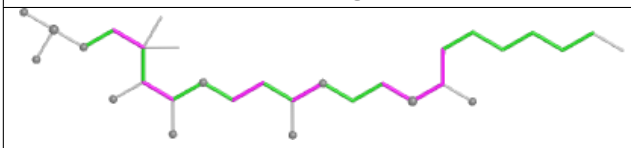
Ligand 66S B 101



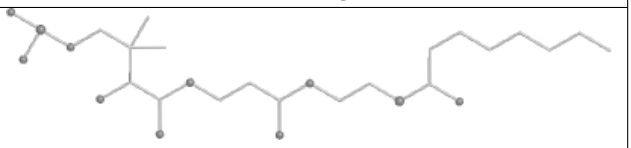
Bond lengths



Bond angles

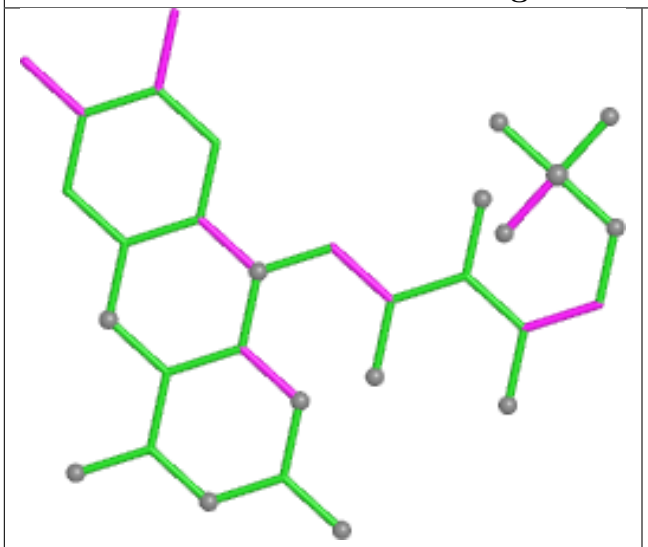


Torsions

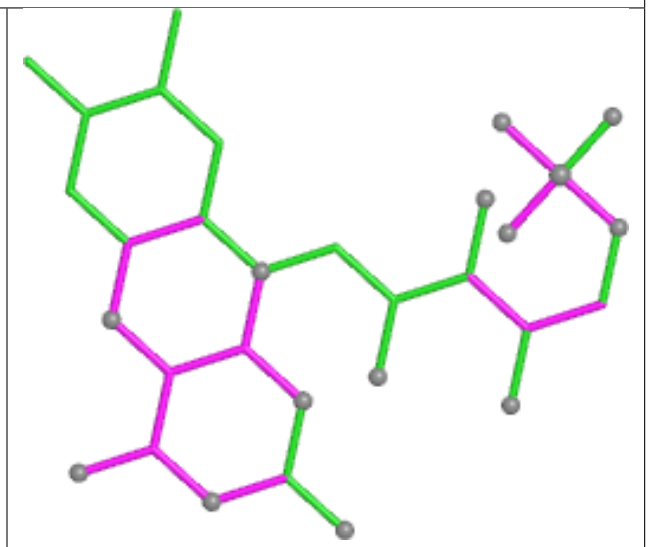


Rings

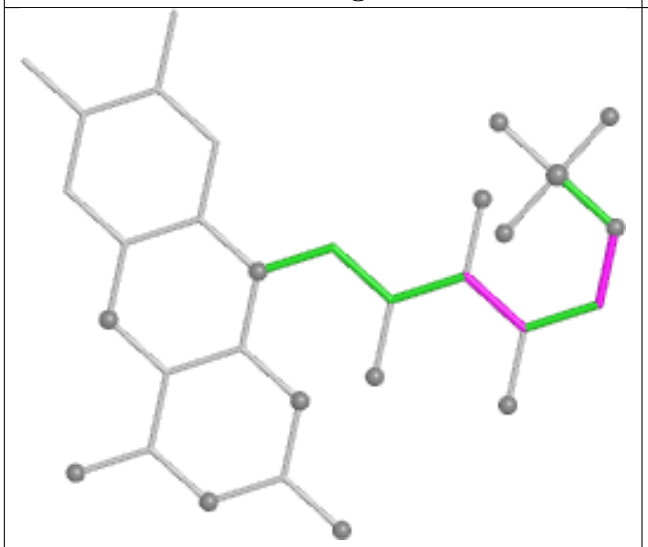
Ligand FMN A 1001



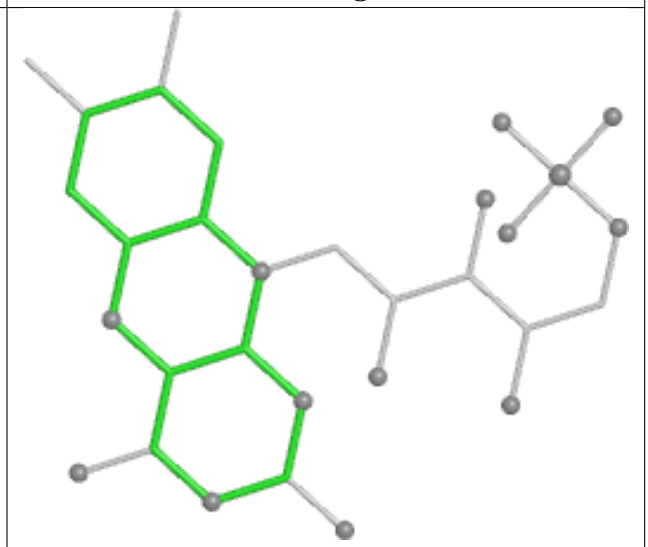
Bond lengths



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	366/372 (98%)	1.04	34 (9%)	14	16	30, 42, 65, 85	1 (0%)
1	C	366/372 (98%)	0.86	16 (4%)	39	41	24, 37, 52, 66	1 (0%)
2	B	72/86 (83%)	1.80	27 (37%)	1	0	44, 61, 81, 82	0
2	D	22/86 (25%)	2.53	15 (68%)	0	0	58, 68, 88, 95	0
All	All	826/916 (90%)	1.07	92 (11%)	10	11	24, 41, 71, 95	2 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	TYR	6.3
2	D	52	ILE	5.0
2	D	50	PHE	4.8
2	D	46	LEU	4.7
2	B	7	ILE	4.1
2	B	72	ILE	3.9
2	B	63	VAL	3.9
2	B	62	ILE	3.9
2	B	50	PHE	3.8
2	B	2	ALA	3.7
1	C	56	ASN	3.6
1	C	64	VAL	3.6
2	B	54	ILE	3.6
1	A	186	LYS	3.4
1	A	-2	HIS	3.4
2	D	48	GLU	3.2
1	A	63	ILE	3.1
2	B	65	VAL	3.1
2	B	70	LYS	3.1
2	D	54	ILE	3.1
2	B	52	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	279	ALA	3.1
1	A	34	ALA	2.9
1	C	334	GLU	2.9
2	B	51	GLY	2.9
1	A	112	ARG	2.9
2	B	3	LEU	2.9
2	B	1	MET	2.9
2	D	53	GLU	2.9
1	C	85	ALA	2.9
2	B	71	TYR	2.8
2	B	46	LEU	2.8
1	A	93	ASN	2.8
2	D	49	LYS	2.8
1	C	138	ASP	2.7
1	A	64	VAL	2.7
1	A	353	VAL	2.7
2	D	40	VAL	2.7
1	C	27	GLY	2.7
1	A	188	GLU	2.7
2	D	55	PRO	2.7
1	C	112	ARG	2.7
1	A	79	ALA	2.7
2	B	66	GLY	2.7
1	A	138	ASP	2.6
1	A	62	ARG	2.6
2	B	59	ALA	2.6
2	B	42	LEU	2.5
2	D	51	GLY	2.5
1	A	59	PHE	2.5
1	A	0	HIS	2.5
1	A	168	ILE	2.5
1	A	259	LEU	2.5
1	A	290	ILE	2.4
1	A	60	VAL	2.4
1	A	83	ILE	2.3
2	D	43	ILE	2.3
2	D	45	ALA	2.3
2	B	48	GLU	2.3
1	A	27	GLY	2.3
1	A	41	GLY	2.3
1	A	67	LYS	2.3
2	D	42	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	47	GLU	2.3
1	A	69	PHE	2.2
1	A	72	LEU	2.2
1	A	1	MET	2.2
2	B	69	VAL	2.2
2	B	67	ASP	2.2
1	A	180	GLY	2.2
1	C	44	GLY	2.2
2	B	68	VAL	2.2
1	C	180	GLY	2.2
1	C	103	ALA	2.2
1	A	33	LEU	2.1
1	C	28	ILE	2.1
1	C	294	ASN	2.1
1	C	136	ALA	2.1
1	A	56	ASN	2.1
2	B	25	GLU	2.1
1	C	26	VAL	2.1
2	B	4	PHE	2.1
1	A	189	ASP	2.1
2	B	6	ASP	2.1
2	B	58	GLN	2.1
1	A	38	ALA	2.0
1	A	65	ALA	2.0
2	D	56	ASP	2.0
2	B	57	GLU	2.0
1	A	85	ALA	2.0
1	C	330	LEU	2.0
1	C	83	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 oligosaccharides in this entry.

6.4 Ligands (i)

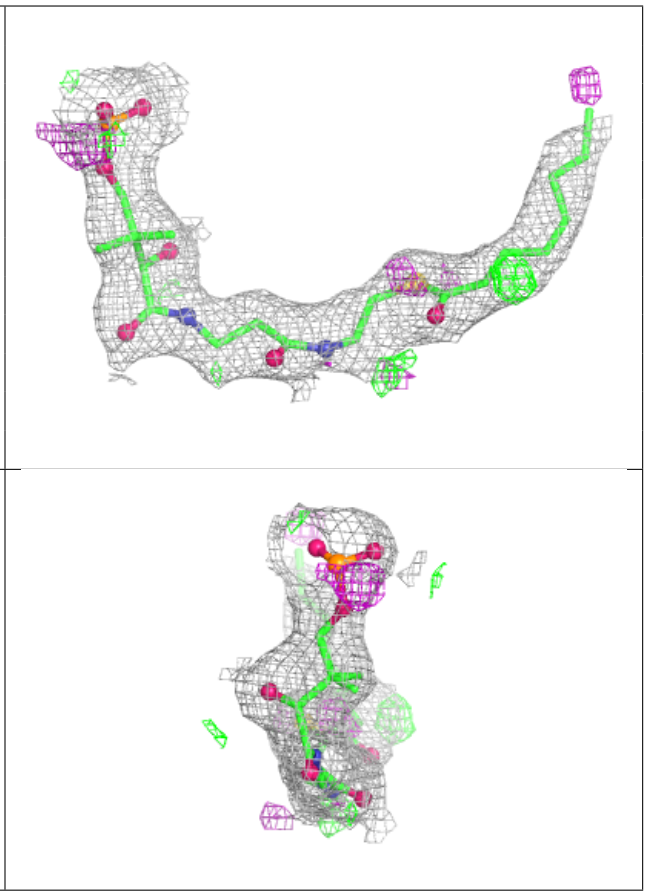
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	66S	D	101	30/31	0.85	0.13	30,40,53,56	0
5	66S	B	101	30/31	0.87	0.12	34,40,53,56	0
3	FMN	C	1001	31/31	0.90	0.10	8,10,12,14	0
3	FMN	A	1001	31/31	0.92	0.10	28,33,37,39	0
4	SF4	A	1002	8/8	0.95	0.08	39,42,47,48	0
4	SF4	C	1002	8/8	0.96	0.06	30,35,38,39	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.

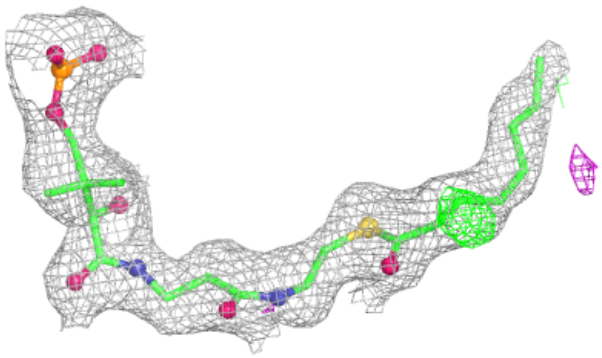
Electron density around 66S D 101:

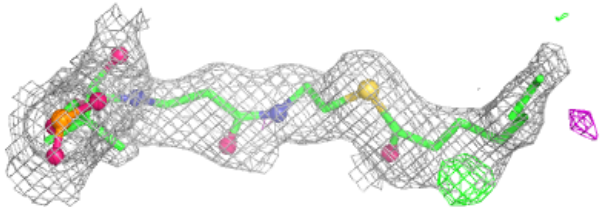
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

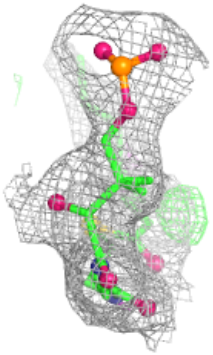


Electron density around 66S B 101:

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

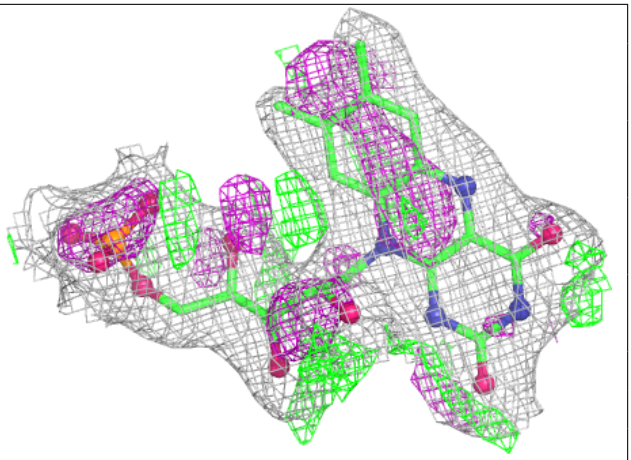


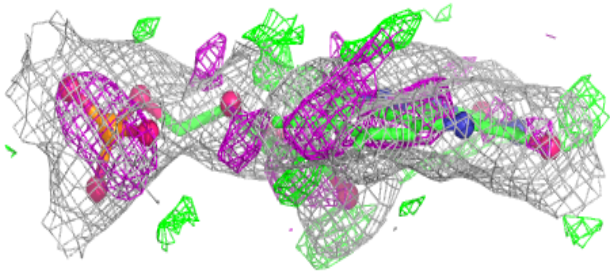


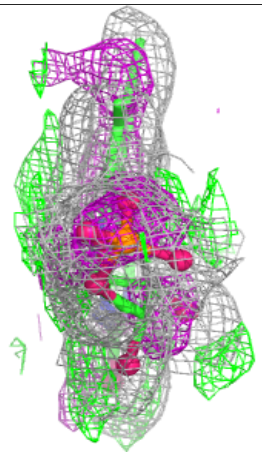


Electron density around FMN C 1001:

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

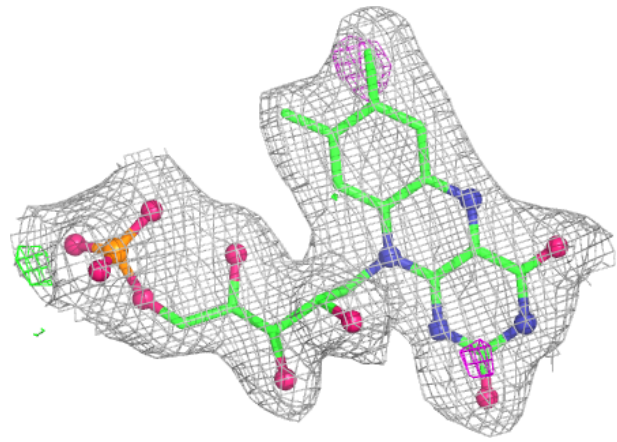


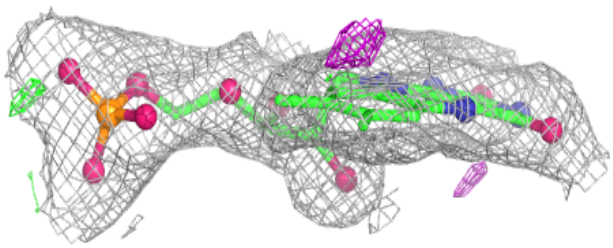


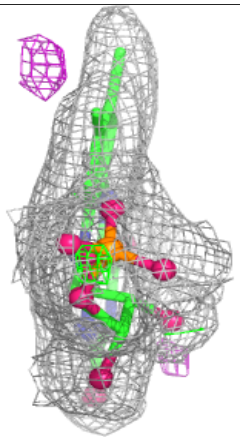


Electron density around FMN A 1001:

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







6.5 Other polymers (i)

There are no such residues in this entry.