Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 02:17 PM EDT

PDB ID	:	7TBQ
Title	:	LOV2-DARPIN fusion : D7
Authors	:	Mittl, P.
Deposited on	:	2021-12-22
Resolution	:	2.68 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

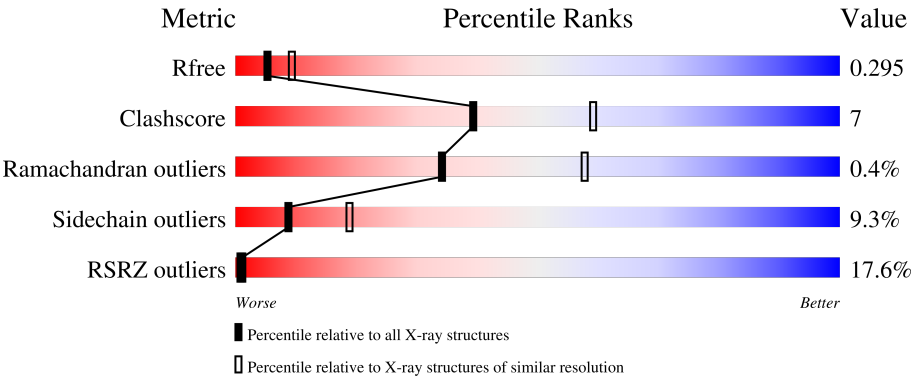
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	377	5% 76% 21%
1	B	377	3% 75% 23%
1	C	377	3% 76% 21%
1	D	377	3% 76% 21%
1	E	377	74% 73% 23%

2 Entry composition

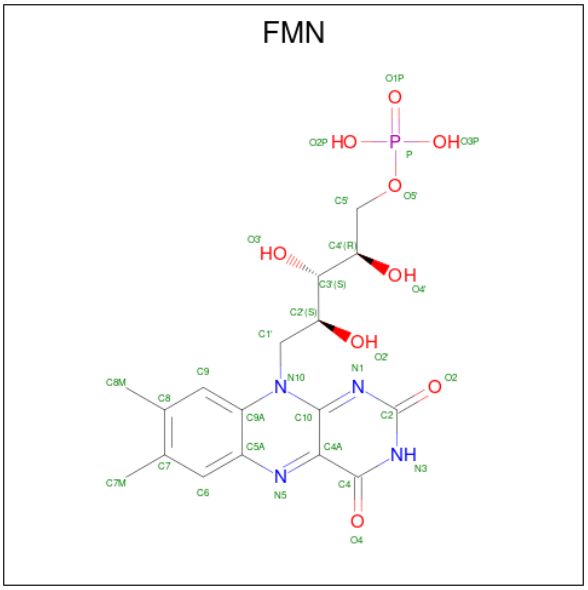
There are 6 unique types of molecules in this entry. The entry contains 17568 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D7 LOV2-DARPin fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2897	1829	505	559	4			
1	B	375	Total	C	N	O	S	0	0	0
			2897	1829	505	559	4			
1	C	375	Total	C	N	O	S	0	0	0
			2897	1829	505	559	4			
1	D	375	Total	C	N	O	S	0	0	0
			2897	1829	505	559	4			
1	E	371	Total	C	N	O	S	0	371	0
			5744	3626	1002	1108	8			

- 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		

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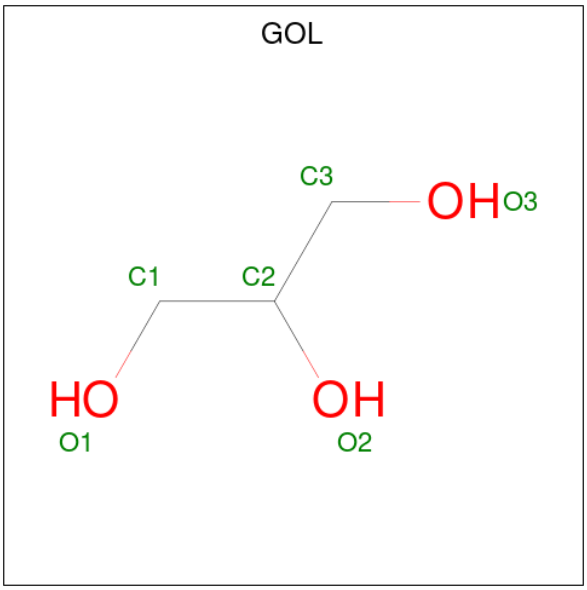
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O P 31 17 4 9 1	0	0
2	C	1	Total C N O P 31 17 4 9 1	0	0
2	D	1	Total C N O P 31 17 4 9 1	0	0
2	E	1	Total C N O P 62 34 8 18 2	0	1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is water.

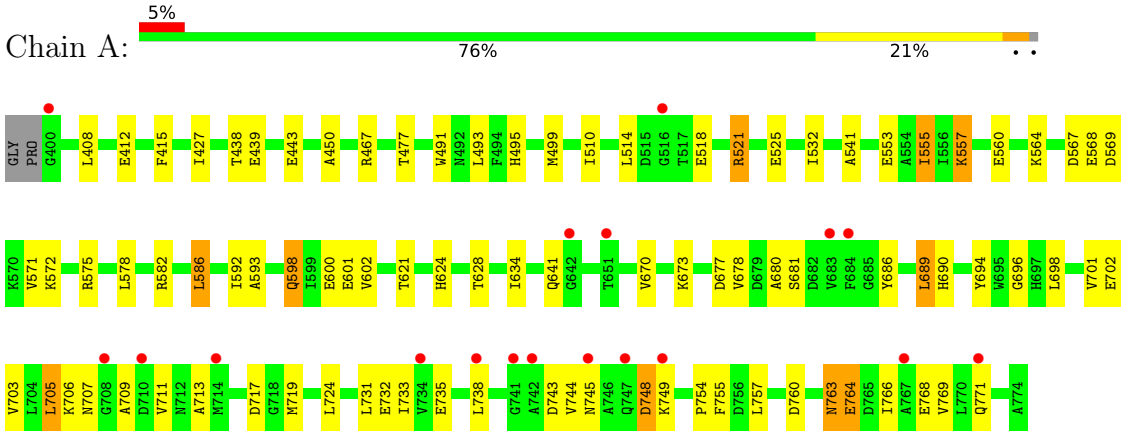
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	3	Total O 3 3	0	0
6	C	5	Total O 5 5	0	0
6	D	4	Total O 4 4	0	0
6	E	1	Total O 1 1	0	0

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.

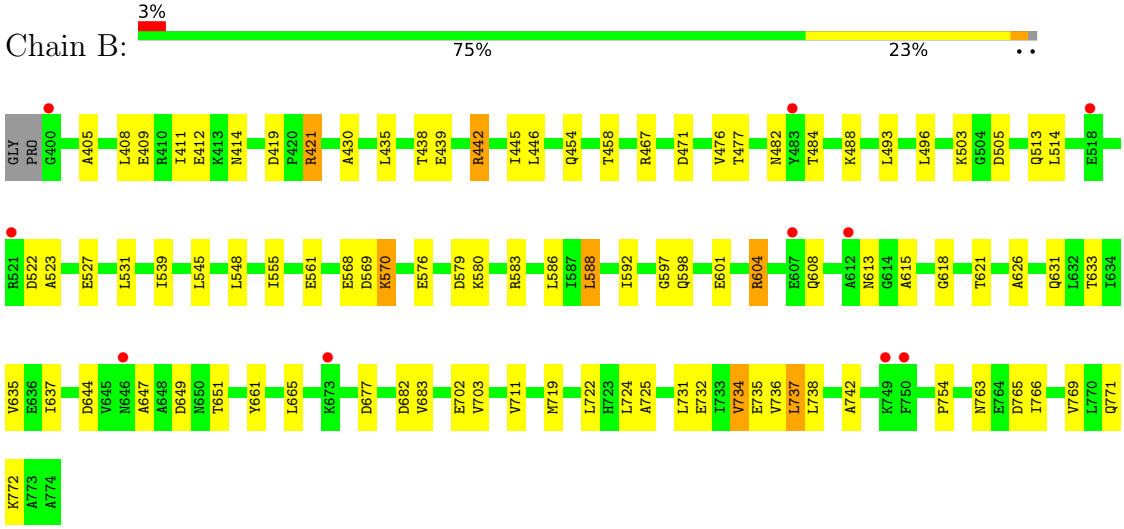
• Molecule 1: D7 LOV2-DARPin fusion

Chain A:



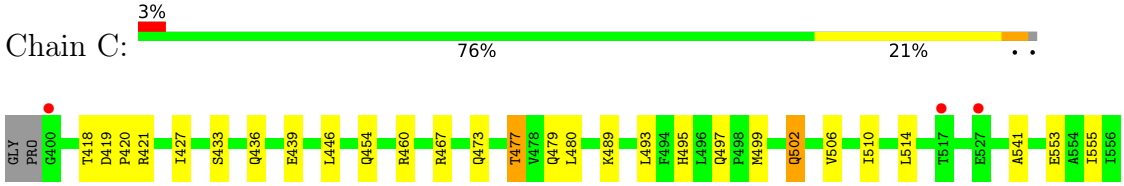
• Molecule 1: D7 LOV2-DARPin fusion

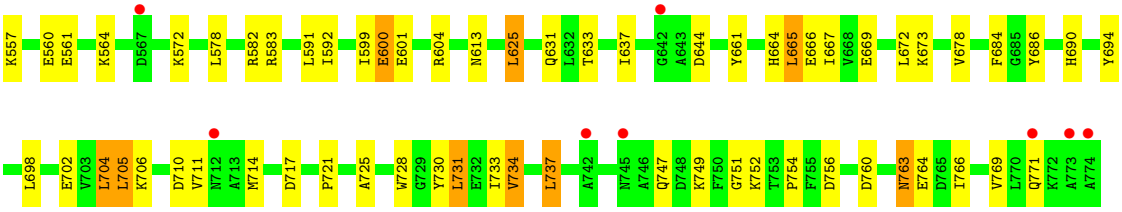
Chain B:



• Molecule 1: D7 LOV2-DARPin fusion

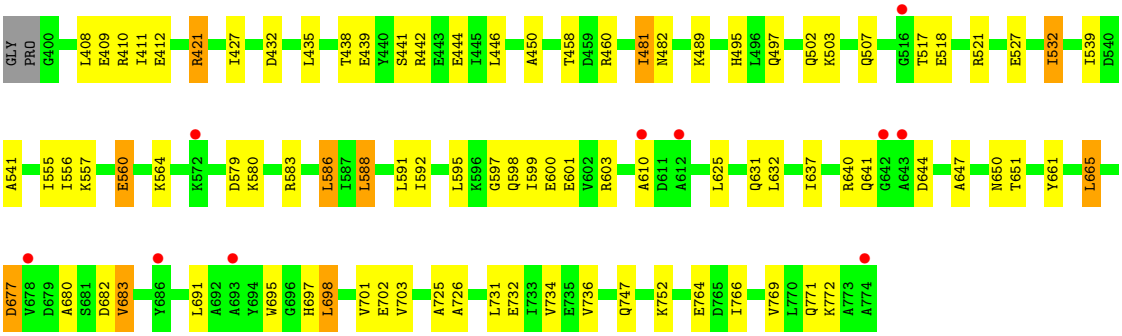
Chain C:





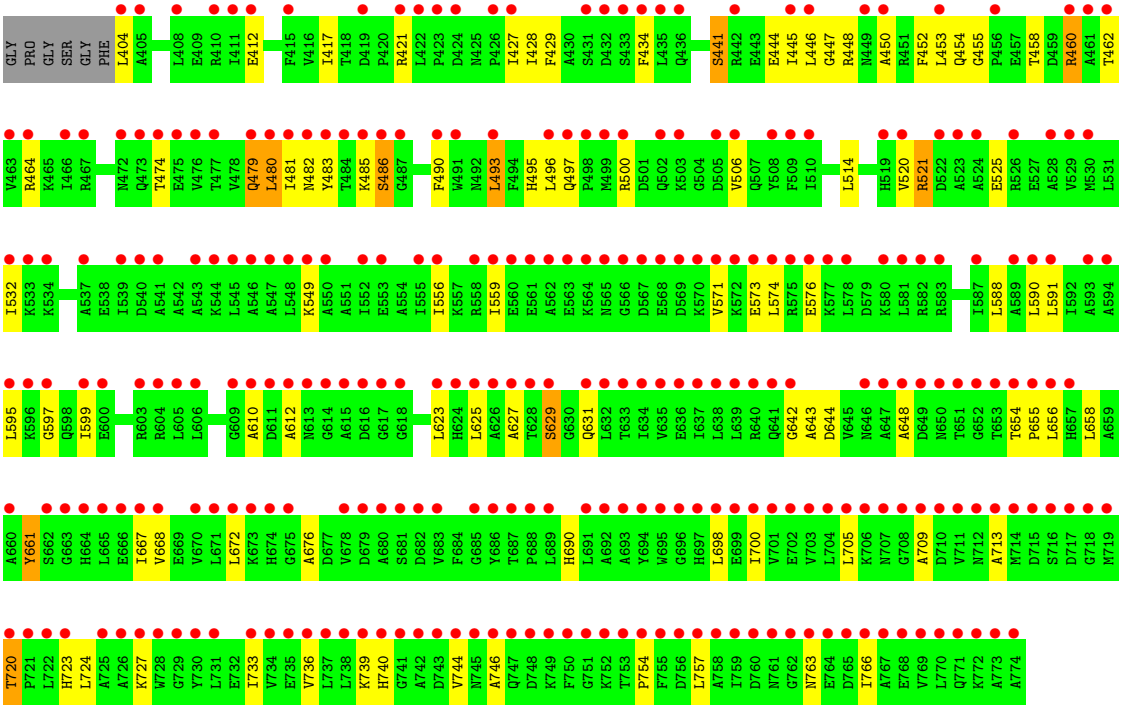
• Molecule 1: D7 LOV2-DARPin fusion

Chain D:



• Molecule 1: D7 LOV2-DARPin fusion

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	93.21Å 93.21Å 233.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.14 – 2.68 38.14 – 2.68	Depositor EDS
% Data completeness (in resolution range)	88.1 (38.14-2.68) 88.1 (38.14-2.68)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.239 , 0.295 0.232 , 0.295	Depositor DCC
R_{free} test set	2665 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	81.5	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.447 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17568	wwPDB-VP
Average B, all atoms (Å^2)	104.0	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 66.03 % 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 6.4521e-06. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, FMN, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.47	0/2941	0.64	0/3980
1	B	0.45	0/2941	0.61	0/3980
1	C	0.47	0/2941	0.63	0/3980
1	D	0.47	0/2941	0.64	0/3980
1	E	0.30	0/5830	0.45	0/7892
All	All	0.42	0/17594	0.58	0/23812

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2897	0	2915	60	0
1	B	2897	0	2915	54	0
1	C	2897	0	2915	54	0
1	D	2897	0	2915	48	0
1	E	5744	0	5790	73	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	31	0	19	0	0
2	E	62	0	38	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	7	0	0	0	0
6	B	3	0	0	0	0
6	C	5	0	0	0	0
6	D	4	0	0	0	0
6	E	1	0	0	0	0
All	All	17568	0	17596	259	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 7.

All (259) 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:C:560:GLU:HB3	1:C:564:LYS:NZ	1.82	0.94
1:C:613:ASN:HD21	1:C:644:ASP:H	1.12	0.92
1:E:690[B]:HIS:HE1	1:E:713[B]:ALA:HB3	1.35	0.90
1:A:702:GLU:O	1:A:706:LYS:HG2	1.72	0.89
1:E:720[A]:THR:HG22	1:E:723[A]:HIS:ND1	1.87	0.89
1:C:763:ASN:HB3	1:C:766:ILE:HD13	1.55	0.87
1:E:723[B]:HIS:HE1	1:E:746[B]:ALA:HB3	1.38	0.86
1:A:560:GLU:HB3	1:A:564:LYS:NZ	1.93	0.84
1:E:723[B]:HIS:CE1	1:E:746[B]:ALA:HB3	2.16	0.81
1:C:560:GLU:HB3	1:C:564:LYS:HZ1	1.44	0.81
1:C:454:GLN:HE21	1:C:460:ARG:NH2	1.80	0.80
1:C:454:GLN:NE2	1:C:460:ARG:HH22	1.80	0.80
1:E:705[B]:LEU:HD13	1:E:740[B]:HIS:CE1	2.17	0.79
1:E:493[B]:LEU:HB3	1:E:514[B]:LEU:HB3	1.63	0.79
1:E:495[B]:HIS:HB2	1:E:532[B]:ILE:HD13	1.65	0.78
1:A:557:LYS:NZ	1:B:771:GLN:HG3	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:GLU:HG2	1:D:772:LYS:NZ	2.00	0.76
1:E:720[A]:THR:HG22	1:E:723[A]:HIS:CE1	2.22	0.74
1:E:690[B]:HIS:CE1	1:E:713[B]:ALA:HB3	2.23	0.73
1:D:495:HIS:HB2	1:D:532:ILE:HD12	1.73	0.70
1:D:541:ALA:HB1	1:D:592:ILE:HD12	1.73	0.69
1:C:454:GLN:NE2	1:C:460:ARG:NH2	2.39	0.69
1:C:560:GLU:HB3	1:C:564:LYS:HZ2	1.55	0.69
1:A:560:GLU:HB3	1:A:564:LYS:HZ1	1.56	0.69
1:C:560:GLU:HG2	1:D:772:LYS:HZ1	1.57	0.68
1:A:499:MET:HG3	1:A:510:ILE:HD11	1.75	0.68
1:E:705[A]:LEU:HD13	1:E:740[A]:HIS:CE1	2.29	0.67
1:E:690[B]:HIS:HE1	1:E:713[B]:ALA:CB	2.07	0.67
1:E:720[B]:THR:HG22	1:E:723[B]:HIS:ND1	2.09	0.67
1:E:495[A]:HIS:HB2	1:E:532[A]:ILE:HD13	1.75	0.66
1:C:730:TYR:HB3	1:C:733:ILE:HD13	1.77	0.66
1:E:590[A]:LEU:HD11	1:E:610[A]:ALA:HB1	1.78	0.65
1:B:604:ARG:NH2	1:B:608:GLN:HE22	1.95	0.64
1:A:557:LYS:HZ3	1:B:771:GLN:HG3	1.63	0.63
1:D:588:LEU:O	1:D:592:ILE:HG12	1.98	0.63
1:D:458:THR:HG22	1:D:481:ILE:O	1.99	0.63
1:E:690[A]:HIS:CD2	1:E:724[A]:LEU:HD13	2.33	0.63
1:B:633:THR:O	1:B:637:ILE:HG13	1.99	0.62
1:C:731:LEU:HD12	1:C:731:LEU:H	1.64	0.62
1:E:705[A]:LEU:HD13	1:E:740[A]:HIS:ND1	2.15	0.62
1:A:560:GLU:HB3	1:A:564:LYS:HZ2	1.63	0.61
1:C:664:HIS:HB3	1:C:667:ILE:HD13	1.81	0.61
1:D:644:ASP:HB3	1:D:647:ALA:HB2	1.82	0.61
1:E:705[B]:LEU:HD13	1:E:740[B]:HIS:ND1	2.16	0.61
1:B:421:ARG:HG2	1:D:507:GLN:HB3	1.82	0.60
1:E:723[B]:HIS:HE1	1:E:746[B]:ALA:CB	2.11	0.60
1:C:702:GLU:O	1:C:706:LYS:HG2	2.00	0.60
1:B:419:ASP:CG	1:D:421:ARG:HH12	2.05	0.60
1:A:670:VAL:HA	1:A:673:LYS:HE2	1.84	0.60
1:D:651:THR:O	1:D:682:ASP:HB2	2.02	0.60
1:C:502:GLN:CD	1:C:502:GLN:H	2.05	0.59
1:A:412:GLU:O	1:A:412:GLU:HG3	2.01	0.59
1:E:521[A]:ARG:H	1:E:521[A]:ARG:HH11	1.51	0.59
1:E:736[A]:VAL:HA	1:E:739[A]:LYS:HE2	1.85	0.58
1:E:656[B]:LEU:HD22	1:E:676[B]:ALA:HB1	1.86	0.58
1:A:696:GLY:HA2	1:A:733:ILE:HD11	1.85	0.57
1:A:602:VAL:HG21	1:A:634:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:GLU:OE2	1:C:604:ARG:NH1	2.37	0.57
1:B:414:ASN:HB2	1:B:513:GLN:O	2.04	0.56
1:D:683:VAL:HG12	1:E:428[A]:ILE:HG22	1.87	0.56
1:A:569:ASP:HA	1:A:572:LYS:HD2	1.87	0.56
1:A:698:LEU:O	1:A:702:GLU:OE2	2.24	0.56
1:C:600:GLU:CD	1:C:600:GLU:H	2.09	0.56
1:A:557:LYS:HZ2	1:B:771:GLN:HG3	1.69	0.55
1:D:595:LEU:HD13	1:D:625:LEU:HD22	1.87	0.55
1:C:493:LEU:HB3	1:C:514:LEU:HB3	1.88	0.55
1:B:683:VAL:HG12	1:E:428[B]:ILE:HG22	1.89	0.54
1:B:421:ARG:NH1	1:D:421:ARG:HD3	2.22	0.54
1:E:460[A]:ARG:NE	1:E:460[A]:ARG:H	2.06	0.54
1:A:764:GLU:O	1:A:768:GLU:HG3	2.06	0.54
1:B:763:ASN:HB3	1:B:766:ILE:HD13	1.88	0.54
1:E:705[B]:LEU:HD23	1:E:709[B]:ALA:HB3	1.90	0.54
1:E:763[A]:ASN:HB3	1:E:766[A]:ILE:HD13	1.88	0.54
1:B:411:ILE:O	1:B:412:GLU:HG2	2.07	0.54
1:A:690:HIS:CE1	1:A:713:ALA:HB3	2.43	0.54
1:E:462[B]:THR:HG21	1:E:480[B]:LEU:HB3	1.90	0.54
1:A:438:THR:O	1:A:439:GLU:HB2	2.08	0.54
1:B:598:GLN:HB3	1:B:601:GLU:HB2	1.90	0.54
1:E:559[B]:ILE:HD11	1:E:574[B]:LEU:HB3	1.90	0.53
1:B:503:LYS:HB2	1:E:486[A]:SER:HA	1.91	0.53
1:B:644:ASP:HB3	1:B:647:ALA:HB2	1.90	0.53
1:D:588:LEU:HD23	1:D:592:ILE:HD11	1.89	0.53
1:E:698[B]:LEU:HG	1:E:733[B]:ILE:HG12	1.90	0.53
1:B:738:LEU:HD23	1:B:742:ALA:HB3	1.91	0.52
1:D:435:LEU:HD11	1:D:442:ARG:HG2	1.91	0.52
1:A:560:GLU:CB	1:A:564:LYS:HZ1	2.22	0.52
1:A:568:GLU:HG3	1:A:572:LYS:HE3	1.92	0.52
1:A:763:ASN:HB3	1:A:766:ILE:HD13	1.91	0.52
1:D:541:ALA:HB1	1:D:592:ILE:CD1	2.38	0.52
1:A:686:TYR:HD1	1:A:690:HIS:HB3	1.74	0.51
1:D:438:THR:O	1:D:439:GLU:HB2	2.11	0.51
1:E:690[A]:HIS:HD2	1:E:724[A]:LEU:HD13	1.74	0.51
1:A:696:GLY:HA2	1:A:733:ILE:CD1	2.41	0.51
1:E:629[B]:SER:HB2	1:E:631[B]:GLN:HG2	1.93	0.51
1:A:593:ALA:HA	1:A:598:GLN:HG3	1.93	0.50
1:B:711:VAL:HG23	1:B:737:LEU:HD12	1.93	0.50
1:D:665:LEU:HD21	1:D:703:VAL:HG21	1.94	0.50
1:A:555:ILE:HG21	1:A:578:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:ILE:HD12	1:C:766:ILE:H	1.77	0.50
1:C:473:GLN:HB3	1:C:506:VAL:HG21	1.94	0.50
1:D:599:ILE:O	1:D:603:ARG:HG3	2.12	0.50
1:A:495:HIS:HB2	1:A:532:ILE:HD12	1.93	0.49
1:D:600:GLU:CD	1:D:600:GLU:H	2.14	0.49
1:A:560:GLU:HG2	1:A:564:LYS:HZ1	1.77	0.49
1:A:755:PHE:HE2	1:A:771:GLN:HB2	1.77	0.49
1:B:725:ALA:HB1	1:B:734:VAL:HG12	1.92	0.49
1:A:621:THR:OG1	1:A:624:HIS:ND1	2.39	0.49
1:B:545:LEU:HD22	1:B:592:ILE:HD12	1.94	0.49
1:E:427[B]:ILE:HD11	1:E:450[B]:ALA:HB2	1.95	0.49
1:E:672[A]:LEU:HD23	1:E:676[A]:ALA:HB3	1.94	0.49
1:B:597:GLY:HA2	1:B:631:GLN:HG3	1.95	0.49
1:C:578:LEU:O	1:C:582:ARG:HG3	2.13	0.49
1:C:599:ILE:HD12	1:E:464[B]:ARG:NE	2.28	0.49
1:A:694:TYR:HD2	1:A:724:LEU:HD22	1.77	0.48
1:B:467:ARG:NH1	1:B:471:ASP:OD1	2.46	0.48
1:C:752:LYS:HE3	1:C:756:ASP:HB3	1.96	0.48
1:D:725:ALA:HB1	1:D:734:VAL:HG12	1.95	0.48
1:A:600:GLU:OE1	1:E:464[A]:ARG:NH2	2.34	0.48
1:D:698:LEU:HD21	1:D:732:GLU:HB3	1.94	0.48
1:A:439:GLU:HG2	1:E:599[B]:ILE:HG21	1.95	0.48
1:B:503:LYS:HE3	1:E:485[A]:LYS:O	2.13	0.48
1:D:435:LEU:CD1	1:D:442:ARG:HG2	2.44	0.48
1:D:637:ILE:HG23	1:D:640:ARG:HH21	1.77	0.48
1:E:427[A]:ILE:HD11	1:E:450[A]:ALA:HB2	1.94	0.48
1:C:560:GLU:HG2	1:D:772:LYS:HZ2	1.75	0.48
1:C:747:GLN:HB3	1:C:751:GLY:HA2	1.95	0.48
1:E:612[A]:ALA:HB1	1:E:643[A]:ALA:HB2	1.94	0.48
1:A:553:GLU:HB3	1:B:771:GLN:HE22	1.79	0.48
1:B:651:THR:O	1:B:682:ASP:HB2	2.14	0.48
1:B:421:ARG:HD2	1:D:421:ARG:CZ	2.43	0.48
1:D:731:LEU:HD11	1:D:769:VAL:HG21	1.96	0.48
1:E:705[A]:LEU:HD23	1:E:709[A]:ALA:HB3	1.96	0.48
1:D:691:LEU:O	1:D:695:TRP:HD1	1.97	0.47
1:C:427:ILE:HG22	1:C:446:LEU:HD23	1.96	0.47
1:C:686:TYR:CD1	1:C:690:HIS:HB3	2.48	0.47
1:C:717:ASP:HA	1:C:749:LYS:HG3	1.94	0.47
1:D:586:LEU:HD23	1:D:610:ALA:HB2	1.96	0.47
1:E:434[B]:PHE:HZ	1:E:453[B]:LEU:HD11	1.79	0.47
1:A:557:LYS:HD2	1:B:771:GLN:HE21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:TYR:CB	1:C:733:ILE:HD13	2.43	0.47
1:E:500[B]:ARG:H	1:E:500[B]:ARG:HG3	1.49	0.47
1:A:600:GLU:CD	1:A:600:GLU:H	2.18	0.47
1:A:689:LEU:HD12	1:A:709:ALA:HB1	1.97	0.47
1:C:667:ILE:H	1:C:667:ILE:HD12	1.79	0.47
1:D:441:SER:HB3	1:D:444:GLU:HG3	1.97	0.47
1:E:744[A]:VAL:O	1:E:754[A]:PRO:HD2	2.14	0.47
1:A:690:HIS:HE1	1:A:713:ALA:CB	2.27	0.47
1:E:672[B]:LEU:HD23	1:E:676[B]:ALA:HB3	1.96	0.47
1:B:476:VAL:HG12	1:B:496:LEU:HB3	1.97	0.46
1:E:479[B]:GLN:HE22	1:E:520[B]:VAL:H	1.61	0.46
1:A:521:ARG:HA	1:A:525:GLU:HB2	1.97	0.46
1:A:703:VAL:O	1:A:707:ASN:OD1	2.33	0.46
1:B:454:GLN:HG2	1:B:458:THR:HG21	1.96	0.46
1:A:427:ILE:HD11	1:A:450:ALA:HB2	1.97	0.46
1:C:666:GLU:CD	1:C:666:GLU:H	2.18	0.46
1:E:623[A]:LEU:HD23	1:E:655[A]:PRO:HG2	1.97	0.46
1:A:598:GLN:HB2	1:A:601:GLU:HB2	1.96	0.46
1:D:579:ASP:O	1:D:583:ARG:HG2	2.15	0.46
1:A:717:ASP:HA	1:A:749:LYS:HG2	1.97	0.46
1:B:503:LYS:HE2	1:B:505:ASP:OD2	2.15	0.46
1:D:702:GLU:HG2	1:D:736:VAL:HG11	1.98	0.46
1:B:665:LEU:HD11	1:B:703:VAL:HG21	1.98	0.45
1:E:595[B]:LEU:HD22	1:E:625[B]:LEU:HD23	1.98	0.45
1:A:705:LEU:HD21	1:A:711:VAL:HB	1.97	0.45
1:A:582:ARG:O	1:A:586:LEU:HD22	2.17	0.45
1:D:409:GLU:HG3	1:D:410:ARG:HG3	1.99	0.45
1:A:560:GLU:CG	1:B:772:LYS:NZ	2.80	0.45
1:B:408:LEU:HD22	1:B:539:ILE:HG23	1.99	0.45
1:C:672:LEU:HD22	1:C:678:VAL:HG13	1.99	0.45
1:C:678:VAL:HG12	1:C:704:LEU:HD13	1.97	0.45
1:C:439:GLU:HG2	1:E:599[A]:ILE:HD13	1.99	0.45
1:C:665:LEU:H	1:C:665:LEU:HD12	1.81	0.45
1:C:702:GLU:HB3	1:C:706:LYS:NZ	2.32	0.45
1:A:560:GLU:HG2	1:B:772:LYS:NZ	2.31	0.45
1:B:548:LEU:HD12	1:B:588:LEU:HD12	1.99	0.45
1:A:689:LEU:HD21	1:A:701:VAL:HG13	1.99	0.45
1:E:627[A]:ALA:HA	1:E:667[A]:ILE:HD13	1.98	0.45
1:B:722:LEU:HD23	1:B:754:PRO:HG2	1.98	0.44
1:E:668[B]:VAL:HG11	1:E:700[B]:ILE:HG23	1.97	0.44
1:D:650:ASN:HB3	1:E:447[A]:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:ALA:CB	1:B:734:VAL:HG12	2.48	0.44
1:D:408:LEU:HD22	1:D:539:ILE:HG23	1.99	0.44
1:C:694:TYR:CE2	1:C:728:TRP:NE1	2.86	0.44
1:C:721:PRO:HB2	1:C:737:LEU:HD11	1.98	0.44
1:B:615:ALA:HB2	1:B:621:THR:HG22	2.00	0.44
1:C:702:GLU:C	1:C:706:LYS:HZ2	2.21	0.44
1:D:597:GLY:HA2	1:D:631:GLN:HG3	1.99	0.43
1:D:598:GLN:HB3	1:D:601:GLU:HB3	1.99	0.43
1:E:441[B]:SER:HB3	1:E:444[B]:GLU:HG3	1.99	0.43
1:E:705[A]:LEU:CD1	1:E:740[A]:HIS:CE1	3.00	0.43
1:A:690:HIS:CE1	1:A:713:ALA:CB	3.00	0.43
1:B:604:ARG:HH21	1:B:608:GLN:HE22	1.65	0.43
1:C:686:TYR:HD1	1:C:690:HIS:HB3	1.84	0.43
1:E:727[A]:LYS:HB2	1:E:757[A]:LEU:HD23	1.99	0.43
1:D:427:ILE:HD11	1:D:450:ALA:HB2	2.00	0.43
1:E:417[B]:ILE:HB	1:E:429[B]:PHE:HB3	2.01	0.43
1:A:560:GLU:CG	1:B:772:LYS:HZ2	2.32	0.43
1:B:719:MET:HE2	1:B:724:LEU:HD12	2.01	0.43
1:C:418:THR:HG22	1:C:427:ILE:HA	1.99	0.43
1:A:571:VAL:O	1:A:575:ARG:HG3	2.18	0.43
1:B:731:LEU:HD11	1:B:769:VAL:HG21	2.01	0.43
1:C:454:GLN:HE21	1:C:460:ARG:HH21	1.65	0.43
1:C:633:THR:O	1:C:637:ILE:HG13	2.19	0.43
1:B:493:LEU:HB3	1:B:514:LEU:HB3	2.00	0.43
1:B:430:ALA:CB	1:B:445:ILE:HD11	2.49	0.42
1:C:557:LYS:CD	1:D:771:GLN:HE21	2.32	0.42
1:A:766:ILE:HD12	1:A:766:ILE:H	1.85	0.42
1:E:454[B]:GLN:HG2	1:E:458[B]:THR:HG21	2.00	0.42
1:C:499:MET:HG3	1:C:510:ILE:HD11	2.01	0.42
1:A:705:LEU:HA	1:A:709:ALA:HB3	2.00	0.42
1:A:744:VAL:O	1:A:754:PRO:HD2	2.20	0.42
1:C:705:LEU:HD21	1:C:711:VAL:HB	2.02	0.42
1:B:405:ALA:O	1:B:409:GLU:HB3	2.19	0.42
1:B:626:ALA:HB1	1:B:635:VAL:HG23	2.02	0.42
1:E:705[B]:LEU:CD1	1:E:740[B]:HIS:CE1	2.98	0.42
1:E:588[A]:LEU:HD12	1:E:591[A]:LEU:HD12	2.02	0.42
1:B:618:GLY:O	1:B:649:ASP:HB2	2.19	0.42
1:B:702:GLU:HG3	1:B:736:VAL:HG11	2.01	0.42
1:D:677:ASP:HB3	1:D:680:ALA:HB2	2.00	0.42
1:E:520[A]:VAL:HG13	1:E:525[A]:GLU:HG3	2.01	0.42
1:E:763[B]:ASN:HB3	1:E:766[B]:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ASP:HB3	1:A:680:ALA:HB2	2.00	0.42
1:B:570:LYS:NZ	1:D:460:ARG:HH21	2.18	0.42
1:C:541:ALA:HB1	1:C:592:ILE:HG12	2.01	0.42
1:D:747:GLN:HA	1:D:752:LYS:O	2.19	0.42
1:C:477:THR:HG23	1:C:495:HIS:HB2	2.01	0.42
1:C:591:LEU:HD22	1:C:625:LEU:HD22	2.02	0.42
1:C:725:ALA:HB1	1:C:734:VAL:HG12	2.02	0.42
1:E:648[A]:ALA:HB2	1:E:654[A]:THR:HG22	2.02	0.42
1:E:532[A]:ILE:H	1:E:532[A]:ILE:HG13	1.72	0.41
1:E:454[A]:GLN:HG2	1:E:458[A]:THR:HG21	2.01	0.41
1:A:493:LEU:HD23	1:A:514:LEU:HD23	2.01	0.41
1:D:697:HIS:O	1:D:701:VAL:HG23	2.20	0.41
1:B:419:ASP:OD1	1:D:421:ARG:NH1	2.52	0.41
1:D:411:ILE:O	1:D:412:GLU:HB2	2.21	0.41
1:E:427[A]:ILE:HG22	1:E:446[A]:LEU:HD23	2.02	0.41
1:E:658[A]:LEU:HA	1:E:661[A]:TYR:HB2	2.02	0.41
1:B:435:LEU:HD11	1:B:442:ARG:HG3	2.03	0.41
1:E:493[B]:LEU:HD12	1:E:532[B]:ILE:HG12	2.02	0.41
1:C:419:ASP:OD1	1:C:421:ARG:HB2	2.21	0.41
1:C:667:ILE:HD12	1:C:667:ILE:N	2.36	0.41
1:E:559[A]:ILE:HD12	1:E:571[A]:VAL:HG13	2.03	0.41
1:E:445[A]:ILE:HG23	1:E:452[A]:PHE:HZ	1.84	0.41
1:A:541:ALA:HB1	1:A:592:ILE:HG12	2.03	0.41
1:B:438:THR:O	1:B:439:GLU:HB2	2.21	0.41
1:B:503:LYS:CB	1:E:486[A]:SER:HA	2.50	0.41
1:A:408:LEU:HB3	1:A:415:PHE:HZ	1.86	0.41
1:B:484:THR:OG1	1:B:488:LYS:HB3	2.21	0.41
1:B:523:ALA:O	1:B:527:GLU:HG3	2.21	0.41
1:C:436:GLN:OE1	1:E:597[A]:GLY:O	2.39	0.41
1:E:455[A]:GLY:HA3	1:E:483[A]:TYR:CE1	2.56	0.41
1:E:493[A]:LEU:HD12	1:E:532[A]:ILE:HG12	2.03	0.41
1:C:557:LYS:HD2	1:D:771:GLN:HE21	1.85	0.40
1:D:726:ALA:HA	1:D:766:ILE:HG21	2.03	0.40
1:A:719:MET:HG3	1:A:748:ASP:HB2	2.03	0.40
1:A:749:LYS:HD3	1:A:749:LYS:HA	1.84	0.40
1:D:556:ILE:O	1:D:560:GLU:HG2	2.21	0.40
1:A:491:TRP:CD1	1:A:518:GLU:HA	2.56	0.40
1:A:690:HIS:HE1	1:A:713:ALA:HB1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	373/377 (99%)	352 (94%)	18 (5%)	3 (1%)	19 40
1	B	373/377 (99%)	349 (94%)	23 (6%)	1 (0%)	41 64
1	C	373/377 (99%)	346 (93%)	24 (6%)	3 (1%)	19 40
1	D	373/377 (99%)	356 (95%)	17 (5%)	0	100 100
1	E	738/377 (196%)	658 (89%)	78 (11%)	2 (0%)	41 64
All	All	2230/1885 (118%)	2061 (92%)	160 (7%)	9 (0%)	34 58

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	567	ASP
1	C	763	ASN
1	A	763	ASN
1	B	522	ASP
1	E	642[A]	GLY
1	E	642[B]	GLY
1	C	710	ASP
1	A	769	VAL
1	C	769	VAL

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	298/299 (100%)	274 (92%)	24 (8%)	11 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	298/299 (100%)	272 (91%)	26 (9%)	10 21
1	C	298/299 (100%)	265 (89%)	33 (11%)	6 13
1	D	298/299 (100%)	268 (90%)	30 (10%)	7 16
1	E	592/299 (198%)	540 (91%)	52 (9%)	10 21
All	All	1784/1495 (119%)	1619 (91%)	165 (9%)	9 19

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	GLU
1	A	467	ARG
1	A	477	THR
1	A	521	ARG
1	A	555	ILE
1	A	557	LYS
1	A	586	LEU
1	A	598	GLN
1	A	628	THR
1	A	641	GLN
1	A	678	VAL
1	A	681	SER
1	A	689	LEU
1	A	705	LEU
1	A	731	LEU
1	A	732	GLU
1	A	735	GLU
1	A	738	LEU
1	A	743	ASP
1	A	745	ASN
1	A	748	ASP
1	A	757	LEU
1	A	760	ASP
1	A	764	GLU
1	B	421	ARG
1	B	442	ARG
1	B	446	LEU
1	B	477	THR
1	B	482	ASN
1	B	531	LEU
1	B	555	ILE
1	B	561	GLU

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Mol	Chain	Res	Type
1	B	568	GLU
1	B	569	ASP
1	B	570	LYS
1	B	576	GLU
1	B	579	ASP
1	B	580	LYS
1	B	583	ARG
1	B	586	LEU
1	B	588	LEU
1	B	604	ARG
1	B	613	ASN
1	B	661	TYR
1	B	677	ASP
1	B	732	GLU
1	B	734	VAL
1	B	735	GLU
1	B	737	LEU
1	B	765	ASP
1	C	420	PRO
1	C	433	SER
1	C	467	ARG
1	C	477	THR
1	C	479	GLN
1	C	480	LEU
1	C	489	LYS
1	C	497	GLN
1	C	502	GLN
1	C	553	GLU
1	C	555	ILE
1	C	561	GLU
1	C	572	LYS
1	C	583	ARG
1	C	600	GLU
1	C	625	LEU
1	C	631	GLN
1	C	661	TYR
1	C	665	LEU
1	C	669	GLU
1	C	673	LYS
1	C	684	PHE
1	C	698	LEU
1	C	704	LEU

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Mol	Chain	Res	Type
1	C	705	LEU
1	C	714	MET
1	C	731	LEU
1	C	734	VAL
1	C	737	LEU
1	C	754	PRO
1	C	760	ASP
1	C	764	GLU
1	C	771	GLN
1	D	421	ARG
1	D	432	ASP
1	D	446	LEU
1	D	481	ILE
1	D	482	ASN
1	D	489	LYS
1	D	497	GLN
1	D	502	GLN
1	D	503	LYS
1	D	517	THR
1	D	518	GLU
1	D	521	ARG
1	D	527	GLU
1	D	532	ILE
1	D	555	ILE
1	D	557	LYS
1	D	560	GLU
1	D	564	LYS
1	D	580	LYS
1	D	586	LEU
1	D	588	LEU
1	D	591	LEU
1	D	632	LEU
1	D	641	GLN
1	D	661	TYR
1	D	665	LEU
1	D	677	ASP
1	D	683	VAL
1	D	698	LEU
1	D	764	GLU
1	E	404[A]	LEU
1	E	404[B]	LEU
1	E	412[A]	GLU

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Mol	Chain	Res	Type
1	E	412[B]	GLU
1	E	421[A]	ARG
1	E	421[B]	ARG
1	E	441[A]	SER
1	E	441[B]	SER
1	E	448[A]	ARG
1	E	448[B]	ARG
1	E	460[A]	ARG
1	E	460[B]	ARG
1	E	474[A]	THR
1	E	474[B]	THR
1	E	479[A]	GLN
1	E	479[B]	GLN
1	E	480[A]	LEU
1	E	480[B]	LEU
1	E	481[A]	ILE
1	E	481[B]	ILE
1	E	482[A]	ASN
1	E	482[B]	ASN
1	E	486[A]	SER
1	E	486[B]	SER
1	E	490[A]	PHE
1	E	490[B]	PHE
1	E	493[A]	LEU
1	E	493[B]	LEU
1	E	496[A]	LEU
1	E	496[B]	LEU
1	E	497[A]	GLN
1	E	497[B]	GLN
1	E	506[A]	VAL
1	E	506[B]	VAL
1	E	521[A]	ARG
1	E	521[B]	ARG
1	E	549[A]	LYS
1	E	549[B]	LYS
1	E	556[A]	ILE
1	E	556[B]	ILE
1	E	573[A]	GLU
1	E	573[B]	GLU
1	E	576[A]	GLU
1	E	576[B]	GLU
1	E	629[A]	SER

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Mol	Chain	Res	Type
1	E	629[B]	SER
1	E	644[A]	ASP
1	E	644[B]	ASP
1	E	661[A]	TYR
1	E	661[B]	TYR
1	E	720[A]	THR
1	E	720[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	GLN
1	A	707	ASN
1	B	608	GLN
1	B	747	GLN
1	B	771	GLN
1	C	454	GLN
1	C	613	ASN
1	D	414	ASN
1	D	454	GLN
1	D	497	GLN
1	D	502	GLN
1	D	565	ASN
1	D	608	GLN
1	D	740	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	D	801	-	33,33,33	0.33	0	48,50,50	0.68	0
3	GOL	D	802	-	5,5,5	0.10	0	5,5,5	0.19	0
2	FMN	E	801[A]	-	33,33,33	0.28	0	48,50,50	0.68	2 (4%)
2	FMN	A	801	-	33,33,33	0.37	0	48,50,50	0.56	0
3	GOL	A	802	-	5,5,5	0.09	0	5,5,5	0.19	0
3	GOL	B	802	-	5,5,5	0.10	0	5,5,5	0.26	0
3	GOL	C	802	-	5,5,5	0.09	0	5,5,5	0.19	0
2	FMN	C	801	-	33,33,33	0.47	0	48,50,50	0.73	1 (2%)
2	FMN	E	801[B]	-	33,33,33	0.33	0	48,50,50	0.56	0
2	FMN	B	801	-	33,33,33	0.43	0	48,50,50	0.83	3 (6%)

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	801	-	-	1/18/18/18	0/3/3/3
3	GOL	D	802	-	-	0/4/4/4	-
2	FMN	E	801[A]	-	-	10/18/18/18	0/3/3/3
2	FMN	A	801	-	-	2/18/18/18	0/3/3/3
3	GOL	A	802	-	-	0/4/4/4	-
3	GOL	B	802	-	-	2/4/4/4	-
3	GOL	C	802	-	-	0/4/4/4	-
2	FMN	C	801	-	-	2/18/18/18	0/3/3/3
2	FMN	E	801[B]	-	-	9/18/18/18	0/3/3/3
2	FMN	B	801	-	-	1/18/18/18	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	FMN	P-O5'-C5'	2.58	125.41	118.30
2	B	801	FMN	P-O5'-C5'	2.35	124.78	118.30
2	B	801	FMN	C5'-C4'-C3'	2.24	116.53	112.20
2	E	801[A]	FMN	O5'-P-O1P	2.08	112.31	106.47
2	E	801[A]	FMN	C4'-C3'-C2'	2.07	117.66	113.36
2	B	801	FMN	O3'-C3'-C4'	2.02	113.68	108.81

There are no chirality outliers.

All (27) torsion outliers are listed below:

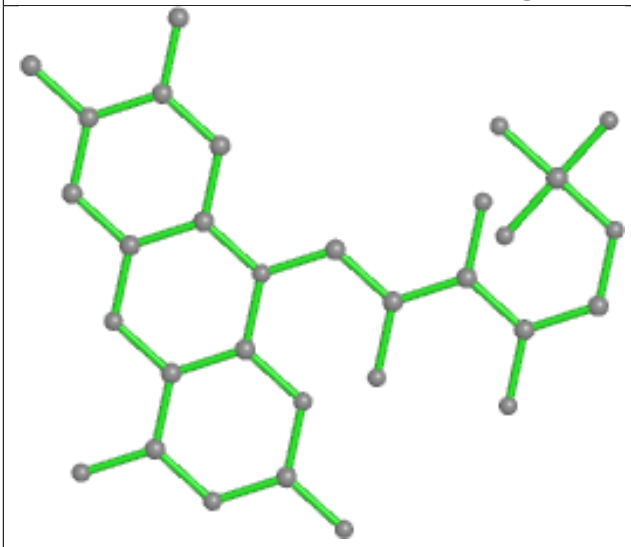
Mol	Chain	Res	Type	Atoms
2	E	801[A]	FMN	C1'-C2'-C3'-O3'
2	E	801[A]	FMN	C1'-C2'-C3'-C4'
2	E	801[A]	FMN	O2'-C2'-C3'-O3'
2	E	801[A]	FMN	O2'-C2'-C3'-C4'
2	E	801[A]	FMN	C3'-C4'-C5'-O5'
2	E	801[A]	FMN	O4'-C4'-C5'-O5'
2	E	801[A]	FMN	C5'-O5'-P-O1P
2	E	801[A]	FMN	C5'-O5'-P-O2P
2	E	801[A]	FMN	C5'-O5'-P-O3P
2	E	801[B]	FMN	C1'-C2'-C3'-O3'
2	E	801[B]	FMN	C1'-C2'-C3'-C4'
2	E	801[B]	FMN	C5'-O5'-P-O1P
2	E	801[B]	FMN	C5'-O5'-P-O2P
2	E	801[B]	FMN	C5'-O5'-P-O3P
3	B	802	GOL	C1-C2-C3-O3
2	E	801[B]	FMN	O2'-C2'-C3'-O3'
2	E	801[B]	FMN	O2'-C2'-C3'-C4'
2	B	801	FMN	C4'-C5'-O5'-P
2	C	801	FMN	C4'-C5'-O5'-P
3	B	802	GOL	O2-C2-C3-O3
2	D	801	FMN	C4'-C5'-O5'-P
2	E	801[B]	FMN	C3'-C4'-C5'-O5'
2	A	801	FMN	C4'-C5'-O5'-P
2	A	801	FMN	O2'-C2'-C3'-C4'
2	E	801[A]	FMN	C4'-C5'-O5'-P
2	E	801[B]	FMN	C4'-C5'-O5'-P
2	C	801	FMN	O2'-C2'-C3'-C4'

There are no ring outliers.

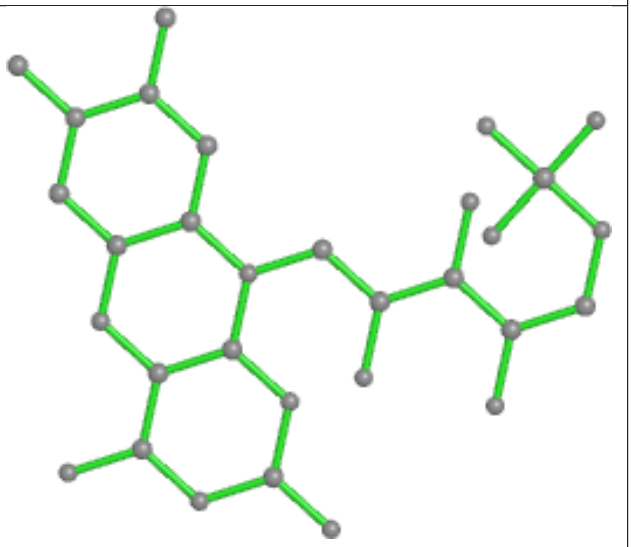
No monomer is involved in short contacts.

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.

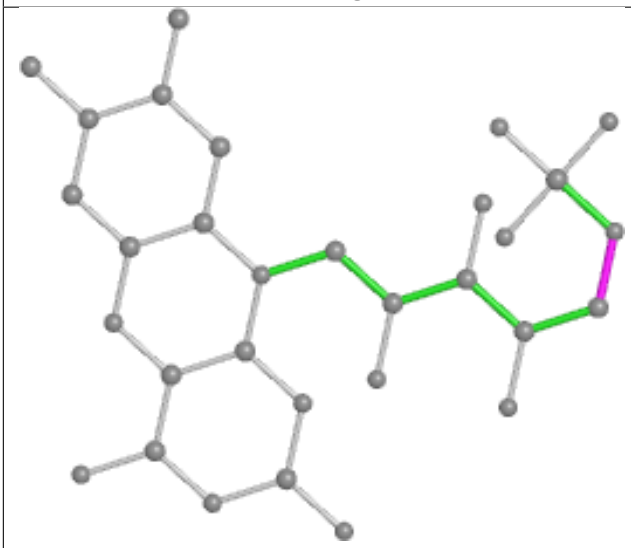
Ligand FMN D 801



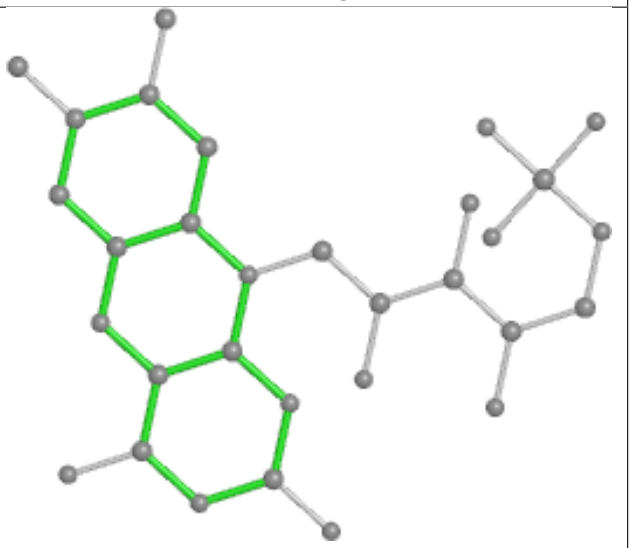
Bond lengths



Bond angles

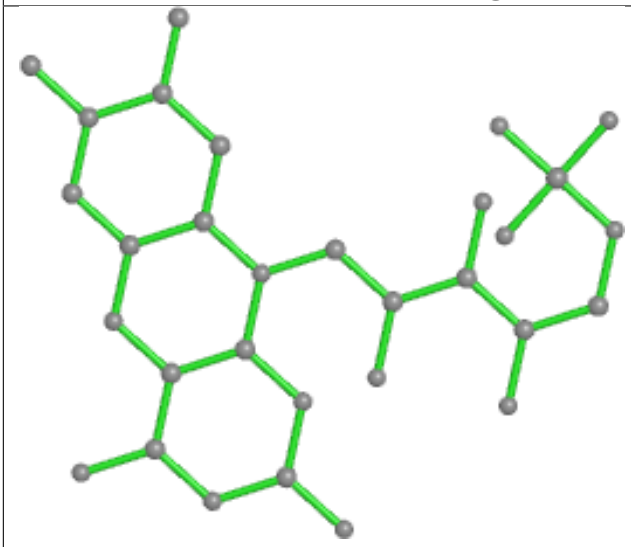


Torsions

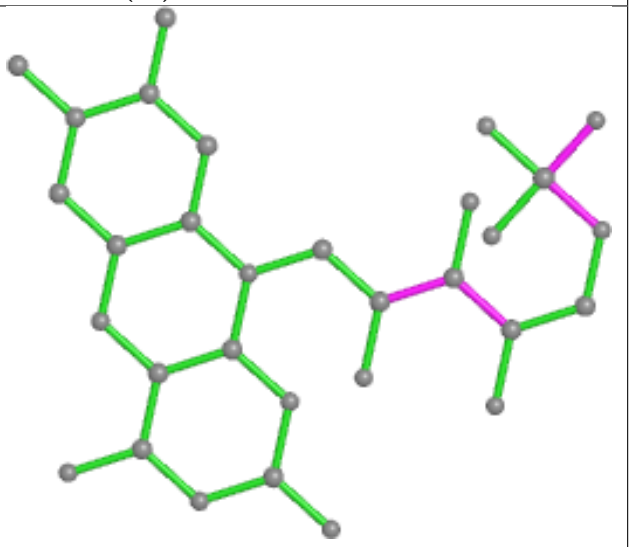


Rings

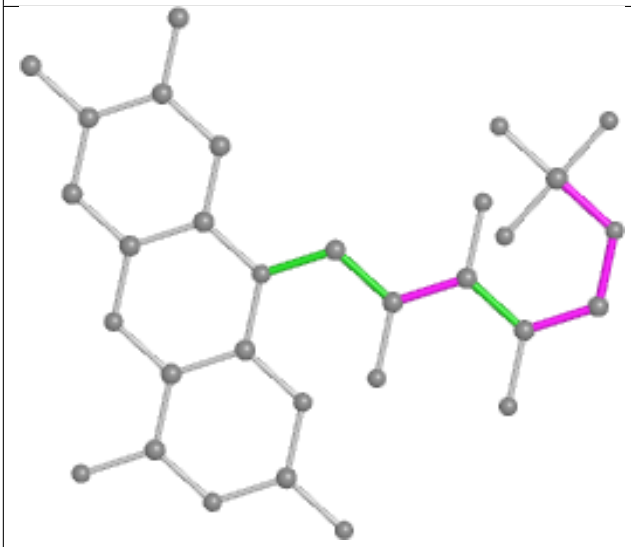
Ligand FMN E 801 (A)



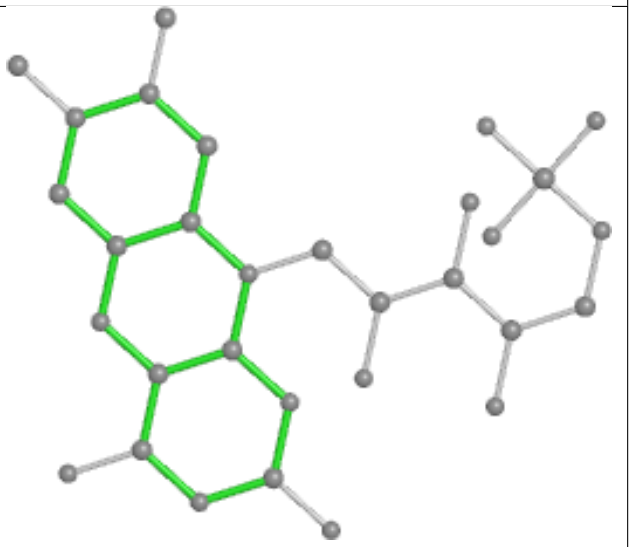
Bond lengths



Bond angles

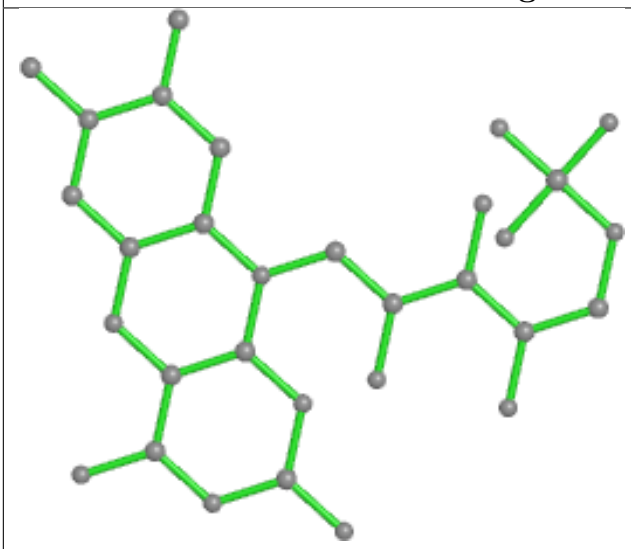


Torsions

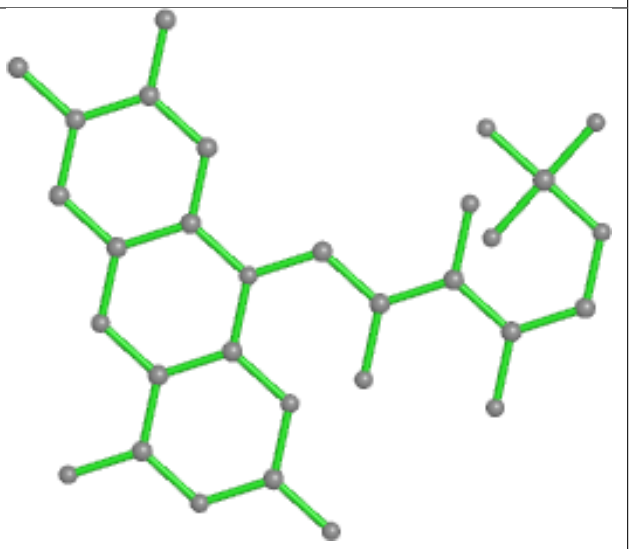


Rings

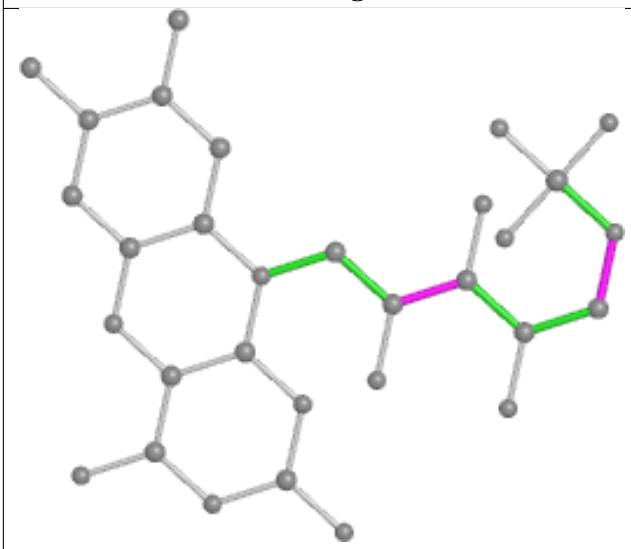
Ligand FMN A 801



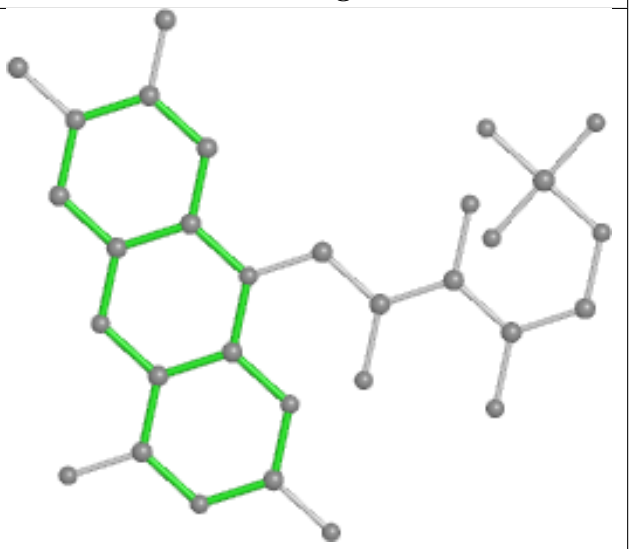
Bond lengths



Bond angles

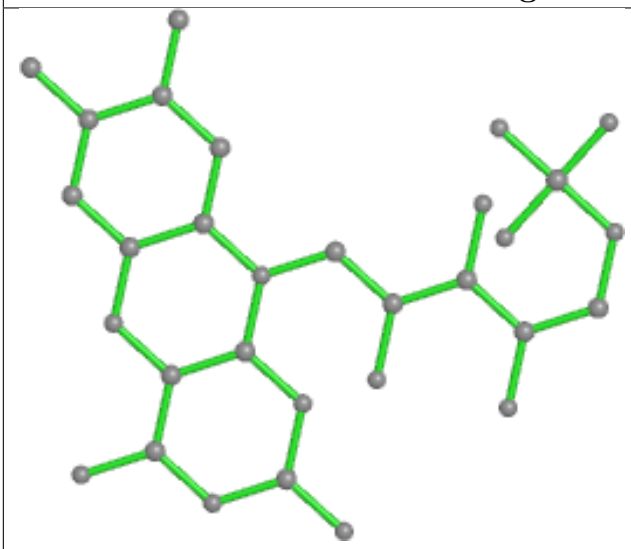


Torsions

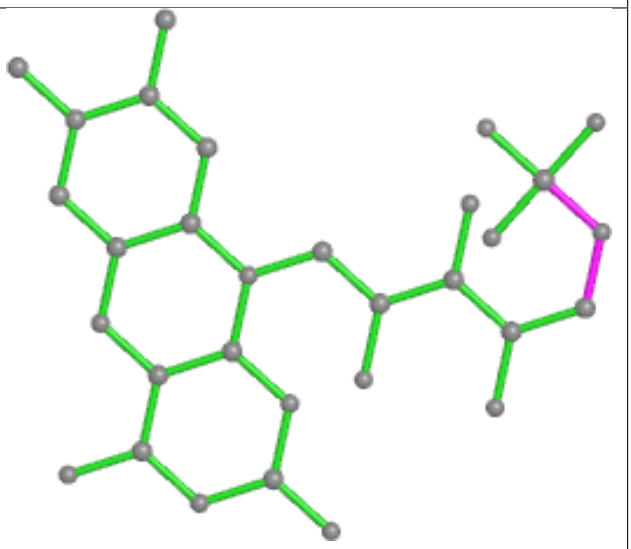


Rings

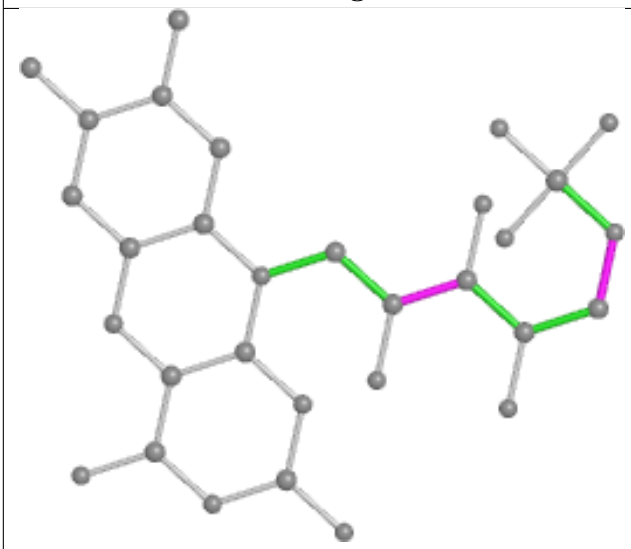
Ligand FMN C 801



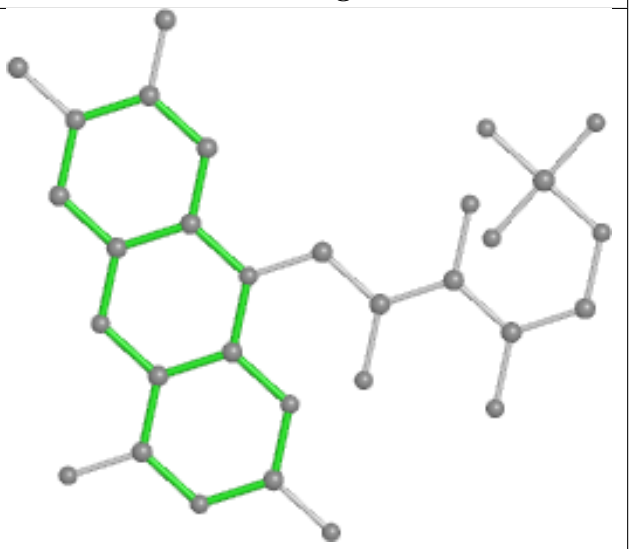
Bond lengths



Bond angles

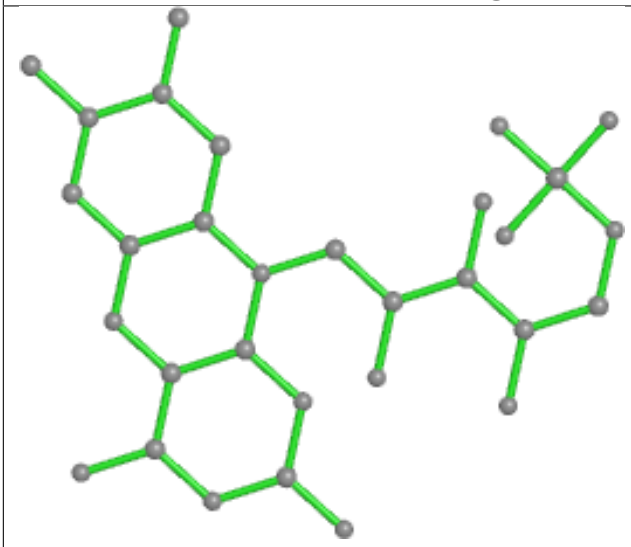


Torsions

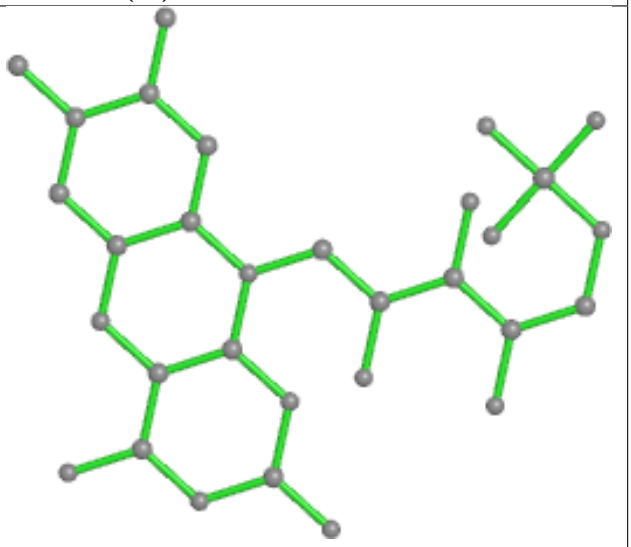


Rings

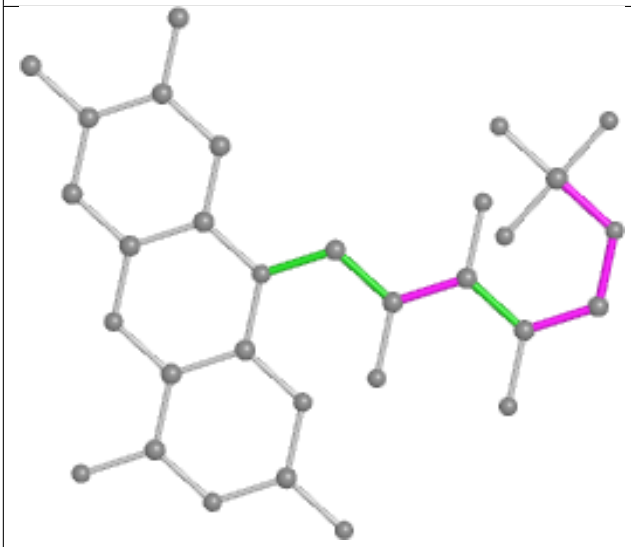
Ligand FMN E 801 (B)



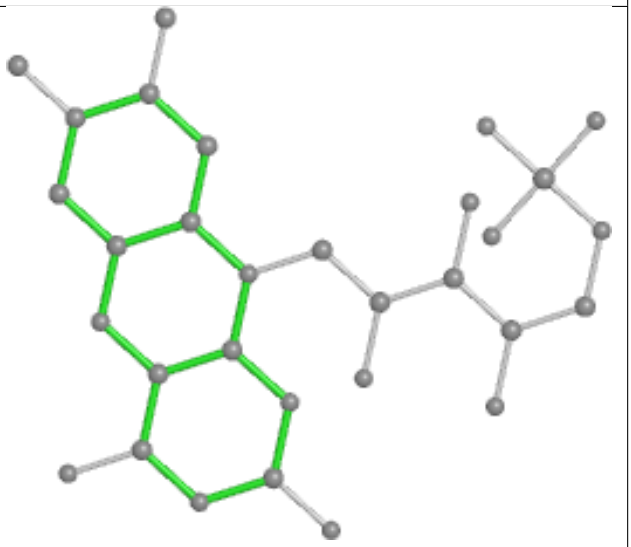
Bond lengths



Bond angles

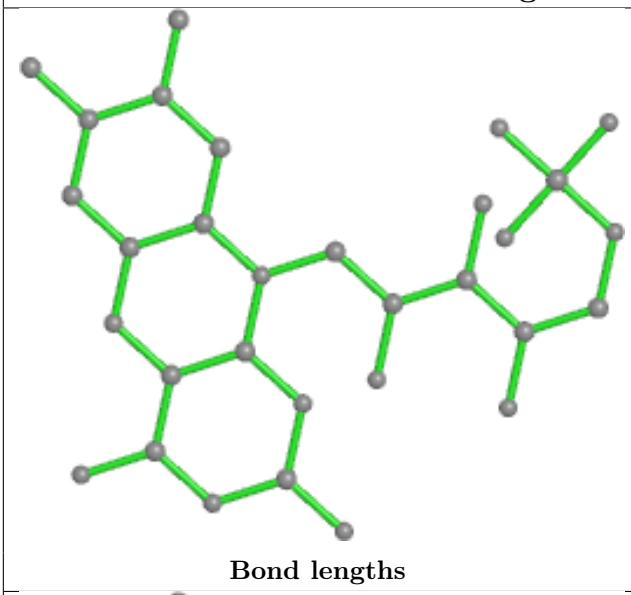


Torsions

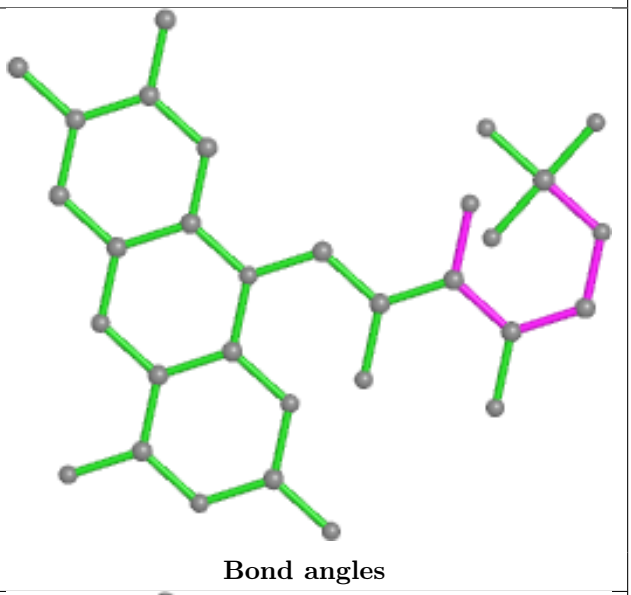


Rings

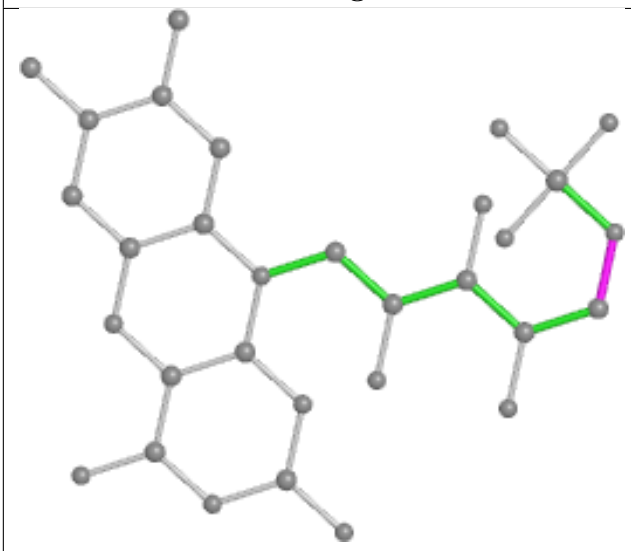
Ligand FMN B 801



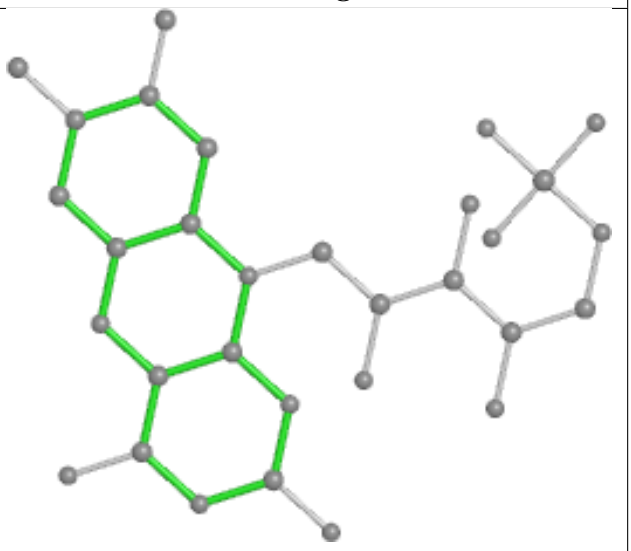
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	375/377 (99%)	0.02	18 (4%)	30	28	53, 92, 131, 152	2 (0%)
1	B	375/377 (99%)	-0.05	10 (2%)	54	54	49, 92, 117, 125	1 (0%)
1	C	375/377 (99%)	-0.04	11 (2%)	51	51	54, 90, 131, 152	1 (0%)
1	D	375/377 (99%)	-0.09	10 (2%)	54	54	46, 93, 118, 129	1 (0%)
1	E	371/377 (98%)	4.28	280 (75%)	0	0	59, 141, 194, 203	0
All	All	1871/1885 (99%)	0.82	329 (17%)	1	1	46, 95, 173, 203	5 (0%)

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	763[A]	ASN	20.2
1	E	759[A]	ILE	19.3
1	E	748[A]	ASP	18.7
1	E	751[A]	GLY	16.5
1	E	772[A]	LYS	15.1
1	E	709[A]	ALA	14.3
1	E	708[A]	GLY	14.3
1	E	760[A]	ASP	14.1
1	E	665[A]	LEU	13.9
1	E	758[A]	ALA	13.8
1	E	683[A]	VAL	13.5
1	E	706[A]	LYS	13.0
1	E	697[A]	HIS	11.7
1	E	666[A]	GLU	11.1
1	E	612[A]	ALA	11.0
1	E	678[A]	VAL	11.0
1	E	558[A]	ARG	10.3
1	E	717[A]	ASP	10.3
1	E	738[A]	LEU	10.2
1	E	613[A]	ASN	10.1

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Mol	Chain	Res	Type	RSRZ
1	E	731[A]	LEU	10.0
1	E	740[A]	HIS	9.8
1	E	562[A]	ALA	9.7
1	E	653[A]	THR	9.5
1	E	750[A]	PHE	9.5
1	E	739[A]	LYS	9.4
1	E	766[A]	ILE	9.4
1	E	773[A]	ALA	9.1
1	E	698[A]	LEU	9.1
1	E	674[A]	HIS	9.0
1	E	667[A]	ILE	8.8
1	E	745[A]	ASN	8.8
1	E	774[A]	ALA	8.7
1	E	769[A]	VAL	8.5
1	E	736[A]	VAL	8.5
1	E	633[A]	THR	8.4
1	E	728[A]	TRP	8.4
1	E	704[A]	LEU	8.2
1	E	446[A]	LEU	8.2
1	E	694[A]	TYR	8.2
1	E	768[A]	GLU	8.2
1	E	648[A]	ALA	8.1
1	E	640[A]	ARG	8.0
1	E	771[A]	GLN	8.0
1	E	528[A]	ALA	8.0
1	E	609[A]	GLY	7.9
1	E	611[A]	ASP	7.9
1	E	625[A]	LEU	7.9
1	E	682[A]	ASP	7.9
1	E	744[A]	VAL	7.8
1	E	681[A]	SER	7.8
1	E	719[A]	MET	7.7
1	E	632[A]	LEU	7.7
1	E	656[A]	LEU	7.7
1	E	565[A]	ASN	7.7
1	E	624[A]	HIS	7.7
1	E	729[A]	GLY	7.7
1	E	730[A]	TYR	7.6
1	E	654[A]	THR	7.5
1	E	707[A]	ASN	7.4
1	E	560[A]	GLU	7.2
1	E	655[A]	PRO	7.2

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Mol	Chain	Res	Type	RSRZ
1	E	741[A]	GLY	7.2
1	E	481[A]	ILE	7.2
1	E	651[A]	THR	7.1
1	E	679[A]	ASP	7.1
1	E	662[A]	SER	7.1
1	E	641[A]	GLN	7.0
1	E	716[A]	SER	7.0
1	E	705[A]	LEU	6.9
1	E	668[A]	VAL	6.9
1	E	688[A]	PRO	6.8
1	E	408[A]	LEU	6.8
1	E	743[A]	ASP	6.8
1	E	703[A]	VAL	6.7
1	E	532[A]	ILE	6.7
1	E	722[A]	LEU	6.6
1	E	561[A]	GLU	6.6
1	A	642	GLY	6.5
1	E	647[A]	ALA	6.5
1	E	564[A]	LYS	6.5
1	E	757[A]	LEU	6.5
1	E	754[A]	PRO	6.4
1	E	529[A]	VAL	6.4
1	E	755[A]	PHE	6.4
1	E	548[A]	LEU	6.4
1	E	752[A]	LYS	6.3
1	E	747[A]	GLN	6.3
1	E	566[A]	GLY	6.2
1	E	742[A]	ALA	6.1
1	E	723[A]	HIS	6.0
1	E	636[A]	GLU	6.0
1	E	650[A]	ASN	5.9
1	E	770[A]	LEU	5.9
1	E	720[A]	THR	5.6
1	E	675[A]	GLY	5.6
1	E	574[A]	LEU	5.6
1	E	410[A]	ARG	5.6
1	E	733[A]	ILE	5.5
1	E	435[A]	LEU	5.5
1	E	526[A]	ARG	5.5
1	E	762[A]	GLY	5.4
1	E	687[A]	THR	5.4
1	E	530[A]	MET	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	718[A]	GLY	5.3
1	E	503[A]	LYS	5.3
1	E	749[A]	LYS	5.3
1	E	614[A]	GLY	5.3
1	E	631[A]	GLN	5.2
1	E	672[A]	LEU	5.2
1	E	701[A]	VAL	5.2
1	E	710[A]	ASP	5.1
1	E	700[A]	ILE	5.1
1	E	559[A]	ILE	5.1
1	E	583[A]	ARG	5.1
1	E	476[A]	VAL	5.1
1	E	555[A]	ILE	5.1
1	E	635[A]	VAL	5.0
1	C	771	GLN	4.9
1	E	502[A]	GLN	4.9
1	E	575[A]	ARG	4.9
1	E	604[A]	ARG	4.8
1	E	637[A]	ILE	4.8
1	E	649[A]	ASP	4.8
1	E	510[A]	ILE	4.8
1	E	767[A]	ALA	4.7
1	E	673[A]	LYS	4.7
1	E	670[A]	VAL	4.7
1	E	746[A]	ALA	4.7
1	E	433[A]	SER	4.6
1	E	590[A]	LEU	4.6
1	E	524[A]	ALA	4.6
1	E	714[A]	MET	4.6
1	E	411[A]	ILE	4.6
1	E	570[A]	LYS	4.6
1	E	711[A]	VAL	4.6
1	E	550[A]	ALA	4.5
1	E	764[A]	GLU	4.5
1	E	639[A]	LEU	4.4
1	E	715[A]	ASP	4.4
1	E	699[A]	GLU	4.4
1	E	726[A]	ALA	4.3
1	E	405[A]	ALA	4.3
1	E	474[A]	THR	4.3
1	E	573[A]	GLU	4.3
1	A	683	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	761[A]	ASN	4.2
1	B	607	GLU	4.2
1	E	616[A]	ASP	4.2
1	E	449[A]	ASN	4.2
1	E	753[A]	THR	4.2
1	B	673	LYS	4.1
1	E	505[A]	ASP	4.1
1	E	493[A]	LEU	4.1
1	E	450[A]	ALA	4.1
1	E	594[A]	ALA	4.1
1	E	484[A]	THR	4.0
1	E	628[A]	THR	4.0
1	E	547[A]	ALA	4.0
1	E	735[A]	GLU	4.0
1	E	404[A]	LEU	4.0
1	E	634[A]	ILE	4.0
1	E	692[A]	ALA	4.0
1	A	400	GLY	4.0
1	E	461[A]	ALA	4.0
1	E	587[A]	ILE	4.0
1	E	589[A]	ALA	4.0
1	E	617[A]	GLY	3.9
1	E	626[A]	ALA	3.9
1	E	593[A]	ALA	3.9
1	E	445[A]	ILE	3.9
1	E	734[A]	VAL	3.8
1	E	571[A]	VAL	3.8
1	E	680[A]	ALA	3.8
1	E	534[A]	LYS	3.8
1	E	581[A]	LEU	3.7
1	E	442[A]	ARG	3.7
1	E	725[A]	ALA	3.7
1	E	642[A]	GLY	3.7
1	D	643	ALA	3.7
1	E	646[A]	ASN	3.7
1	E	523[A]	ALA	3.7
1	E	691[A]	LEU	3.7
1	E	463[A]	VAL	3.7
1	E	615[A]	ALA	3.7
1	E	541[A]	ALA	3.6
1	E	693[A]	ALA	3.6
1	E	491[A]	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	533[A]	LYS	3.5
1	E	721[A]	PRO	3.5
1	E	756[A]	ASP	3.5
1	A	745	ASN	3.4
1	E	553[A]	GLU	3.4
1	E	685[A]	GLY	3.4
1	D	693	ALA	3.4
1	E	496[A]	LEU	3.4
1	E	595[A]	LEU	3.3
1	E	537[A]	ALA	3.3
1	E	432[A]	ASP	3.3
1	E	702[A]	GLU	3.3
1	A	742	ALA	3.3
1	A	516	GLY	3.3
1	C	773	ALA	3.2
1	E	431[A]	SER	3.2
1	E	671[A]	LEU	3.2
1	E	629[A]	SER	3.2
1	E	765[A]	ASP	3.2
1	E	713[A]	ALA	3.2
1	E	623[A]	LEU	3.2
1	E	466[A]	ILE	3.1
1	E	473[A]	GLN	3.1
1	E	549[A]	LYS	3.1
1	E	490[A]	PHE	3.1
1	E	652[A]	GLY	3.1
1	E	480[A]	LEU	3.1
1	E	712[A]	ASN	3.1
1	E	486[A]	SER	3.1
1	E	519[A]	HIS	3.1
1	E	597[A]	GLY	3.1
1	E	663[A]	GLY	3.1
1	E	689[A]	LEU	3.1
1	E	539[A]	ILE	3.1
1	E	415[A]	PHE	3.1
1	E	472[A]	ASN	3.1
1	E	618[A]	GLY	3.0
1	E	567[A]	ASP	3.0
1	E	498[A]	PRO	3.0
1	E	627[A]	ALA	3.0
1	D	612	ALA	3.0
1	E	421[A]	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	545[A]	LEU	3.0
1	E	657[A]	HIS	2.9
1	E	487[A]	GLY	2.9
1	E	506[A]	VAL	2.9
1	E	603[A]	ARG	2.9
1	E	556[A]	ILE	2.9
1	D	686	TYR	2.9
1	E	520[A]	VAL	2.9
1	E	453[A]	LEU	2.9
1	E	460[A]	ARG	2.9
1	E	427[A]	ILE	2.9
1	E	509[A]	PHE	2.9
1	D	774	ALA	2.8
1	E	423[A]	PRO	2.8
1	E	569[A]	ASP	2.8
1	E	479[A]	GLN	2.8
1	E	695[A]	TRP	2.8
1	C	517	THR	2.8
1	E	499[A]	MET	2.7
1	B	521	ARG	2.7
1	E	606[A]	LEU	2.7
1	E	552[A]	ILE	2.7
1	E	599[A]	ILE	2.7
1	E	580[A]	LYS	2.7
1	E	456[A]	PRO	2.7
1	E	563[A]	GLU	2.7
1	D	642	GLY	2.7
1	C	642	GLY	2.7
1	E	540[A]	ASP	2.7
1	C	742	ALA	2.6
1	A	734	VAL	2.6
1	E	426[A]	PRO	2.6
1	E	600[A]	GLU	2.6
1	E	591[A]	LEU	2.6
1	E	638[A]	LEU	2.6
1	A	771	GLN	2.5
1	E	660[A]	ALA	2.5
1	E	543[A]	ALA	2.5
1	E	664[A]	HIS	2.5
1	E	727[A]	LYS	2.5
1	C	400	GLY	2.5
1	A	710	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	612	ALA	2.5
1	B	483	TYR	2.4
1	E	422[A]	LEU	2.4
1	E	582[A]	ARG	2.4
1	D	610	ALA	2.4
1	E	500[A]	ARG	2.4
1	C	774	ALA	2.4
1	A	684	PHE	2.4
1	E	467[A]	ARG	2.4
1	E	424[A]	ASP	2.4
1	A	741	GLY	2.4
1	E	482[A]	ASN	2.4
1	D	678	VAL	2.4
1	A	714	MET	2.3
1	E	544[A]	LYS	2.3
1	A	767	ALA	2.3
1	E	737[A]	LEU	2.3
1	E	576[A]	GLU	2.3
1	B	400	GLY	2.3
1	E	477[A]	THR	2.3
1	B	749	LYS	2.3
1	E	497[A]	GLN	2.3
1	B	750	PHE	2.3
1	E	434[A]	PHE	2.3
1	A	749	LYS	2.3
1	D	516	GLY	2.3
1	E	546[A]	ALA	2.3
1	E	610[A]	ALA	2.3
1	E	462[A]	THR	2.3
1	E	605[A]	LEU	2.2
1	E	464[A]	ARG	2.2
1	A	651	THR	2.2
1	E	485[A]	LYS	2.2
1	E	572[A]	LYS	2.2
1	E	577[A]	LYS	2.2
1	E	436[A]	GLN	2.2
1	E	412[A]	GLU	2.1
1	A	708	GLY	2.1
1	E	475[A]	GLU	2.1
1	E	419[A]	ASP	2.1
1	E	596[A]	LYS	2.1
1	B	518	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	567	ASP	2.1
1	E	483[A]	TYR	2.1
1	E	696[A]	GLY	2.1
1	A	747	GLN	2.0
1	C	527	GLU	2.0
1	E	508[A]	TYR	2.0
1	E	568[A]	GLU	2.0
1	B	646	ASN	2.0
1	C	745	ASN	2.0
1	D	572	LYS	2.0
1	E	522[A]	ASP	2.0
1	A	738	LEU	2.0
1	E	578[A]	LEU	2.0
1	C	712	ASN	2.0
1	E	686[A]	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	802	6/6	0.62	0.33	112,112,112,112	0
5	CL	B	803	1/1	0.68	0.18	96,96,96,96	0
3	GOL	D	802	6/6	0.70	0.24	114,116,116,116	0
5	CL	D	803	1/1	0.80	0.15	105,105,105,105	0
2	FMN	E	801[A]	31/31	0.81	0.28	68,68,70,70	31
2	FMN	E	801[B]	31/31	0.81	0.28	57,58,60,61	31
3	GOL	B	802	6/6	0.85	0.23	106,107,107,107	0
3	GOL	A	802	6/6	0.88	0.17	118,118,119,119	0

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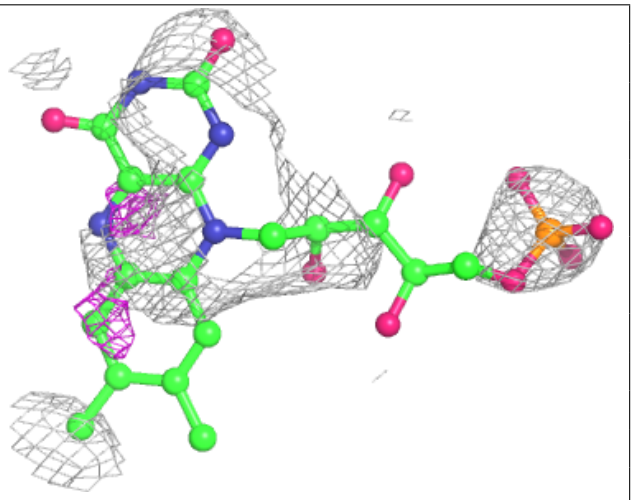
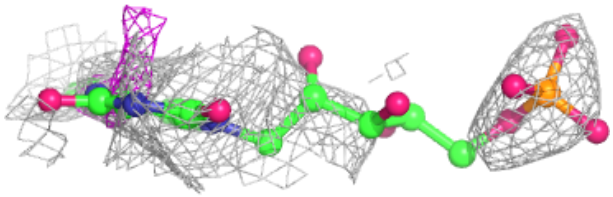
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FMN	B	801	31/31	0.95	0.12	56,63,69,70	0
2	FMN	C	801	31/31	0.95	0.12	60,64,69,69	0
4	MG	C	803	1/1	0.96	0.06	46,46,46,46	0
2	FMN	A	801	31/31	0.96	0.14	63,66,70,70	0
2	FMN	D	801	31/31	0.96	0.13	60,66,71,71	0
4	MG	B	804	1/1	0.97	0.15	48,48,48,48	0
4	MG	A	803	1/1	0.99	0.15	42,42,42,42	0
4	MG	D	804	1/1	0.99	0.04	43,43,43,43	0

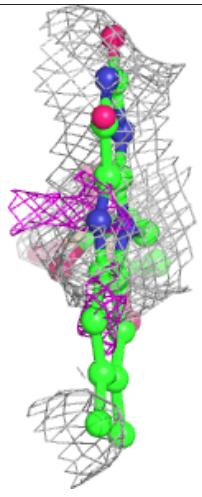
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN E 801 (A):

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

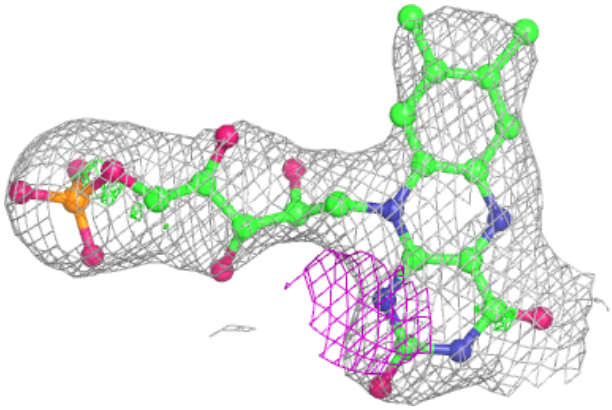


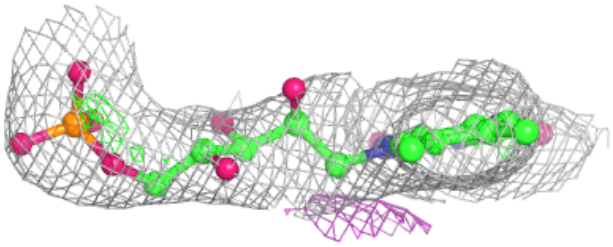


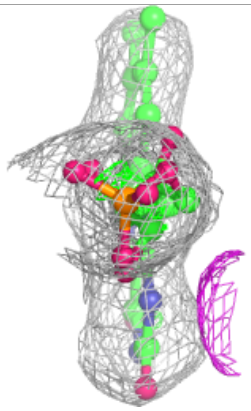


Electron density around FMN E 801 (B):

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

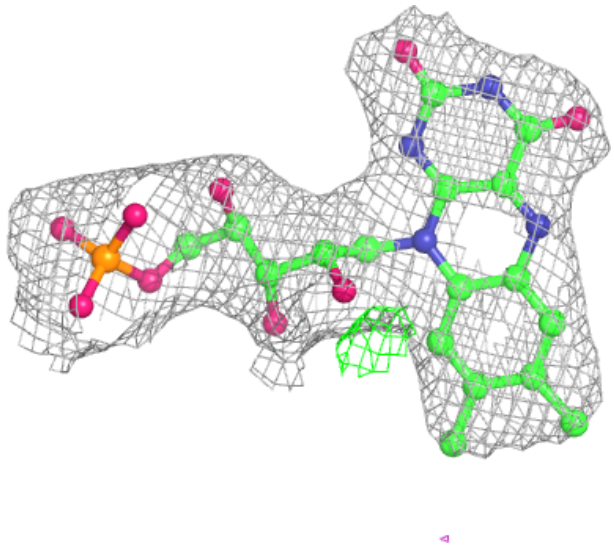


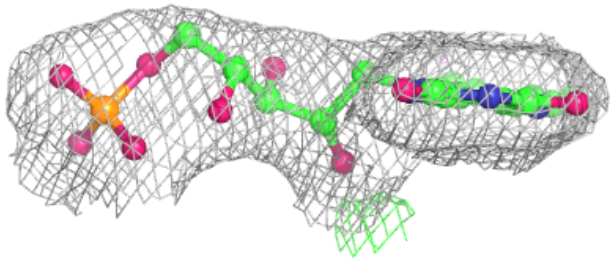


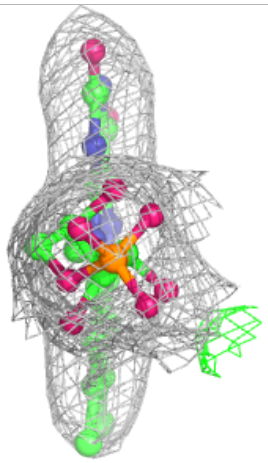


Electron density around FMN B 801:

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

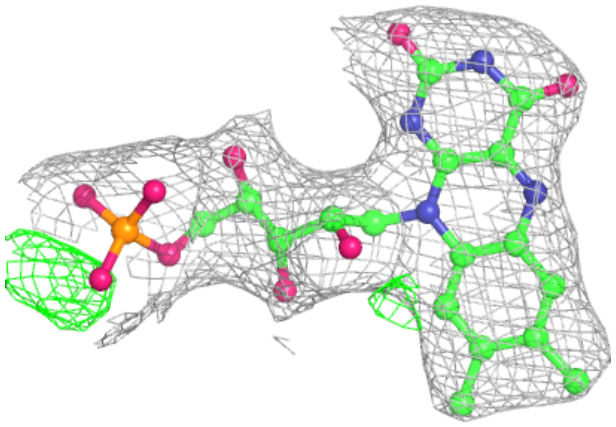


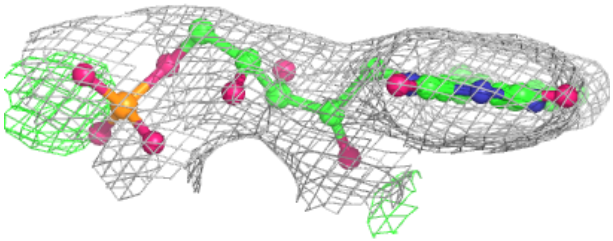


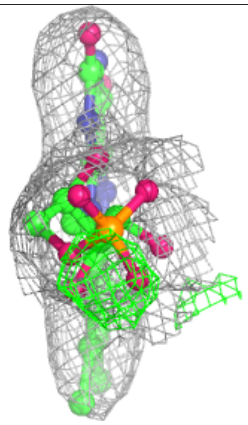


Electron density around FMN C 801:

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

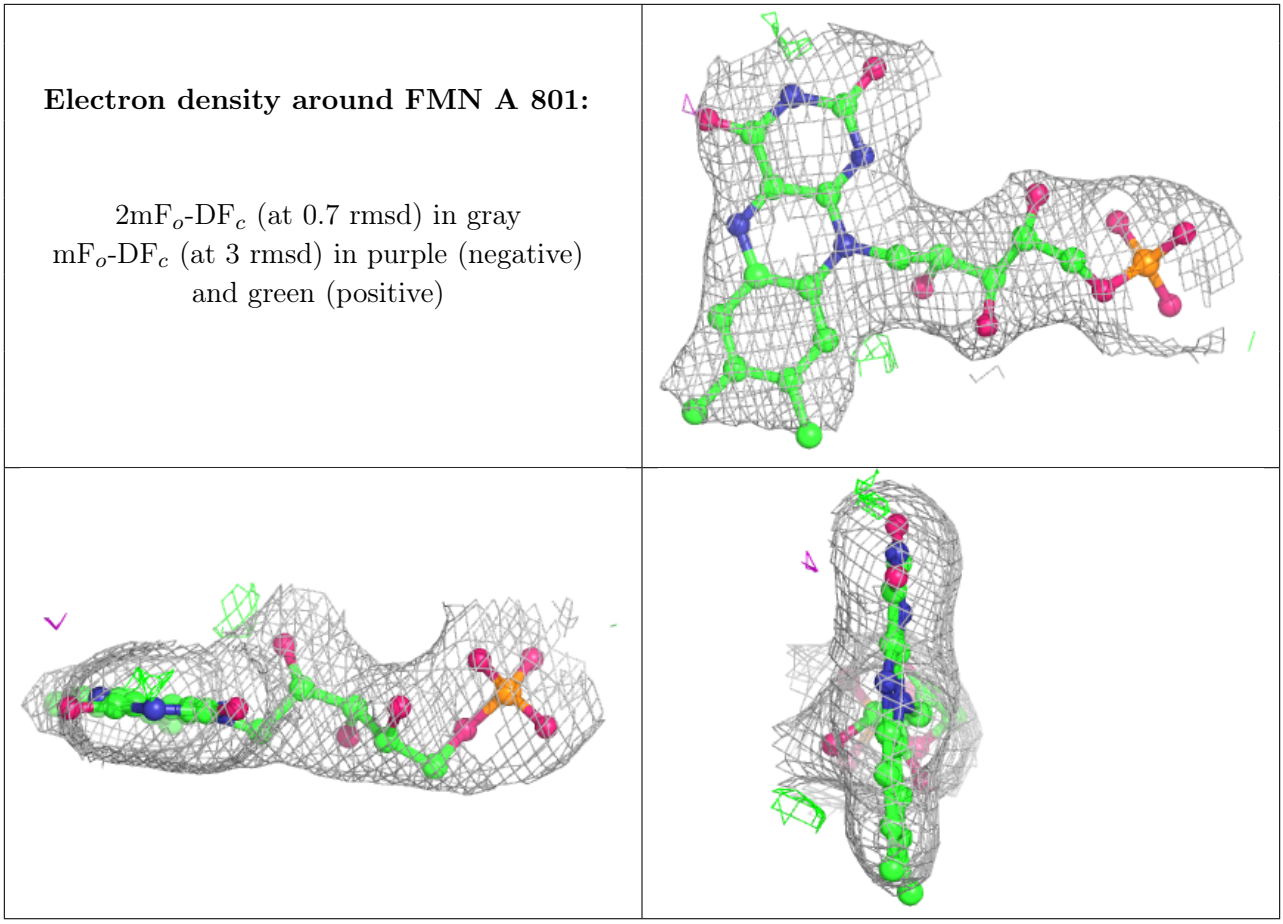






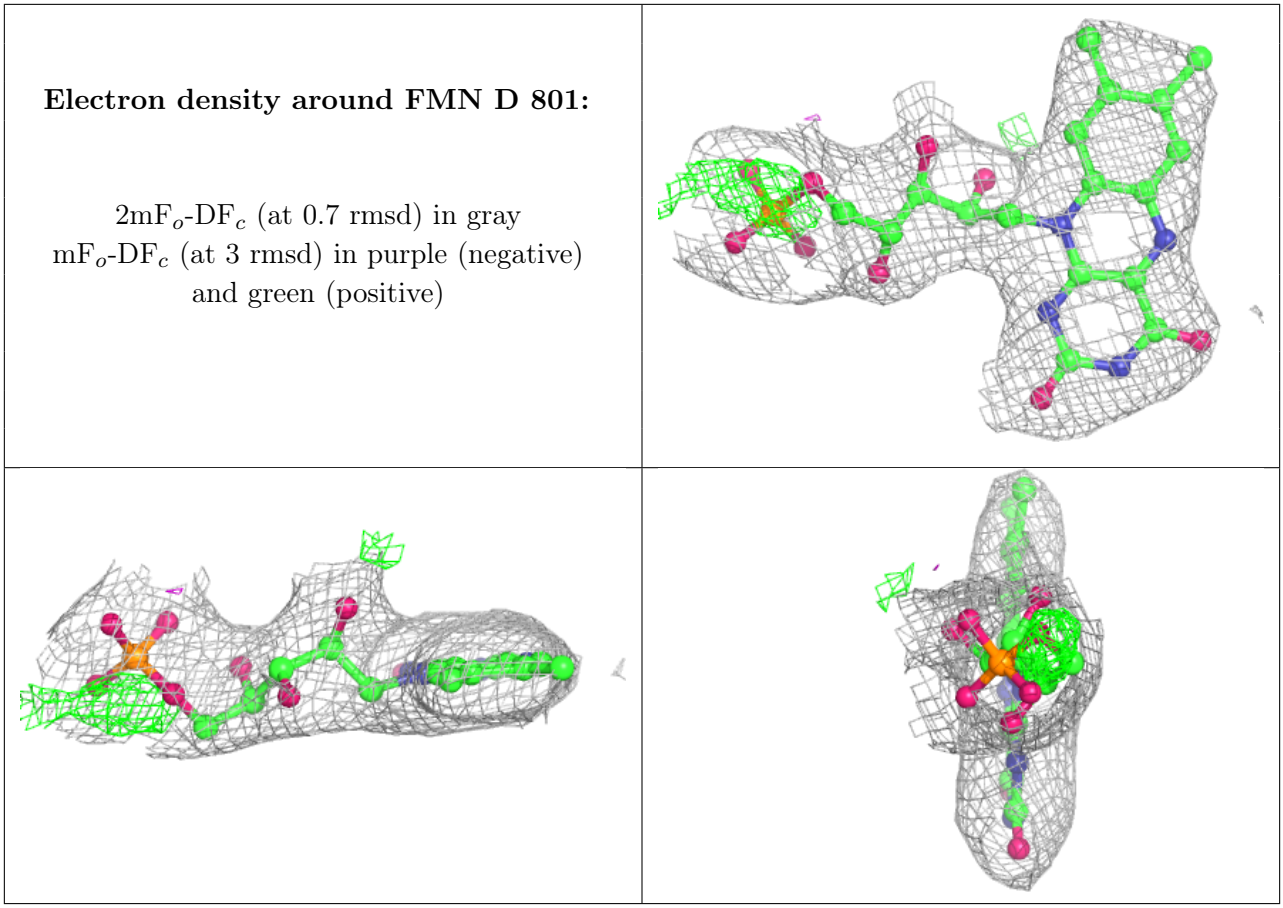
Electron density around FMN A 801:

$2mF_o$-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 801:

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



6.5 Other polymers

There are no such residues in this entry.