Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 08:15 AM EDT

PDB ID	:	7ABO
Title	:	Structure of the N318H variant of the reversible pyrrole-2-carboxylic acid decarboxylase PA0254/HudA in complex with FMN
Authors	:	Leys, D.; Marshall, S.A.
Deposited on	:	2020-09-08
Resolution	:	1.95 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:

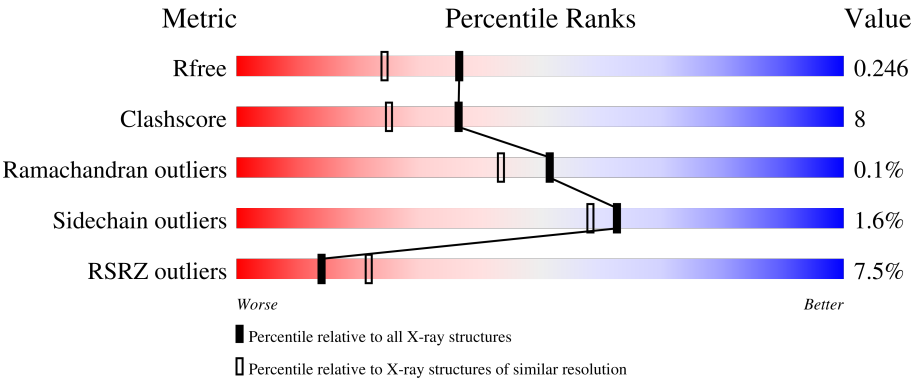
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	499	9% 83% 16%
1	B	499	10% 82% 18%
1	C	499	6% 82% 17%
1	D	499	5% 84% 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16551 atoms, of which 76 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.

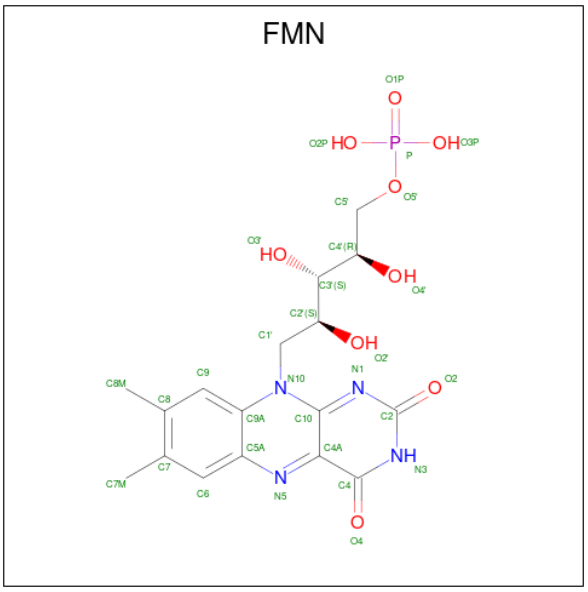
- Molecule 1 is a protein called UbiD-like decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	499	Total	C	N	O	S	0	0	0
			3808	2422	683	688	15			
1	B	496	Total	C	N	O	S	0	0	0
			3822	2428	690	689	15			
1	D	497	Total	C	N	O	S	0	0	0
			3816	2425	691	685	15			
1	A	498	Total	C	N	O	S	0	0	0
			3837	2435	698	689	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	expression tag	UNP A0A5F1BUV8
C	-1	GLN	-	expression tag	UNP A0A5F1BUV8
C	0	SER	-	expression tag	UNP A0A5F1BUV8
C	318	HIS	ASN	engineered mutation	UNP A0A5F1BUV8
B	-2	PHE	-	expression tag	UNP A0A5F1BUV8
B	-1	GLN	-	expression tag	UNP A0A5F1BUV8
B	0	SER	-	expression tag	UNP A0A5F1BUV8
B	318	HIS	ASN	engineered mutation	UNP A0A5F1BUV8
D	-2	PHE	-	expression tag	UNP A0A5F1BUV8
D	-1	GLN	-	expression tag	UNP A0A5F1BUV8
D	0	SER	-	expression tag	UNP A0A5F1BUV8
D	318	HIS	ASN	engineered mutation	UNP A0A5F1BUV8
A	-2	PHE	-	expression tag	UNP A0A5F1BUV8
A	-1	GLN	-	expression tag	UNP A0A5F1BUV8
A	0	SER	-	expression tag	UNP A0A5F1BUV8
A	318	HIS	ASN	engineered mutation	UNP A0A5F1BUV8

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	B	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	D	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	A	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0

- Molecule 5 is water.

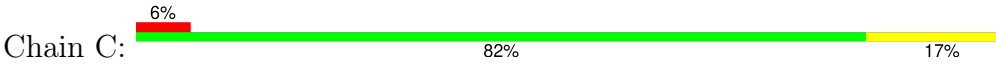
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	221	Total O 221 221	0	0
5	B	244	Total O 244 244	0	0
5	D	303	Total O 303 303	0	0
5	A	292	Total O 292 292	0	0

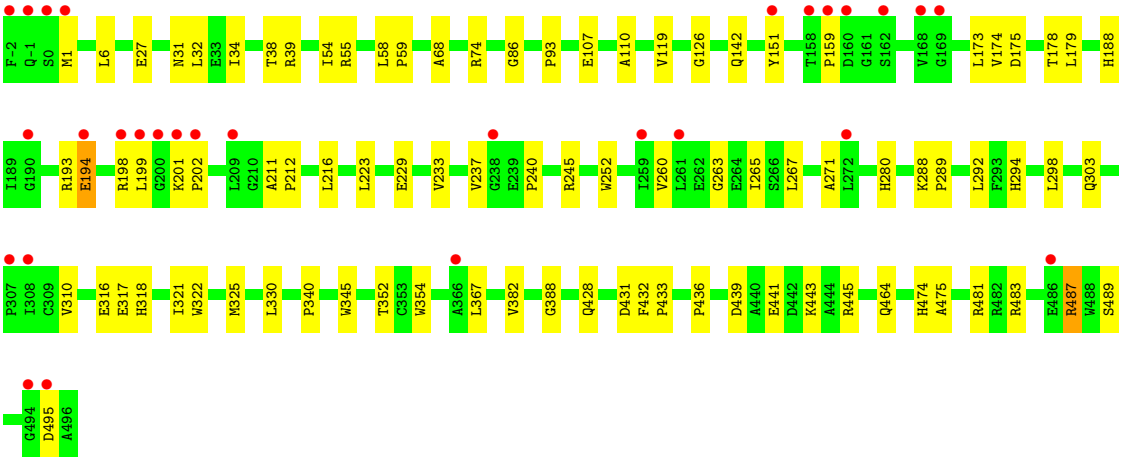
3 Residue-property plots (i)

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: UbiD-like decarboxylase

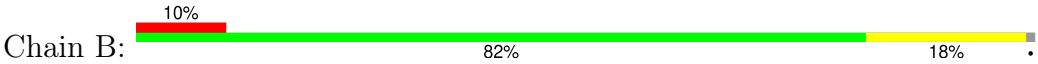
Chain C:

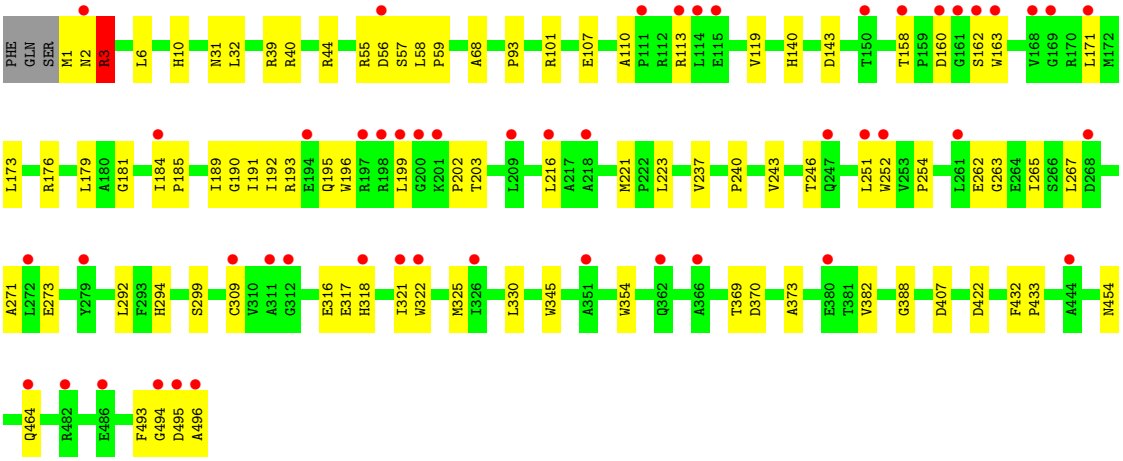




• Molecule 1: UbiD-like decarboxylase

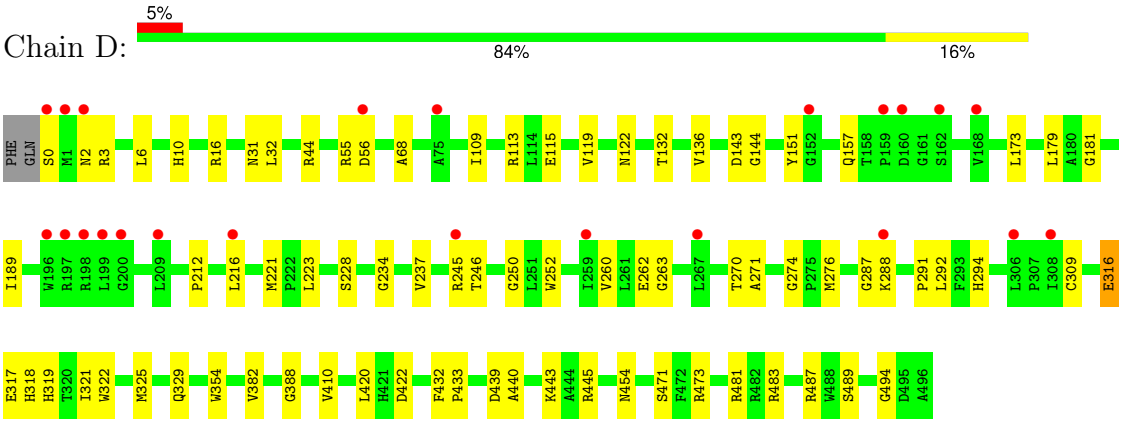
Chain B:





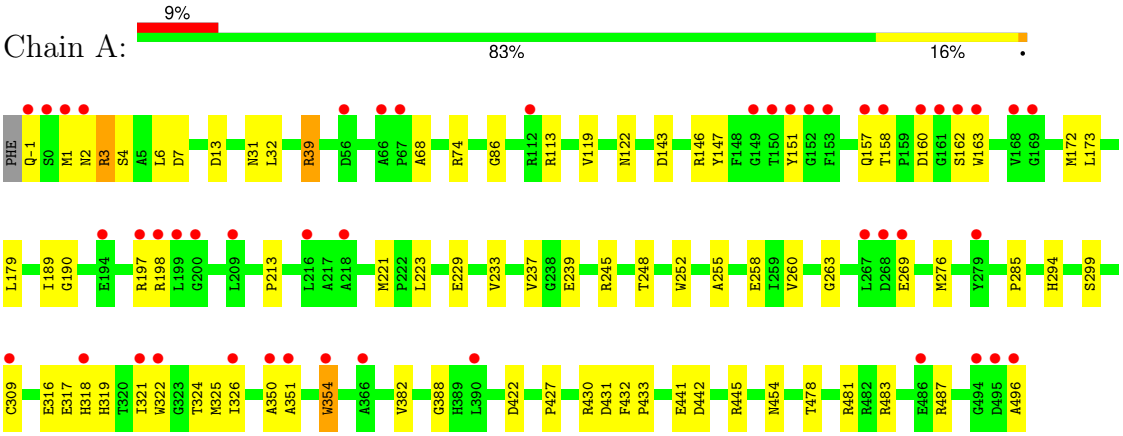
• Molecule 1: UbiD-like decarboxylase

Chain D:



- Molecule 1: UbiD-like decarboxylase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.88Å 55.57Å 198.88Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	40.93 – 1.95 40.93 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.93-1.95) 99.2 (40.93-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.214 , 0.246 0.215 , 0.246	Depositor DCC
R_{free} test set	8445 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16551	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 39.99 % 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 2.9237e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MN, 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	0.30	0/3946	0.49	0/5393
1	B	0.30	0/3931	0.50	2/5373 (0.0%)
1	C	0.28	0/3917	0.48	0/5359
1	D	0.29	0/3925	0.50	0/5366
All	All	0.29	0/15719	0.49	2/21491 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	B	107	GLU	OE1-CD-OE2	5.31	129.68	123.30

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	3837	0	3732	63	0
1	B	3822	0	3716	57	0
1	C	3808	0	3678	57	0
1	D	3816	0	3709	66	0
2	A	31	19	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	19	19	1	0
2	C	31	19	19	0	0
2	D	31	19	19	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	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	A	292	0	0	13	1
5	B	244	0	0	6	0
5	C	221	0	0	10	0
5	D	303	0	0	7	1
All	All	16475	76	14911	240	1

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 8.

All (240) 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:475:ALA:HA	5:C:601:HOH:O	1.15	1.32
1:C:474:HIS:O	5:C:601:HOH:O	1.78	1.00
1:C:194:GLU:OE2	1:C:194:GLU:O	1.82	0.96
1:D:316:GLU:OE2	1:D:317:GLU:N	2.02	0.93
1:D:316:GLU:OE1	1:D:318:HIS:ND1	2.04	0.90
1:D:294:HIS:ND1	5:D:601:HOH:O	2.13	0.82
1:D:316:GLU:OE2	1:D:318:HIS:N	2.11	0.82
1:A:245:ARG:O	5:A:601:HOH:O	1.99	0.81
1:A:6:LEU:HD21	1:A:237:VAL:HG21	1.63	0.80
1:C:288:LYS:HG2	1:C:289:PRO:HD2	1.65	0.78
1:B:58:LEU:HD12	1:B:59:PRO:HD2	1.65	0.78
2:B:501:FMN:O3P	5:B:601:HOH:O	2.03	0.76
1:B:6:LEU:HD21	1:B:237:VAL:HG21	1.67	0.74
1:A:239:GLU:OE1	5:A:604:HOH:O	2.05	0.74
1:A:431:ASP:OD1	5:A:603:HOH:O	2.05	0.74
1:A:3:ARG:HH21	1:A:7:ASP:HB2	1.53	0.74
1:A:113:ARG:HD3	1:A:252:TRP:CZ2	2.23	0.73
1:A:321:ILE:O	1:A:325:MET:HG2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:GLY:O	1:D:288:LYS:HD3	1.89	0.73
1:B:3:ARG:NH2	5:B:605:HOH:O	2.22	0.71
1:D:270:THR:HG23	5:D:851:HOH:O	1.91	0.71
1:B:158:THR:CG2	1:B:163:TRP:HB3	2.21	0.70
1:B:68:ALA:HB3	1:B:317:GLU:HG3	1.73	0.70
1:A:269:GLU:OE1	5:A:605:HOH:O	2.09	0.70
1:C:6:LEU:HD21	1:C:237:VAL:HG21	1.72	0.70
1:B:173:LEU:HA	1:B:179:LEU:HD23	1.75	0.69
1:B:55:ARG:HD3	1:B:56:ASP:HB2	1.75	0.68
1:A:-1:GLN:N	1:A:2:ASN:OD1	2.26	0.68
1:B:191:ILE:O	1:B:195:GLN:HG3	1.92	0.68
1:D:113:ARG:HD3	1:D:252:TRP:CZ2	2.29	0.67
1:B:318:HIS:O	1:B:322:TRP:HB3	1.93	0.67
1:C:431:ASP:OD2	5:C:602:HOH:O	2.11	0.67
1:B:202:PRO:HA	1:B:267:LEU:HD21	1.76	0.67
1:D:316:GLU:OE1	1:D:318:HIS:HB2	1.95	0.66
1:B:199:LEU:HD23	1:B:199:LEU:O	1.95	0.66
1:A:483:ARG:NH2	5:A:613:HOH:O	2.28	0.66
1:B:321:ILE:O	1:B:325:MET:HG2	1.95	0.65
1:A:318:HIS:O	1:A:322:TRP:HB3	1.97	0.65
1:D:119:VAL:HG21	1:D:260:VAL:HG23	1.79	0.65
1:D:489:SER:HA	1:D:494:GLY:H	1.62	0.65
1:B:407:ASP:HB2	5:B:760:HOH:O	1.97	0.64
1:B:158:THR:HG23	1:B:163:TRP:HB3	1.79	0.64
1:C:107:GLU:O	5:C:604:HOH:O	2.15	0.64
1:B:113:ARG:HB3	1:B:252:TRP:CZ3	2.33	0.64
1:A:74:ARG:HG3	5:A:830:HOH:O	1.98	0.63
1:A:119:VAL:HG21	1:A:260:VAL:HG23	1.80	0.63
1:C:445:ARG:HD3	5:C:644:HOH:O	1.97	0.63
1:C:321:ILE:O	1:C:325:MET:HG2	1.98	0.63
1:D:6:LEU:HD21	1:D:237:VAL:HG21	1.81	0.62
1:B:160:ASP:OD1	1:B:162:SER:HB2	1.99	0.62
1:D:321:ILE:O	1:D:325:MET:HG2	1.99	0.62
1:A:158:THR:CG2	1:A:163:TRP:HB3	2.30	0.62
1:B:273:GLU:OE2	5:B:602:HOH:O	2.15	0.60
1:C:481:ARG:NH1	5:C:603:HOH:O	2.15	0.60
1:A:158:THR:HG23	1:A:163:TRP:HB3	1.84	0.60
1:C:119:VAL:HG21	1:C:260:VAL:HG23	1.82	0.60
1:D:113:ARG:HB3	1:D:252:TRP:CZ3	2.37	0.59
1:A:119:VAL:HG21	1:A:260:VAL:CG2	2.32	0.59
1:C:194:GLU:OE2	1:C:194:GLU:C	2.40	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ALA:HB2	1:D:292:LEU:HD21	1.84	0.59
1:D:316:GLU:CD	1:D:318:HIS:H	2.06	0.59
1:C:201:LYS:O	1:C:267:LEU:HD21	2.03	0.58
1:A:487:ARG:NH2	5:A:618:HOH:O	2.37	0.58
1:C:263:GLY:HA3	1:C:294:HIS:O	2.03	0.58
1:B:263:GLY:HA3	1:B:294:HIS:O	2.04	0.58
1:C:1:MET:HE3	1:C:86:GLY:O	2.04	0.57
1:B:1:MET:H3	1:B:3:ARG:HH21	1.52	0.57
1:B:246:THR:HB	1:B:262:GLU:OE2	2.03	0.57
1:C:288:LYS:HG2	1:C:289:PRO:CD	2.33	0.57
1:D:318:HIS:O	1:D:322:TRP:HB3	2.03	0.57
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.70	0.56
1:A:432:PHE:CD1	1:A:433:PRO:HD2	2.41	0.56
1:B:432:PHE:CD1	1:B:433:PRO:HD2	2.40	0.56
1:B:93:PRO:HB3	1:B:345:TRP:CH2	2.41	0.56
1:B:158:THR:HG21	1:B:163:TRP:HB3	1.87	0.56
1:C:31:ASN:O	1:C:32:LEU:HB2	2.05	0.56
1:C:58:LEU:HD12	1:C:59:PRO:HD2	1.87	0.56
1:B:101:ARG:HD3	5:B:758:HOH:O	2.06	0.55
1:B:493:PHE:HB3	1:B:496:ALA:HB3	1.88	0.55
1:C:68:ALA:HB3	1:C:317:GLU:HG3	1.88	0.55
1:C:173:LEU:HA	1:C:179:LEU:HD23	1.88	0.55
1:D:68:ALA:HB3	1:D:317:GLU:HG3	1.88	0.55
1:D:119:VAL:HG21	1:D:260:VAL:CG2	2.37	0.55
1:C:318:HIS:O	1:C:322:TRP:HB3	2.07	0.54
1:D:473:ARG:HA	1:D:481:ARG:HD3	1.88	0.54
1:C:245:ARG:HG3	1:C:252:TRP:CE2	2.42	0.54
1:A:160:ASP:OD2	1:A:162:SER:HB2	2.08	0.54
1:A:324:THR:HB	1:A:325:MET:HE2	1.89	0.53
1:A:113:ARG:HD3	1:A:252:TRP:CH2	2.44	0.53
1:A:248:THR:HG22	1:A:248:THR:O	2.08	0.53
1:A:13:ASP:OD2	5:A:606:HOH:O	2.18	0.53
1:B:140:HIS:HB2	1:B:143:ASP:OD1	2.08	0.53
1:C:382:VAL:O	1:C:388:GLY:HA3	2.08	0.53
1:B:246:THR:HG23	1:B:251:LEU:O	2.09	0.53
1:C:198:ARG:C	1:C:199:LEU:HD23	2.30	0.52
1:B:464:GLN:HA	1:B:464:GLN:OE1	2.08	0.52
1:B:119:VAL:HG22	1:B:299:SER:OG	2.10	0.52
1:A:68:ALA:HB3	1:A:317:GLU:HG3	1.91	0.52
1:B:2:ASN:H	1:B:3:ARG:NH2	2.08	0.52
1:A:263:GLY:HA3	1:A:294:HIS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ARG:HG3	1:C:252:TRP:CZ2	2.44	0.52
1:D:316:GLU:OE1	1:D:318:HIS:CG	2.61	0.52
1:A:258:GLU:OE2	5:A:607:HOH:O	2.19	0.52
1:C:159:PRO:HD2	5:C:651:HOH:O	2.10	0.51
1:C:202:PRO:HA	1:C:267:LEU:HD21	1.91	0.51
1:B:243:VAL:HG12	1:B:254:PRO:HA	1.91	0.51
1:B:369:THR:OG1	1:B:373:ALA:HB3	2.11	0.51
1:A:382:VAL:O	1:A:388:GLY:HA3	2.10	0.51
1:D:245:ARG:HG2	1:D:252:TRP:CD2	2.46	0.50
1:C:193:ARG:HD2	1:C:265:ILE:HG21	1.92	0.50
1:D:157:GLN:N	5:D:603:HOH:O	2.17	0.50
1:D:3:ARG:HB3	1:D:10:HIS:CD2	2.47	0.50
1:A:119:VAL:HG12	1:A:255:ALA:O	2.12	0.50
1:D:173:LEU:HA	1:D:179:LEU:HD23	1.93	0.49
1:B:1:MET:N	1:B:3:ARG:HH21	2.10	0.49
1:D:144:GLY:HA3	1:D:274:GLY:O	2.13	0.49
1:D:432:PHE:CD1	1:D:433:PRO:HD2	2.47	0.49
1:A:422:ASP:HB3	1:A:454:ASN:O	2.13	0.49
1:C:34:ILE:HD11	1:C:54:ILE:HG12	1.95	0.49
1:B:246:THR:HB	1:B:262:GLU:CD	2.33	0.49
1:B:221:MET:HG2	1:B:223:LEU:HG	1.94	0.49
1:B:382:VAL:O	1:B:388:GLY:HA3	2.13	0.49
1:C:441:GLU:HG3	1:C:445:ARG:HE	1.78	0.49
1:D:316:GLU:OE2	1:D:316:GLU:C	2.51	0.49
1:C:432:PHE:CD1	1:C:433:PRO:HD2	2.48	0.48
1:B:31:ASN:O	1:B:32:LEU:HB2	2.13	0.48
1:D:31:ASN:O	1:D:32:LEU:HB2	2.12	0.48
1:C:74:ARG:NH2	5:C:617:HOH:O	2.46	0.48
1:D:3:ARG:HD3	1:D:10:HIS:CG	2.47	0.48
1:C:119:VAL:HG21	1:C:260:VAL:CG2	2.43	0.48
1:D:136:VAL:O	1:D:136:VAL:HG13	2.13	0.48
1:D:316:GLU:OE1	1:D:318:HIS:CB	2.61	0.48
1:D:439:ASP:O	1:D:443:LYS:HG3	2.14	0.48
1:B:271:ALA:HB2	1:B:292:LEU:HD21	1.96	0.47
1:A:197:ARG:HG3	1:A:197:ARG:NH1	2.28	0.47
1:C:340:PRO:HG3	1:C:367:LEU:HD11	1.96	0.47
1:C:174:VAL:HB	1:C:178:THR:OG1	2.15	0.47
1:A:1:MET:O	1:A:86:GLY:HA2	2.14	0.47
1:A:442:ASP:OD1	1:A:445:ARG:NH2	2.47	0.47
1:C:439:ASP:O	1:C:443:LYS:HG3	2.15	0.47
1:D:44:ARG:NE	1:A:496:ALA:O	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ARG:HG2	1:D:252:TRP:CE2	2.50	0.47
1:C:229:GLU:O	1:C:233:VAL:HG23	2.15	0.47
1:B:2:ASN:H	1:B:3:ARG:CZ	2.28	0.47
1:A:430:ARG:HD3	5:A:844:HOH:O	2.15	0.47
1:C:288:LYS:CG	1:C:289:PRO:HD2	2.42	0.46
1:C:27:GLU:CD	1:C:55:ARG:HG3	2.35	0.46
1:A:478:THR:OG1	1:A:481:ARG:NH2	2.49	0.46
1:B:192:ILE:O	1:B:196:TRP:HD1	1.99	0.46
1:B:422:ASP:HB3	1:B:454:ASN:O	2.15	0.46
1:A:3:ARG:NH2	1:A:7:ASP:HB2	2.26	0.46
1:B:176:ARG:NH2	5:B:623:HOH:O	2.48	0.46
1:D:6:LEU:HA	1:D:212:PRO:HB3	1.98	0.46
1:C:271:ALA:HB2	1:C:292:LEU:HD21	1.97	0.45
1:B:3:ARG:NE	1:B:3:ARG:H	2.13	0.45
1:A:-1:GLN:H2	1:A:2:ASN:CG	2.16	0.45
1:D:245:ARG:NE	1:D:250:GLY:HA2	2.31	0.45
1:D:445:ARG:HD3	5:D:605:HOH:O	2.16	0.45
1:C:93:PRO:HB3	1:C:345:TRP:CH2	2.51	0.45
1:C:495:ASP:N	1:D:16:ARG:HD3	2.32	0.45
1:B:3:ARG:HB2	1:B:10:HIS:CE1	2.51	0.45
1:B:110:ALA:O	1:B:240:PRO:HB3	2.17	0.45
1:D:250:GLY:N	5:D:609:HOH:O	2.39	0.45
1:A:158:THR:HG21	1:A:163:TRP:HB3	1.99	0.44
1:A:441:GLU:O	1:A:445:ARG:HG3	2.17	0.44
1:D:0:SER:HA	1:D:10:HIS:NE2	2.31	0.44
1:D:382:VAL:O	1:D:388:GLY:HA3	2.18	0.44
1:D:471:SER:HA	1:A:39:ARG:HD3	1.99	0.44
1:A:350:ALA:HB2	1:A:354:TRP:CE2	2.52	0.44
1:C:303:GLN:NE2	5:C:605:HOH:O	2.18	0.44
1:B:193:ARG:HD2	1:B:265:ILE:HG21	1.98	0.44
1:C:110:ALA:O	1:C:240:PRO:HB3	2.18	0.44
1:D:115:GLU:H	1:D:115:GLU:CD	2.21	0.44
1:D:143:ASP:OD1	1:D:276:MET:HA	2.18	0.44
1:A:245:ARG:HG2	1:A:252:TRP:CZ3	2.52	0.44
1:A:157:GLN:HG2	1:A:158:THR:O	2.18	0.44
1:C:298:LEU:C	1:C:298:LEU:HD12	2.37	0.44
1:B:369:THR:OG1	1:B:370:ASP:N	2.50	0.44
1:D:122:ASN:HA	5:D:741:HOH:O	2.18	0.44
1:A:285:PRO:HD2	5:A:715:HOH:O	2.18	0.43
1:B:40:ARG:HG2	1:B:44:ARG:HD3	2.00	0.43
1:D:263:GLY:HA3	1:D:294:HIS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.82	0.43
1:A:350:ALA:HB2	1:A:354:TRP:NE1	2.33	0.43
1:A:229:GLU:O	1:A:233:VAL:HG23	2.19	0.43
1:B:3:ARG:H	1:B:3:ARG:CD	2.32	0.43
1:A:31:ASN:O	1:A:32:LEU:HB2	2.18	0.43
1:A:147:TYR:CE2	1:A:172:MET:HB2	2.53	0.43
1:D:136:VAL:HG11	1:D:173:LEU:HD22	1.99	0.43
1:C:175:ASP:OD1	1:C:178:THR:HG23	2.18	0.43
1:D:410:VAL:HG13	1:A:354:TRP:CZ2	2.53	0.43
1:C:151:TYR:CZ	1:C:216:LEU:HD22	2.54	0.42
1:C:39:ARG:HG2	1:C:310:VAL:HG11	2.00	0.42
1:C:151:TYR:CE1	1:C:317:GLU:HG2	2.54	0.42
1:D:422:ASP:HB3	1:D:454:ASN:O	2.19	0.42
1:C:211:ALA:HB1	1:C:212:PRO:HD2	2.02	0.42
1:A:146:ARG:NE	5:A:628:HOH:O	2.52	0.42
1:C:38:THR:HG21	5:C:609:HOH:O	2.18	0.42
1:C:464:GLN:OE1	1:C:464:GLN:HA	2.19	0.42
1:D:151:TYR:CZ	1:D:216:LEU:HD22	2.55	0.42
1:A:221:MET:HG2	1:A:223:LEU:HG	2.01	0.42
1:B:171:LEU:HD23	1:B:181:GLY:HA3	2.00	0.42
1:B:330:LEU:HD22	1:B:382:VAL:HG13	2.01	0.42
1:D:246:THR:HB	1:D:262:GLU:CD	2.40	0.42
1:A:173:LEU:HA	1:A:179:LEU:HD23	2.01	0.42
1:B:184:ILE:HG23	1:B:185:PRO:HD2	2.02	0.42
1:D:246:THR:HB	1:D:262:GLU:OE2	2.19	0.42
1:D:113:ARG:HD3	1:D:252:TRP:CH2	2.54	0.42
1:D:189:ILE:HG22	5:D:667:HOH:O	2.19	0.42
1:D:221:MET:HE2	1:D:329:GLN:HG2	2.02	0.42
1:D:420:LEU:HD11	1:A:427:PRO:HB3	2.02	0.42
1:B:216:LEU:HD13	1:B:216:LEU:C	2.40	0.41
1:A:223:LEU:N	5:A:617:HOH:O	2.53	0.41
1:C:280:HIS:HB2	1:C:436:PRO:HG3	2.02	0.41
1:D:181:GLY:O	1:D:291:PRO:HD2	2.20	0.41
1:D:440:ALA:HA	1:D:443:LYS:HD2	2.03	0.41
1:A:350:ALA:CB	1:A:354:TRP:NE1	2.83	0.41
1:D:316:GLU:HG3	1:D:319:HIS:CE1	2.56	0.41
1:A:4:SER:O	1:A:213:PRO:HG2	2.20	0.41
1:A:143:ASP:OD1	1:A:276:MET:HA	2.19	0.41
1:C:483:ARG:HG3	1:C:487:ARG:HD2	2.03	0.41
1:D:113:ARG:HB3	1:D:252:TRP:CH2	2.55	0.41
1:D:483:ARG:HG3	1:D:487:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ARG:HG3	1:B:203:THR:OG1	2.21	0.41
1:B:494:GLY:O	1:B:495:ASP:HB2	2.20	0.41
1:A:322:TRP:NE1	1:A:326:ILE:HD11	2.35	0.41
2:D:501:FMN:H2'	2:D:501:FMN:H5'2	1.89	0.41
1:A:151:TYR:CE1	1:A:317:GLU:HG2	2.55	0.41
1:B:189:ILE:HG23	1:B:190:GLY:N	2.35	0.41
1:D:109:ILE:HB	1:D:234:GLY:HA3	2.02	0.41
1:A:189:ILE:HG23	1:A:190:GLY:N	2.36	0.41
1:D:221:MET:HG2	1:D:223:LEU:HG	2.01	0.41
1:C:330:LEU:HD21	1:C:388:GLY:CA	2.51	0.40
1:D:132:THR:HG22	1:D:173:LEU:HD21	2.02	0.40
1:C:188:HIS:HE1	1:C:223:LEU:O	2.04	0.40
1:D:55:ARG:HG2	1:D:56:ASP:OD1	2.22	0.40
1:A:122:ASN:O	1:A:299:SER:HA	2.22	0.40
1:D:245:ARG:CZ	1:D:250:GLY:HA2	2.51	0.40
1:C:352:THR:HG22	1:C:352:THR:O	2.20	0.40
1:A:319:HIS:CD2	1:A:351:ALA:HA	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:721:HOH:O	5:A:805:HOH:O[1_545]	2.18	0.02

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	496/499 (99%)	475 (96%)	21 (4%)	0	100	100
1	B	494/499 (99%)	472 (96%)	22 (4%)	0	100	100
1	C	497/499 (100%)	480 (97%)	16 (3%)	1 (0%)	47	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	495/499 (99%)	478 (97%)	17 (3%)	0	100 100
All	All	1982/1996 (99%)	1905 (96%)	76 (4%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	389/396 (98%)	383 (98%)	6 (2%)	65 60
1	B	388/396 (98%)	382 (98%)	6 (2%)	65 60
1	C	383/396 (97%)	376 (98%)	7 (2%)	59 53
1	D	386/396 (98%)	381 (99%)	5 (1%)	69 65
All	All	1546/1584 (98%)	1522 (98%)	24 (2%)	62 58

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	142	GLN
1	C	194	GLU
1	C	316	GLU
1	C	354	TRP
1	C	428	GLN
1	C	487	ARG
1	C	489	SER
1	B	3	ARG
1	B	39	ARG
1	B	57	SER
1	B	309	CYS
1	B	316	GLU
1	B	354	TRP

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Mol	Chain	Res	Type
1	D	2	ASN
1	D	228	SER
1	D	309	CYS
1	D	316	GLU
1	D	354	TRP
1	A	3	ARG
1	A	39	ARG
1	A	198	ARG
1	A	309	CYS
1	A	316	GLU
1	A	354	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2	ASN
1	A	31	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	B	501	3,4	33,33,33	1.01	2 (6%)	48,50,50	1.46	8 (16%)
2	FMN	A	501	3,4	33,33,33	1.02	2 (6%)	48,50,50	1.21	5 (10%)
2	FMN	D	501	3,4	33,33,33	1.04	2 (6%)	48,50,50	1.21	7 (14%)
2	FMN	C	501	3,4	33,33,33	1.04	2 (6%)	48,50,50	1.29	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	501	3,4	-	0/18/18/18	0/3/3/3
2	FMN	A	501	3,4	-	0/18/18/18	0/3/3/3
2	FMN	D	501	3,4	-	2/18/18/18	0/3/3/3
2	FMN	C	501	3,4	-	1/18/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FMN	C4A-N5	3.47	1.38	1.30
2	B	501	FMN	C4A-N5	3.37	1.38	1.30
2	C	501	FMN	C4A-N5	3.22	1.37	1.30
2	D	501	FMN	C4A-N5	3.14	1.37	1.30
2	D	501	FMN	C10-N1	2.67	1.38	1.33
2	C	501	FMN	C10-N1	2.64	1.38	1.33
2	A	501	FMN	C10-N1	2.53	1.38	1.33
2	B	501	FMN	C10-N1	2.43	1.38	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FMN	C4'-C3'-C2'	-4.26	106.49	113.57
2	C	501	FMN	C4'-C3'-C2'	-3.40	107.91	113.57
2	D	501	FMN	C4-N3-C2	-3.17	120.02	125.64
2	A	501	FMN	C4-N3-C2	-3.15	120.04	125.64
2	C	501	FMN	C4-N3-C2	-3.10	120.14	125.64
2	B	501	FMN	C4-N3-C2	-3.02	120.28	125.64
2	B	501	FMN	C4A-C10-N10	2.86	120.58	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FMN	O4-C4-C4A	-2.86	118.98	126.53
2	A	501	FMN	C4A-C10-N10	2.85	120.56	116.48
2	B	501	FMN	C10-C4A-N5	-2.58	119.55	124.81
2	B	501	FMN	C4A-C4-N3	2.57	119.80	113.25
2	A	501	FMN	O4-C4-C4A	-2.55	119.79	126.53
2	C	501	FMN	C4A-C10-N10	2.53	120.11	116.48
2	A	501	FMN	C4A-C4-N3	2.53	119.69	113.25
2	D	501	FMN	C4A-C10-N10	2.47	120.01	116.48
2	A	501	FMN	C10-C4A-N5	-2.46	119.78	124.81
2	C	501	FMN	C4A-C4-N3	2.46	119.51	113.25
2	C	501	FMN	C10-C4A-N5	-2.44	119.82	124.81
2	D	501	FMN	C4A-C4-N3	2.38	119.31	113.25
2	C	501	FMN	O4-C4-C4A	-2.34	120.37	126.53
2	B	501	FMN	O4-C4-C4A	-2.33	120.38	126.53
2	B	501	FMN	O2'-C2'-C3'	2.32	114.67	109.25
2	D	501	FMN	C4-C4A-C10	2.27	120.83	116.93
2	B	501	FMN	O3'-C3'-C2'	2.18	113.88	108.93
2	D	501	FMN	C10-C4A-N5	-2.11	120.50	124.81
2	D	501	FMN	C4A-C10-N1	-2.01	119.66	124.59

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	FMN	C2'-C3'-C4'-C5'
2	D	501	FMN	C4'-C5'-O5'-P
2	C	501	FMN	C2'-C3'-C4'-C5'

There are no ring outliers.

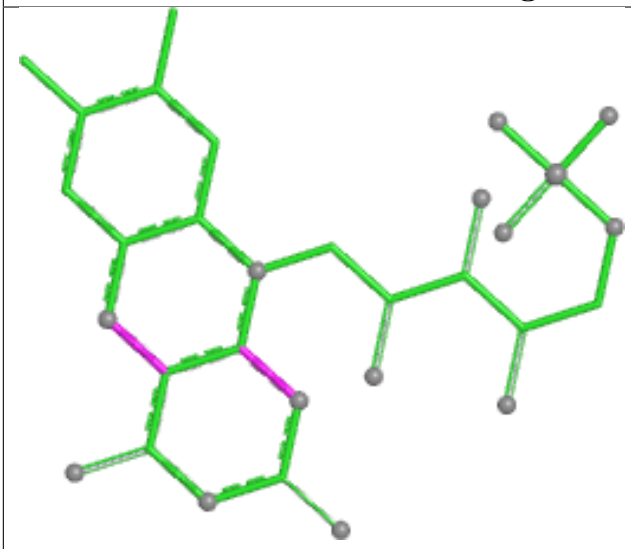
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FMN	1	0
2	D	501	FMN	1	0

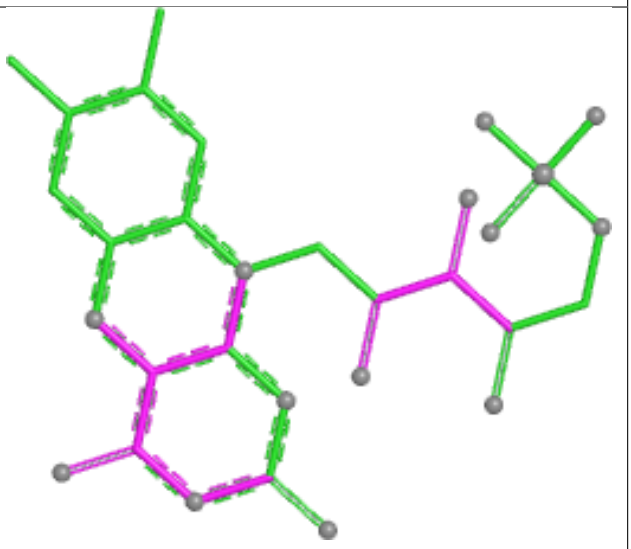
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

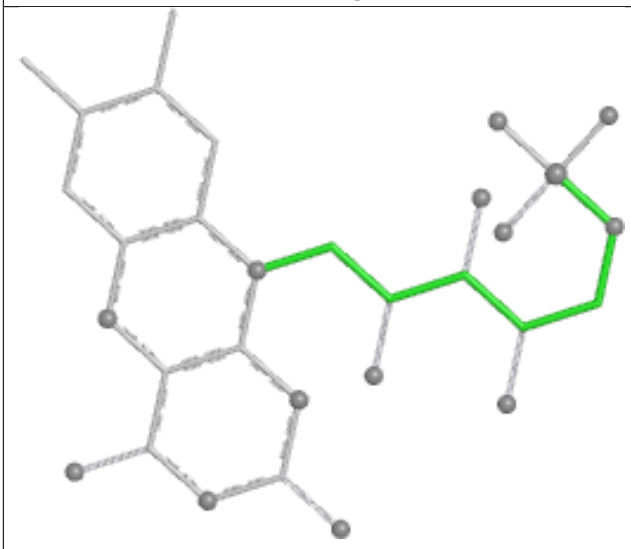
Ligand FMN B 501



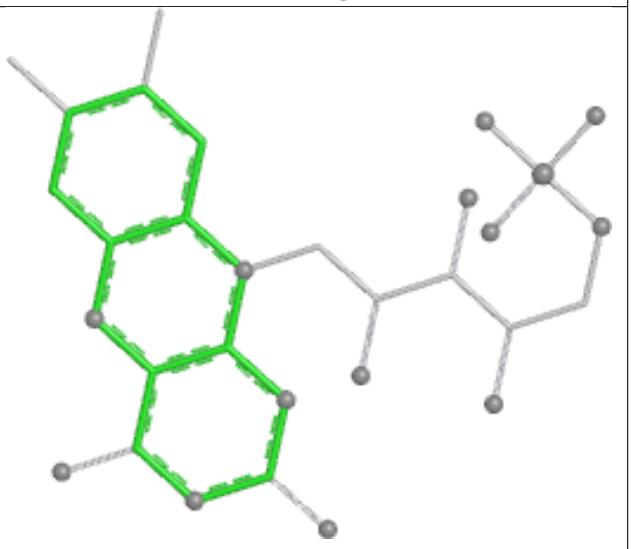
Bond lengths



Bond angles

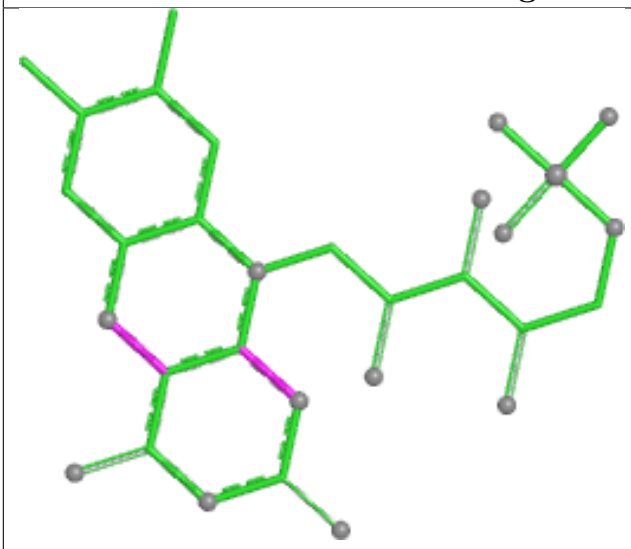


Torsions

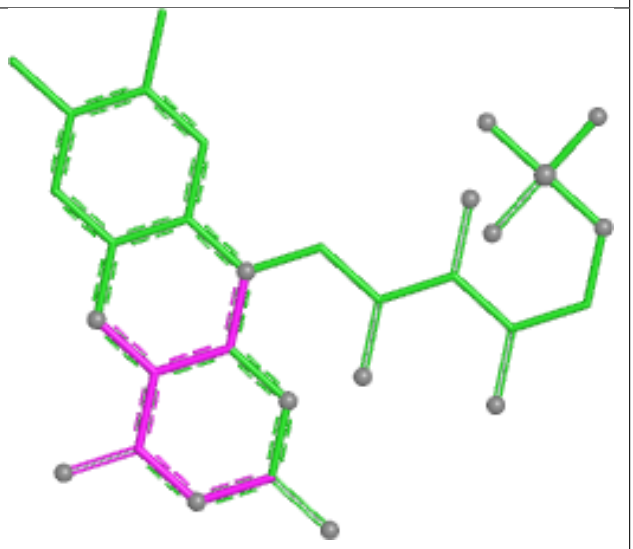


Rings

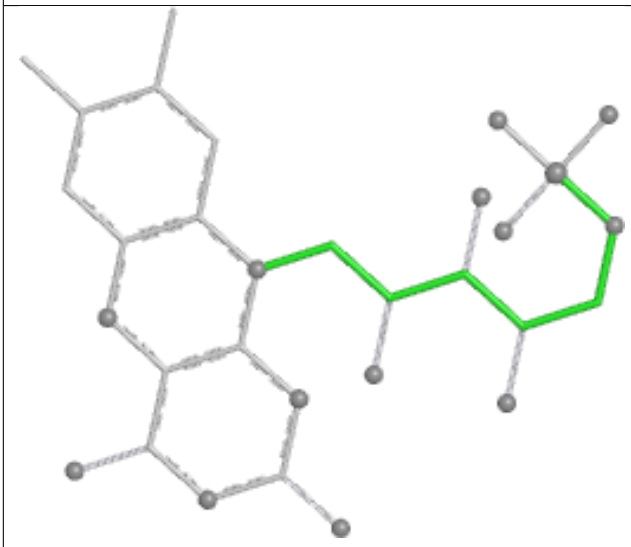
Ligand FMN A 501



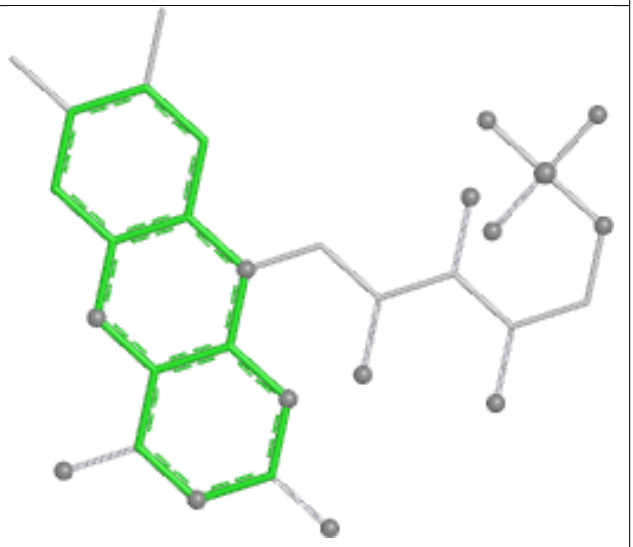
Bond lengths



Bond angles

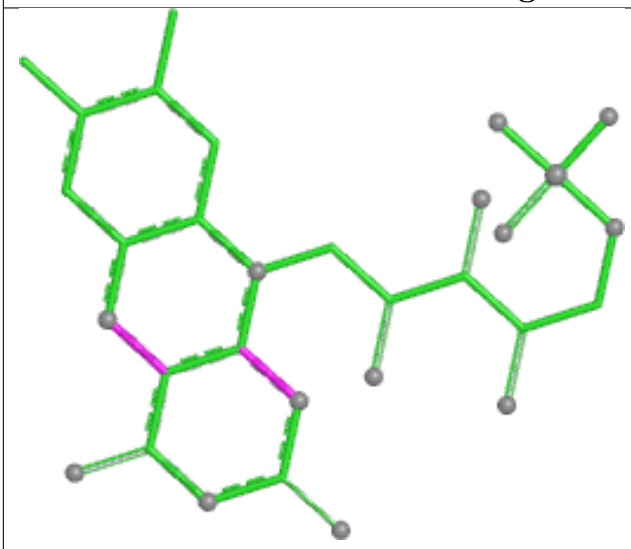


Torsions

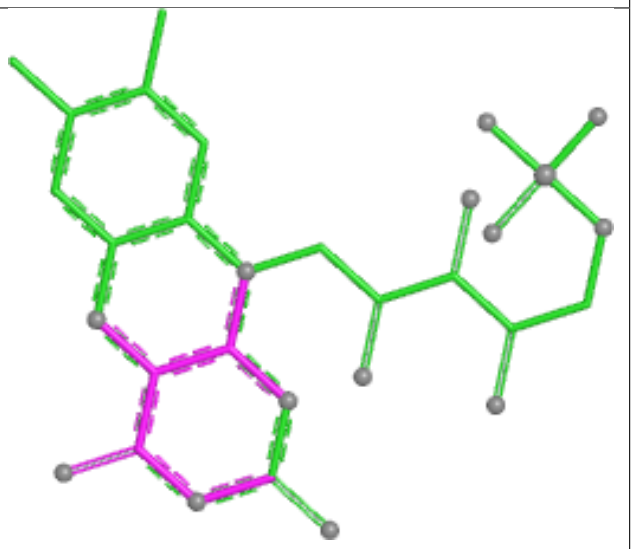


Rings

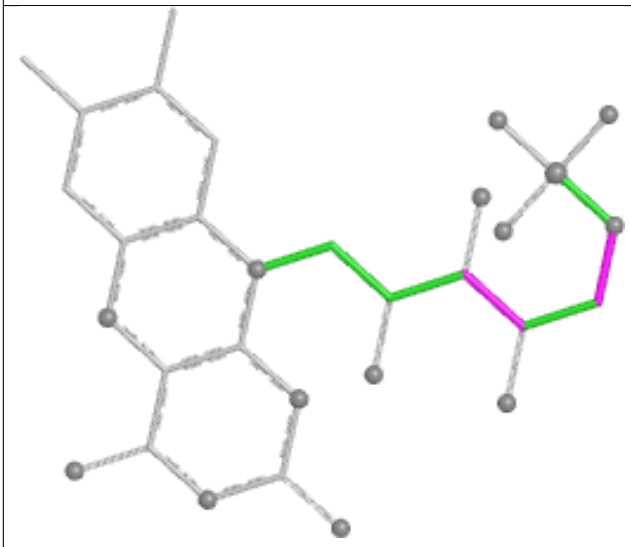
Ligand FMN D 501



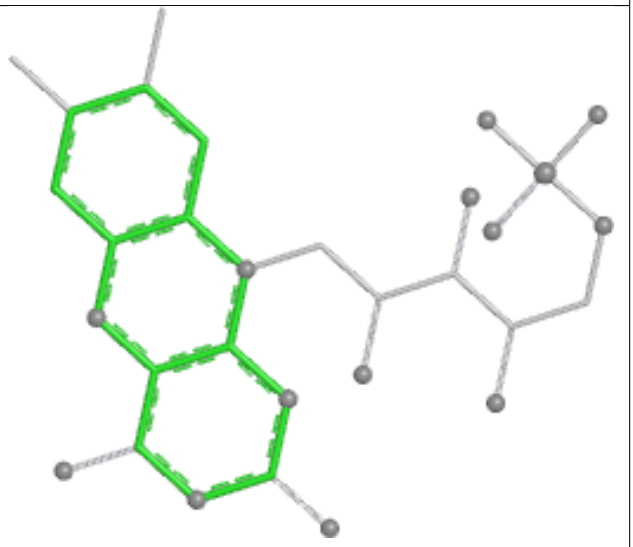
Bond lengths



Bond angles

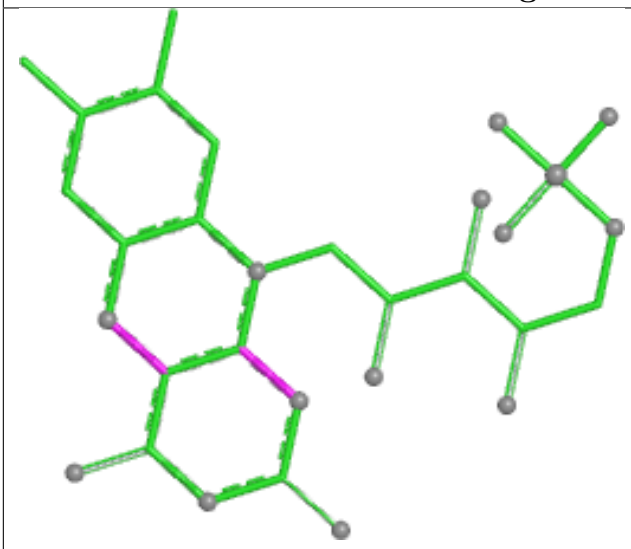


Torsions

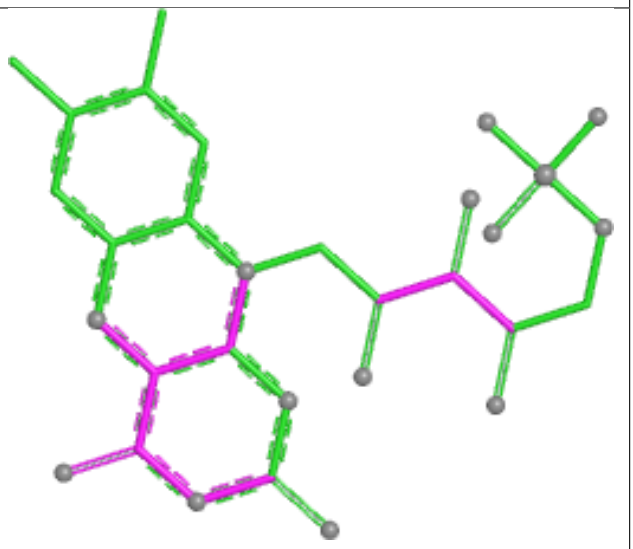


Rings

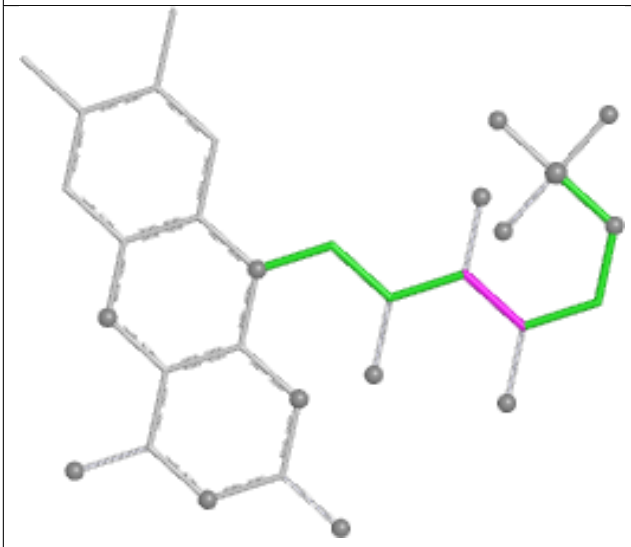
Ligand FMN C 501



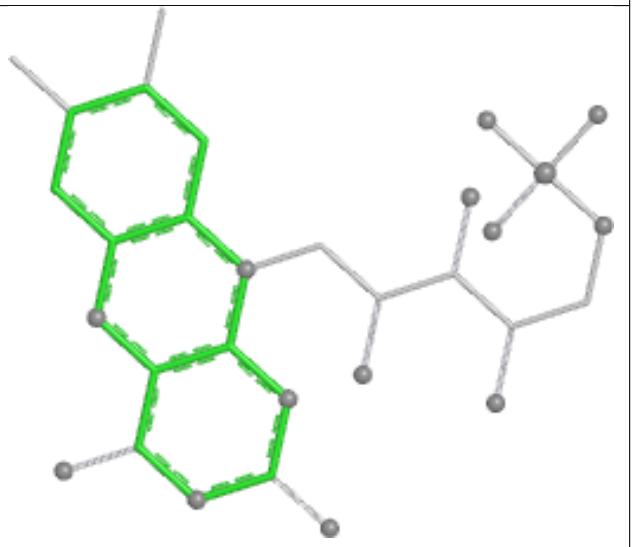
Bond lengths



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	498/499 (99%)	0.62	47 (9%)	8 13	19, 36, 58, 73	0
1	B	496/499 (99%)	0.66	50 (10%)	7 11	23, 39, 62, 89	0
1	C	499/499 (100%)	0.41	29 (5%)	23 31	23, 37, 57, 78	0
1	D	497/499 (99%)	0.33	23 (4%)	32 42	20, 34, 54, 65	0
All	All	1990/1996 (99%)	0.50	149 (7%)	14 22	19, 36, 57, 89	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	ASP	7.2
1	C	200	GLY	5.9
1	A	198	ARG	5.8
1	C	-2	PHE	5.7
1	A	495	ASP	5.5
1	B	200	GLY	5.0
1	A	168	VAL	4.9
1	B	201	LYS	4.8
1	A	0	SER	4.7
1	D	267	LEU	4.4
1	B	366	ALA	4.3
1	C	1	MET	4.2
1	C	168	VAL	4.2
1	D	1	MET	4.0
1	A	267	LEU	4.0
1	B	168	VAL	3.9
1	B	496	ALA	3.7
1	B	198	ARG	3.6
1	A	216	LEU	3.6
1	B	194	GLU	3.6
1	D	209	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	114	LEU	3.5
1	C	366	ALA	3.5
1	A	321	ILE	3.5
1	C	194	GLU	3.5
1	B	252	TRP	3.5
1	B	251	LEU	3.5
1	B	197	ARG	3.4
1	D	198	ARG	3.4
1	D	199	LEU	3.4
1	D	168	VAL	3.4
1	A	209	LEU	3.4
1	B	115	GLU	3.3
1	A	350	ALA	3.3
1	A	322	TRP	3.3
1	B	184	ILE	3.3
1	B	169	GLY	3.3
1	A	161	GLY	3.2
1	C	308	ILE	3.2
1	A	160	ASP	3.2
1	C	160	ASP	3.2
1	A	-1	GLN	3.2
1	A	1	MET	3.2
1	B	162	SER	3.1
1	A	354	TRP	3.1
1	B	199	LEU	3.0
1	A	268	ASP	3.0
1	A	153	PHE	3.0
1	B	268	ASP	3.0
1	B	160	ASP	3.0
1	A	279	TYR	2.9
1	A	351	ALA	2.9
1	A	309	CYS	2.9
1	B	321	ILE	2.9
1	B	161	GLY	2.9
1	B	494	GLY	2.9
1	C	-1	GLN	2.9
1	A	151	TYR	2.8
1	C	209	LEU	2.8
1	B	482	ARG	2.8
1	B	311	ALA	2.8
1	A	194	GLU	2.8
1	D	308	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	162	SER	2.7
1	B	309	CYS	2.7
1	C	201	LYS	2.7
1	B	158	THR	2.7
1	B	113	ARG	2.7
1	A	486	GLU	2.7
1	C	159	PRO	2.7
1	B	111	PRO	2.7
1	A	163	TRP	2.6
1	D	197	ARG	2.6
1	C	0	SER	2.6
1	A	158	THR	2.6
1	A	197	ARG	2.6
1	B	272	LEU	2.6
1	B	56	ASP	2.6
1	A	318	HIS	2.6
1	C	272	LEU	2.5
1	B	247	GLN	2.5
1	D	0	SER	2.5
1	B	216	LEU	2.5
1	D	160	ASP	2.5
1	D	200	GLY	2.5
1	A	169	GLY	2.5
1	A	162	SER	2.5
1	A	496	ALA	2.5
1	B	322	TRP	2.4
1	D	75	ALA	2.4
1	C	259	ILE	2.4
1	C	199	LEU	2.4
1	A	326	ILE	2.4
1	A	149	GLY	2.4
1	D	2	ASN	2.3
1	B	279	TYR	2.3
1	A	150	THR	2.3
1	B	380	GLU	2.3
1	D	259	ILE	2.3
1	B	351	ALA	2.3
1	A	366	ALA	2.3
1	D	56	ASP	2.3
1	B	209	LEU	2.3
1	D	196	TRP	2.3
1	A	157	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	159	PRO	2.2
1	B	444	ALA	2.2
1	C	151	TYR	2.2
1	A	200	GLY	2.2
1	A	494	GLY	2.2
1	B	261	LEU	2.2
1	A	199	LEU	2.2
1	B	362	GLN	2.2
1	D	288	LYS	2.2
1	B	2	ASN	2.2
1	A	112	ARG	2.2
1	C	307	PRO	2.2
1	D	162	SER	2.2
1	A	67	PRO	2.2
1	B	318	HIS	2.2
1	A	390	LEU	2.2
1	C	202	PRO	2.1
1	D	306	LEU	2.1
1	A	56	ASP	2.1
1	B	486	GLU	2.1
1	A	269	GLU	2.1
1	C	494	GLY	2.1
1	A	66	ALA	2.1
1	C	486	GLU	2.1
1	B	326	ILE	2.1
1	C	261	LEU	2.1
1	A	218	ALA	2.1
1	A	2	ASN	2.1
1	A	152	GLY	2.1
1	B	218	ALA	2.1
1	C	198	ARG	2.1
1	B	171	LEU	2.1
1	D	216	LEU	2.1
1	D	152	GLY	2.1
1	D	245	ARG	2.0
1	C	158	THR	2.0
1	C	495	ASP	2.0
1	C	190	GLY	2.0
1	B	150	THR	2.0
1	C	169	GLY	2.0
1	C	238	GLY	2.0
1	B	312	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	163	TRP	2.0
1	B	464	GLN	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)

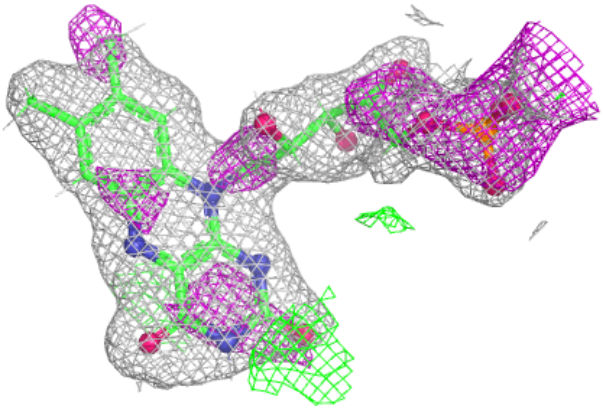
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

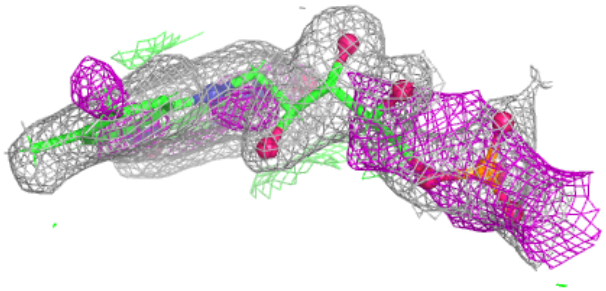
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FMN	A	501	31/31	0.84	0.18	31,41,47,53	0
2	FMN	B	501	31/31	0.89	0.15	35,44,52,62	0
2	FMN	C	501	31/31	0.89	0.12	30,38,45,55	0
2	FMN	D	501	31/31	0.91	0.12	30,37,44,50	0
3	MN	D	502	1/1	0.98	0.04	33,33,33,33	0
4	NA	C	503	1/1	0.98	0.23	28,28,28,28	0
4	NA	D	503	1/1	0.98	0.27	26,26,26,26	0
3	MN	C	502	1/1	0.99	0.09	41,41,41,41	0
4	NA	B	503	1/1	0.99	0.21	31,31,31,31	0
3	MN	A	502	1/1	0.99	0.05	36,36,36,36	0
4	NA	A	503	1/1	0.99	0.25	27,27,27,27	0
3	MN	B	502	1/1	1.00	0.04	43,43,43,43	0

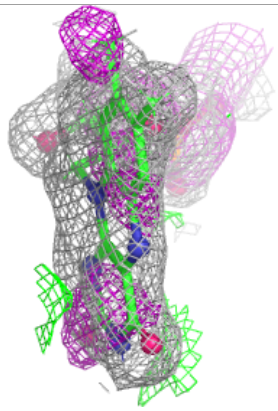
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN A 501:

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

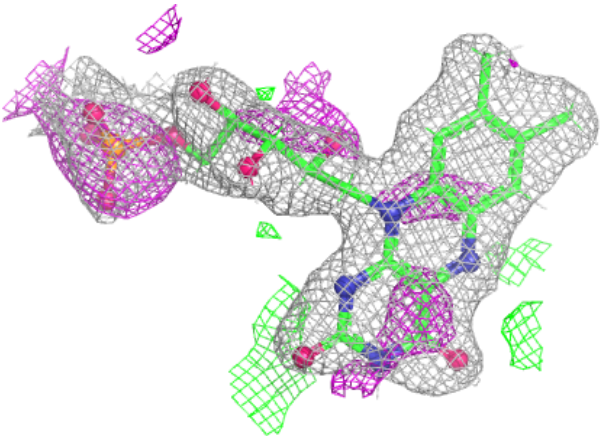


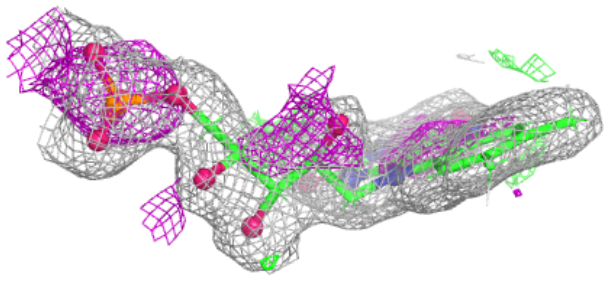


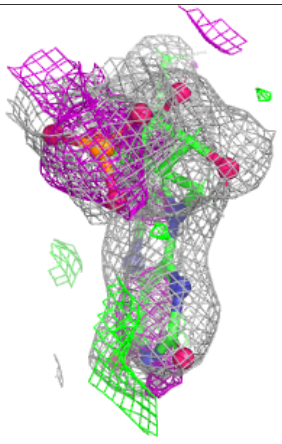


Electron density around FMN B 501:

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

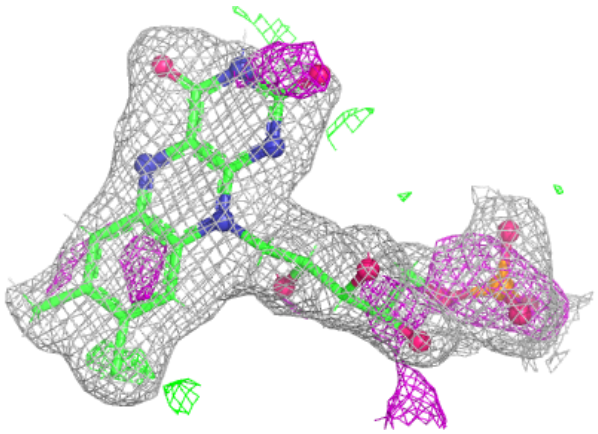


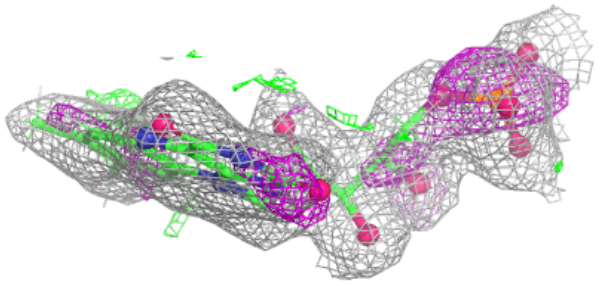


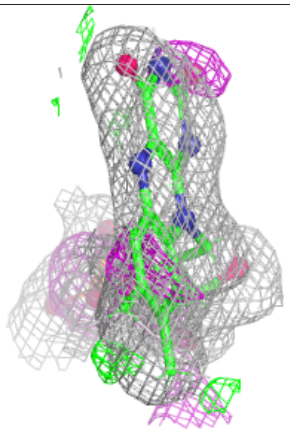


Electron density around FMN C 501:

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

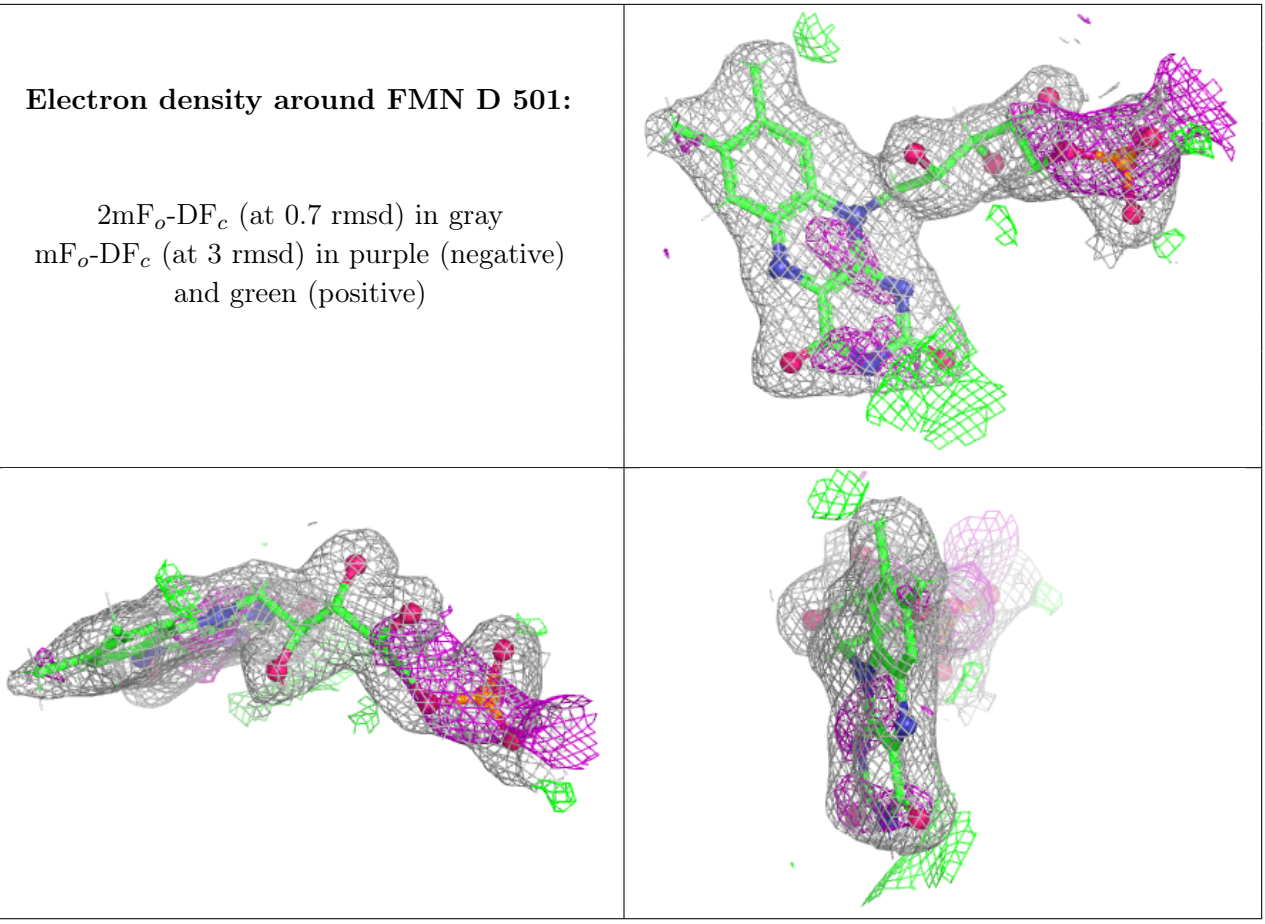






Electron density around FMN D 501:

$2mF_o$-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.