Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 05:36 pm GMT

PDB ID	:	2J6X
Title	:	The crystal structure of lactate oxidase
Authors	:	Leiros, I.; Wang, E.; Rasmussen, T.; Oksanen, E.; Repo, H.; Petersen, S.B.; Heikinheimo, P.; Hough, E.
Deposited on	:	2006-10-05
Resolution	:	2.10 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:

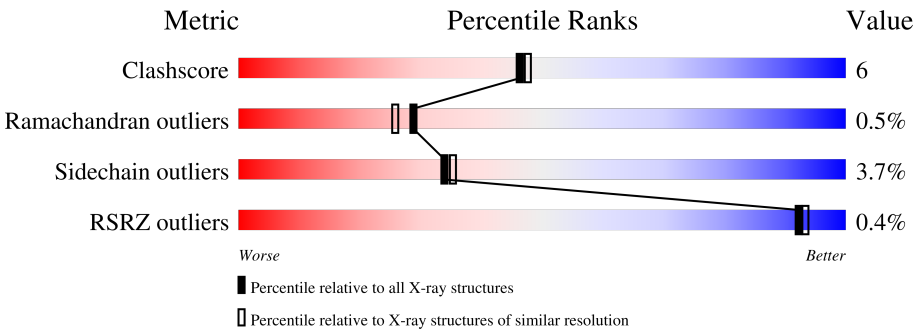
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	374	86% 11% ••
1	B	374	87% 10% ••
1	C	374	84% 13% ••
1	D	374	% 76% 17% • 6%
1	E	374	% 82% 15% ••
1	F	374	% 78% 15% • 5%

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Mol	Chain	Length	Quality of chain
1	G	374	84% 11%
1	H	374	% 83% 9% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23895 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 LACTATE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2852	1802	493	550	7	0	0	0
1	B	367	2827	1787	490	543	7	0	0	0
1	C	368	2836	1792	491	546	7	0	0	0
1	D	353	2717	1721	468	522	6	0	0	0
1	E	367	2827	1787	490	543	7	0	0	0
1	F	357	2748	1739	474	529	6	0	0	0
1	G	367	2827	1787	490	543	7	0	0	0
1	H	348	2682	1697	462	517	6	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	ALA	GLY	conflict	UNP Q44467
A	255	ALA	ARG	conflict	UNP Q44467
B	232	ALA	GLY	conflict	UNP Q44467
B	255	ALA	ARG	conflict	UNP Q44467
C	232	ALA	GLY	conflict	UNP Q44467
C	255	ALA	ARG	conflict	UNP Q44467
D	232	ALA	GLY	conflict	UNP Q44467
D	255	ALA	ARG	conflict	UNP Q44467
E	232	ALA	GLY	conflict	UNP Q44467
E	255	ALA	ARG	conflict	UNP Q44467
F	232	ALA	GLY	conflict	UNP Q44467
F	255	ALA	ARG	conflict	UNP Q44467
G	232	ALA	GLY	conflict	UNP Q44467

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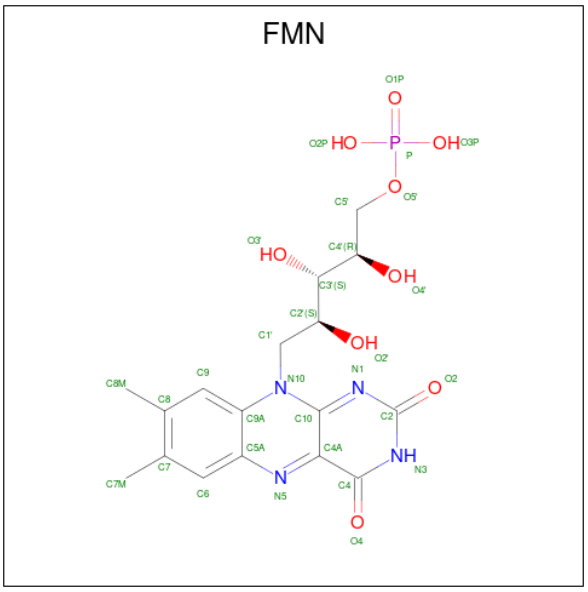
Chain	Residue	Modelled	Actual	Comment	Reference
G	255	ALA	ARG	conflict	UNP Q44467
H	232	ALA	GLY	conflict	UNP Q44467
H	255	ALA	ARG	conflict	UNP Q44467

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



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	D	1	1	1	0	0

- Molecule 4 is water.

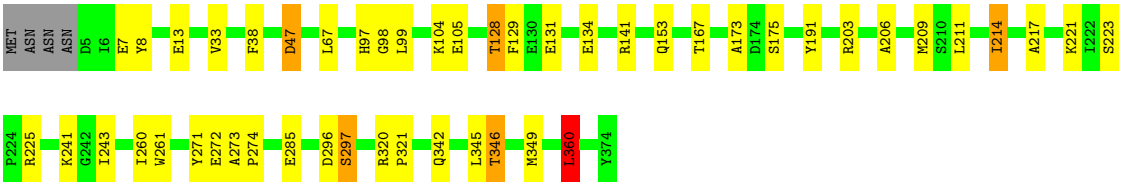
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	199	199	199	0	0
			Total	O		
4	B	185	185	185	0	0
			Total	O		
4	C	203	203	203	0	0
			Total	O		
4	D	145	145	145	0	0
			Total	O		
4	E	132	132	132	0	0
			Total	O		
4	F	148	148	148	0	0
			Total	O		
4	G	158	158	158	0	0
			Total	O		
4	H	160	160	160	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.

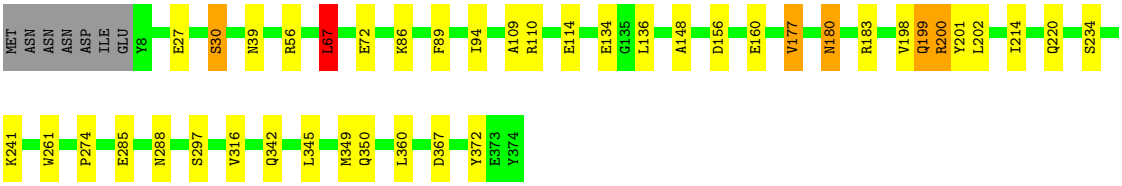
• Molecule 1: LACTATE OXIDASE

Chain A:



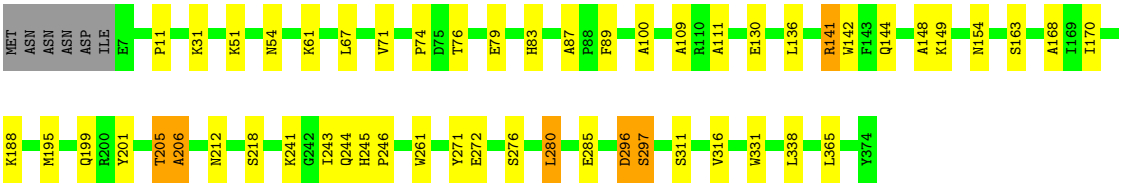
• Molecule 1: LACTATE OXIDASE

Chain B:



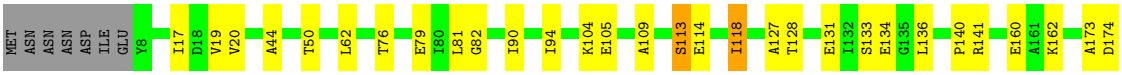
• Molecule 1: LACTATE OXIDASE

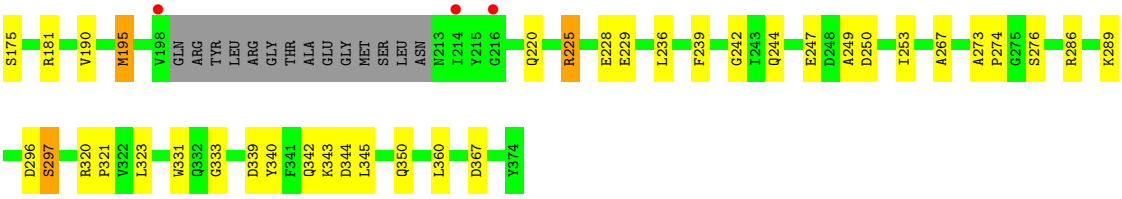
Chain C:



• Molecule 1: LACTATE OXIDASE

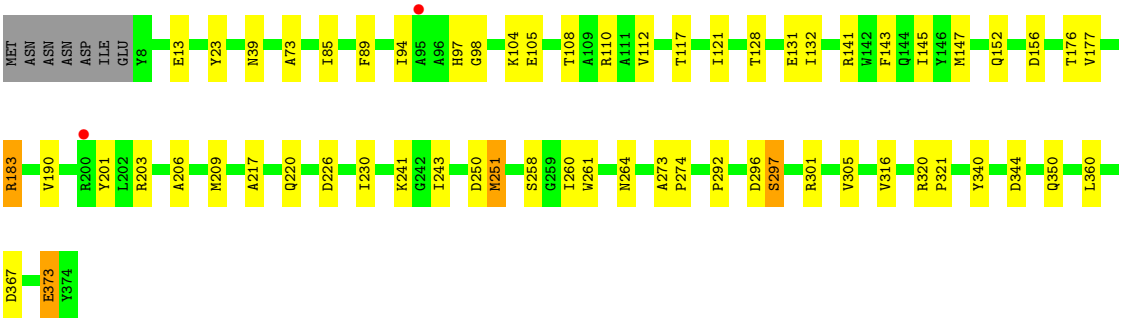
Chain D:





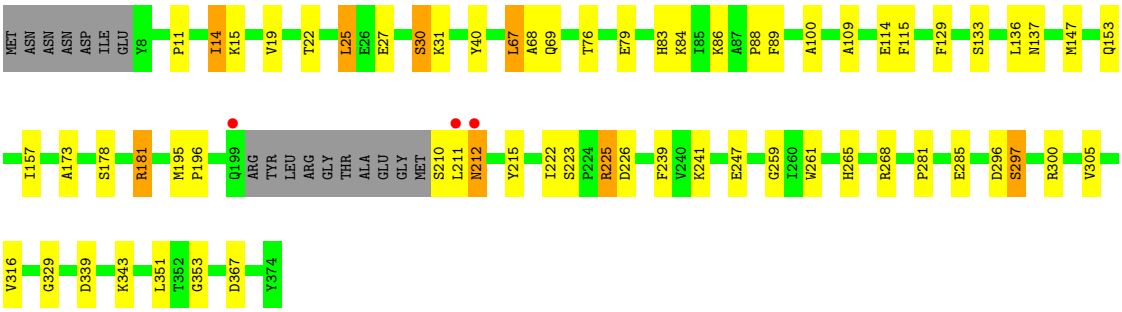
• Molecule 1: LACTATE OXIDASE

Chain E:



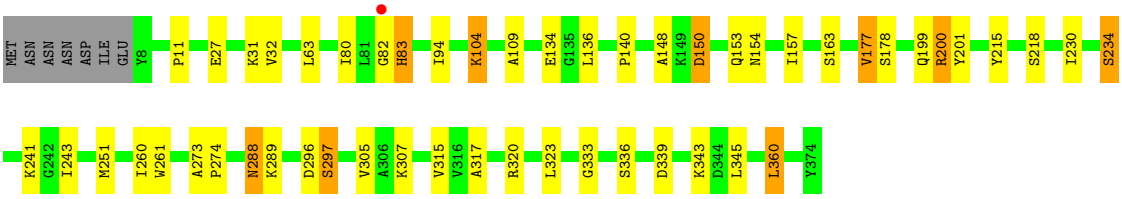
• Molecule 1: LACTATE OXIDASE

Chain F:



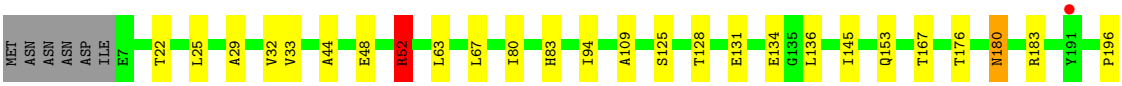
• Molecule 1: LACTATE OXIDASE

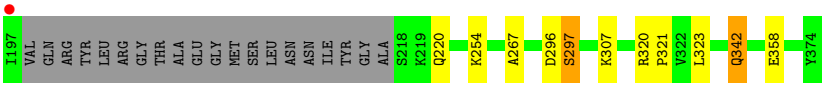
Chain G:



• Molecule 1: LACTATE OXIDASE

Chain H:


MET
ASN
ASN
ASN
ASP
ILE
E7
T22
L25
A29
V32
V33
A44
E48
R52
L63
L67
I80
H83
I94
A109
S125
T128
E131
E134
G135
L136
I145
Q153
T167
T176
N180
R183
Y191
P196


I197
VAL
GLN
ARG
TYR
LEU
ARG
GLY
THR
ALA
GLU
GLY
MET
SER
LEU
ASN
ASN
ILE
TYR
GLY
ALA
S218
K219
Q220
K254
A267
D296
S297
K307
R320
P321
V322
L323
Q342
E358
Y374

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.34Å 134.74Å 185.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.10 46.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.00-2.10) 100.0 (46.54-2.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.257 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	12.8	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23895	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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 30.27 % 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 1.3449e-03. 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: ZN, 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	0.57	0/2916	0.65	1/3952 (0.0%)
1	B	0.52	0/2891	0.67	3/3918 (0.1%)
1	C	0.57	0/2900	0.65	0/3930
1	D	0.52	0/2779	0.63	0/3767
1	E	0.50	0/2891	0.61	0/3918
1	F	0.53	0/2810	0.63	1/3809 (0.0%)
1	G	0.52	0/2891	0.65	2/3918 (0.1%)
1	H	0.55	0/2743	0.65	1/3717 (0.0%)
All	All	0.54	0/22821	0.64	8/30929 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	320	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	G	320	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	199	GLN	C-N-CA	5.72	136.00	121.70
1	F	25	LEU	CA-CB-CG	5.65	128.31	115.30
1	B	199	GLN	N-CA-C	5.52	125.89	111.00
1	H	52	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	67	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	360	LEU	CA-CB-CG	5.01	126.83	115.30

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	2852	0	2779	42	0
1	B	2827	0	2758	29	0
1	C	2836	0	2764	34	0
1	D	2717	0	2648	46	0
1	E	2827	0	2758	42	0
1	F	2748	0	2678	37	0
1	G	2827	0	2758	38	0
1	H	2682	0	2611	23	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	1	0
2	F	31	0	19	0	0
2	G	31	0	19	1	0
2	H	31	0	19	0	0
3	D	1	0	0	0	0
4	A	199	0	0	6	0
4	B	185	0	0	5	0
4	C	203	0	0	8	0
4	D	145	0	0	9	0
4	E	132	0	0	7	0
4	F	148	0	0	6	0
4	G	158	0	0	6	0
4	H	160	0	0	7	0
All	All	23895	0	21906	278	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 6.

All (278) 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:F:40:TYR:O	1:F:268:ARG:NH2	1.82	1.10
1:C:141:ARG:HG2	1:C:141:ARG:HH11	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:GLY:HA3	1:G:83:HIS:HB2	1.51	0.93
1:C:71:VAL:HG13	4:C:2190:HOH:O	1.71	0.90
1:B:180:ASN:HD22	1:B:180:ASN:H	1.19	0.90
1:C:71:VAL:CG1	4:C:2190:HOH:O	2.20	0.89
1:H:180:ASN:H	1:H:180:ASN:HD22	1.20	0.85
1:G:82:GLY:HA3	1:G:83:HIS:CB	2.07	0.85
1:D:289:LYS:HD3	4:D:2102:HOH:O	1.75	0.84
1:E:39:ASN:HD22	1:E:183:ARG:HH11	1.25	0.84
1:A:129:PHE:O	1:A:129:PHE:CD2	2.31	0.84
1:A:209:MET:HE3	1:A:217:ALA:CB	2.10	0.82
1:H:94:ILE:HG21	1:H:323:LEU:HD21	1.62	0.81
1:G:148:ALA:H	1:G:154:ASN:HD21	1.25	0.81
1:D:50:THR:HG21	4:D:2093:HOH:O	1.81	0.81
1:H:128:THR:HG21	4:H:2072:HOH:O	1.81	0.81
1:D:273:ALA:HB3	4:D:2093:HOH:O	1.80	0.80
1:F:86:LYS:HD2	1:F:115:PHE:O	1.82	0.80
1:F:265:HIS:O	1:F:268:ARG:HG3	1.82	0.80
1:C:141:ARG:HG2	1:C:141:ARG:NH1	2.00	0.77
1:G:178:SER:HB3	1:G:215:TYR:HD1	1.51	0.76
1:A:209:MET:HE3	1:A:217:ALA:HB1	1.66	0.76
1:D:19:VAL:CG2	1:D:340:TYR:HB2	2.16	0.75
1:D:195:MET:CE	4:D:2070:HOH:O	2.34	0.75
1:G:82:GLY:CA	1:G:83:HIS:HB2	2.16	0.75
1:A:209:MET:CE	1:A:217:ALA:HB3	2.17	0.74
1:C:74:PRO:HG3	4:C:2190:HOH:O	1.88	0.73
1:D:19:VAL:HG21	1:D:340:TYR:HB2	1.71	0.72
1:B:39:ASN:HD22	1:B:183:ARG:HH11	1.37	0.71
1:D:104:LYS:HE2	4:D:2046:HOH:O	1.90	0.70
1:E:301:ARG:NH2	4:E:2106:HOH:O	2.24	0.69
1:B:27:GLU:O	1:B:30:SER:HB2	1.93	0.69
1:B:288:ASN:ND2	1:G:289:LYS:HD3	2.08	0.68
1:C:285:GLU:HG3	4:C:2160:HOH:O	1.93	0.68
1:D:118:ILE:HG22	1:D:140:PRO:HB2	1.76	0.68
1:B:156:ASP:O	1:B:160:GLU:HG3	1.94	0.68
1:G:178:SER:HB2	4:G:2079:HOH:O	1.93	0.68
1:D:128:THR:HB	4:D:2054:HOH:O	1.95	0.67
1:A:209:MET:CE	1:A:217:ALA:CB	2.73	0.67
1:B:200:ARG:HB2	4:B:2101:HOH:O	1.95	0.67
1:A:285:GLU:HG2	4:A:2153:HOH:O	1.96	0.65
1:E:121:ILE:HD12	1:E:132:ILE:HG21	1.79	0.65
1:F:247:GLU:HG3	4:F:2096:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:SER:CB	4:G:2079:HOH:O	2.46	0.64
1:F:27:GLU:O	1:F:30:SER:HB2	1.96	0.64
1:E:243:ILE:HD13	1:F:67:LEU:HD11	1.80	0.63
1:A:67:LEU:HD12	1:C:243:ILE:HD13	1.80	0.63
1:F:31:LYS:HE2	4:F:2008:HOH:O	1.97	0.63
1:F:211:LEU:O	1:F:212:ASN:HB2	1.98	0.63
1:H:83:HIS:CD2	4:H:2049:HOH:O	2.51	0.63
1:H:48:GLU:OE2	1:H:183:ARG:HD2	1.98	0.63
1:D:195:MET:HE3	4:D:2070:HOH:O	1.94	0.63
1:H:254:LYS:HD3	4:H:2111:HOH:O	1.99	0.63
1:E:243:ILE:HG13	1:E:260:ILE:HG23	1.82	0.62
1:A:241:LYS:NZ	4:A:2134:HOH:O	2.25	0.62
1:A:342:GLN:O	1:A:346:THR:HG23	1.99	0.62
1:E:350:GLN:NE2	4:E:2117:HOH:O	2.33	0.62
1:A:209:MET:HE2	1:A:217:ALA:HB3	1.81	0.62
1:A:173:ALA:HB3	1:B:67:LEU:HD13	1.82	0.61
4:B:2138:HOH:O	1:G:288:ASN:HB3	1.99	0.61
1:G:82:GLY:HA3	1:G:83:HIS:CG	2.35	0.61
1:D:195:MET:HE1	4:D:2070:HOH:O	1.96	0.61
1:D:128:THR:HG23	1:D:131:GLU:H	1.64	0.61
1:E:39:ASN:ND2	1:E:183:ARG:HH11	1.99	0.60
1:H:44:ALA:HB1	1:H:267:ALA:O	2.01	0.60
1:F:79:GLU:HB3	1:F:84:LYS:HD2	1.84	0.59
1:B:285:GLU:HB3	4:B:2133:HOH:O	2.03	0.59
1:G:148:ALA:HB2	1:G:201:TYR:CD2	2.38	0.59
1:G:218:SER:HB2	4:G:2096:HOH:O	2.03	0.58
1:D:345:LEU:HD11	1:D:360:LEU:HD11	1.85	0.58
1:A:47:ASP:HB2	1:A:271:TYR:OH	2.02	0.58
1:B:180:ASN:H	1:B:180:ASN:ND2	1.95	0.58
1:D:94:ILE:HG21	1:D:323:LEU:HD11	1.84	0.57
1:G:63:LEU:HG	1:G:307:LYS:HE2	1.86	0.57
1:F:210:SER:N	4:F:2079:HOH:O	2.37	0.57
1:G:273:ALA:HB1	1:G:274:PRO:HD2	1.87	0.57
1:H:109:ALA:HB1	1:H:136:LEU:HG	1.85	0.57
1:H:358:GLU:HG2	4:H:2148:HOH:O	2.04	0.57
1:H:128:THR:HG23	1:H:131:GLU:H	1.70	0.56
1:A:128:THR:HG22	1:A:131:GLU:H	1.69	0.56
1:A:345:LEU:O	1:A:349:MET:HG3	2.06	0.56
1:F:223:SER:OG	1:F:225:ARG:HG3	2.05	0.56
1:G:83:HIS:CE1	1:G:140:PRO:HB3	2.40	0.56
1:F:76:THR:O	1:F:88:PRO:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PRO:HG2	1:C:100:ALA:O	2.05	0.55
1:E:350:GLN:HG2	1:G:177:VAL:HB	1.87	0.55
1:C:195:MET:O	1:C:199:GLN:HG3	2.06	0.55
1:D:296:ASP:O	1:D:297:SER:HB2	2.07	0.55
1:G:109:ALA:HB1	1:G:136:LEU:HG	1.88	0.55
1:G:11:PRO:HB3	1:G:32:VAL:HG22	1.89	0.54
1:C:148:ALA:H	1:C:154:ASN:HD21	1.54	0.54
1:F:69:GLN:HG3	1:F:353:GLY:HA3	1.90	0.54
1:G:241:LYS:HA	1:G:261:TRP:HB3	1.89	0.54
1:H:63:LEU:HG	1:H:307:LYS:HE2	1.89	0.54
1:A:167:THR:HG22	4:A:2065:HOH:O	2.06	0.54
1:B:177:VAL:HB	1:D:350:GLN:HG2	1.89	0.54
1:G:345:LEU:HD11	1:G:360:LEU:HD21	1.91	0.53
1:H:296:ASP:O	1:H:297:SER:HB2	2.07	0.53
1:D:109:ALA:HB1	1:D:136:LEU:HG	1.91	0.53
1:E:94:ILE:HG23	2:E:1375:FMN:C6	2.39	0.53
1:C:241:LYS:HA	1:C:261:TRP:HB3	1.91	0.53
1:G:243:ILE:HD12	1:G:260:ILE:HG23	1.90	0.52
1:H:29:ALA:O	1:H:33:VAL:HG23	2.09	0.52
1:E:156:ASP:HB3	1:E:201:TYR:CD2	2.45	0.52
1:D:17:ILE:HG12	1:D:333:GLY:HA2	1.92	0.52
1:D:19:VAL:HG21	1:D:340:TYR:CB	2.39	0.52
1:G:199:GLN:HG2	4:G:2089:HOH:O	2.10	0.52
1:A:273:ALA:HB1	1:A:274:PRO:HD2	1.90	0.52
1:G:296:ASP:HB3	1:G:317:ALA:HB3	1.92	0.52
1:A:296:ASP:O	1:A:297:SER:HB2	2.09	0.52
1:B:349:MET:HG2	1:B:360:LEU:HD21	1.91	0.52
1:D:19:VAL:HG23	1:D:340:TYR:CD1	2.45	0.52
1:G:80:ILE:O	1:G:83:HIS:HB2	2.10	0.52
1:F:14:ILE:HD11	4:F:2127:HOH:O	2.08	0.52
1:H:22:THR:O	1:H:25:LEU:HB2	2.10	0.52
1:F:296:ASP:O	1:F:297:SER:HB2	2.10	0.51
1:D:104:LYS:HG3	1:D:105:GLU:H	1.74	0.51
1:F:281:PRO:O	1:F:285:GLU:HG2	2.11	0.51
1:A:67:LEU:HD12	1:C:243:ILE:CD1	2.41	0.51
1:E:73:ALA:HA	4:E:2033:HOH:O	2.10	0.51
1:E:89:PHE:HA	1:E:316:VAL:O	2.10	0.51
1:E:128:THR:HG23	1:E:131:GLU:H	1.76	0.51
1:E:373:GLU:HB2	4:E:2130:HOH:O	2.11	0.51
1:G:230:ILE:O	1:G:234:SER:HB2	2.11	0.51
1:C:244:GLN:HE22	1:C:276:SER:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ALA:HB2	1:B:201:TYR:CD2	2.46	0.50
1:B:56:ARG:HG2	1:B:372:TYR:CD1	2.45	0.50
1:B:198:VAL:C	1:B:200:ARG:HB3	2.31	0.50
1:B:39:ASN:ND2	1:B:183:ARG:HH11	2.08	0.50
1:E:85:ILE:HG22	1:E:117:THR:HA	1.94	0.49
1:A:153:GLN:HE22	1:A:206:ALA:HB3	1.76	0.49
1:A:209:MET:HE3	1:A:217:ALA:HB3	1.80	0.49
1:C:31:LYS:HE3	4:C:2019:HOH:O	2.11	0.49
1:D:113:SER:OG	1:D:136:LEU:O	2.23	0.49
1:G:150:ASP:OD2	1:G:153:GLN:NE2	2.32	0.49
1:C:67:LEU:HD13	1:D:173:ALA:HB3	1.95	0.49
1:E:190:VAL:HG22	4:E:2036:HOH:O	2.11	0.49
1:D:296:ASP:OD1	1:D:296:ASP:C	2.51	0.49
1:G:157:ILE:HD11	1:G:200:ARG:HD3	1.95	0.49
1:A:243:ILE:HD12	1:A:260:ILE:HG23	1.96	0.48
1:D:249:ALA:O	1:D:253:ILE:HG12	2.13	0.48
1:G:150:ASP:HB2	4:G:2066:HOH:O	2.12	0.48
1:A:97:HIS:CD2	1:A:105:GLU:HG3	2.48	0.48
1:B:241:LYS:HA	1:B:261:TRP:HB3	1.95	0.48
1:F:225:ARG:NH1	4:F:2088:HOH:O	2.47	0.48
1:A:13:GLU:HB2	4:A:2171:HOH:O	2.12	0.48
1:A:129:PHE:O	1:A:129:PHE:CG	2.66	0.48
1:F:22:THR:HG22	1:F:300:ARG:HD2	1.96	0.48
1:A:241:LYS:HA	1:A:261:TRP:HB3	1.95	0.48
1:C:205:THR:HG21	4:C:2122:HOH:O	2.13	0.48
1:G:178:SER:HB3	1:G:215:TYR:CD1	2.39	0.48
1:B:199:GLN:O	1:B:202:LEU:HB2	2.14	0.48
1:E:206:ALA:O	1:E:209:MET:HB2	2.14	0.47
1:F:11:PRO:HD2	1:F:100:ALA:O	2.13	0.47
1:G:296:ASP:O	1:G:297:SER:HB2	2.14	0.47
1:E:147:MET:CE	1:E:230:ILE:HD11	2.44	0.47
1:D:339:ASP:OD2	1:D:343:LYS:HE2	2.14	0.47
1:F:129:PHE:O	1:F:133:SER:HB2	2.14	0.47
1:C:280:LEU:HD13	1:C:311:SER:HB2	1.95	0.47
1:E:97:HIS:CD2	1:E:105:GLU:HG3	2.50	0.47
1:F:241:LYS:NZ	4:F:2093:HOH:O	2.43	0.47
1:F:241:LYS:HA	1:F:261:TRP:HB3	1.97	0.47
1:D:104:LYS:HD2	1:D:127:ALA:HB2	1.96	0.47
1:A:285:GLU:HG3	4:A:2150:HOH:O	2.15	0.47
1:E:108:THR:O	1:E:112:VAL:HG23	2.15	0.47
1:D:225:ARG:HA	1:D:228:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:MET:HE3	1:E:217:ALA:HB1	1.97	0.46
1:A:345:LEU:HD11	1:A:360:LEU:HD21	1.95	0.46
1:D:76:THR:OG1	1:D:342:GLN:NE2	2.46	0.46
1:F:173:ALA:HB3	1:H:67:LEU:HD13	1.96	0.46
1:D:273:ALA:HB1	1:D:274:PRO:HD2	1.96	0.46
1:D:90:ILE:HG22	1:D:118:ILE:HG12	1.97	0.46
1:E:147:MET:CE	1:E:226:ASP:HB3	2.46	0.46
1:D:128:THR:HG22	1:D:131:GLU:OE1	2.15	0.46
1:D:225:ARG:NH2	1:D:229:GLU:OE2	2.48	0.46
1:E:340:TYR:O	1:E:344:ASP:HB2	2.16	0.46
1:C:205:THR:O	1:C:206:ALA:CB	2.64	0.45
1:C:296:ASP:O	1:C:297:SER:HB2	2.16	0.45
1:D:114:GLU:OE1	1:D:331:TRP:CZ3	2.69	0.45
1:H:180:ASN:H	1:H:180:ASN:ND2	1.99	0.45
1:A:221:LYS:HB2	1:B:72:GLU:HB2	1.97	0.45
1:E:176:THR:O	1:E:220:GLN:HG3	2.17	0.45
1:C:89:PHE:HA	1:C:316:VAL:O	2.17	0.45
1:D:79:GLU:OE2	1:D:82:GLY:HA2	2.17	0.45
1:D:174:ASP:HB3	1:D:242:GLY:HA3	1.99	0.45
1:B:350:GLN:NE2	4:B:2161:HOH:O	2.49	0.45
1:E:320:ARG:N	1:E:321:PRO:HD2	2.32	0.45
1:A:129:PHE:O	1:A:129:PHE:HD2	1.97	0.45
1:G:333:GLY:O	1:G:336:SER:HB2	2.16	0.44
1:G:27:GLU:OE2	1:G:31:LYS:HE2	2.17	0.44
1:A:342:GLN:O	1:A:346:THR:CG2	2.66	0.44
1:B:202:LEU:HD21	1:B:214:ILE:HG23	2.00	0.44
1:G:94:ILE:HG23	2:G:1375:FMN:C6	2.47	0.44
1:B:345:LEU:O	1:B:349:MET:HG3	2.17	0.44
1:F:241:LYS:HD2	1:F:261:TRP:CE2	2.53	0.44
1:G:148:ALA:N	1:G:154:ASN:HD21	2.02	0.44
1:H:125:SER:O	1:H:196:PRO:HD2	2.18	0.44
1:A:8:TYR:CE2	1:A:99:LEU:HA	2.53	0.44
1:B:274:PRO:HA	1:D:62:LEU:HD13	2.00	0.44
1:F:222:ILE:HA	1:F:226:ASP:OD2	2.18	0.44
1:D:44:ALA:HB1	1:D:267:ALA:O	2.18	0.43
1:E:209:MET:HE3	1:E:217:ALA:CB	2.48	0.43
1:F:153:GLN:O	1:F:157:ILE:HG13	2.18	0.43
1:G:339:ASP:OD2	1:G:343:LYS:HE2	2.17	0.43
1:F:79:GLU:HA	1:F:83:HIS:O	2.18	0.43
1:H:296:ASP:OD1	1:H:296:ASP:C	2.56	0.43
1:B:110:ARG:O	1:B:114:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:LYS:HD3	4:G:2058:HOH:O	2.18	0.43
1:H:52:ARG:CD	4:H:2028:HOH:O	2.65	0.43
1:C:271:TYR:CE2	1:C:272:GLU:HG3	2.53	0.43
1:E:296:ASP:O	1:E:297:SER:HB2	2.17	0.43
1:D:104:LYS:HG3	1:D:105:GLU:N	2.34	0.43
1:D:320:ARG:N	1:D:321:PRO:HD2	2.34	0.43
1:H:52:ARG:HD2	4:H:2028:HOH:O	2.17	0.43
1:B:86:LYS:HD2	4:B:2063:HOH:O	2.18	0.43
1:C:148:ALA:HB2	1:C:201:TYR:CD2	2.53	0.43
1:A:223:SER:OG	1:A:225:ARG:HG2	2.19	0.43
1:A:320:ARG:N	1:A:321:PRO:HD2	2.34	0.43
1:C:79:GLU:HA	1:C:83:HIS:O	2.19	0.43
1:D:128:THR:HG21	4:D:2055:HOH:O	2.19	0.43
1:E:177:VAL:HG12	1:F:351:LEU:CD1	2.48	0.43
1:C:142:TRP:CG	1:C:168:ALA:HB3	2.54	0.43
1:C:212:ASN:HB2	4:C:2127:HOH:O	2.18	0.43
1:E:98:GLY:CA	1:E:104:LYS:HG2	2.49	0.43
1:F:109:ALA:HB1	1:F:136:LEU:HG	2.01	0.43
1:F:339:ASP:OD2	1:F:343:LYS:HE2	2.19	0.43
1:C:109:ALA:HB1	1:C:136:LEU:HG	2.01	0.43
1:E:128:THR:HG21	4:E:2048:HOH:O	2.19	0.43
1:A:97:HIS:CG	1:A:105:GLU:HG3	2.53	0.42
1:C:245:HIS:HA	1:C:246:PRO:HD3	1.95	0.42
1:E:209:MET:CE	1:E:217:ALA:HB3	2.49	0.42
1:E:305:VAL:HG22	1:E:316:VAL:HG21	2.01	0.42
1:E:296:ASP:C	1:E:296:ASP:OD1	2.58	0.42
1:B:110:ARG:O	1:B:114:GLU:CG	2.67	0.42
1:H:320:ARG:N	1:H:321:PRO:HD2	2.34	0.42
1:C:51:LYS:NZ	4:C:2033:HOH:O	2.52	0.42
1:D:81:LEU:HD11	1:D:239:PHE:CE2	2.55	0.42
1:A:98:GLY:HA2	1:A:104:LYS:HG2	2.02	0.42
1:E:258:SER:O	1:E:292:PRO:HD2	2.19	0.42
1:G:148:ALA:H	1:G:154:ASN:ND2	2.05	0.42
1:E:145:ILE:HD11	1:E:230:ILE:HD13	2.02	0.42
1:E:273:ALA:HB1	1:E:274:PRO:HD2	2.00	0.42
1:D:244:GLN:HE22	1:D:276:SER:HA	1.85	0.41
1:H:342:GLN:NE2	4:H:2140:HOH:O	2.53	0.41
1:B:199:GLN:O	1:B:199:GLN:HG3	2.21	0.41
1:F:178:SER:HB2	1:F:215:TYR:HD1	1.85	0.41
1:F:305:VAL:HG22	1:F:316:VAL:HG21	2.02	0.41
1:A:191:TYR:CE1	1:A:211:LEU:HD12	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LYS:O	1:C:54:ASN:HB2	2.20	0.41
1:C:61:LYS:HB3	1:C:365:LEU:HD13	2.02	0.41
1:C:144:GLN:HA	1:C:170:ILE:HB	2.02	0.41
1:G:305:VAL:HB	1:G:345:LEU:HD13	2.02	0.41
1:B:156:ASP:HB3	1:B:200:ARG:HH21	1.85	0.41
1:C:149:LYS:NZ	1:C:218:SER:O	2.54	0.41
1:D:162:LYS:HE3	1:D:236:LEU:HD21	2.01	0.41
1:E:264:ASN:HA	4:E:2058:HOH:O	2.20	0.41
1:H:176:THR:O	1:H:220:GLN:HG2	2.21	0.41
1:F:181:ARG:H	1:F:181:ARG:HG2	1.67	0.41
1:D:247:GLU:OE1	1:D:286:ARG:NH1	2.50	0.41
1:B:109:ALA:HB1	1:B:136:LEU:HG	2.03	0.41
1:F:195:MET:HA	1:F:196:PRO:HD2	1.87	0.41
1:A:342:GLN:HG3	4:A:2177:HOH:O	2.20	0.41
1:E:152:GLN:HB3	1:E:203:ARG:HH21	1.85	0.41
1:F:89:PHE:HA	1:F:316:VAL:O	2.20	0.41
1:C:111:ALA:HB2	1:C:331:TRP:O	2.20	0.41
1:B:89:PHE:HA	1:B:316:VAL:O	2.20	0.40
1:E:251:MET:CE	1:F:68:ALA:HB3	2.51	0.40
1:D:273:ALA:HB1	1:D:274:PRO:CD	2.52	0.40
1:A:33:VAL:HB	1:A:38:PHE:HB2	2.02	0.40
1:A:153:GLN:NE2	1:A:203:ARG:H	2.18	0.40
1:A:296:ASP:C	1:A:296:ASP:OD1	2.60	0.40
1:A:271:TYR:CG	1:A:272:GLU:N	2.89	0.40
1:C:76:THR:O	1:C:87:ALA:HA	2.22	0.40
1:E:147:MET:HE3	1:E:226:ASP:HB3	2.01	0.40
1:E:241:LYS:HA	1:E:261:TRP:HB3	2.03	0.40
1:A:209:MET:SD	1:A:214:ILE:HG12	2.61	0.40
1:E:23:TYR:CE2	1:E:301:ARG:NH1	2.89	0.40
1:F:239:PHE:CE1	1:F:259:GLY:HA3	2.55	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	368/374 (98%)	359 (98%)	8 (2%)	1 (0%)	41	41
1	B	365/374 (98%)	352 (96%)	11 (3%)	2 (0%)	29	26
1	C	366/374 (98%)	352 (96%)	12 (3%)	2 (0%)	29	26
1	D	349/374 (93%)	338 (97%)	10 (3%)	1 (0%)	41	41
1	E	365/374 (98%)	351 (96%)	13 (4%)	1 (0%)	41	41
1	F	353/374 (94%)	339 (96%)	10 (3%)	4 (1%)	14	9
1	G	365/374 (98%)	350 (96%)	13 (4%)	2 (0%)	29	26
1	H	344/374 (92%)	335 (97%)	8 (2%)	1 (0%)	41	41
All	All	2875/2992 (96%)	2776 (97%)	85 (3%)	14 (0%)	29	26

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	B	200	ARG
1	B	297	SER
1	C	297	SER
1	D	297	SER
1	E	297	SER
1	F	297	SER
1	G	83	HIS
1	G	297	SER
1	H	297	SER
1	C	206	ALA
1	F	212	ASN
1	F	19	VAL
1	F	329	GLY

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	293/297 (99%)	284 (97%)	9 (3%)	40	43
1	B	290/297 (98%)	280 (97%)	10 (3%)	37	39
1	C	291/297 (98%)	283 (97%)	8 (3%)	44	48
1	D	279/297 (94%)	263 (94%)	16 (6%)	20	18
1	E	290/297 (98%)	280 (97%)	10 (3%)	37	39
1	F	283/297 (95%)	272 (96%)	11 (4%)	32	33
1	G	290/297 (98%)	278 (96%)	12 (4%)	30	31
1	H	276/297 (93%)	267 (97%)	9 (3%)	38	40
All	All	2292/2376 (96%)	2207 (96%)	85 (4%)	34	35

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	47	ASP
1	A	128	THR
1	A	134	GLU
1	A	141	ARG
1	A	175	SER
1	A	214	ILE
1	A	346	THR
1	A	360	LEU
1	B	30	SER
1	B	67	LEU
1	B	94	ILE
1	B	134	GLU
1	B	177	VAL
1	B	180	ASN
1	B	220	GLN
1	B	234	SER
1	B	342	GLN
1	B	367	ASP
1	C	130	GLU
1	C	141	ARG
1	C	163	SER
1	C	188	LYS
1	C	205	THR
1	C	280	LEU
1	C	296	ASP
1	C	338	LEU

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Mol	Chain	Res	Type
1	D	20	VAL
1	D	113	SER
1	D	118	ILE
1	D	133	SER
1	D	134	GLU
1	D	141	ARG
1	D	160	GLU
1	D	175	SER
1	D	181	ARG
1	D	190	VAL
1	D	195	MET
1	D	220	GLN
1	D	225	ARG
1	D	250	ASP
1	D	344	ASP
1	D	367	ASP
1	E	13	GLU
1	E	110	ARG
1	E	141	ARG
1	E	143	PHE
1	E	183	ARG
1	E	250	ASP
1	E	251	MET
1	E	360	LEU
1	E	367	ASP
1	E	373	GLU
1	F	14	ILE
1	F	15	LYS
1	F	25	LEU
1	F	30	SER
1	F	67	LEU
1	F	114	GLU
1	F	137	ASN
1	F	147	MET
1	F	181	ARG
1	F	225	ARG
1	F	367	ASP
1	G	104	LYS
1	G	134	GLU
1	G	150	ASP
1	G	163	SER
1	G	177	VAL

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Mol	Chain	Res	Type
1	G	200	ARG
1	G	234	SER
1	G	251	MET
1	G	288	ASN
1	G	315	VAL
1	G	323	LEU
1	G	360	LEU
1	H	32	VAL
1	H	52	ARG
1	H	80	ILE
1	H	134	GLU
1	H	145	ILE
1	H	153	GLN
1	H	167	THR
1	H	180	ASN
1	H	342	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	153	GLN
1	B	39	ASN
1	B	180	ASN
1	B	288	ASN
1	B	350	GLN
1	B	355	GLN
1	C	69	GLN
1	C	154	ASN
1	C	244	GLN
1	D	244	GLN
1	E	39	ASN
1	E	350	GLN
1	F	137	ASN
1	G	154	ASN
1	G	187	ASN
1	G	244	GLN
1	H	35	HIS
1	H	180	ASN
1	H	187	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	FMN	C	1375	-	33,33,33	1.18	2 (6%)	48,50,50	1.37	6 (12%)
2	FMN	H	1375	-	33,33,33	1.07	2 (6%)	48,50,50	1.21	7 (14%)
2	FMN	B	1375	-	33,33,33	1.02	2 (6%)	48,50,50	1.33	5 (10%)
2	FMN	E	1375	-	33,33,33	1.06	2 (6%)	48,50,50	1.29	8 (16%)
2	FMN	F	1375	-	33,33,33	1.06	2 (6%)	48,50,50	1.34	6 (12%)
2	FMN	A	1375	-	33,33,33	1.20	2 (6%)	48,50,50	1.23	7 (14%)
2	FMN	G	1375	-	33,33,33	1.12	2 (6%)	48,50,50	1.10	5 (10%)
2	FMN	D	1375	-	33,33,33	1.10	2 (6%)	48,50,50	1.36	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
2	FMN	C	1375	-	-	1/18/18/18	0/3/3/3
2	FMN	H	1375	-	-	1/18/18/18	0/3/3/3
2	FMN	B	1375	-	-	4/18/18/18	0/3/3/3
2	FMN	E	1375	-	-	4/18/18/18	0/3/3/3
2	FMN	F	1375	-	-	2/18/18/18	0/3/3/3
2	FMN	A	1375	-	-	1/18/18/18	0/3/3/3
2	FMN	G	1375	-	-	1/18/18/18	0/3/3/3
2	FMN	D	1375	-	-	1/18/18/18	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1375	FMN	C4A-N5	4.52	1.39	1.30
2	C	1375	FMN	C4A-N5	4.34	1.39	1.30
2	D	1375	FMN	C4A-N5	4.13	1.38	1.30
2	E	1375	FMN	C4A-N5	4.07	1.38	1.30
2	H	1375	FMN	C4A-N5	3.93	1.38	1.30
2	B	1375	FMN	C4A-N5	3.90	1.38	1.30
2	G	1375	FMN	C4A-N5	3.86	1.38	1.30
2	F	1375	FMN	C4A-N5	3.68	1.37	1.30
2	G	1375	FMN	C10-N1	3.39	1.40	1.33
2	A	1375	FMN	C10-N1	3.17	1.39	1.33
2	C	1375	FMN	C10-N1	3.07	1.39	1.33
2	H	1375	FMN	C10-N1	2.88	1.39	1.33
2	D	1375	FMN	C10-N1	2.78	1.38	1.33
2	E	1375	FMN	C10-N1	2.71	1.38	1.33
2	F	1375	FMN	C10-N1	2.55	1.38	1.33
2	B	1375	FMN	C10-N1	2.16	1.37	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1375	FMN	C4A-C10-N10	3.31	121.32	116.48
2	F	1375	FMN	C4A-C10-N10	3.24	121.21	116.48
2	B	1375	FMN	C4A-C10-N10	3.23	121.20	116.48
2	F	1375	FMN	C4-N3-C2	-3.12	119.88	125.64
2	B	1375	FMN	C10-C4A-N5	-3.02	118.45	124.86
2	D	1375	FMN	C9A-C5A-N5	-2.97	119.21	122.43
2	B	1375	FMN	C4-N3-C2	-2.93	120.23	125.64
2	A	1375	FMN	C4-N3-C2	-2.89	120.30	125.64
2	E	1375	FMN	C4A-C4-N3	2.87	120.47	113.19
2	D	1375	FMN	C4A-C4-N3	2.79	120.27	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1375	FMN	C10-C4A-N5	-2.78	118.97	124.86
2	A	1375	FMN	C4A-C4-N3	2.76	120.20	113.19
2	H	1375	FMN	C4-N3-C2	-2.76	120.54	125.64
2	D	1375	FMN	C4-N3-C2	-2.76	120.55	125.64
2	F	1375	FMN	C10-C4A-N5	-2.75	119.01	124.86
2	E	1375	FMN	C4-N3-C2	-2.71	120.63	125.64
2	D	1375	FMN	C4A-C10-N10	2.70	120.42	116.48
2	H	1375	FMN	C4A-C4-N3	2.69	120.03	113.19
2	E	1375	FMN	C4A-C10-N10	2.61	120.29	116.48
2	F	1375	FMN	C4A-C4-N3	2.60	119.80	113.19
2	C	1375	FMN	C9A-C5A-N5	-2.58	119.63	122.43
2	D	1375	FMN	C10-C4A-N5	-2.55	119.44	124.86
2	B	1375	FMN	C4A-C10-N1	-2.50	118.94	124.73
2	E	1375	FMN	C10-N1-C2	2.41	121.71	116.90
2	C	1375	FMN	C4A-C4-N3	2.40	119.30	113.19
2	G	1375	FMN	C4A-C4-N3	2.40	119.30	113.19
2	H	1375	FMN	C9A-C5A-N5	-2.39	119.83	122.43
2	D	1375	FMN	C5A-C9A-N10	2.39	120.42	117.95
2	A	1375	FMN	C10-C4A-N5	-2.38	119.80	124.86
2	E	1375	FMN	C10-C4A-N5	-2.37	119.83	124.86
2	B	1375	FMN	C4A-C4-N3	2.35	119.16	113.19
2	D	1375	FMN	C5'-C4'-C3'	-2.35	107.66	112.20
2	A	1375	FMN	C4A-C10-N1	-2.33	119.32	124.73
2	F	1375	FMN	C4A-C10-N1	-2.29	119.41	124.73
2	C	1375	FMN	C4A-C10-N1	-2.27	119.46	124.73
2	H	1375	FMN	O4-C4-C4A	-2.27	120.58	126.60
2	C	1375	FMN	C4-N3-C2	-2.27	121.45	125.64
2	G	1375	FMN	C4A-C10-N10	2.26	119.79	116.48
2	A	1375	FMN	C4A-C10-N10	2.26	119.79	116.48
2	A	1375	FMN	C10-N1-C2	2.26	121.42	116.90
2	A	1375	FMN	O4-C4-C4A	-2.25	120.62	126.60
2	E	1375	FMN	C4A-C10-N1	-2.25	119.51	124.73
2	G	1375	FMN	C10-C4A-N5	-2.23	120.13	124.86
2	H	1375	FMN	C10-C4A-N5	-2.21	120.16	124.86
2	E	1375	FMN	O4-C4-C4A	-2.19	120.78	126.60
2	H	1375	FMN	C4A-C10-N10	2.19	119.68	116.48
2	D	1375	FMN	C4A-C10-N1	-2.15	119.75	124.73
2	D	1375	FMN	C4-C4A-N5	2.15	121.29	118.23
2	H	1375	FMN	C4A-C10-N1	-2.13	119.80	124.73
2	G	1375	FMN	C4-N3-C2	-2.12	121.73	125.64
2	G	1375	FMN	C4A-C10-N1	-2.10	119.86	124.73
2	E	1375	FMN	C4-C4A-N5	2.05	121.14	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1375	FMN	O4-C4-C4A	-2.04	121.19	126.60
2	F	1375	FMN	C4-C4A-N5	2.02	121.10	118.23

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1375	FMN	C1'-C2'-C3'-C4'
2	E	1375	FMN	O2'-C2'-C3'-C4'
2	F	1375	FMN	O2'-C2'-C3'-C4'
2	C	1375	FMN	C4'-C5'-O5'-P
2	D	1375	FMN	C4'-C5'-O5'-P
2	E	1375	FMN	C4'-C5'-O5'-P
2	H	1375	FMN	C4'-C5'-O5'-P
2	G	1375	FMN	C4'-C5'-O5'-P
2	A	1375	FMN	C4'-C5'-O5'-P
2	F	1375	FMN	C4'-C5'-O5'-P
2	E	1375	FMN	O2'-C2'-C3'-O3'
2	B	1375	FMN	C2'-C3'-C4'-C5'
2	B	1375	FMN	C2'-C3'-C4'-O4'
2	B	1375	FMN	C4'-C5'-O5'-P
2	B	1375	FMN	O3'-C3'-C4'-C5'

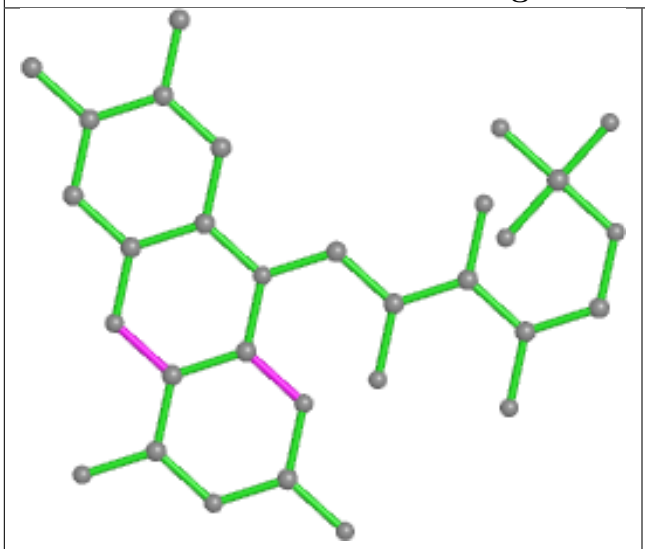
There are no ring outliers.

2 monomers are involved in 2 short contacts:

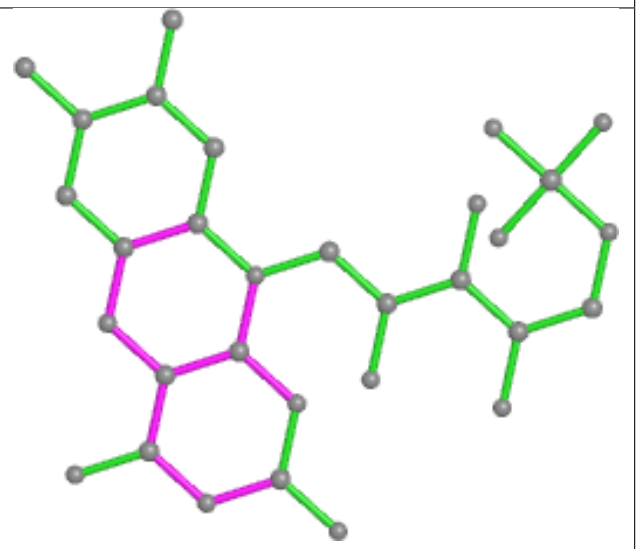
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1375	FMN	1	0
2	G	1375	FMN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and 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.

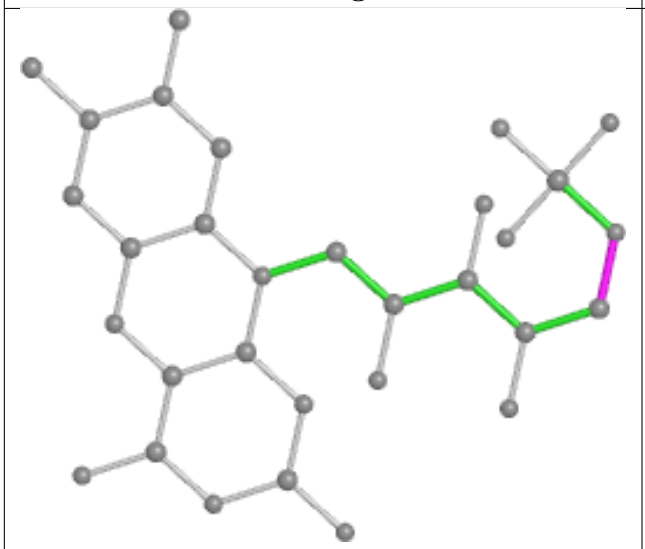
Ligand FMN C 1375



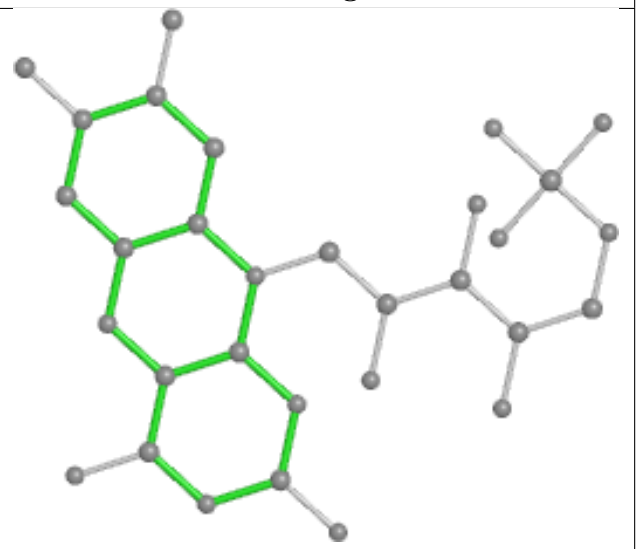
Bond lengths



Bond angles

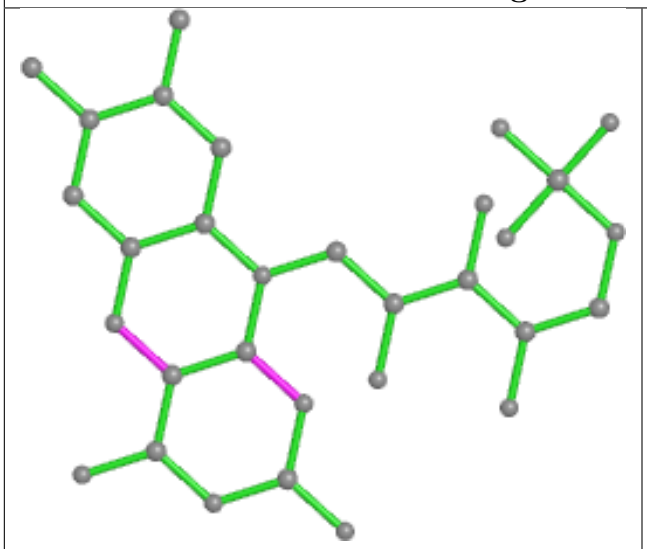


Torsions



Rings

Ligand FMN H 1375



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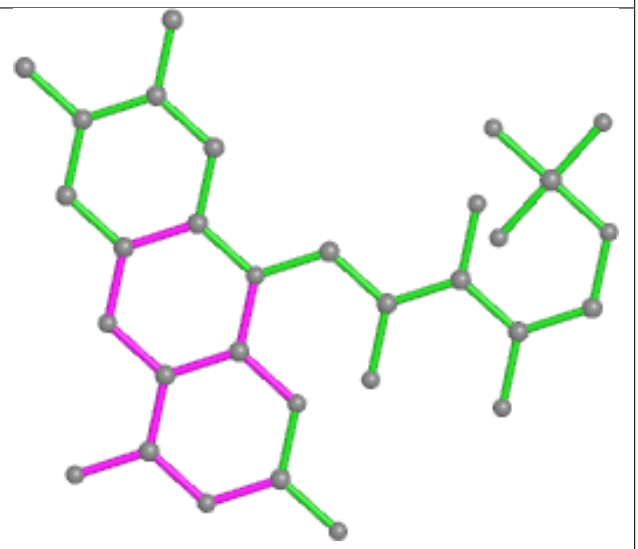

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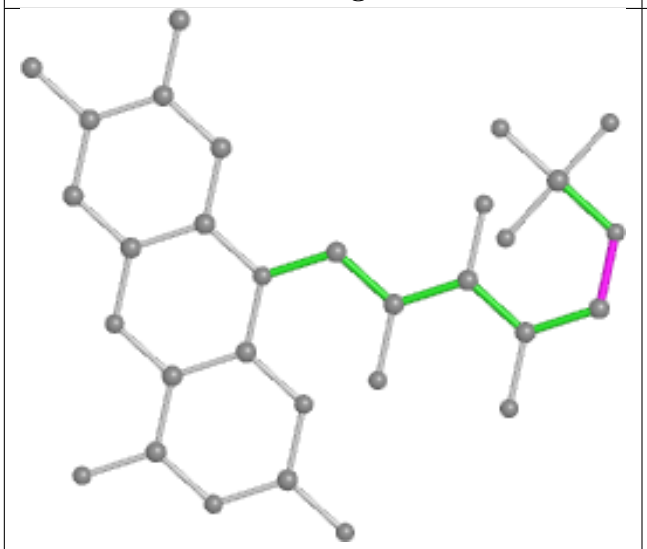

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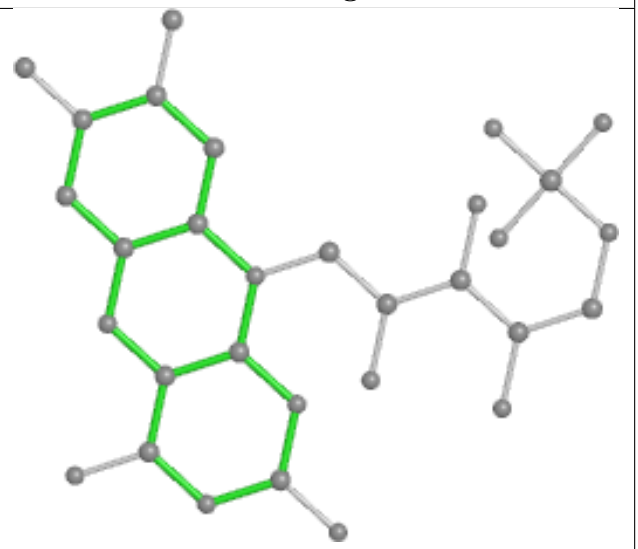
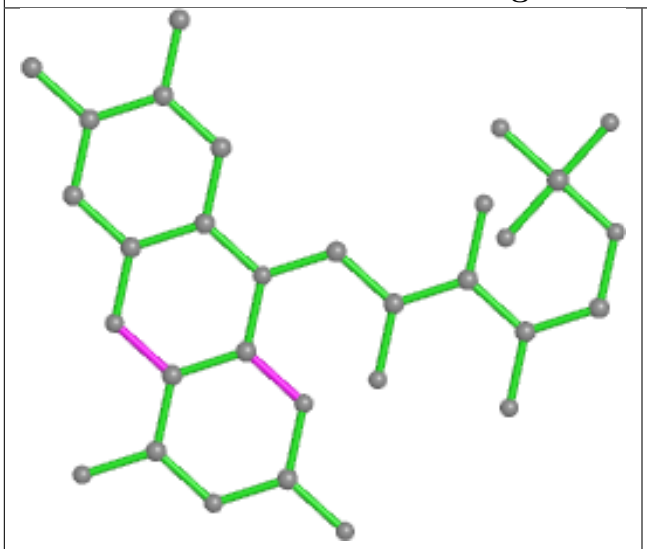
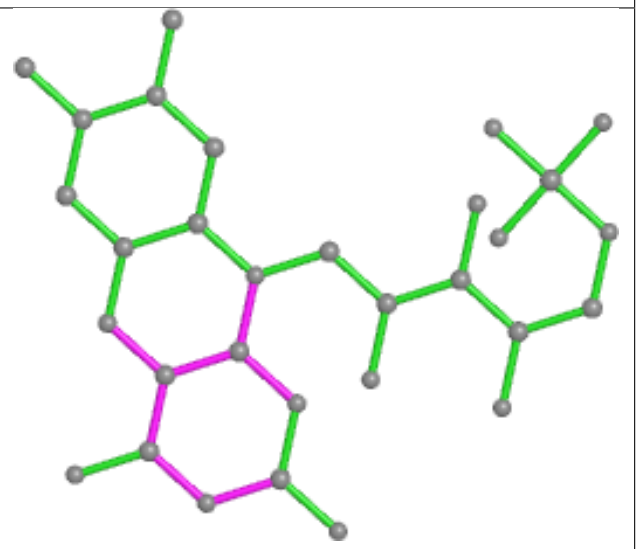


Rings

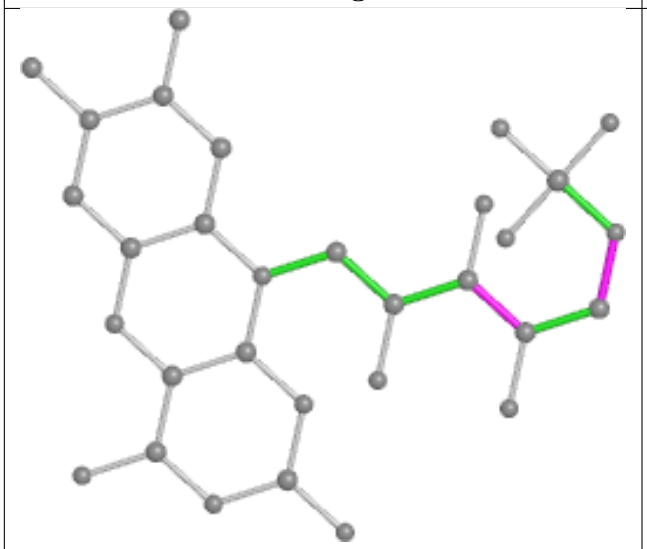
Ligand FMN B 1375



Bond lengths



Bond angles



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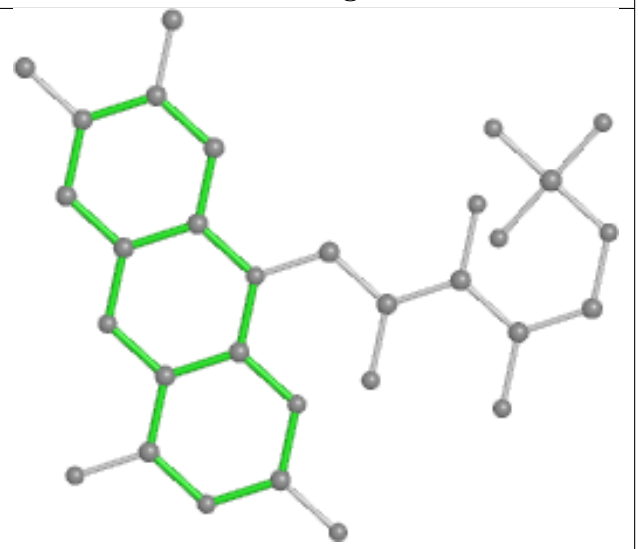
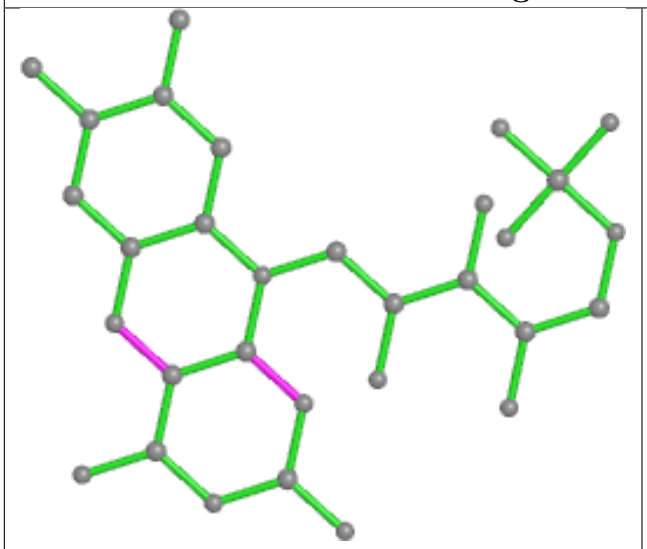
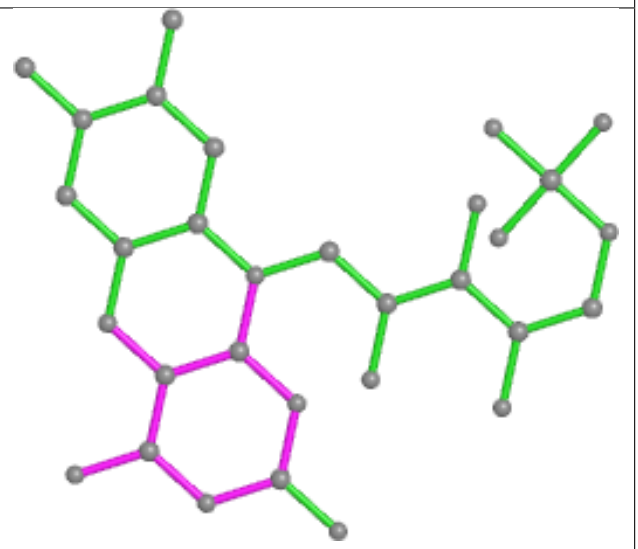


Rings

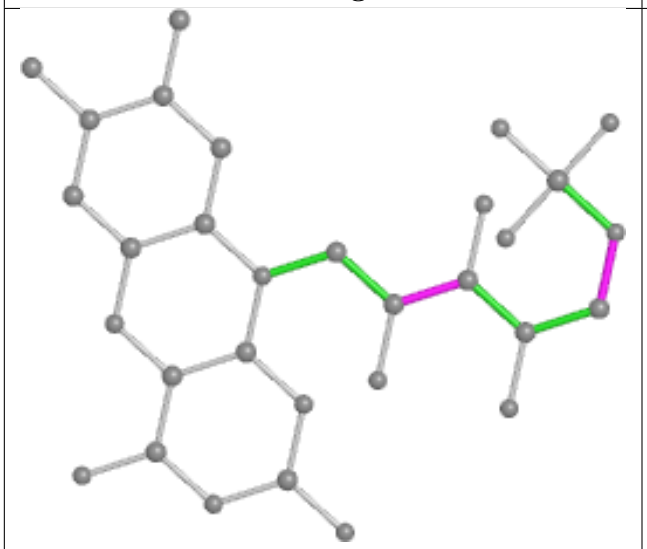
Ligand FMN E 1375



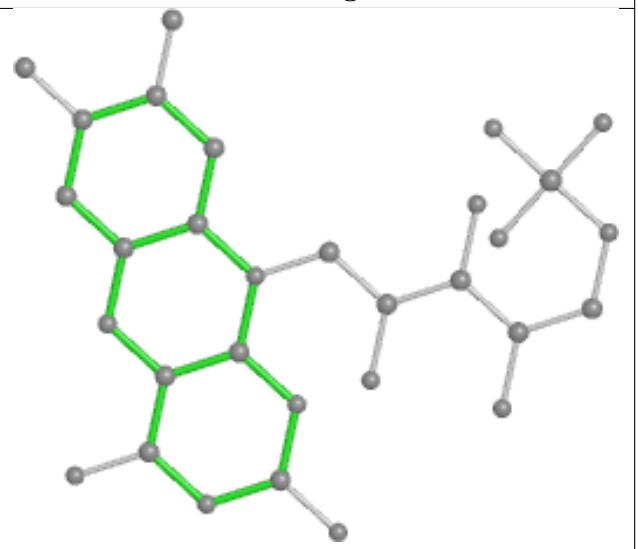
Bond lengths



Bond angles

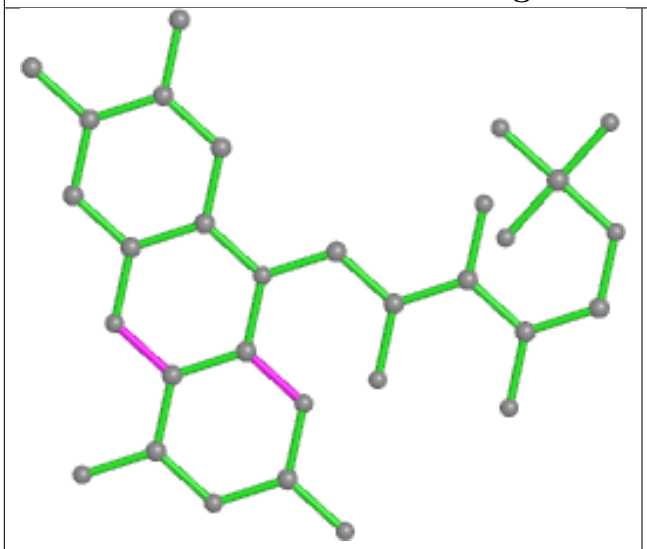


Torsions

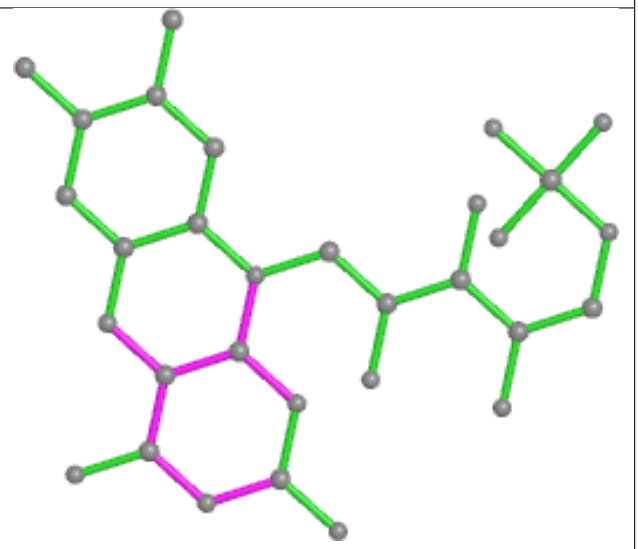


Rings

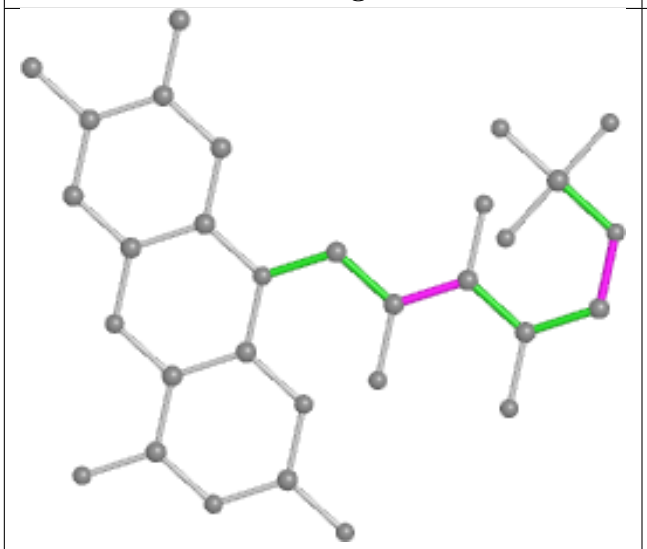
Ligand FMN F 1375



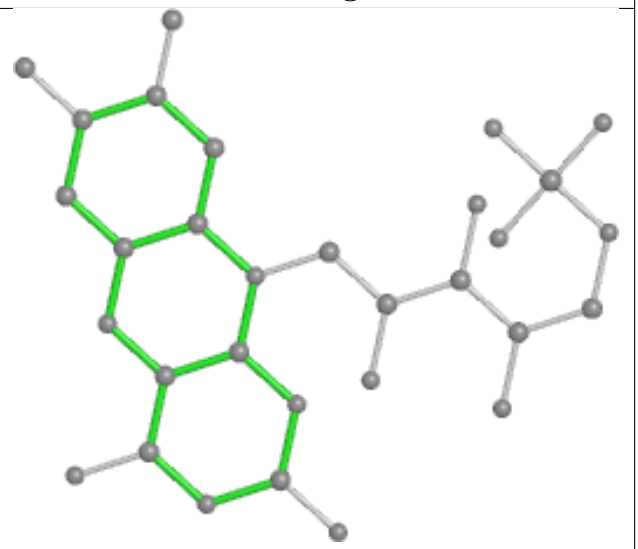
Bond lengths



Bond angles

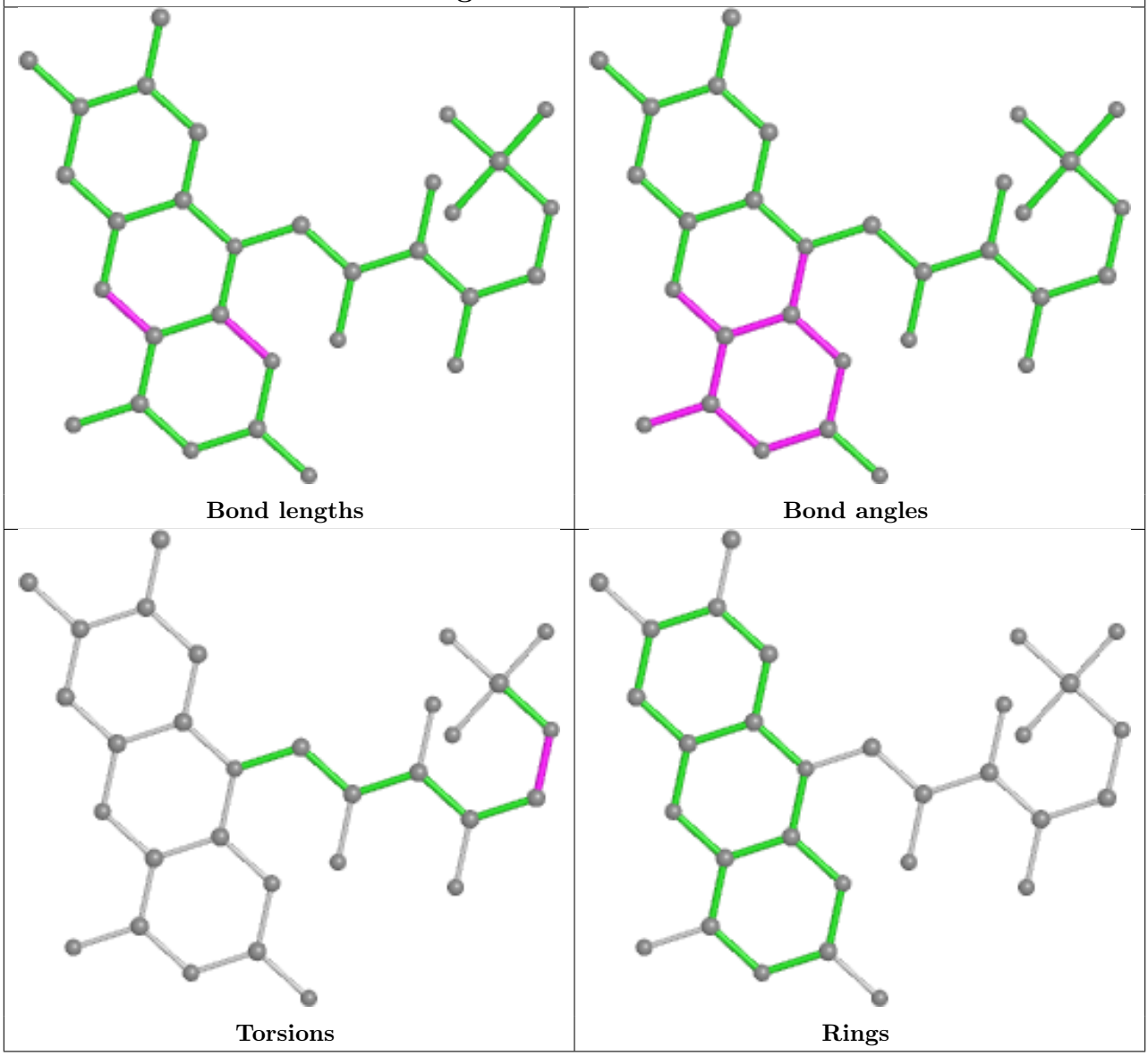


Torsions

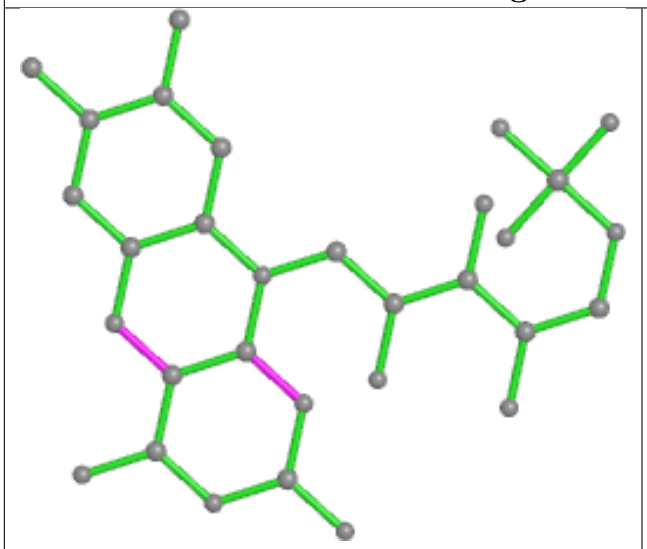


Rings

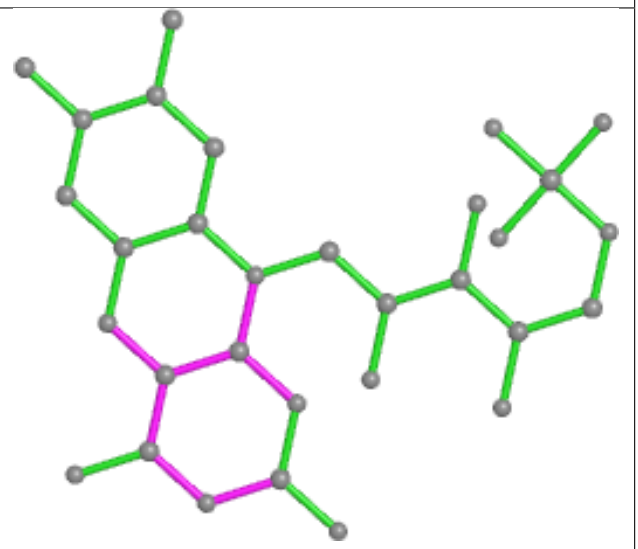
Ligand FMN A 1375



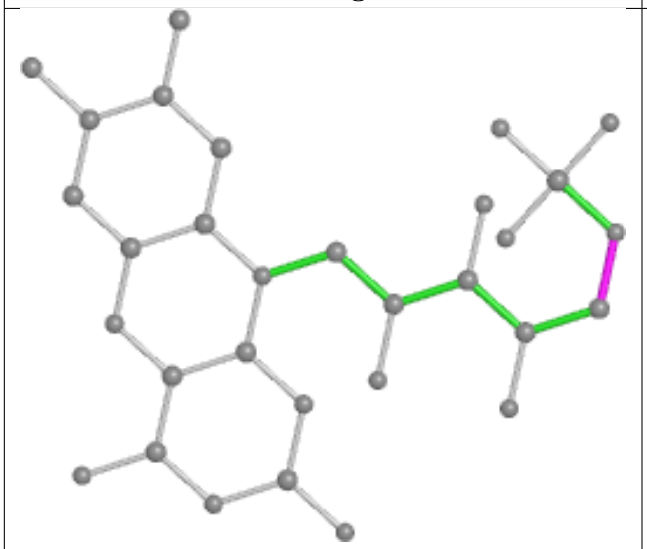
Ligand FMN G 1375



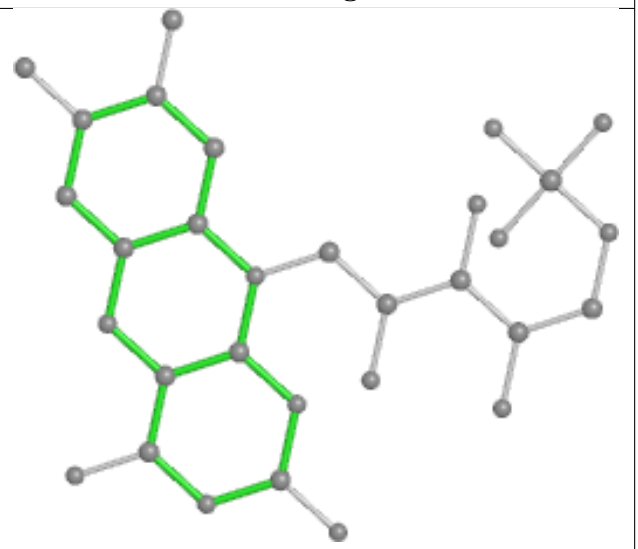
Bond lengths



Bond angles

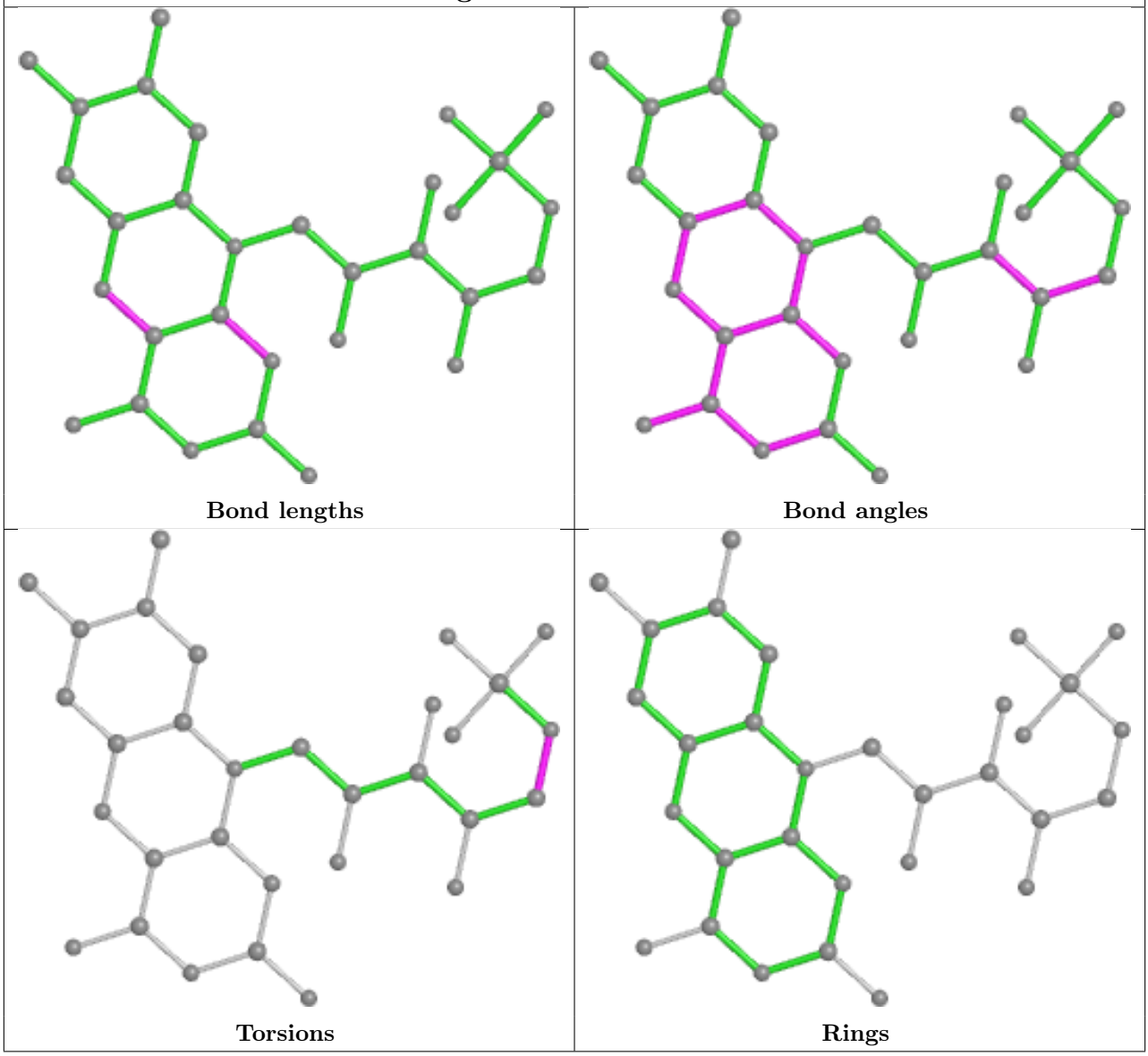


Torsions



Rings

Ligand FMN D 1375



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	370/374 (98%)	-0.62	0	100	100	2, 9, 20, 27	0
1	B	367/374 (98%)	-0.55	0	100	100	3, 11, 21, 25	0
1	C	368/374 (98%)	-0.59	0	100	100	2, 8, 19, 28	0
1	D	353/374 (94%)	-0.32	3 (0%)	86	88	3, 14, 34, 49	0
1	E	367/374 (98%)	-0.30	2 (0%)	91	92	5, 17, 31, 40	0
1	F	357/374 (95%)	-0.37	3 (0%)	86	88	3, 12, 24, 43	0
1	G	367/374 (98%)	-0.48	1 (0%)	94	94	4, 13, 25, 29	0
1	H	348/374 (93%)	-0.48	2 (0%)	89	91	3, 11, 26, 35	0
All	All	2897/2992 (96%)	-0.46	11 (0%)	92	93	2, 12, 26, 49	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	198	VAL	3.7
1	H	197	ILE	2.9
1	D	216	GLY	2.8
1	F	199	GLN	2.4
1	F	211	LEU	2.3
1	D	214	ILE	2.2
1	H	191	TYR	2.2
1	E	95	ALA	2.1
1	F	212	ASN	2.1
1	E	200	ARG	2.1
1	G	82	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

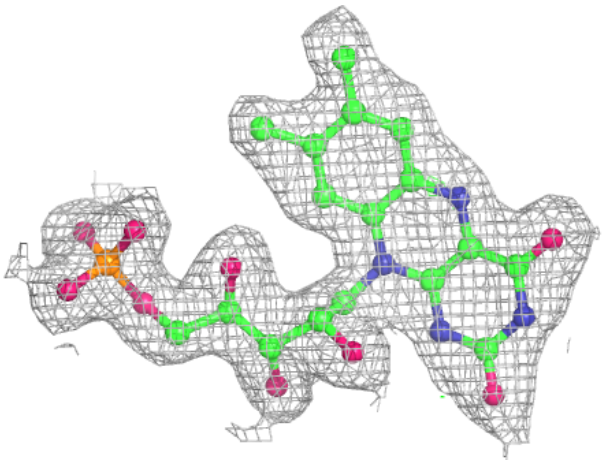
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

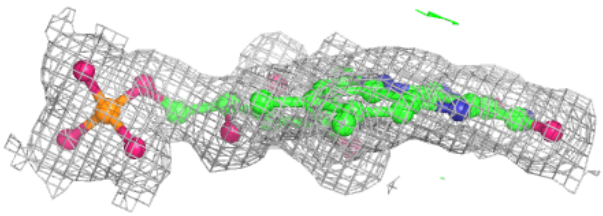
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FMN	C	1375	31/31	0.97	0.08	2,5,7,8	0
2	FMN	E	1375	31/31	0.97	0.10	9,11,13,13	0
2	FMN	F	1375	31/31	0.97	0.08	3,7,8,9	0
2	FMN	G	1375	31/31	0.97	0.10	5,9,11,11	0
2	FMN	H	1375	31/31	0.97	0.08	5,8,10,13	0
2	FMN	A	1375	31/31	0.98	0.07	2,6,8,9	0
2	FMN	D	1375	31/31	0.98	0.07	5,8,11,12	0
2	FMN	B	1375	31/31	0.98	0.08	5,7,9,9	0
3	ZN	D	1376	1/1	0.99	0.08	26,26,26,26	0

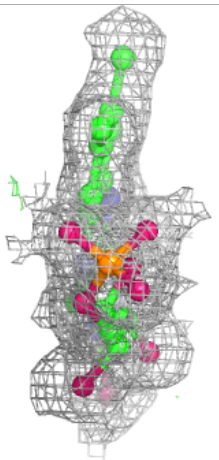
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN C 1375:

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

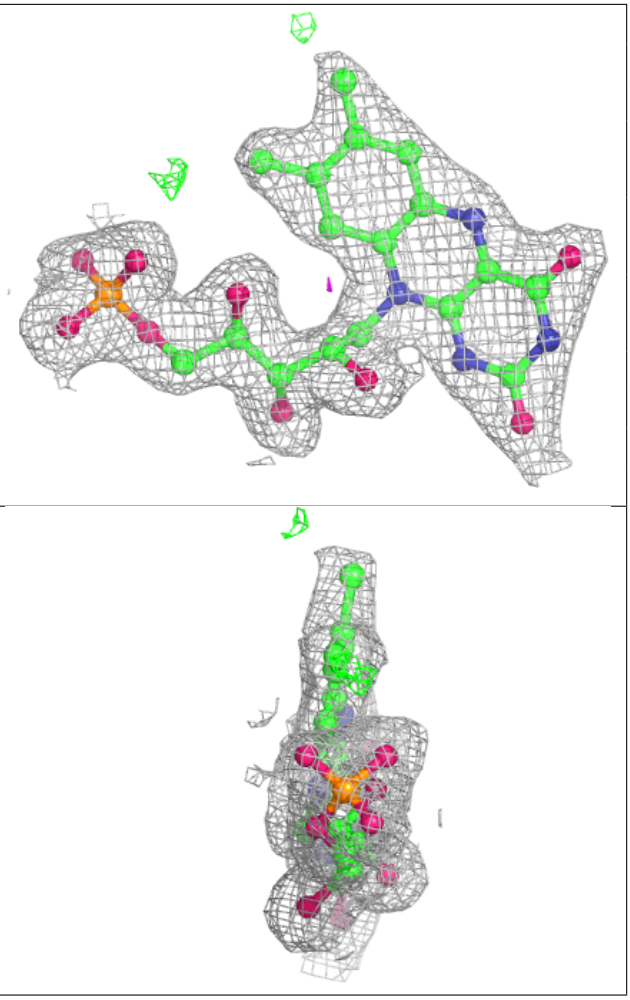






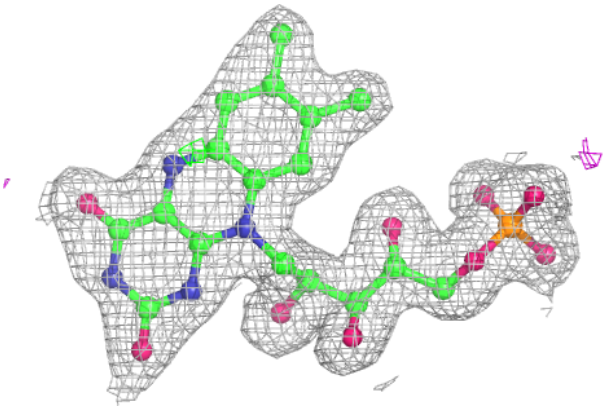
Electron density around FMN E 1375:

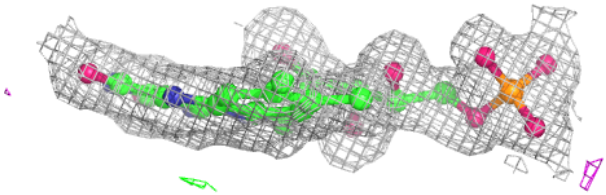
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

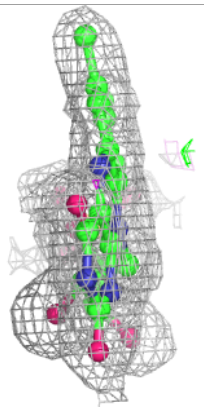


Electron density around FMN F 1375:

$2mF_o$-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 1375:

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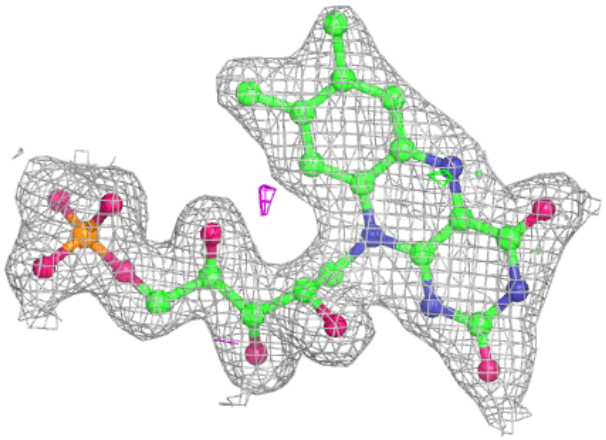
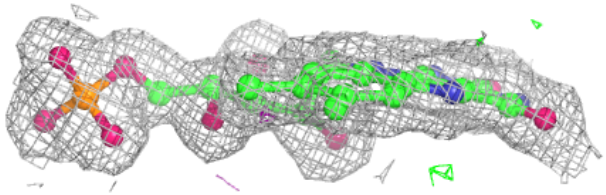
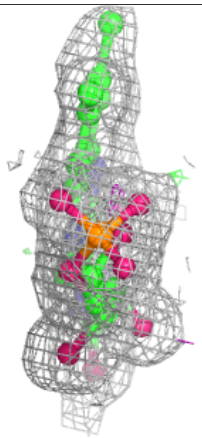
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

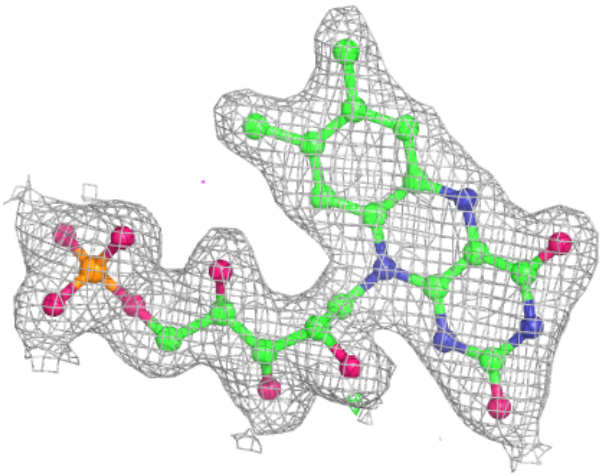


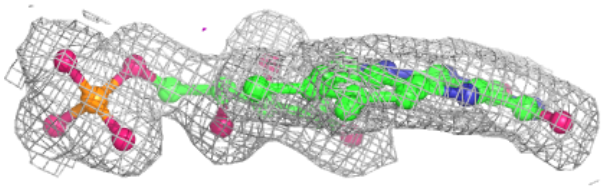


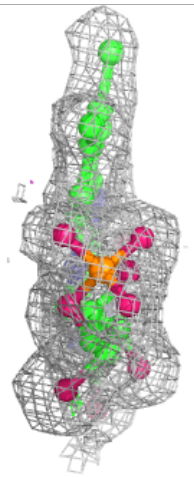


Electron density around FMN H 1375:

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

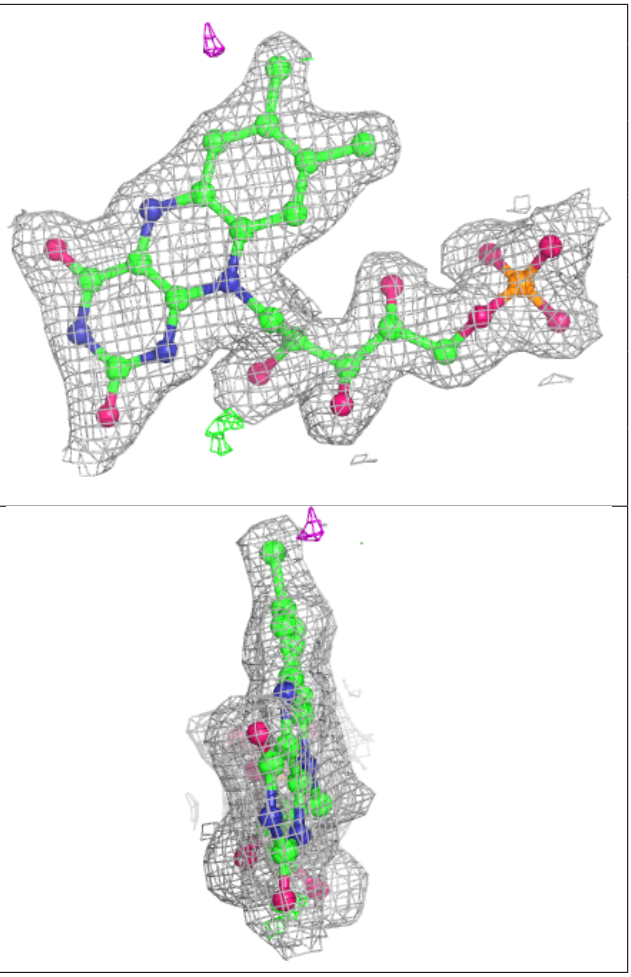






Electron density around FMN A 1375:

$2mF_o$-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 1375:

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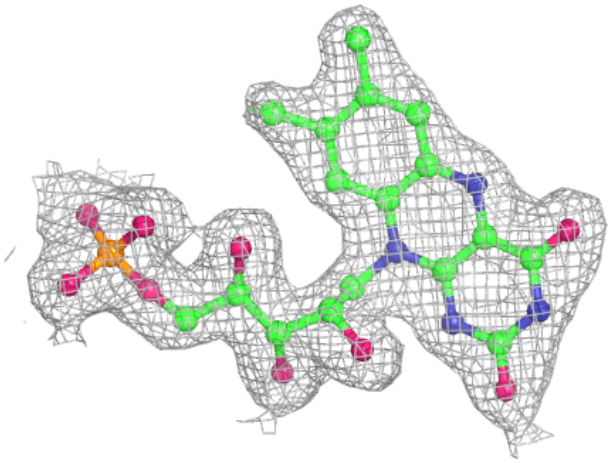
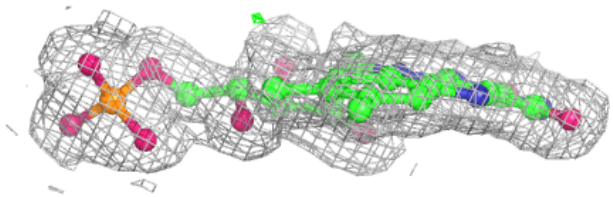
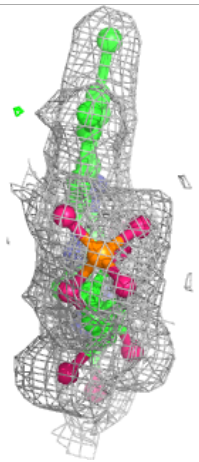
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around FMN B 1375:

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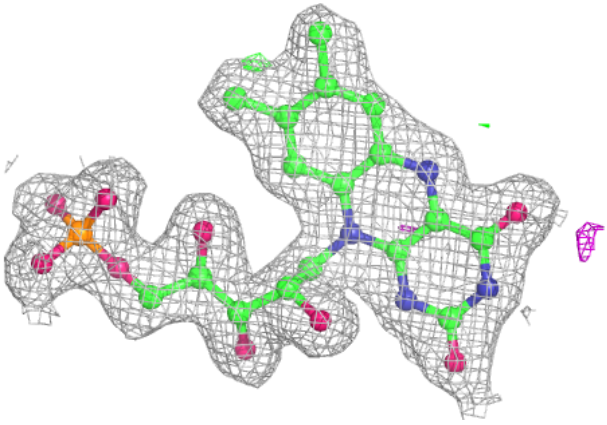
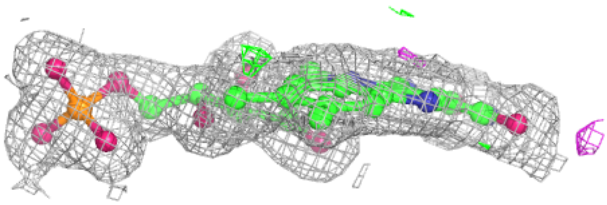
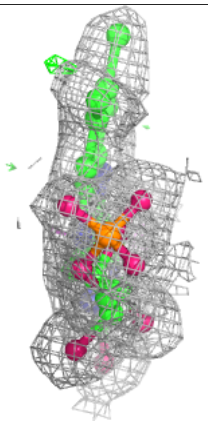
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.