



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:57 am BST

PDB ID : 1QZU
Title : crystal structure of human phosphopantothienoylcysteine decarboxylase
Authors : Manoj, N.; Ealick, S.E.
Deposited on : 2003-09-17
Resolution : 2.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

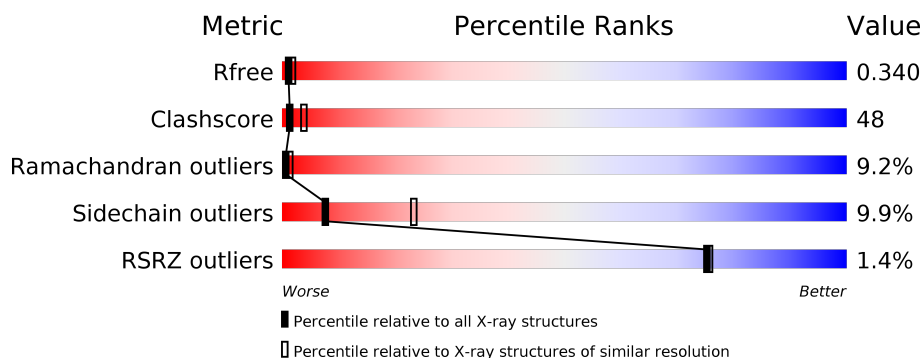
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	206	<div> <div>%</div> <div> <div></div> <div>33%</div> <div>35%</div> <div>9%</div> <div>22%</div> </div> </div>
1	B	206	<div> <div>%</div> <div> <div></div> <div>30%</div> <div>37%</div> <div>8%</div> <div>25%</div> </div> </div>
1	C	206	<div> <div></div> <div> <div>33%</div> <div>37%</div> <div>8%</div> <div>22%</div> </div> </div>
1	D	206	<div> <div>%</div> <div> <div></div> <div>31%</div> <div>35%</div> <div>9%</div> <div>25%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4558 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 hypothetical protein MDS018.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1127	720	196	204	7			
1	B	155	Total	C	N	O	S	0	0	0
			1101	705	188	202	6			
1	C	160	Total	C	N	O	S	0	0	0
			1117	714	193	204	6			
1	D	155	Total	C	N	O	S	0	0	0
			1090	699	183	202	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q96CD2
A	0	ALA	-	CLONING ARTIFACT	UNP Q96CD2
B	-1	GLY	-	CLONING ARTIFACT	UNP Q96CD2
B	0	ALA	-	CLONING ARTIFACT	UNP Q96CD2
C	-1	GLY	-	CLONING ARTIFACT	UNP Q96CD2
C	0	ALA	-	CLONING ARTIFACT	UNP Q96CD2
D	-1	GLY	-	CLONING ARTIFACT	UNP Q96CD2
D	0	ALA	-	CLONING ARTIFACT	UNP Q96CD2

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

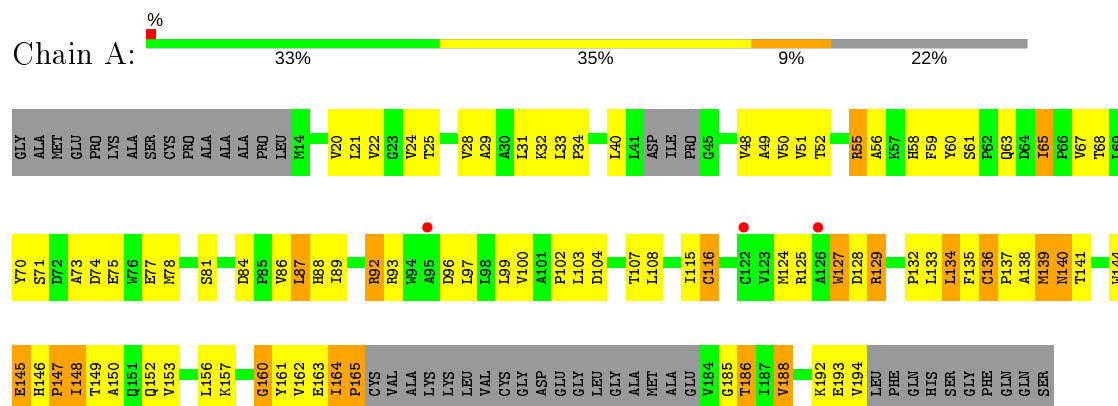


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			30	17	4	8	1		

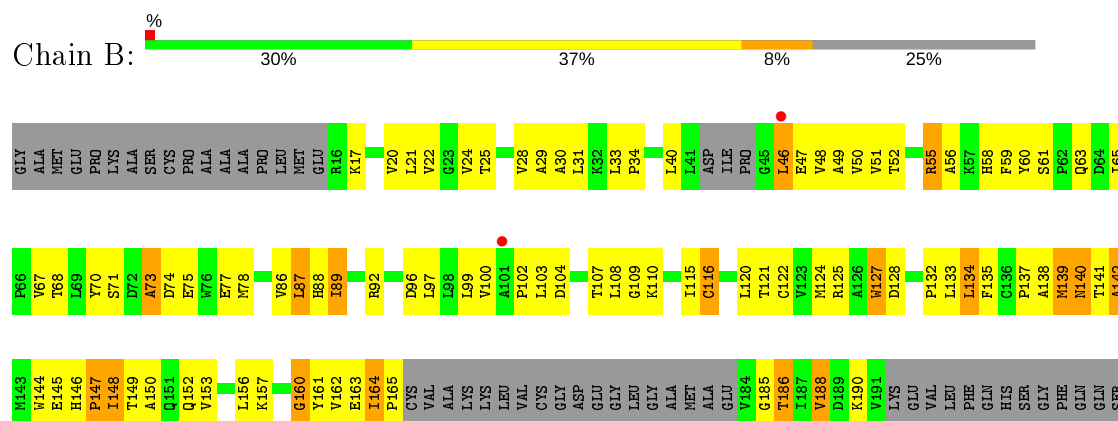
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

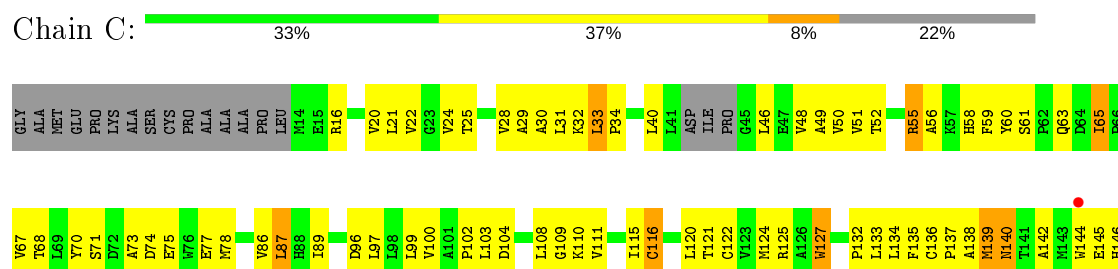
• Molecule 1: hypothetical protein MDS018

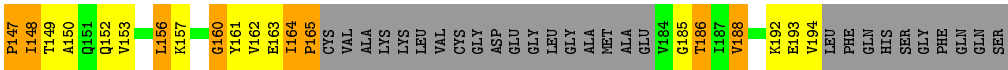


• Molecule 1: hypothetical protein MDS018

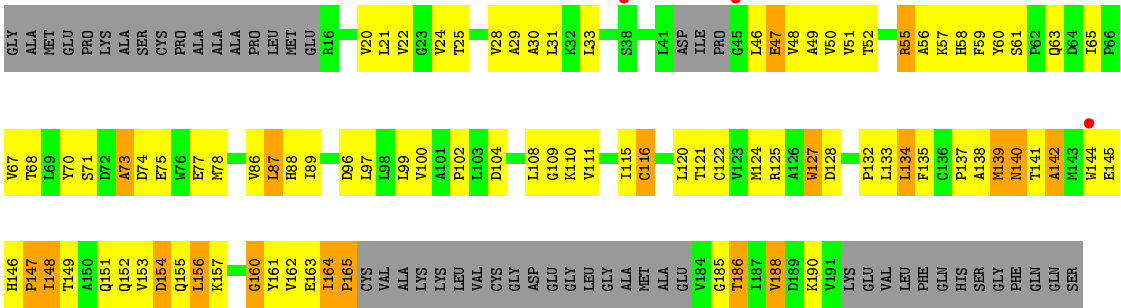


• Molecule 1: hypothetical protein MDS018





• Molecule 1: hypothetical protein MDS018



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	124.78Å 124.78Å 153.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.48 – 2.91 25.48 – 2.91	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.48-2.91) 95.9 (25.48-2.91)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.293 , 0.342 0.285 , 0.340	Depositor DCC
R_{free} test set	1284 reflections (6.87%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.000 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.000 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.000 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.000 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.477 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4558	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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 39.95 % 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 2.9431e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/1151	0.78	1/1581 (0.1%)
1	B	0.57	1/1125 (0.1%)	0.75	1/1547 (0.1%)
1	C	0.53	0/1141	0.75	1/1569 (0.1%)
1	D	0.57	1/1113 (0.1%)	0.75	1/1532 (0.1%)
All	All	0.56	2/4530 (0.0%)	0.76	4/6229 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	ALA	CA-CB	-5.36	1.41	1.52
1	D	73	ALA	CA-CB	-5.05	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	PRO	N-CA-CB	5.75	110.19	103.30
1	D	165	PRO	N-CA-CB	5.69	110.13	103.30
1	C	165	PRO	N-CA-CB	5.49	109.88	103.30
1	A	165	PRO	N-CA-CB	5.45	109.84	103.30

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	1127	0	1007	108	0
1	B	1101	0	989	103	0
1	C	1117	0	984	98	0
1	D	1090	0	973	106	0
2	A	31	0	19	1	0
2	B	31	0	19	3	0
2	C	31	0	19	2	0
2	D	30	0	19	2	0
All	All	4558	0	4029	416	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 48.

All (416) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:HB	1:B:52:THR:HG22	1.40	1.00
1:C:24:VAL:HB	1:C:52:THR:HG22	1.44	0.98
1:D:24:VAL:HB	1:D:52:THR:HG22	1.45	0.96
1:A:24:VAL:HB	1:A:52:THR:HG22	1.43	0.96
1:C:20:VAL:CG1	1:C:48:VAL:HG22	1.99	0.93
1:A:20:VAL:HG13	1:A:48:VAL:HG22	1.52	0.90
1:D:146:HIS:HE1	1:D:148:ILE:HG13	1.36	0.90
1:A:146:HIS:HE1	1:A:148:ILE:HG13	1.38	0.88
1:A:20:VAL:CG1	1:A:48:VAL:HG22	2.02	0.88
1:C:146:HIS:HE1	1:C:148:ILE:HG13	1.38	0.88
1:C:52:THR:HG21	1:C:60:TYR:OH	1.72	0.88
1:D:20:VAL:CG1	1:D:48:VAL:HG22	2.05	0.87
1:A:52:THR:HG21	1:A:60:TYR:OH	1.74	0.87
1:B:52:THR:HG21	1:B:60:TYR:OH	1.75	0.86
1:B:146:HIS:HE1	1:B:148:ILE:HG13	1.39	0.86
1:D:52:THR:HG21	1:D:60:TYR:OH	1.76	0.86
1:C:75:GLU:HG3	1:C:87:LEU:HB3	1.57	0.86
1:A:28:VAL:O	1:A:31:LEU:HB2	1.76	0.85
1:C:28:VAL:O	1:C:31:LEU:HB2	1.76	0.85
1:A:75:GLU:HG3	1:A:87:LEU:HB3	1.57	0.85
1:D:20:VAL:HG13	1:D:48:VAL:HG22	1.59	0.85
1:D:75:GLU:HG3	1:D:87:LEU:HB3	1.58	0.85
1:A:48:VAL:HG12	1:A:49:ALA:H	1.41	0.84
1:B:75:GLU:HG3	1:B:87:LEU:HB3	1.59	0.84
1:C:48:VAL:HG12	1:C:49:ALA:H	1.42	0.83
1:C:133:LEU:HD13	1:C:161:TYR:CE1	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:VAL:O	1:B:31:LEU:HB2	1.79	0.82
1:B:48:VAL:HG12	1:B:49:ALA:H	1.45	0.81
1:A:133:LEU:HD13	1:A:161:TYR:CE1	2.16	0.81
1:D:48:VAL:HG12	1:D:49:ALA:H	1.43	0.81
1:D:28:VAL:O	1:D:31:LEU:HB2	1.81	0.79
1:C:135:PHE:CD1	1:C:137:PRO:HD3	2.17	0.79
1:B:133:LEU:HD13	1:B:161:TYR:CE1	2.19	0.78
1:A:48:VAL:HG12	1:A:49:ALA:N	1.97	0.78
1:B:48:VAL:HG12	1:B:49:ALA:N	1.98	0.78
1:C:48:VAL:HG12	1:C:49:ALA:N	1.98	0.77
1:D:133:LEU:HD13	1:D:161:TYR:CE1	2.20	0.77
1:B:97:LEU:HD11	1:B:134:LEU:HG	1.64	0.77
1:D:48:VAL:HG12	1:D:49:ALA:N	1.98	0.77
1:C:139:MET:HA	2:C:803:FMN:HN3	1.49	0.76
1:D:139:MET:HA	2:D:804:FMN:HN3	1.49	0.75
1:B:139:MET:HA	2:B:802:FMN:HN3	1.54	0.73
1:A:157:LYS:O	1:A:160:GLY:N	2.20	0.73
1:B:157:LYS:O	1:B:160:GLY:N	2.19	0.73
1:C:157:LYS:O	1:C:160:GLY:N	2.18	0.72
1:A:135:PHE:CD1	1:A:137:PRO:HD3	2.24	0.72
1:D:135:PHE:CD1	1:D:137:PRO:HD3	2.24	0.72
1:D:63:GLN:OE1	1:D:63:GLN:N	2.21	0.72
1:A:129:ARG:HA	1:A:129:ARG:NE	2.05	0.71
1:B:65:ILE:O	1:B:65:ILE:HG22	1.88	0.71
1:B:21:LEU:HD12	1:B:49:ALA:O	1.90	0.71
1:D:65:ILE:HG22	1:D:65:ILE:O	1.91	0.71
1:A:63:GLN:OE1	1:A:63:GLN:N	2.23	0.71
1:B:164:ILE:O	1:B:164:ILE:HG22	1.91	0.71
1:D:164:ILE:HG22	1:D:164:ILE:O	1.90	0.71
1:B:63:GLN:N	1:B:63:GLN:OE1	2.23	0.70
1:B:135:PHE:CD1	1:B:137:PRO:HD3	2.26	0.70
1:A:25:THR:HB	1:A:104:ASP:OD2	1.91	0.70
1:A:65:ILE:O	1:A:65:ILE:HG22	1.91	0.70
1:A:21:LEU:HD12	1:A:49:ALA:O	1.92	0.69
1:D:157:LYS:O	1:D:160:GLY:N	2.20	0.69
1:D:21:LEU:HD12	1:D:49:ALA:O	1.92	0.69
1:A:164:ILE:HG22	1:A:164:ILE:O	1.93	0.69
1:C:164:ILE:O	1:C:164:ILE:HG22	1.91	0.69
1:C:65:ILE:HG22	1:C:65:ILE:O	1.93	0.69
1:D:97:LEU:HD11	1:D:134:LEU:HG	1.73	0.68
1:C:25:THR:HB	1:C:104:ASP:OD2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:SER:HB3	1:D:63:GLN:NE2	2.08	0.68
1:C:63:GLN:N	1:C:63:GLN:OE1	2.23	0.68
1:C:20:VAL:HG13	1:C:48:VAL:HG13	1.74	0.68
1:C:61:SER:HB3	1:C:63:GLN:NE2	2.09	0.66
1:D:24:VAL:HG11	1:D:33:LEU:HD22	1.77	0.66
1:B:147:PRO:O	1:B:149:THR:N	2.30	0.65
1:C:127:TRP:CD1	1:C:133:LEU:HD12	2.31	0.65
1:A:86:VAL:O	1:A:89:ILE:N	2.30	0.65
1:D:127:TRP:CD1	1:D:133:LEU:HD12	2.31	0.65
1:B:22:VAL:HA	1:B:99:LEU:O	1.98	0.64
1:C:24:VAL:HG21	1:C:33:LEU:HD22	1.78	0.64
1:D:134:LEU:HD23	1:D:134:LEU:N	2.12	0.64
1:B:25:THR:HB	1:B:104:ASP:OD2	1.98	0.64
1:D:147:PRO:O	1:D:149:THR:N	2.31	0.64
1:C:21:LEU:HD12	1:C:49:ALA:O	1.98	0.64
1:A:147:PRO:O	1:A:149:THR:N	2.31	0.63
1:D:25:THR:HB	1:D:104:ASP:OD2	1.98	0.63
1:A:61:SER:HB3	1:A:63:GLN:NE2	2.12	0.63
1:A:51:VAL:HG22	1:A:70:TYR:HB2	1.79	0.63
1:B:46:LEU:HD23	1:B:46:LEU:H	1.63	0.63
1:A:127:TRP:CD1	1:A:133:LEU:HD12	2.34	0.63
1:C:51:VAL:HG22	1:C:70:TYR:HB2	1.79	0.63
1:A:139:MET:HA	2:A:801:FMN:HN3	1.63	0.63
1:D:51:VAL:HG22	1:D:70:TYR:HB2	1.79	0.63
1:D:61:SER:HB3	1:D:63:GLN:HE22	1.62	0.63
1:B:127:TRP:CD1	1:B:133:LEU:HD12	2.34	0.63
1:B:97:LEU:HD11	1:B:134:LEU:CG	2.29	0.63
1:B:73:ALA:O	1:B:77:GLU:HG3	2.00	0.62
1:B:51:VAL:HG22	1:B:70:TYR:HB2	1.80	0.62
1:B:61:SER:HB3	1:B:63:GLN:NE2	2.14	0.62
1:D:97:LEU:HD11	1:D:134:LEU:CG	2.29	0.62
1:C:96:ASP:O	1:C:132:PRO:HD2	2.00	0.62
1:C:86:VAL:O	1:C:89:ILE:N	2.30	0.62
1:D:67:VAL:HG12	1:D:68:THR:N	2.15	0.62
1:A:29:ALA:HB3	1:A:102:PRO:HG3	1.82	0.61
1:A:96:ASP:O	1:A:132:PRO:HD2	2.00	0.61
1:C:147:PRO:O	1:C:149:THR:N	2.33	0.61
1:D:22:VAL:HA	1:D:99:LEU:O	2.01	0.61
1:B:185:GLY:O	1:B:188:VAL:N	2.32	0.61
1:B:29:ALA:HB3	1:B:102:PRO:HG3	1.82	0.61
1:A:137:PRO:CB	1:A:144:TRP:HZ3	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:GLY:O	1:D:188:VAL:N	2.34	0.61
1:C:48:VAL:CG1	1:C:49:ALA:H	2.13	0.61
1:D:48:VAL:CG1	1:D:49:ALA:H	2.12	0.61
1:B:96:ASP:O	1:B:132:PRO:HD2	2.01	0.60
1:C:20:VAL:HG13	1:C:48:VAL:HG22	1.80	0.60
1:D:73:ALA:O	1:D:77:GLU:HG3	2.00	0.60
1:A:100:VAL:HG21	1:A:124:MET:CE	2.30	0.60
1:B:100:VAL:HG21	1:B:124:MET:HE1	1.83	0.60
1:B:100:VAL:HG21	1:B:124:MET:CE	2.31	0.60
1:B:67:VAL:HG12	1:B:68:THR:N	2.16	0.60
1:C:67:VAL:HG12	1:C:68:THR:N	2.17	0.60
1:A:133:LEU:HD13	1:A:161:TYR:CD1	2.36	0.60
1:A:67:VAL:HG12	1:A:68:THR:N	2.16	0.60
1:C:133:LEU:HD13	1:C:161:TYR:CD1	2.35	0.60
1:D:96:ASP:O	1:D:132:PRO:HD2	2.02	0.60
1:A:48:VAL:CG1	1:A:49:ALA:H	2.11	0.60
1:D:29:ALA:HB3	1:D:102:PRO:HG3	1.82	0.59
1:C:100:VAL:HG21	1:C:124:MET:CE	2.32	0.59
1:D:137:PRO:HB2	1:D:144:TRP:HZ3	1.68	0.59
1:D:67:VAL:HG12	1:D:68:THR:H	1.68	0.59
1:D:100:VAL:HG21	1:D:124:MET:CE	2.33	0.59
1:D:86:VAL:O	1:D:89:ILE:N	2.34	0.58
1:B:48:VAL:CG1	1:B:49:ALA:H	2.13	0.58
1:A:137:PRO:HB2	1:A:144:TRP:HZ3	1.67	0.58
1:B:97:LEU:HD11	1:B:134:LEU:CD1	2.33	0.58
1:C:78:MET:HE1	1:C:87:LEU:HD13	1.86	0.58
1:D:132:PRO:HB2	1:D:134:LEU:HD21	1.85	0.58
1:C:135:PHE:CE1	1:C:137:PRO:HD3	2.39	0.58
1:A:100:VAL:HG21	1:A:124:MET:HE3	1.85	0.57
1:B:67:VAL:HG12	1:B:68:THR:H	1.69	0.57
1:A:48:VAL:CG1	1:A:49:ALA:N	2.67	0.57
1:B:133:LEU:HD13	1:B:161:TYR:CD1	2.39	0.57
1:A:137:PRO:HB2	1:A:144:TRP:CZ3	2.38	0.57
1:C:29:ALA:HB3	1:C:102:PRO:HG3	1.85	0.57
1:D:137:PRO:HB2	1:D:144:TRP:CZ3	2.40	0.57
1:B:137:PRO:CB	1:B:144:TRP:HZ3	2.18	0.57
1:B:20:VAL:O	1:B:48:VAL:HG13	2.05	0.57
1:D:137:PRO:CB	1:D:144:TRP:HZ3	2.18	0.57
1:C:24:VAL:HG11	1:C:33:LEU:HD22	1.87	0.57
1:D:149:THR:O	1:D:153:VAL:HG23	2.05	0.57
1:D:78:MET:HE1	1:D:87:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:PRO:CB	1:C:144:TRP:HZ3	2.17	0.56
1:C:48:VAL:CG1	1:C:49:ALA:N	2.68	0.56
1:C:67:VAL:HG12	1:C:68:THR:H	1.71	0.56
1:A:67:VAL:HG12	1:A:68:THR:H	1.71	0.56
1:B:116:CYS:SG	1:B:116:CYS:O	2.63	0.56
1:C:22:VAL:HA	1:C:99:LEU:O	2.05	0.56
1:C:135:PHE:HD1	1:C:137:PRO:HD3	1.67	0.56
1:C:185:GLY:O	1:C:188:VAL:N	2.39	0.56
1:B:56:ALA:C	1:B:58:HIS:H	2.08	0.56
1:D:56:ALA:C	1:D:58:HIS:H	2.07	0.56
1:C:61:SER:HB3	1:C:63:GLN:HE22	1.71	0.55
1:A:73:ALA:O	1:A:77:GLU:HG3	2.07	0.55
1:C:73:ALA:O	1:C:77:GLU:HG3	2.06	0.55
1:C:97:LEU:CD1	1:C:132:PRO:HG2	2.37	0.55
1:B:149:THR:O	1:B:153:VAL:HG23	2.07	0.55
1:B:86:VAL:O	1:B:89:ILE:N	2.37	0.55
1:A:92:ARG:HD3	1:A:93:ARG:HG3	1.89	0.54
1:B:20:VAL:CG2	1:B:46:LEU:HD12	2.37	0.54
1:A:185:GLY:O	1:A:188:VAL:N	2.39	0.54
1:A:97:LEU:HD13	1:A:132:PRO:HG2	1.89	0.54
1:B:137:PRO:HB2	1:B:144:TRP:HZ3	1.70	0.54
1:B:137:PRO:HB2	1:B:144:TRP:CZ3	2.41	0.54
1:C:137:PRO:HB2	1:C:144:TRP:HZ3	1.73	0.54
1:C:137:PRO:HB2	1:C:144:TRP:CZ3	2.43	0.54
1:A:33:LEU:HG	1:A:65:ILE:HD11	1.90	0.54
1:B:78:MET:HE1	1:B:87:LEU:HD13	1.89	0.54
1:D:116:CYS:SG	1:D:116:CYS:O	2.66	0.54
1:A:135:PHE:CE1	1:A:137:PRO:HD3	2.43	0.54
1:B:33:LEU:HG	1:B:65:ILE:HD11	1.88	0.54
1:C:97:LEU:HD13	1:C:132:PRO:HG2	1.89	0.53
1:B:97:LEU:CD1	1:B:132:PRO:HG2	2.38	0.53
1:A:116:CYS:O	1:A:116:CYS:SG	2.66	0.53
1:C:139:MET:HA	2:C:803:FMN:N3	2.22	0.53
1:D:31:LEU:HD12	1:D:59:PHE:O	2.08	0.53
1:A:97:LEU:CD1	1:A:132:PRO:HG2	2.38	0.53
1:C:24:VAL:HG21	1:C:33:LEU:CD2	2.38	0.53
1:D:135:PHE:CE1	1:D:137:PRO:HD3	2.44	0.53
1:D:133:LEU:HD13	1:D:161:TYR:CD1	2.42	0.53
1:A:56:ALA:C	1:A:58:HIS:H	2.10	0.53
1:C:116:CYS:O	1:C:116:CYS:SG	2.67	0.53
1:D:164:ILE:CG2	1:D:164:ILE:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:GLU:O	1:D:47:GLU:HG3	2.07	0.53
1:D:33:LEU:HG	1:D:65:ILE:HD11	1.91	0.52
1:B:133:LEU:O	1:B:161:TYR:O	2.27	0.52
1:B:24:VAL:HG11	1:B:33:LEU:HD22	1.90	0.52
1:B:22:VAL:O	1:B:50:VAL:HG13	2.10	0.52
1:D:133:LEU:O	1:D:161:TYR:O	2.27	0.52
1:B:20:VAL:HG23	1:B:46:LEU:HD12	1.91	0.52
1:B:97:LEU:HD13	1:B:132:PRO:HG2	1.91	0.51
1:A:24:VAL:HG21	1:A:33:LEU:HD22	1.92	0.51
1:A:33:LEU:CG	1:A:65:ILE:HD11	2.41	0.51
1:A:22:VAL:HA	1:A:99:LEU:O	2.10	0.51
1:C:133:LEU:O	1:C:161:TYR:O	2.29	0.51
1:A:135:PHE:C	1:A:136:CYS:SG	2.87	0.51
1:A:133:LEU:O	1:A:161:TYR:O	2.27	0.51
1:C:56:ALA:C	1:C:58:HIS:H	2.12	0.51
1:A:129:ARG:HB2	1:A:129:ARG:CZ	2.39	0.51
1:D:22:VAL:O	1:D:50:VAL:HG13	2.10	0.51
1:B:31:LEU:HD12	1:B:59:PHE:O	2.11	0.51
1:C:100:VAL:HG21	1:C:124:MET:HE1	1.92	0.51
1:C:164:ILE:O	1:C:164:ILE:CG2	2.59	0.51
1:D:100:VAL:HG21	1:D:124:MET:HE3	1.93	0.51
1:A:31:LEU:HD12	1:A:59:PHE:O	2.11	0.51
1:A:78:MET:HE1	1:A:87:LEU:HD13	1.93	0.51
1:A:147:PRO:O	1:A:148:ILE:C	2.49	0.50
1:A:61:SER:HB3	1:A:63:GLN:HE22	1.75	0.50
1:B:24:VAL:HB	1:B:52:THR:CG2	2.27	0.50
1:D:56:ALA:C	1:D:58:HIS:N	2.65	0.50
1:A:149:THR:O	1:A:153:VAL:HG23	2.11	0.50
1:B:61:SER:HB3	1:B:63:GLN:HE22	1.76	0.50
1:D:97:LEU:CD1	1:D:132:PRO:HG2	2.41	0.50
1:B:135:PHE:CE1	1:B:137:PRO:HD3	2.46	0.50
1:C:149:THR:O	1:C:153:VAL:HG23	2.10	0.50
1:C:55:ARG:O	1:C:58:HIS:HB2	2.11	0.50
1:A:55:ARG:O	1:A:58:HIS:HB2	2.11	0.50
1:A:146:HIS:CE1	1:A:148:ILE:HG13	2.30	0.50
1:C:185:GLY:O	1:C:186:THR:C	2.50	0.50
1:D:97:LEU:HD13	1:D:132:PRO:HG2	1.93	0.50
1:A:185:GLY:O	1:A:186:THR:C	2.50	0.50
1:A:22:VAL:O	1:A:50:VAL:HG13	2.12	0.49
1:C:31:LEU:HD12	1:C:59:PHE:O	2.12	0.49
1:B:164:ILE:O	1:B:164:ILE:CG2	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:PRO:O	1:C:148:ILE:C	2.51	0.49
1:D:139:MET:HA	2:D:804:FMN:N3	2.24	0.49
1:C:100:VAL:HG21	1:C:124:MET:HE3	1.94	0.49
1:C:33:LEU:HG	1:C:65:ILE:HD11	1.95	0.49
1:B:132:PRO:HB2	1:B:134:LEU:HD21	1.95	0.49
1:D:30:ALA:O	1:D:33:LEU:HB3	2.12	0.49
1:B:33:LEU:HD23	1:B:60:TYR:CD1	2.47	0.49
1:D:185:GLY:O	1:D:186:THR:C	2.50	0.49
1:D:55:ARG:O	1:D:58:HIS:HB2	2.13	0.48
1:C:52:THR:HG21	1:C:60:TYR:HH	1.72	0.48
1:D:135:PHE:HD1	1:D:137:PRO:HD3	1.77	0.48
1:D:146:HIS:CG	1:D:147:PRO:HD2	2.48	0.48
1:D:102:PRO:HB2	1:D:138:ALA:HB3	1.95	0.48
1:B:146:HIS:CG	1:B:147:PRO:HD2	2.48	0.48
1:B:185:GLY:O	1:B:186:THR:C	2.52	0.48
1:B:33:LEU:CG	1:B:65:ILE:HD11	2.44	0.48
1:D:65:ILE:CG2	1:D:65:ILE:O	2.61	0.48
1:A:164:ILE:CG2	1:A:164:ILE:O	2.60	0.48
1:A:71:SER:O	1:A:74:ASP:HB2	2.13	0.48
1:B:146:HIS:ND1	1:B:147:PRO:N	2.62	0.47
1:D:100:VAL:HG21	1:D:124:MET:HE1	1.95	0.47
1:A:129:ARG:HB2	1:A:129:ARG:NH1	2.29	0.47
1:D:147:PRO:O	1:D:148:ILE:C	2.53	0.47
1:B:24:VAL:HG21	1:B:33:LEU:HD22	1.96	0.47
1:C:108:LEU:HG	1:C:152:GLN:OE1	2.14	0.47
1:B:56:ALA:C	1:B:58:HIS:N	2.67	0.47
1:D:139:MET:HB2	1:D:140:ASN:H	1.50	0.47
1:D:154:ASP:O	1:D:157:LYS:N	2.48	0.47
1:D:33:LEU:HD23	1:D:60:TYR:CD1	2.49	0.47
1:D:125:ARG:O	1:D:125:ARG:HG3	2.14	0.47
1:A:124:MET:O	1:A:127:TRP:HB2	2.15	0.47
1:A:135:PHE:HD1	1:A:137:PRO:HD3	1.74	0.47
1:B:147:PRO:O	1:B:148:ILE:C	2.52	0.47
1:C:102:PRO:HB2	1:C:138:ALA:HB3	1.96	0.47
1:C:124:MET:O	1:C:127:TRP:HB2	2.15	0.47
1:D:20:VAL:HG11	1:D:48:VAL:HG22	1.93	0.47
1:B:127:TRP:HA	1:B:127:TRP:CE3	2.50	0.47
1:B:102:PRO:HB2	1:B:138:ALA:HB3	1.95	0.47
1:B:55:ARG:O	1:B:58:HIS:HB2	2.14	0.47
1:A:33:LEU:HD21	1:A:65:ILE:HD11	1.97	0.47
1:B:140:ASN:O	1:B:141:THR:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:VAL:O	1:C:50:VAL:HG13	2.15	0.47
1:C:71:SER:O	1:C:74:ASP:HB2	2.15	0.47
1:B:71:SER:N	1:B:74:ASP:OD2	2.40	0.47
1:C:146:HIS:CG	1:C:147:PRO:HD2	2.50	0.47
1:A:56:ALA:C	1:A:58:HIS:N	2.68	0.46
1:A:92:ARG:HH11	1:A:92:ARG:HG2	1.80	0.46
1:A:97:LEU:HD11	1:A:134:LEU:CD2	2.45	0.46
1:D:127:TRP:CE3	1:D:127:TRP:HA	2.50	0.46
1:A:102:PRO:HB2	1:A:138:ALA:HB3	1.96	0.46
1:C:139:MET:HB2	1:C:140:ASN:H	1.49	0.46
1:C:99:LEU:HD12	1:C:134:LEU:O	2.16	0.46
1:A:146:HIS:CG	1:A:147:PRO:HD2	2.51	0.46
1:C:20:VAL:HG11	1:C:48:VAL:HG22	1.90	0.46
1:C:146:HIS:HE1	1:C:148:ILE:CG1	2.20	0.46
1:A:129:ARG:CZ	1:A:129:ARG:CB	2.94	0.46
1:C:127:TRP:HA	1:C:127:TRP:CE3	2.51	0.46
1:C:56:ALA:C	1:C:58:HIS:N	2.69	0.46
1:A:86:VAL:O	1:A:87:LEU:C	2.54	0.45
1:B:120:LEU:O	1:B:122:CYS:N	2.50	0.45
1:B:140:ASN:OD1	1:B:142:ALA:N	2.49	0.45
1:C:163:GLU:O	1:C:164:ILE:HG13	2.16	0.45
1:B:92:ARG:C	1:B:92:ARG:HD2	2.37	0.45
1:C:115:ILE:HG22	1:C:115:ILE:O	2.16	0.45
1:D:86:VAL:O	1:D:87:LEU:C	2.54	0.45
1:B:86:VAL:O	1:B:87:LEU:C	2.54	0.45
1:C:193:GLU:O	1:C:194:VAL:C	2.54	0.45
1:A:100:VAL:HG21	1:A:124:MET:HE1	1.99	0.45
1:A:99:LEU:HD12	1:A:134:LEU:O	2.17	0.45
1:B:30:ALA:O	1:B:33:LEU:HB3	2.16	0.45
1:B:125:ARG:O	1:B:125:ARG:HG3	2.16	0.45
1:B:148:ILE:O	1:B:152:GLN:N	2.50	0.45
1:C:32:LYS:C	1:C:34:PRO:HD2	2.36	0.45
1:B:157:LYS:C	1:B:160:GLY:H	2.15	0.45
1:A:157:LYS:C	1:A:160:GLY:H	2.16	0.45
1:A:97:LEU:HD11	1:A:134:LEU:HD21	1.98	0.45
1:C:86:VAL:O	1:C:87:LEU:C	2.55	0.45
1:D:140:ASN:OD1	1:D:142:ALA:N	2.49	0.45
1:A:129:ARG:CA	1:A:129:ARG:NE	2.74	0.44
1:A:108:LEU:HG	1:A:152:GLN:OE1	2.18	0.44
1:C:61:SER:HB3	1:C:63:GLN:CD	2.37	0.44
1:D:127:TRP:CG	1:D:128:ASP:N	2.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:VAL:HB	1:D:52:THR:CG2	2.31	0.44
1:D:61:SER:CB	1:D:63:GLN:NE2	2.79	0.44
1:B:97:LEU:HD11	1:B:134:LEU:HD11	2.00	0.44
1:D:110:LYS:HG2	1:D:115:ILE:HG21	2.00	0.44
1:A:125:ARG:HG3	1:A:125:ARG:O	2.17	0.44
1:D:140:ASN:O	1:D:141:THR:C	2.56	0.44
1:B:135:PHE:HD1	1:B:137:PRO:HD3	1.78	0.44
1:A:61:SER:HB3	1:A:63:GLN:CD	2.38	0.44
1:A:71:SER:N	1:A:74:ASP:OD2	2.43	0.44
1:A:25:THR:C	1:A:56:ALA:HB2	2.38	0.44
1:A:33:LEU:CD2	1:A:65:ILE:HD11	2.48	0.44
1:C:30:ALA:O	1:C:33:LEU:HB3	2.18	0.43
1:D:56:ALA:O	1:D:58:HIS:N	2.50	0.43
1:A:127:TRP:CE3	1:A:127:TRP:HA	2.53	0.43
1:D:24:VAL:HG21	1:D:33:LEU:HD22	2.00	0.43
1:B:124:MET:O	1:B:127:TRP:HB2	2.18	0.43
1:B:163:GLU:O	1:B:164:ILE:HG13	2.18	0.43
1:D:111:VAL:HG12	1:D:156:LEU:HD11	2.00	0.43
1:B:109:GLY:HA2	1:B:152:GLN:NE2	2.34	0.43
1:B:163:GLU:O	1:B:164:ILE:CG1	2.66	0.43
1:B:89:ILE:HD12	1:B:89:ILE:HA	1.78	0.43
1:C:25:THR:C	1:C:56:ALA:HB2	2.38	0.43
1:C:31:LEU:HD12	1:C:31:LEU:HA	1.89	0.43
1:D:148:ILE:O	1:D:152:GLN:HB2	2.18	0.43
1:D:22:VAL:O	1:D:50:VAL:HA	2.19	0.43
1:A:144:TRP:C	1:A:146:HIS:H	2.22	0.43
1:D:148:ILE:O	1:D:152:GLN:N	2.51	0.43
1:A:115:ILE:HG22	1:A:115:ILE:O	2.18	0.43
1:A:139:MET:HB2	1:A:140:ASN:H	1.52	0.43
1:C:110:LYS:HG2	1:C:115:ILE:HG21	2.01	0.43
1:D:146:HIS:ND1	1:D:147:PRO:N	2.66	0.43
1:D:89:ILE:HA	1:D:89:ILE:HD13	1.81	0.43
1:A:127:TRP:CG	1:A:128:ASP:N	2.87	0.43
1:D:124:MET:O	1:D:127:TRP:HB2	2.19	0.43
1:A:146:HIS:HE1	1:A:148:ILE:CG1	2.18	0.43
1:A:193:GLU:O	1:A:194:VAL:C	2.58	0.42
1:C:137:PRO:HB3	1:C:144:TRP:HZ3	1.84	0.42
1:A:137:PRO:HB3	1:A:144:TRP:HZ3	1.84	0.42
1:D:163:GLU:O	1:D:164:ILE:HG13	2.19	0.42
1:A:86:VAL:HG12	1:A:88:HIS:ND1	2.34	0.42
1:D:144:TRP:C	1:D:146:HIS:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:SER:N	1:D:74:ASP:OD2	2.40	0.42
1:B:144:TRP:C	1:B:146:HIS:H	2.22	0.42
1:B:47:GLU:HG3	1:B:47:GLU:O	2.19	0.42
1:C:150:ALA:C	1:C:152:GLN:H	2.23	0.42
1:C:61:SER:CB	1:C:63:GLN:NE2	2.81	0.42
1:A:28:VAL:HG12	1:A:31:LEU:HD22	2.01	0.42
1:B:139:MET:HA	2:B:802:FMN:N3	2.29	0.42
1:B:108:LEU:HG	1:B:152:GLN:OE1	2.20	0.42
1:C:109:GLY:HA2	1:C:152:GLN:NE2	2.34	0.42
1:C:140:ASN:OD1	1:C:142:ALA:N	2.51	0.42
1:D:157:LYS:C	1:D:160:GLY:H	2.16	0.42
1:A:163:GLU:O	1:A:164:ILE:HG13	2.20	0.42
1:C:157:LYS:C	1:C:160:GLY:H	2.15	0.42
1:C:22:VAL:O	1:C:50:VAL:HA	2.20	0.42
1:A:141:THR:O	1:A:145:GLU:N	2.44	0.42
1:A:163:GLU:O	1:A:164:ILE:CG1	2.68	0.42
1:B:127:TRP:CG	1:B:128:ASP:N	2.87	0.42
1:B:75:GLU:OE1	1:B:88:HIS:ND1	2.51	0.42
1:C:163:GLU:O	1:C:164:ILE:CG1	2.68	0.42
1:A:86:VAL:HG12	1:A:88:HIS:HD1	1.84	0.42
1:C:125:ARG:HG3	1:C:125:ARG:O	2.19	0.42
1:C:144:TRP:C	1:C:146:HIS:H	2.23	0.42
1:D:120:LEU:O	1:D:122:CYS:N	2.53	0.42
1:D:75:GLU:OE1	1:D:88:HIS:ND1	2.53	0.42
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.90	0.41
1:B:61:SER:HB3	1:B:63:GLN:CD	2.40	0.41
1:C:111:VAL:HG12	1:C:156:LEU:HD11	2.02	0.41
1:D:109:GLY:HA2	1:D:152:GLN:NE2	2.35	0.41
1:D:164:ILE:O	1:D:165:PRO:C	2.59	0.41
1:A:150:ALA:C	1:A:152:GLN:H	2.23	0.41
1:C:164:ILE:O	1:C:165:PRO:C	2.59	0.41
1:A:146:HIS:ND1	1:A:147:PRO:N	2.68	0.41
1:B:110:LYS:HG2	1:B:115:ILE:HG21	2.03	0.41
1:B:33:LEU:N	1:B:34:PRO:CD	2.84	0.41
1:C:120:LEU:O	1:C:122:CYS:N	2.53	0.41
1:C:28:VAL:HG12	1:C:31:LEU:HD22	2.03	0.41
1:D:108:LEU:HG	1:D:152:GLN:OE1	2.20	0.41
1:B:148:ILE:O	1:B:152:GLN:HB2	2.20	0.41
1:B:22:VAL:O	1:B:50:VAL:HA	2.21	0.41
1:A:136:CYS:SG	1:A:164:ILE:HB	2.61	0.41
1:D:163:GLU:O	1:D:164:ILE:CG1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:LEU:HD12	1:D:33:LEU:O	2.20	0.41
1:D:151:GLN:O	1:D:155:GLN:CB	2.69	0.41
1:D:25:THR:C	1:D:56:ALA:HB2	2.41	0.41
1:A:100:VAL:HG12	1:A:100:VAL:O	2.20	0.41
1:A:32:LYS:C	1:A:34:PRO:HD2	2.40	0.41
1:A:81:SER:N	1:A:84:ASP:OD1	2.54	0.41
1:B:150:ALA:C	1:B:152:GLN:N	2.75	0.41
1:B:55:ARG:HD2	1:B:55:ARG:HA	1.86	0.41
1:B:56:ALA:O	1:B:58:HIS:N	2.54	0.41
2:B:802:FMN:H9	2:B:802:FMN:H1'1	1.94	0.41
1:B:146:HIS:CG	1:B:147:PRO:CD	3.04	0.40
1:B:28:VAL:HG12	1:B:31:LEU:HD22	2.02	0.40
1:A:164:ILE:O	1:A:165:PRO:C	2.59	0.40
1:A:55:ARG:HH11	1:A:55:ARG:HG2	1.86	0.40
1:D:86:VAL:HB	1:D:89:ILE:HB	2.04	0.40
1:B:31:LEU:HD12	1:B:31:LEU:HA	1.91	0.40
1:D:146:HIS:HE1	1:D:148:ILE:CG1	2.19	0.40
1:D:146:HIS:CE1	1:D:148:ILE:HG13	2.29	0.40
1:A:20:VAL:HG13	1:A:48:VAL:CG2	2.37	0.40
1:D:28:VAL:HG12	1:D:31:LEU:HD22	2.04	0.40
1:C:136:CYS:O	1:C:137:PRO:C	2.60	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	154/206 (75%)	115 (75%)	27 (18%)	12 (8%)	1	2
1	B	149/206 (72%)	115 (77%)	19 (13%)	15 (10%)	0	1
1	C	154/206 (75%)	111 (72%)	28 (18%)	15 (10%)	0	1
1	D	149/206 (72%)	114 (76%)	21 (14%)	14 (9%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	606/824 (74%)	455 (75%)	95 (16%)	56 (9%)	1 1

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	148	ILE
1	A	192	LYS
1	B	147	PRO
1	B	148	ILE
1	C	147	PRO
1	C	148	ILE
1	C	192	LYS
1	D	147	PRO
1	D	148	ILE
1	A	162	VAL
1	B	127	TRP
1	B	162	VAL
1	C	162	VAL
1	D	127	TRP
1	D	162	VAL
1	A	127	TRP
1	A	164	ILE
1	A	186	THR
1	B	17	LYS
1	B	121	THR
1	B	164	ILE
1	B	186	THR
1	C	127	TRP
1	C	164	ILE
1	C	186	THR
1	D	164	ILE
1	D	186	THR
1	A	40	LEU
1	A	87	LEU
1	B	87	LEU
1	B	142	ALA
1	B	190	LYS
1	C	16	ARG
1	C	40	LEU
1	C	87	LEU
1	C	121	THR

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Mol	Chain	Res	Type
1	D	87	LEU
1	A	145	GLU
1	B	40	LEU
1	B	145	GLU
1	C	145	GLU
1	C	188	VAL
1	D	57	LYS
1	D	121	THR
1	D	142	ALA
1	D	145	GLU
1	D	190	LYS
1	A	160	GLY
1	A	188	VAL
1	B	160	GLY
1	B	188	VAL
1	C	160	GLY
1	D	160	GLY
1	D	188	VAL
1	C	33	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/172 (58%)	88 (88%)	12 (12%)	5	14
1	B	100/172 (58%)	90 (90%)	10 (10%)	7	22
1	C	97/172 (56%)	89 (92%)	8 (8%)	11	31
1	D	98/172 (57%)	89 (91%)	9 (9%)	9	26
All	All	395/688 (57%)	356 (90%)	39 (10%)	8	23

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	65	ILE

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Mol	Chain	Res	Type
1	A	92	ARG
1	A	103	LEU
1	A	107	THR
1	A	116	CYS
1	A	129	ARG
1	A	134	LEU
1	A	136	CYS
1	A	139	MET
1	A	140	ASN
1	A	156	LEU
1	B	46	LEU
1	B	55	ARG
1	B	89	ILE
1	B	103	LEU
1	B	107	THR
1	B	116	CYS
1	B	134	LEU
1	B	139	MET
1	B	140	ASN
1	B	156	LEU
1	C	46	LEU
1	C	55	ARG
1	C	65	ILE
1	C	103	LEU
1	C	116	CYS
1	C	139	MET
1	C	140	ASN
1	C	156	LEU
1	D	46	LEU
1	D	47	GLU
1	D	55	ARG
1	D	116	CYS
1	D	134	LEU
1	D	139	MET
1	D	140	ASN
1	D	154	ASP
1	D	156	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS

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Mol	Chain	Res	Type
1	A	146	HIS
1	B	146	HIS
1	B	151	GLN
1	C	146	HIS
1	D	146	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	FMN	D	804	-	27,32,33	2.54	8 (29%)	32,47,50	2.77	11 (34%)
2	FMN	B	802	-	31,33,33	2.37	11 (35%)	40,50,50	2.57	12 (30%)
2	FMN	A	801	-	31,33,33	2.74	12 (38%)	40,50,50	2.65	12 (30%)
2	FMN	C	803	-	31,33,33	2.72	13 (41%)	40,50,50	2.61	12 (30%)

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	D	804	-	-	0/15/17/18	0/3/3/3
2	FMN	B	802	-	-	0/18/18/18	0/3/3/3
2	FMN	A	801	-	-	0/18/18/18	0/3/3/3
2	FMN	C	803	-	-	0/18/18/18	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FMN	C4A-C10	6.57	1.45	1.38
2	C	803	FMN	C4A-C10	6.33	1.45	1.38
2	C	803	FMN	C4-C4A	5.69	1.51	1.41
2	D	804	FMN	C4-C4A	5.58	1.51	1.41
2	A	801	FMN	C4-C4A	5.52	1.50	1.41
2	D	804	FMN	C1'-N10	5.45	1.53	1.48
2	A	801	FMN	C1'-N10	5.38	1.53	1.48
2	A	801	FMN	C9A-N10	5.36	1.45	1.38
2	C	803	FMN	C1'-N10	5.35	1.53	1.48
2	B	802	FMN	C4-C4A	5.25	1.50	1.41
2	C	803	FMN	C9A-N10	4.96	1.45	1.38
2	B	802	FMN	C4A-C10	4.85	1.43	1.38
2	D	804	FMN	C9A-N10	4.82	1.45	1.38
2	B	802	FMN	C1'-N10	4.80	1.53	1.48
2	D	804	FMN	C4A-C10	4.79	1.43	1.38
2	C	803	FMN	C4-N3	4.67	1.41	1.33
2	A	801	FMN	C4-N3	4.61	1.41	1.33
2	B	802	FMN	C9A-N10	4.30	1.44	1.38
2	B	802	FMN	C4-N3	4.18	1.40	1.33
2	C	803	FMN	C8-C7	3.95	1.50	1.40
2	D	804	FMN	C4-N3	3.89	1.39	1.33
2	A	801	FMN	C8-C7	3.81	1.50	1.40
2	D	804	FMN	C9-C9A	3.64	1.48	1.40
2	D	804	FMN	C8-C7	3.53	1.49	1.40
2	A	801	FMN	C9-C9A	3.45	1.47	1.40
2	C	803	FMN	C9-C9A	3.42	1.47	1.40
2	B	802	FMN	C8-C7	3.18	1.48	1.40
2	A	801	FMN	P-O1P	-3.16	1.40	1.50
2	B	802	FMN	C9-C9A	2.95	1.46	1.40
2	C	803	FMN	P-O1P	-2.90	1.41	1.50
2	B	802	FMN	P-O1P	-2.80	1.41	1.50
2	B	802	FMN	C2-N3	2.72	1.43	1.38
2	C	803	FMN	C10-N1	2.66	1.36	1.33
2	C	803	FMN	P-O2P	-2.61	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FMN	C2-N3	2.54	1.43	1.38
2	A	801	FMN	P-O2P	-2.46	1.45	1.54
2	A	801	FMN	C10-N1	2.43	1.36	1.33
2	C	803	FMN	C2-N3	2.42	1.43	1.38
2	B	802	FMN	P-O3P	2.36	1.64	1.54
2	D	804	FMN	C2-N3	2.28	1.42	1.38
2	A	801	FMN	P-O3P	2.17	1.63	1.54
2	C	803	FMN	C9A-C5A	2.16	1.46	1.42
2	C	803	FMN	P-O3P	2.09	1.62	1.54
2	B	802	FMN	P-O2P	-2.09	1.46	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FMN	C4-N3-C2	9.93	123.52	115.14
2	C	803	FMN	C4-N3-C2	9.88	123.49	115.14
2	D	804	FMN	C4-N3-C2	9.29	122.99	115.14
2	B	802	FMN	C4-N3-C2	9.05	122.79	115.14
2	D	804	FMN	C4A-N5-C5A	6.39	123.16	116.77
2	B	802	FMN	C4A-N5-C5A	6.27	123.03	116.77
2	A	801	FMN	C4A-N5-C5A	6.19	122.95	116.77
2	C	803	FMN	C4A-N5-C5A	6.03	122.80	116.77
2	D	804	FMN	C1'-N10-C10	5.19	123.06	118.41
2	B	802	FMN	C1'-N10-C10	5.06	122.94	118.41
2	A	801	FMN	C1'-N10-C10	5.02	122.90	118.41
2	A	801	FMN	C4A-C4-N3	-4.97	116.64	123.43
2	C	803	FMN	C4A-C4-N3	-4.93	116.69	123.43
2	C	803	FMN	C1'-N10-C10	4.81	122.71	118.41
2	D	804	FMN	C4A-C4-N3	-4.56	117.20	123.43
2	B	802	FMN	C4A-C4-N3	-4.50	117.27	123.43
2	D	804	FMN	C1'-N10-C9A	-4.10	115.06	118.29
2	B	802	FMN	C1'-N10-C9A	-4.05	115.10	118.29
2	A	801	FMN	O5'-C5'-C4'	-3.99	98.70	109.36
2	C	803	FMN	O5'-C5'-C4'	-3.70	99.47	109.36
2	A	801	FMN	C1'-N10-C9A	-3.61	115.45	118.29
2	B	802	FMN	O5'-C5'-C4'	-3.56	99.85	109.36
2	C	803	FMN	C1'-N10-C9A	-3.24	115.74	118.29
2	C	803	FMN	O3'-C3'-C2'	-3.21	101.05	108.81
2	A	801	FMN	C4A-C10-N10	-3.13	117.08	120.30
2	D	804	FMN	O3'-C3'-C2'	-3.10	101.32	108.81
2	B	802	FMN	O3'-C3'-C2'	-3.09	101.34	108.81
2	A	801	FMN	O3'-C3'-C2'	-2.97	101.64	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	803	FMN	C4A-C10-N10	-2.92	117.30	120.30
2	D	804	FMN	C4-C4A-C10	-2.87	118.05	119.95
2	C	803	FMN	C4-C4A-C10	-2.84	118.07	119.95
2	D	804	FMN	C4A-C10-N10	-2.84	117.38	120.30
2	B	802	FMN	C4A-C10-N10	-2.81	117.42	120.30
2	B	802	FMN	C4-C4A-C10	-2.81	118.09	119.95
2	A	801	FMN	C4-C4A-C10	-2.66	118.19	119.95
2	C	803	FMN	O3'-C3'-C4'	-2.52	102.72	108.81
2	A	801	FMN	O3'-C3'-C4'	-2.51	102.74	108.81
2	B	802	FMN	O3'-C3'-C4'	-2.50	102.78	108.81
2	B	802	FMN	O2'-C2'-C1'	2.46	115.51	109.59
2	D	804	FMN	O3'-C3'-C4'	-2.31	103.22	108.81
2	A	801	FMN	O2'-C2'-C1'	2.31	115.15	109.59
2	D	804	FMN	O2'-C2'-C1'	2.27	115.07	109.59
2	D	804	FMN	C5A-C9A-N10	-2.21	116.11	117.72
2	C	803	FMN	O2P-P-O1P	2.17	119.16	110.68
2	C	803	FMN	O2'-C2'-C1'	2.15	114.77	109.59
2	A	801	FMN	O2P-P-O1P	2.11	118.94	110.68
2	B	802	FMN	C5A-C9A-N10	-2.06	116.22	117.72

There are no chirality outliers.

There are no torsion outliers.

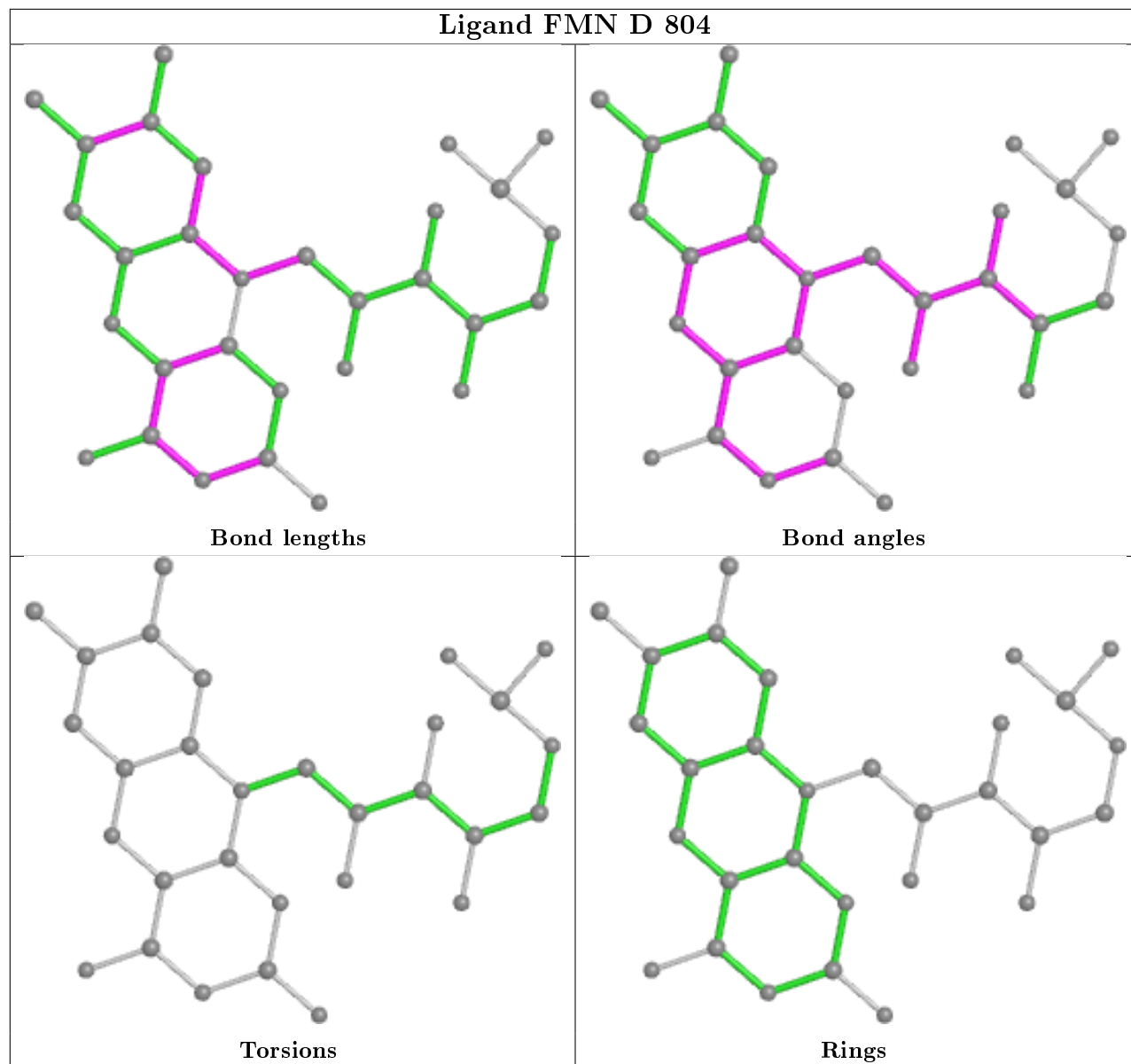
There are no ring outliers.

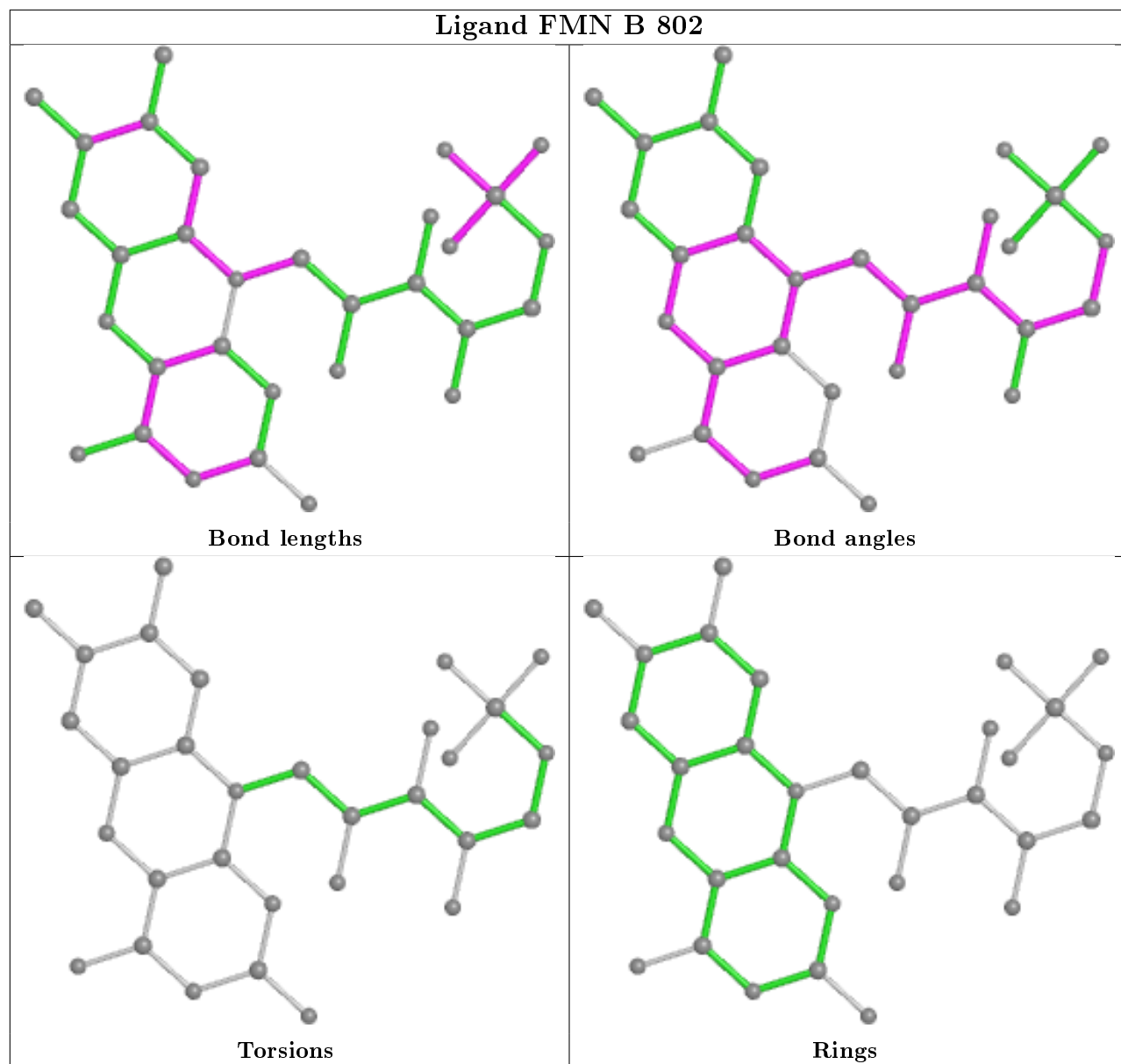
4 monomers are involved in 8 short contacts:

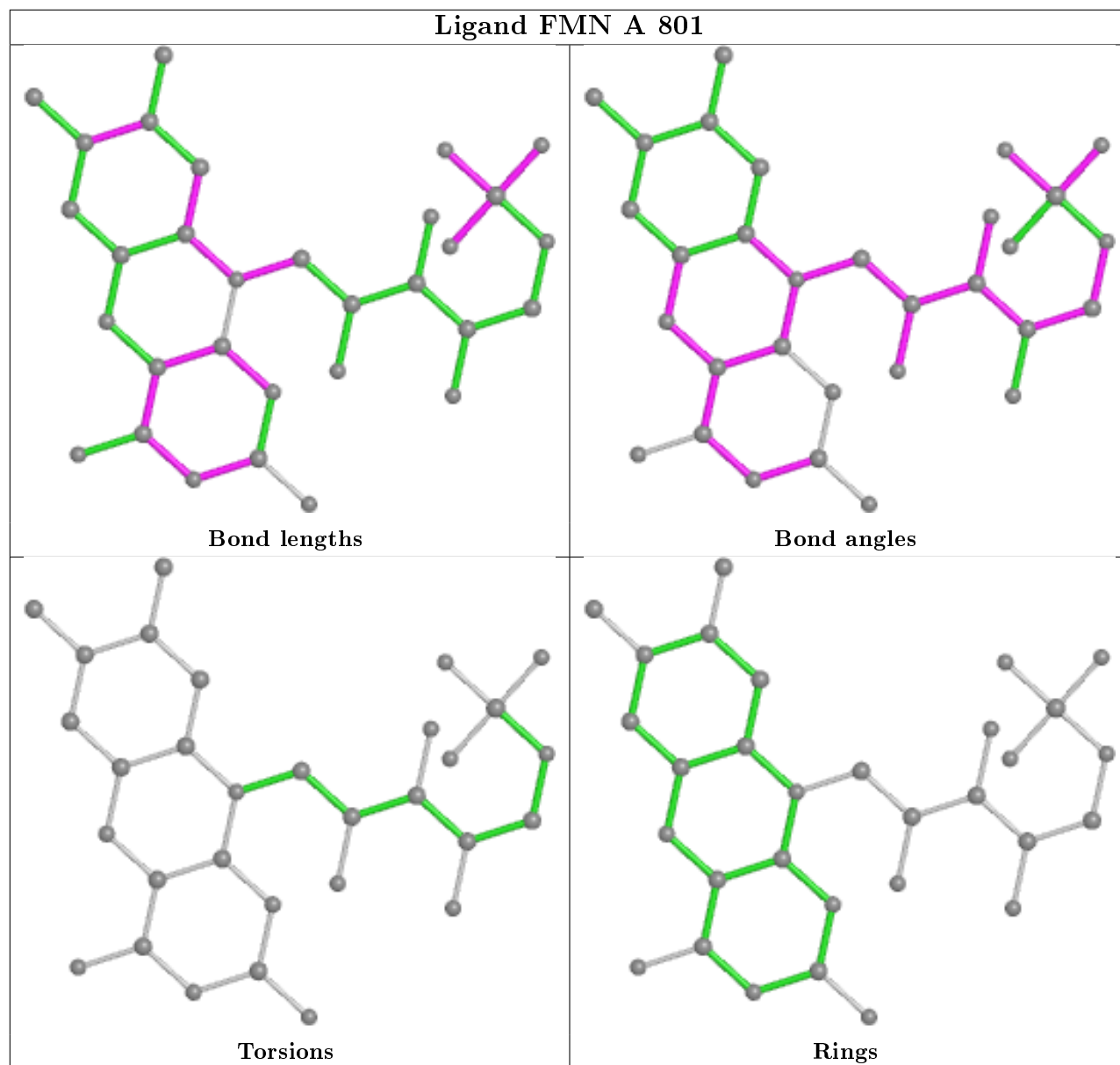
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	804	FMN	2	0
2	B	802	FMN	3	0
2	A	801	FMN	1	0
2	C	803	FMN	2	0

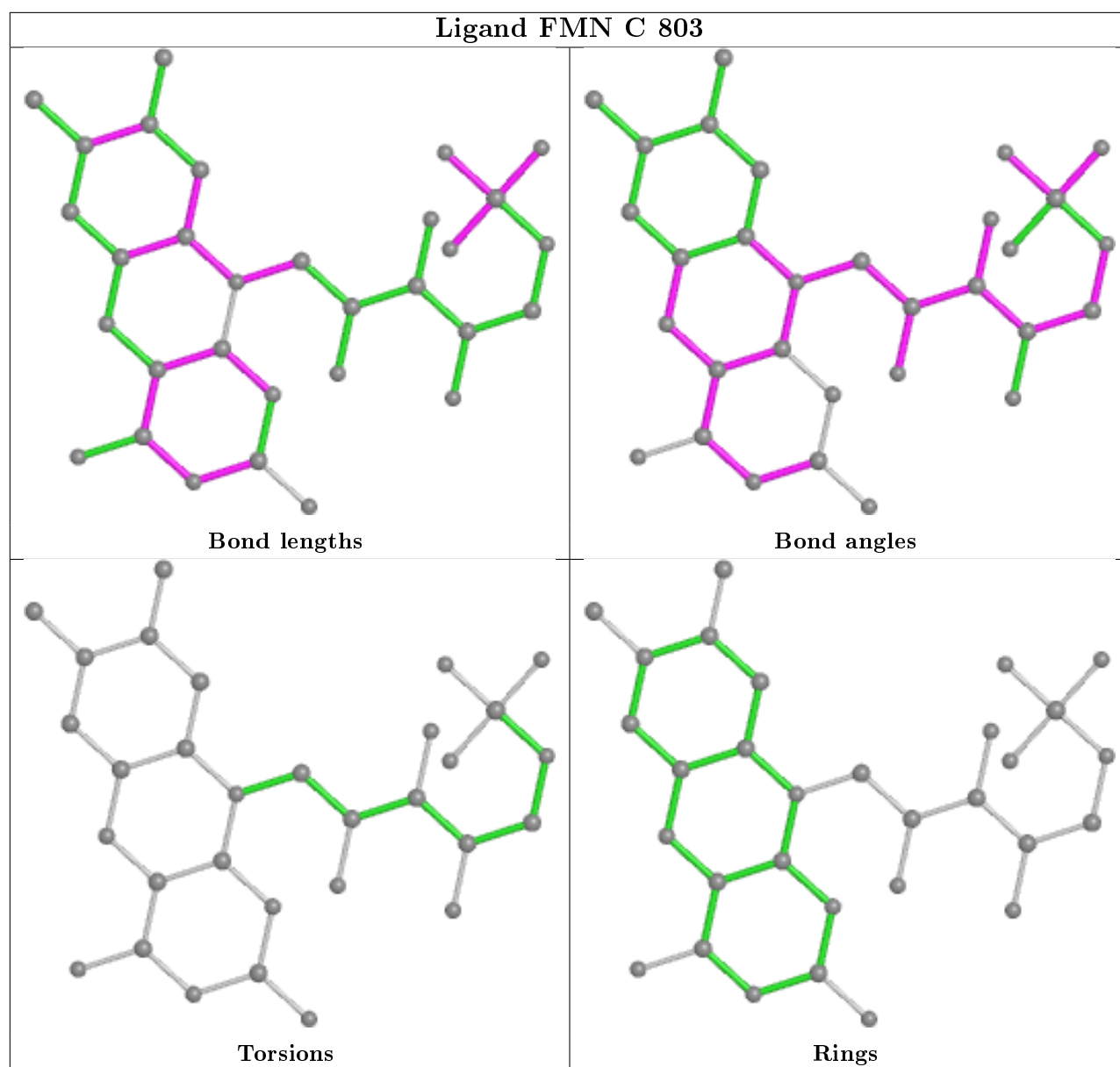
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.









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	160/206 (77%)	-0.05	3 (1%) 66 65	24, 66, 106, 150	0
1	B	155/206 (75%)	0.06	2 (1%) 77 77	22, 68, 114, 150	0
1	C	160/206 (77%)	-0.10	1 (0%) 89 89	23, 65, 114, 149	0
1	D	155/206 (75%)	-0.02	3 (1%) 66 65	19, 65, 118, 151	0
All	All	630/824 (76%)	-0.03	9 (1%) 75 76	19, 66, 115, 151	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	SER	3.5
1	C	144	TRP	2.7
1	A	126	ALA	2.5
1	A	122	CYS	2.3
1	A	95	ALA	2.2
1	D	144	TRP	2.1
1	B	101	ALA	2.0
1	D	45	GLY	2.0
1	B	46	LEU	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 carbohydrates in this entry.

6.4 Ligands ⓘ

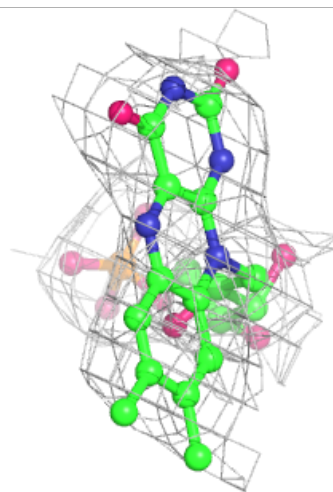
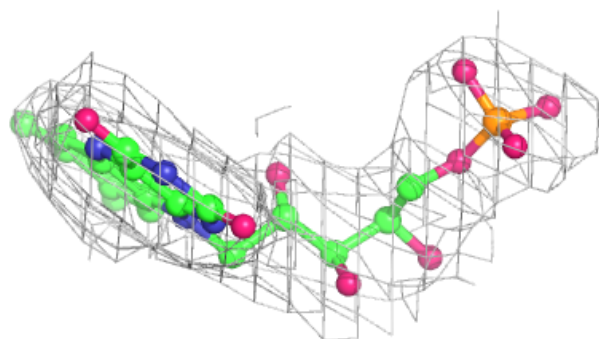
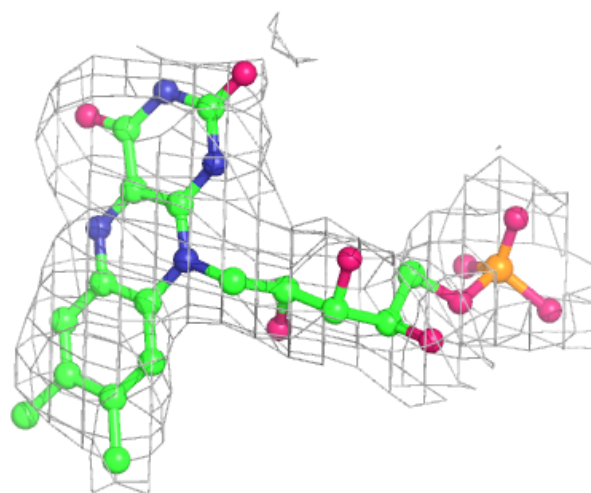
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	C	803	31/31	0.93	0.22	67,67,67,67	0
2	FMN	A	801	31/31	0.93	0.22	63,63,63,63	0
2	FMN	D	804	30/31	0.94	0.22	62,62,62,62	0
2	FMN	B	802	31/31	0.94	0.19	59,59,59,59	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.

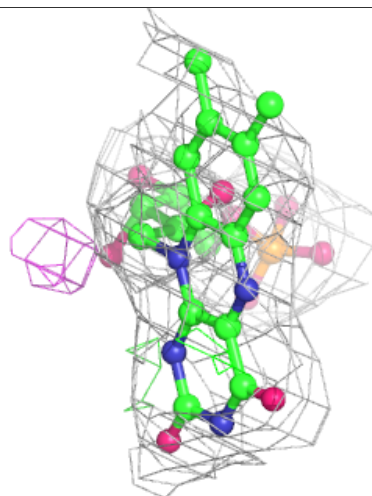
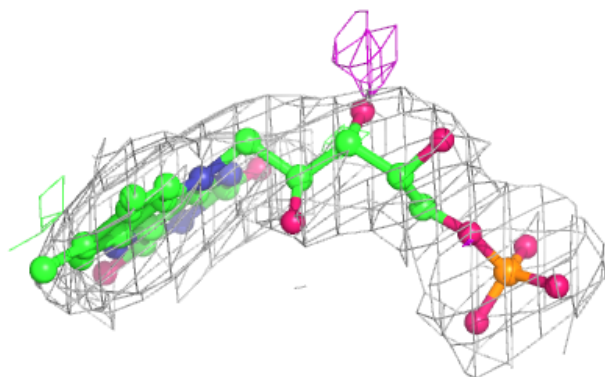
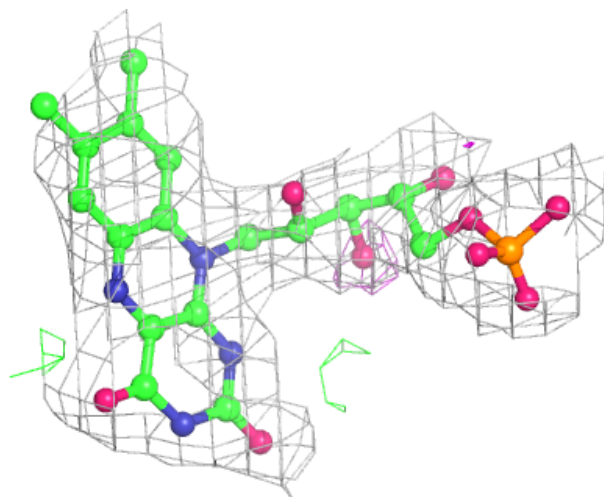
Electron density around FMN C 803:

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



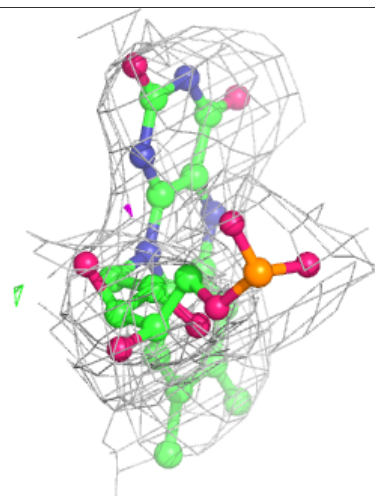
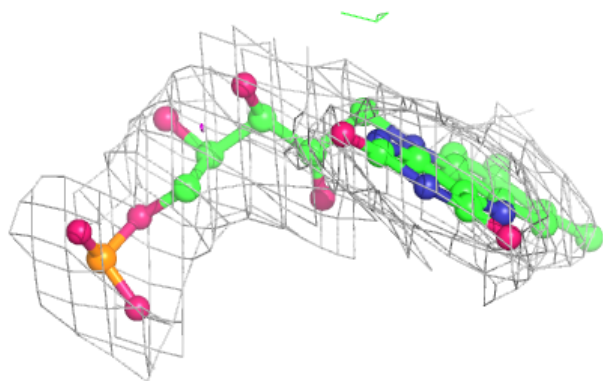
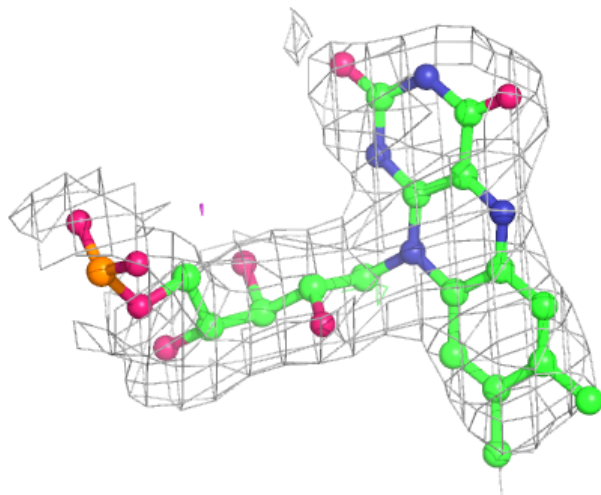
Electron density around FMN A 801:

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



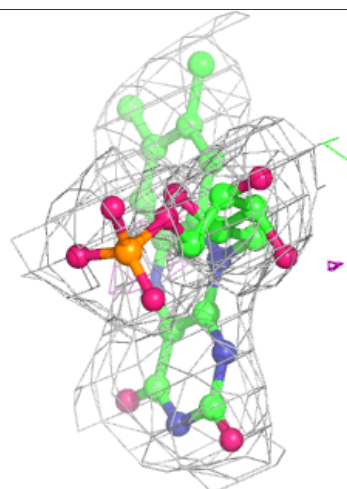
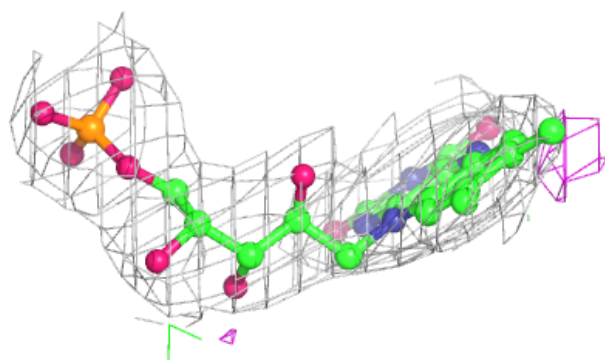
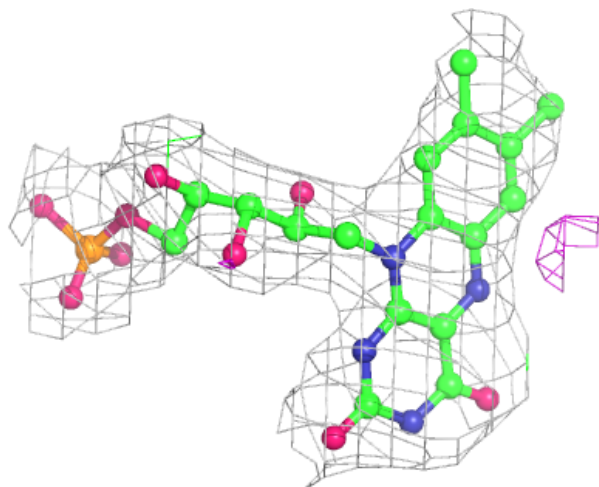
Electron density around FMN D 804:

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



Electron density around FMN B 802:

$2mF_o-DF_c$ (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.