



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:06 PM UTC

PDB ID : 7ABO / pdb_00007abo
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

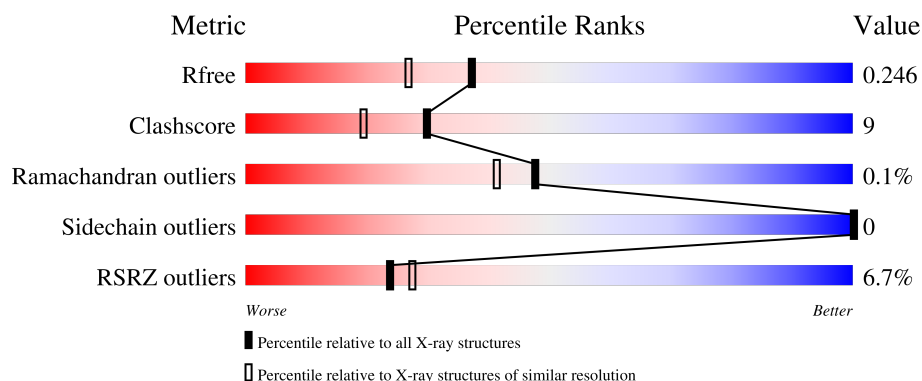
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	499	8% 83% 16%
1	B	499	9% 83% 17% .
1	C	499	6% 82% 18%
1	D	499	4% 84% 15%

2 Entry composition

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.

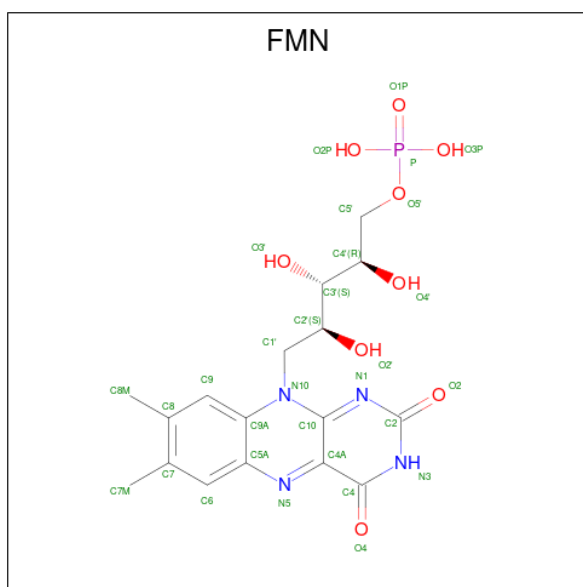
- Molecule 1 is a protein called UbiD-like decarboxylase.

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 (CCD ID: 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	
			50	17	19	4	9	1	
2	B	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	
2	D	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	
2	A	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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

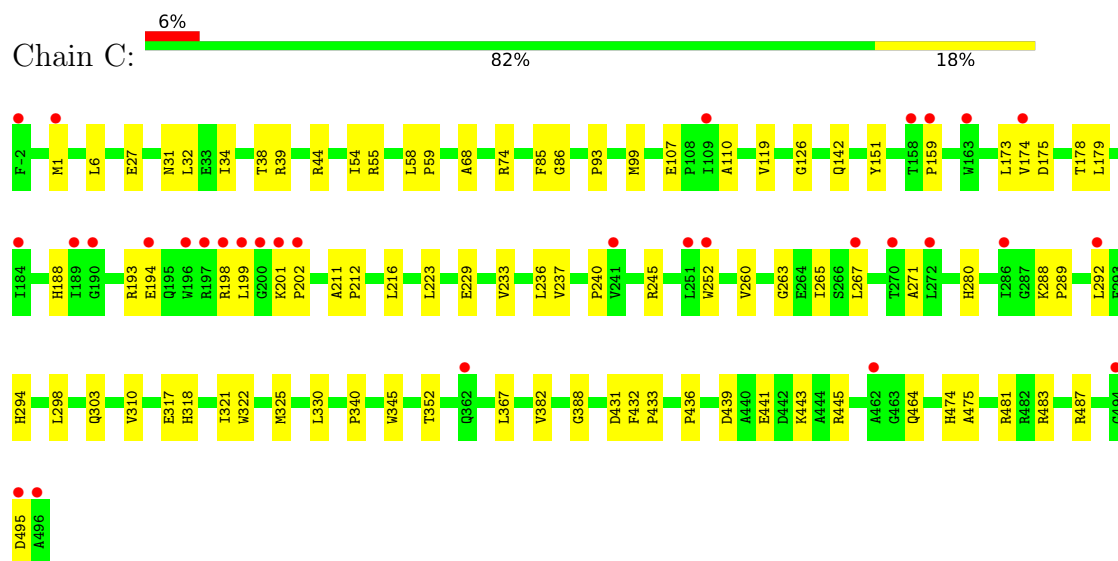
- Molecule 5 is water.

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

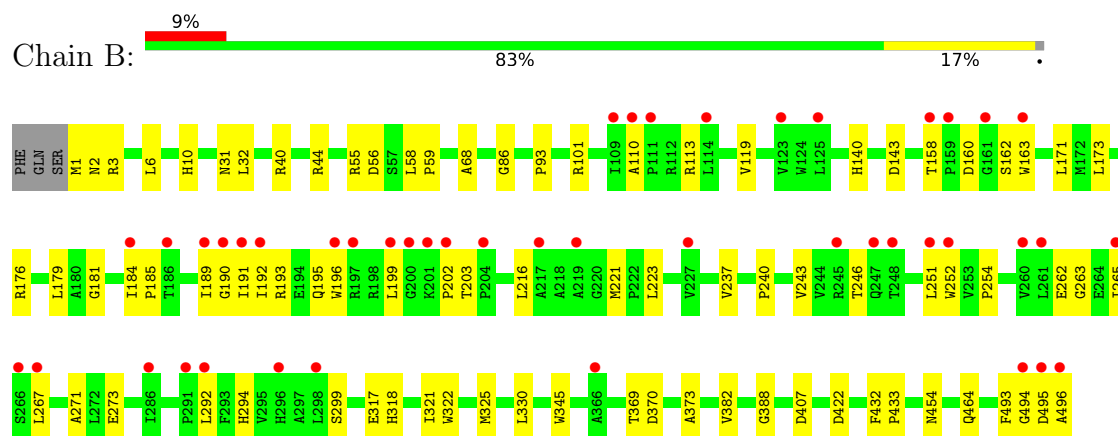
3 Residue-property plots [i](#)

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.

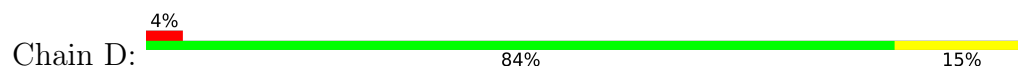
- Molecule 1: UbiD-like decarboxylase

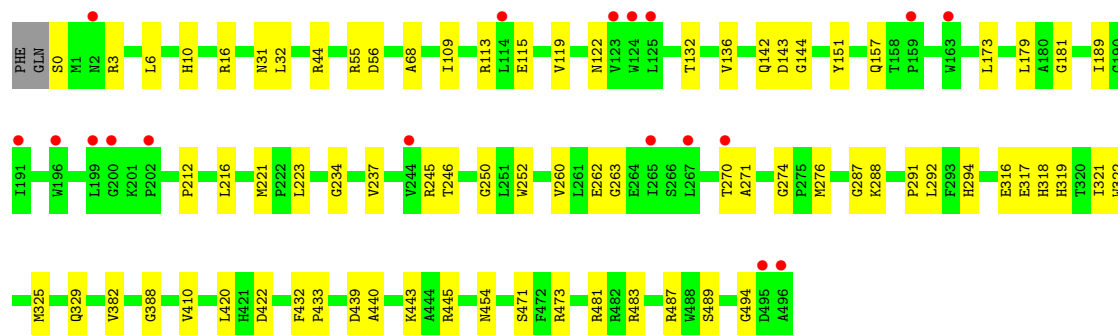


- Molecule 1: UbiD-like decarboxylase

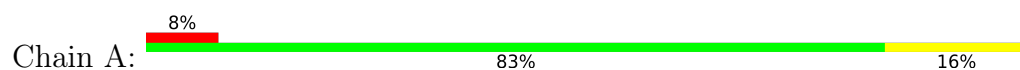


- Molecule 1: UbiD-like decarboxylase





• Molecule 1: UbiD-like decarboxylase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	8446 reflections (4.96%)	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 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, NA, MN

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	0.20	0/3946	0.42	0/5393
1	B	0.22	0/3931	0.43	0/5373
1	C	0.19	0/3917	0.40	0/5359
1	D	0.21	0/3925	0.43	0/5366
All	All	0.20	0/15719	0.42	0/21491

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3837	0	3732	67	0
1	B	3822	0	3716	63	0
1	C	3808	0	3678	64	0
1	D	3816	0	3709	69	0
2	A	31	19	19	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	258	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 9.

All (258) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:99:MET:HE3	1:C:236:LEU:HD11	1.75	0.69
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:1:MET:HE3	1:B:86:GLY:O	1.98	0.64
1:B:407:ASP:HB2	5:B:760:HOH:O	1.97	0.64
1:C:194:GLU:OE2	1:C:194:GLU:C	2.40	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:D:316:GLU:CD	1:D:318:HIS:H	2.06	0.63
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:B:113:ARG:HH21	1:B:252:TRP:CD1	2.19	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

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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: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:113:ARG:HH21	1:B:252:TRP:NE1	2.01	0.58
1:B:263:GLY:HA3	1:B:294:HIS:O	2.04	0.58
1:B:1:MET:H3	1:B:3:ARG:HH21	1.52	0.57
1:C:198:ARG:C	1:C:199:LEU:HD23	2.30	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:85:PHE:HZ	1:A:325:MET:HE1	1.70	0.56
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:C:1:MET:HE3	1:C:86:GLY:O	2.08	0.54
1:D:221:MET:HE2	1:D:329:GLN:HG2	1.90	0.54
1:A:-1:GLN:H2	1:A:2:ASN:CG	2.15	0.54
1:A:160:ASP:OD2	1:A:162:SER:HB2	2.08	0.54
1:B:246:THR:HB	1:B:262:GLU:CD	2.33	0.54
1:C:85:PHE:HB3	1:C:99:MET:HE1	1.90	0.53
1:D:316:GLU:OE2	1:D:316:GLU:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:PHE:CB	1:C:99:MET:HE1	2.39	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
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:D:316:GLU:CD	1:D:318:HIS:HD1	2.15	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:85:PHE:CZ	1:A:325:MET:HE1	2.45	0.51
1:C:27:GLU:CD	1:C:55:ARG:HG3	2.35	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:C:298:LEU:C	1:C:298:LEU:HD12	2.37	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: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:115:GLU:H	1:D:115:GLU:CD	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:245:ARG:HG2	1:D:252:TRP:CE2	2.50	0.47
1:D:246:THR:HB	1:D:262:GLU:CD	2.40	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:B:216:LEU:HD13	1:B:216:LEU:C	2.40	0.46
1:A:221:MET:HE2	1:A:329:GLN:HG2	1.97	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: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:324:THR:HB	1:A:325:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ALA:O	1:C:240:PRO:HB3	2.18	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: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
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.82	0.43
1:C:99:MET:HE2	1:C:99:MET:HB3	1.72	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:A:298:LEU:C	1:A:298:LEU:HD12	2.45	0.42
1:C:38:THR:HG21	5:C:609:HOH:O	2.18	0.42
1:D:115:GLU:CD	1:D:115:GLU:N	2.78	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: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:420:LEU:HD11	1:A:427:PRO:HB3	2.02	0.42
1:A:223:LEU:N	5:A:617:HOH:O	2.53	0.41
1:C:44:ARG:HE	1:B:496:ALA:C	2.28	0.41
1:C:280:HIS:HB2	1:C:436:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLN:H	1:D:142:GLN:CD	2.28	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:C:464:GLN:OE1	1:C:464:GLN:HA	2.19	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
1:C:44:ARG:HH21	1:B:496:ALA:C	2.29	0.41
1:B:113:ARG:HH21	1:B:252:TRP:CG	2.37	0.41
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:C:142:GLN:H	1:C:142:GLN:CD	2.29	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 ⓘ

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	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%)	43	36
1	D	495/499 (99%)	478 (97%)	17 (3%)	0	100	100
All	All	1982/1996 (99%)	1905 (96%)	76 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	GLY

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	389/396 (98%)	389 (100%)	0	100	100
1	B	388/396 (98%)	388 (100%)	0	100	100
1	C	383/396 (97%)	383 (100%)	0	100	100
1	D	386/396 (98%)	386 (100%)	0	100	100
All	All	1546/1584 (98%)	1546 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	421	HIS
1	C	428	GLN
1	B	2	ASN
1	B	14	HIS
1	B	157	GLN
1	D	2	ASN
1	D	421	HIS
1	A	389	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 oligosaccharides 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	D	501	3,4	33,33,33	1.04	2 (6%)	48,50,50	1.21	7 (14%)
2	FMN	B	501	3,4	33,33,33	1.01	2 (6%)	48,50,50	1.46	8 (16%)
2	FMN	C	501	3,4	33,33,33	1.04	2 (6%)	48,50,50	1.29	6 (12%)
2	FMN	A	501	3,4	33,33,33	1.02	2 (6%)	48,50,50	1.21	5 (10%)

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	501	3,4	-	2/18/18/18	0/3/3/3
2	FMN	B	501	3,4	-	0/18/18/18	0/3/3/3
2	FMN	C	501	3,4	-	1/18/18/18	0/3/3/3
2	FMN	A	501	3,4	-	0/18/18/18	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(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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:

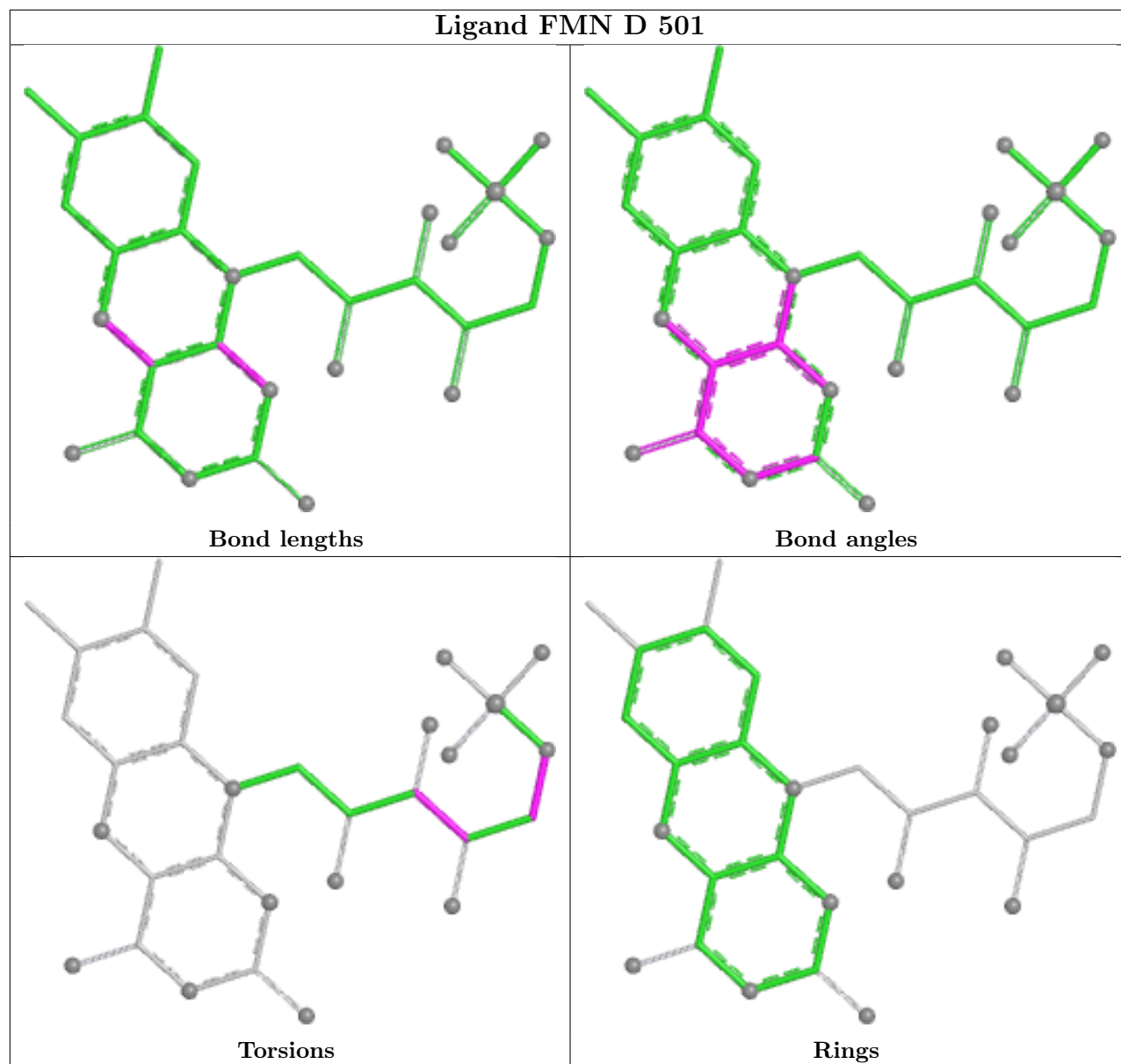
Mol	Chain	Res	Type	Atoms
2	D	501	FMN	C2'-C3'-C4'-C5'
2	D	501	FMN	C4'-C5'-O5'-P
2	C	501	FMN	C2'-C3'-C4'-C5'

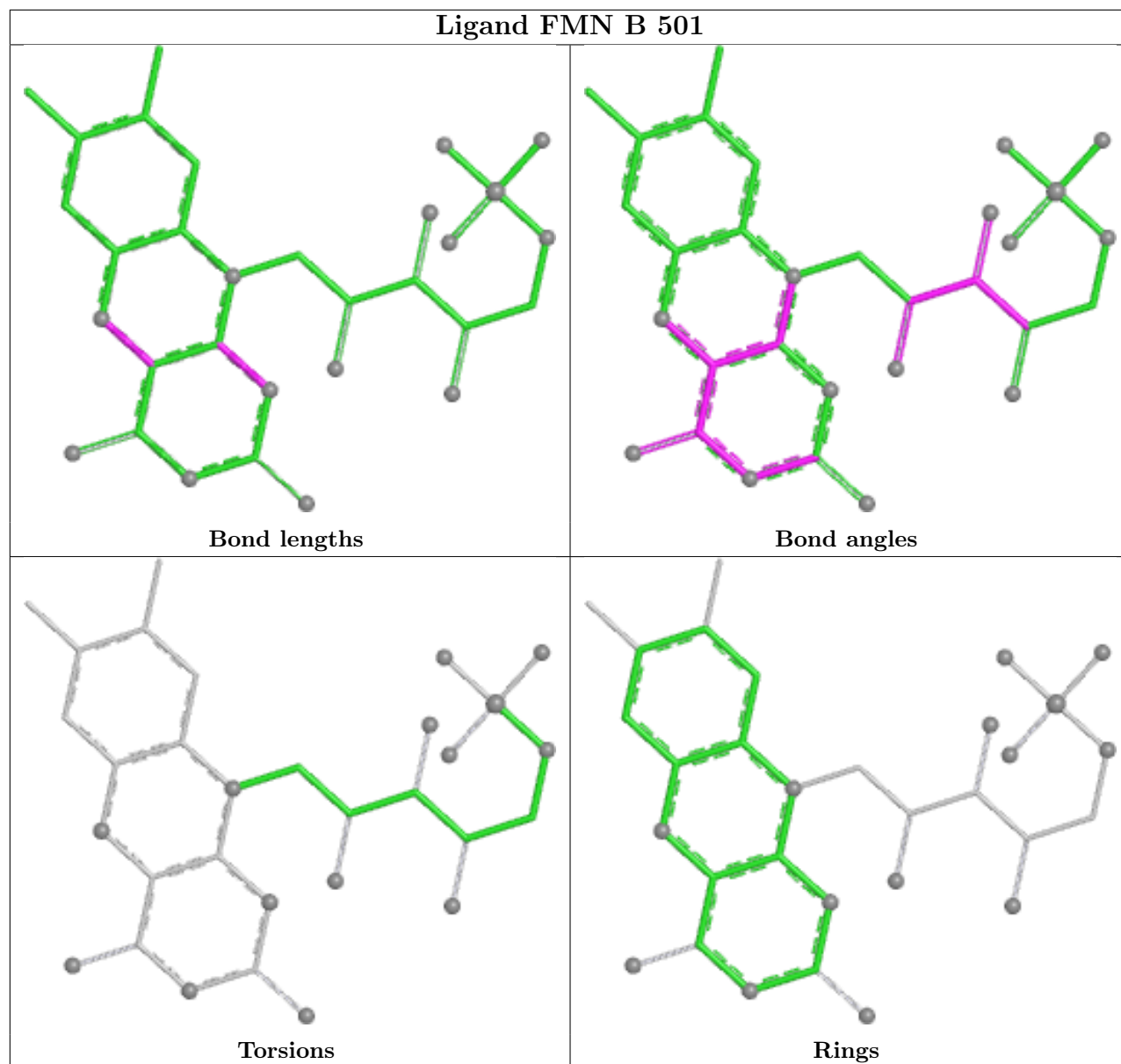
There are no ring outliers.

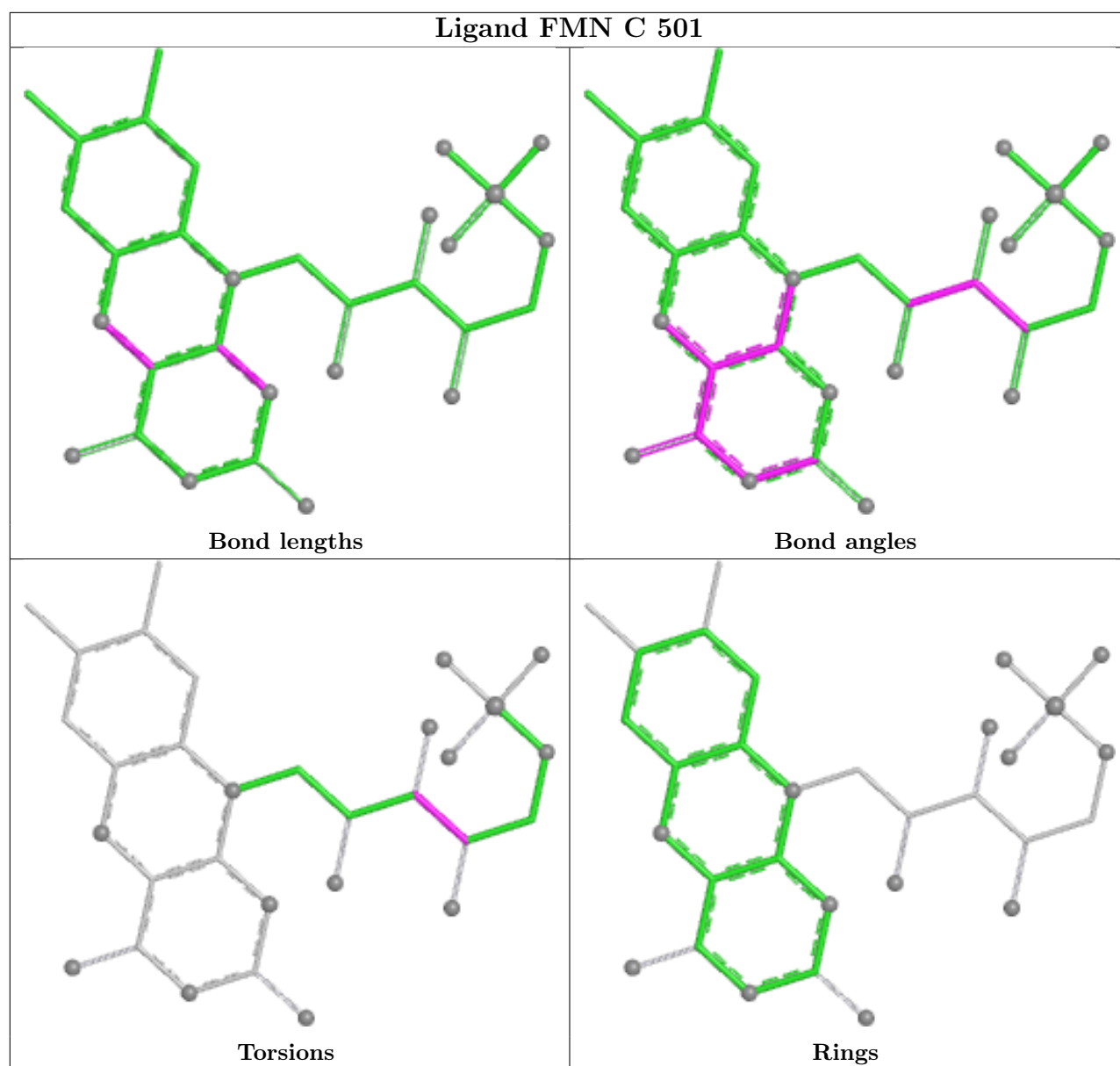
2 monomers are involved in 2 short contacts:

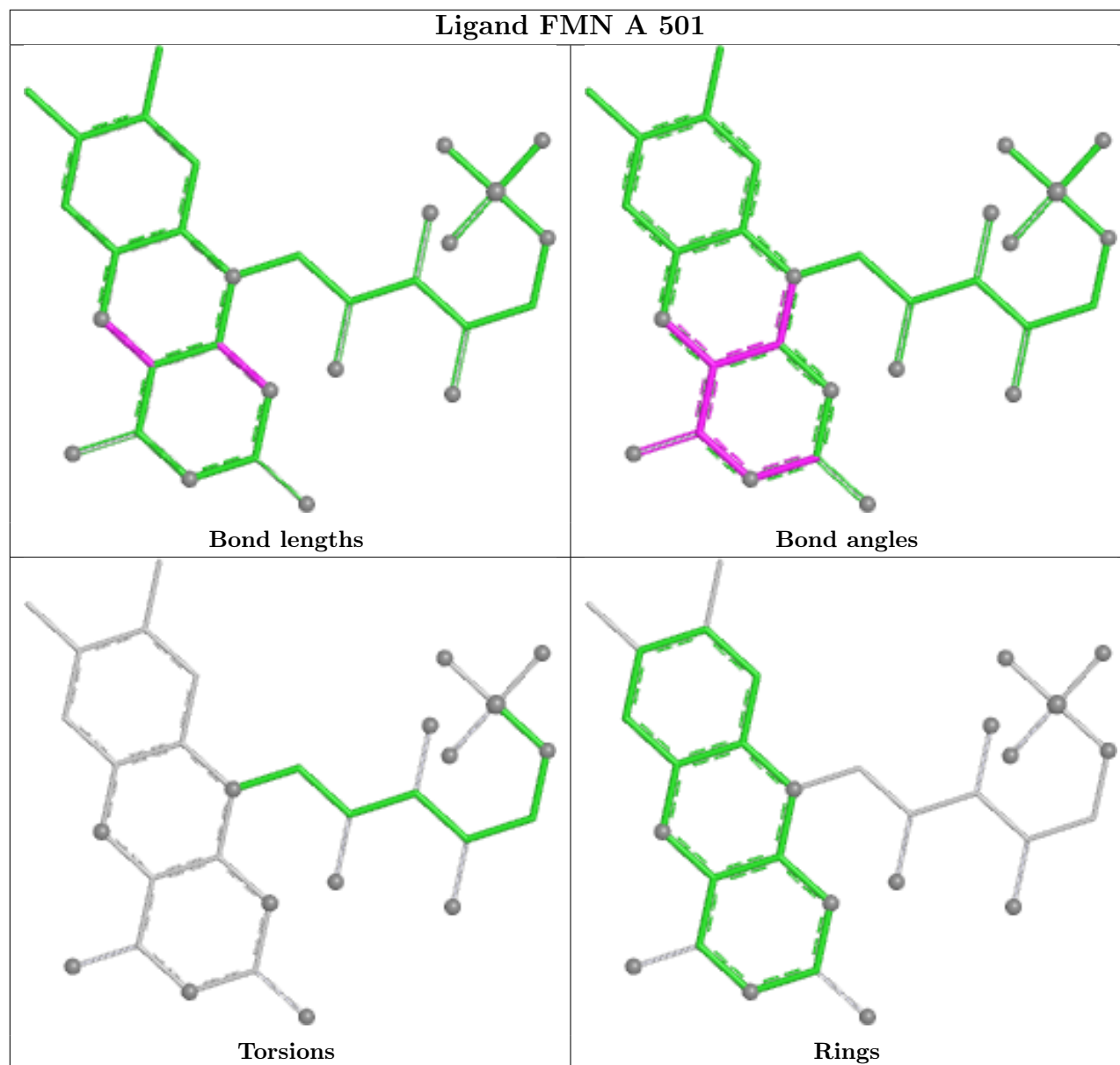
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FMN	1	0
2	B	501	FMN	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	498/499 (99%)	0.59	39 (7%)	19 22	19, 36, 58, 73	0
1	B	496/499 (99%)	0.75	45 (9%)	15 17	23, 39, 62, 89	0
1	C	499/499 (100%)	0.57	31 (6%)	26 31	23, 37, 57, 78	0
1	D	497/499 (99%)	0.39	18 (3%)	46 53	20, 34, 54, 65	0
All	All	1990/1996 (99%)	0.58	133 (6%)	24 27	19, 36, 57, 89	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	TRP	5.2
1	C	200	GLY	5.0
1	B	199	LEU	4.6
1	B	267	LEU	4.5
1	B	200	GLY	4.3
1	C	-2	PHE	4.1
1	A	0	SER	4.0
1	B	184	ILE	3.9
1	A	125	LEU	3.4
1	C	201	LYS	3.3
1	A	163	TRP	3.3
1	A	354	TRP	3.3
1	A	158	THR	3.3
1	A	494	GLY	3.3
1	A	156	VAL	3.3
1	B	247	GLN	3.3
1	B	201	LYS	3.3
1	A	267	LEU	3.3
1	B	251	LEU	3.2
1	A	199	LEU	3.2
1	B	197	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	196	TRP	3.2
1	B	496	ALA	3.2
1	B	191	ILE	3.1
1	C	190	GLY	3.1
1	D	199	LEU	3.0
1	D	202	PRO	3.0
1	C	198	ARG	3.0
1	B	286	ILE	3.0
1	B	192	ILE	3.0
1	B	217	ALA	2.9
1	B	495	ASP	2.9
1	B	227	VAL	2.9
1	A	159	PRO	2.9
1	B	163	TRP	2.9
1	B	189	ILE	2.9
1	A	203	THR	2.8
1	A	184	ILE	2.8
1	B	494	GLY	2.8
1	A	286	ILE	2.8
1	C	252	TRP	2.8
1	C	196	TRP	2.7
1	A	496	ALA	2.7
1	A	202	PRO	2.7
1	C	1	MET	2.7
1	B	186	THR	2.7
1	A	252	TRP	2.6
1	A	248	THR	2.6
1	B	204	PRO	2.6
1	B	109	ILE	2.6
1	B	123	VAL	2.6
1	D	200	GLY	2.6
1	C	194	GLU	2.6
1	A	196	TRP	2.6
1	C	199	LEU	2.6
1	B	292	LEU	2.6
1	B	159	PRO	2.5
1	C	202	PRO	2.5
1	D	125	LEU	2.5
1	C	163	TRP	2.5
1	D	495	ASP	2.5
1	B	158	THR	2.5
1	C	495	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	197	ARG	2.4
1	A	263	GLY	2.4
1	B	114	LEU	2.4
1	D	267	LEU	2.4
1	C	496	ALA	2.4
1	B	245	ARG	2.4
1	B	190	GLY	2.4
1	D	270	THR	2.4
1	B	219	ALA	2.4
1	B	265	ILE	2.4
1	A	204	PRO	2.4
1	B	296	HIS	2.4
1	A	115	GLU	2.3
1	C	267	LEU	2.3
1	B	366	ALA	2.3
1	B	202	PRO	2.3
1	D	159	PRO	2.3
1	C	494	GLY	2.3
1	C	362	GLN	2.3
1	B	125	LEU	2.3
1	D	124	TRP	2.3
1	C	270	THR	2.3
1	A	219	ALA	2.3
1	B	161	GLY	2.3
1	A	228	SER	2.3
1	C	241	VAL	2.3
1	C	251	LEU	2.3
1	A	116	ARG	2.2
1	D	496	ALA	2.2
1	C	189	ILE	2.2
1	A	265	ILE	2.2
1	A	201	LYS	2.2
1	C	158	THR	2.2
1	B	291	PRO	2.2
1	C	109	ILE	2.2
1	D	191	ILE	2.2
1	C	174	VAL	2.2
1	B	260	VAL	2.2
1	A	123	VAL	2.2
1	D	123	VAL	2.2
1	A	186	THR	2.2
1	A	246	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	495	ASP	2.2
1	C	292	LEU	2.2
1	A	200	GLY	2.2
1	B	110	ALA	2.2
1	A	217	ALA	2.2
1	D	265	ILE	2.1
1	A	247	GLN	2.1
1	B	261	LEU	2.1
1	A	58	LEU	2.1
1	A	432	PHE	2.1
1	B	248	THR	2.1
1	A	157	GLN	2.1
1	C	286	ILE	2.1
1	B	266	SER	2.1
1	A	226	GLY	2.1
1	A	1	MET	2.1
1	D	163	TRP	2.1
1	D	196	TRP	2.1
1	D	244	VAL	2.1
1	B	111	PRO	2.1
1	B	298	LEU	2.1
1	D	114	LEU	2.1
1	C	462	ALA	2.1
1	A	109	ILE	2.0
1	D	2	ASN	2.0
1	C	159	PRO	2.0
1	C	272	LEU	2.0
1	C	184	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

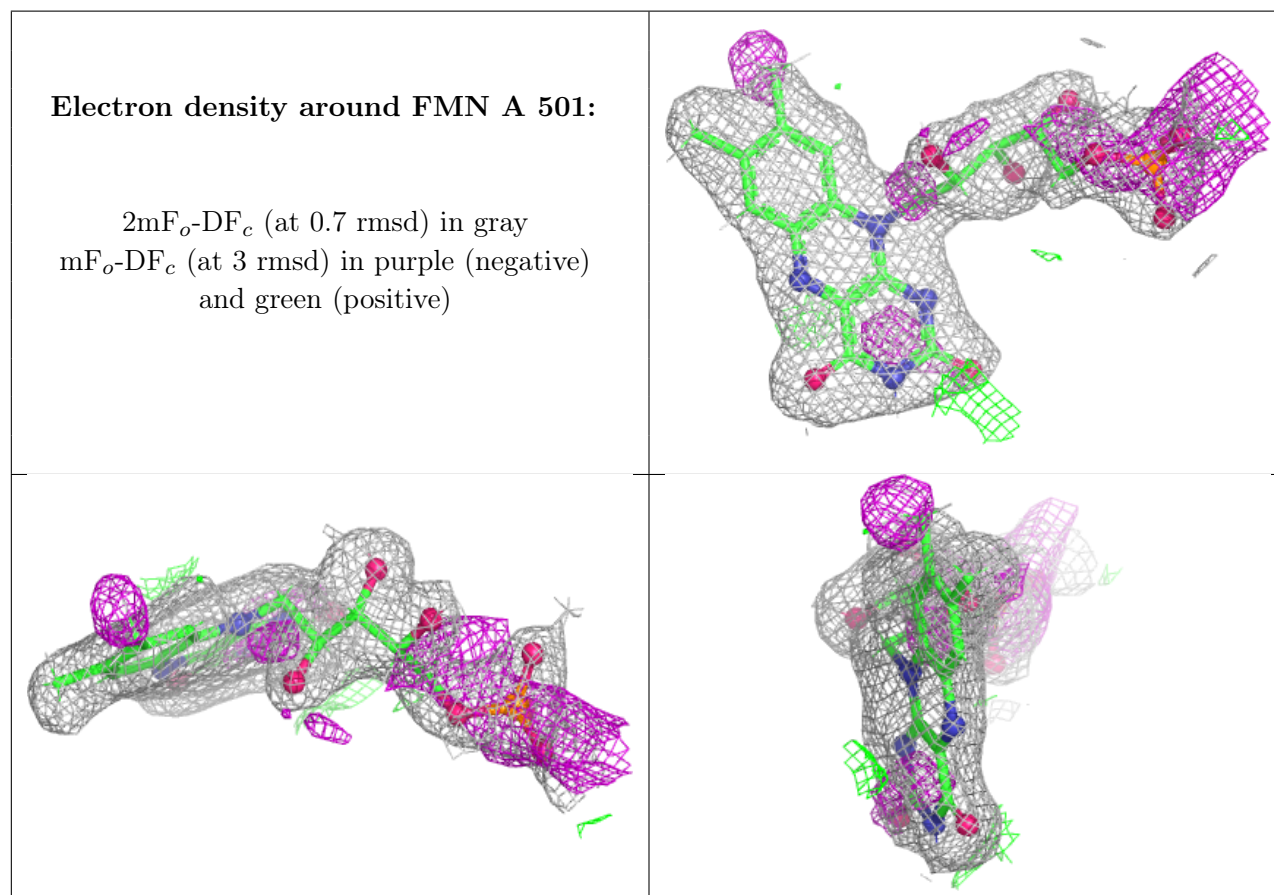
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

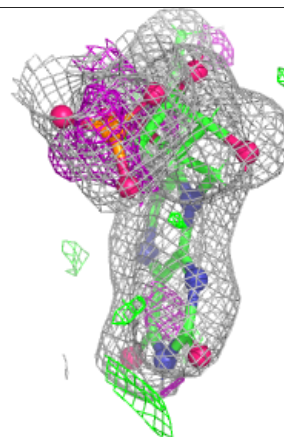
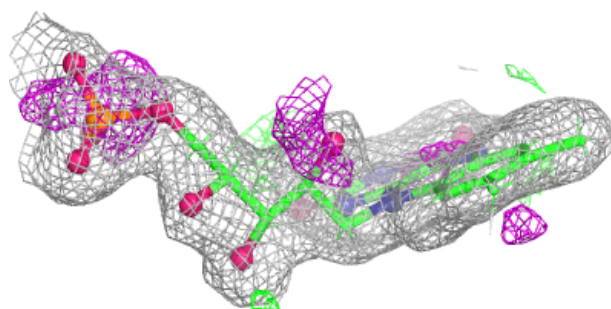
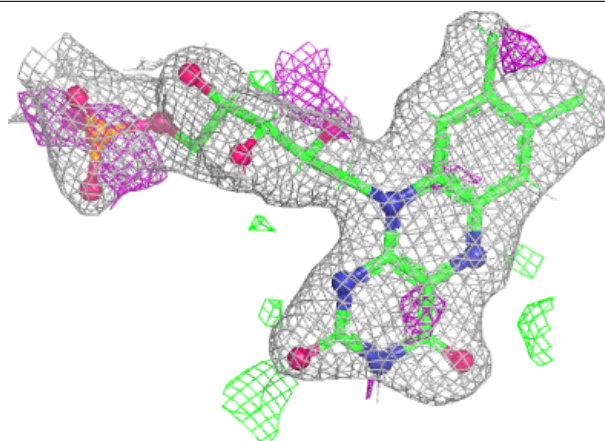
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	A	501	31/31	0.86	0.11	31,41,47,53	0
2	FMN	B	501	31/31	0.88	0.10	35,44,52,62	0
2	FMN	C	501	31/31	0.90	0.10	30,38,45,55	0
2	FMN	D	501	31/31	0.92	0.09	30,37,44,50	0
4	NA	C	503	1/1	0.97	0.10	28,28,28,28	0
4	NA	D	503	1/1	0.97	0.12	26,26,26,26	0
3	MN	D	502	1/1	0.98	0.06	33,33,33,33	0
4	NA	B	503	1/1	0.98	0.08	31,31,31,31	0
3	MN	A	502	1/1	0.98	0.09	36,36,36,36	0
3	MN	B	502	1/1	0.99	0.06	43,43,43,43	0
3	MN	C	502	1/1	0.99	0.03	41,41,41,41	0
4	NA	A	503	1/1	0.99	0.09	27,27,27,27	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.



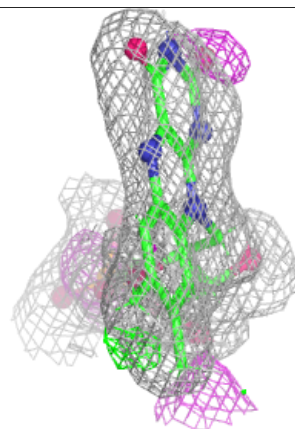
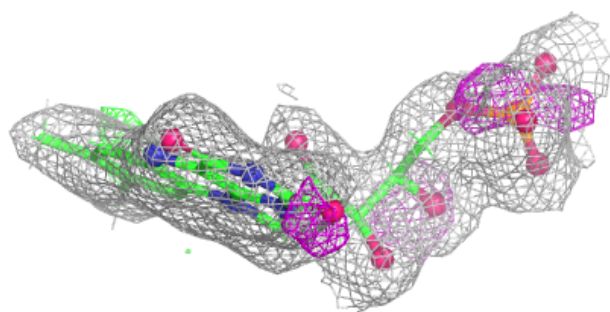
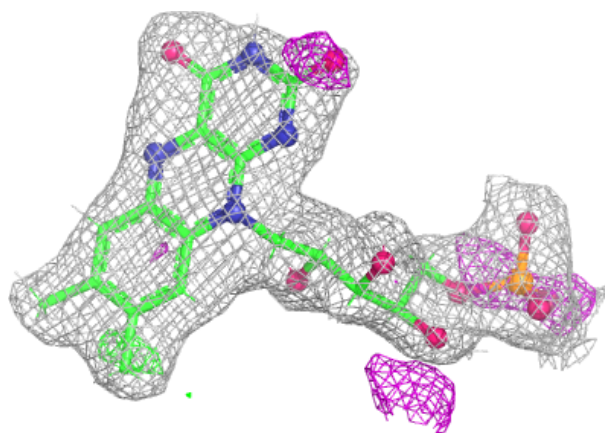
Electron density around FMN B 501:

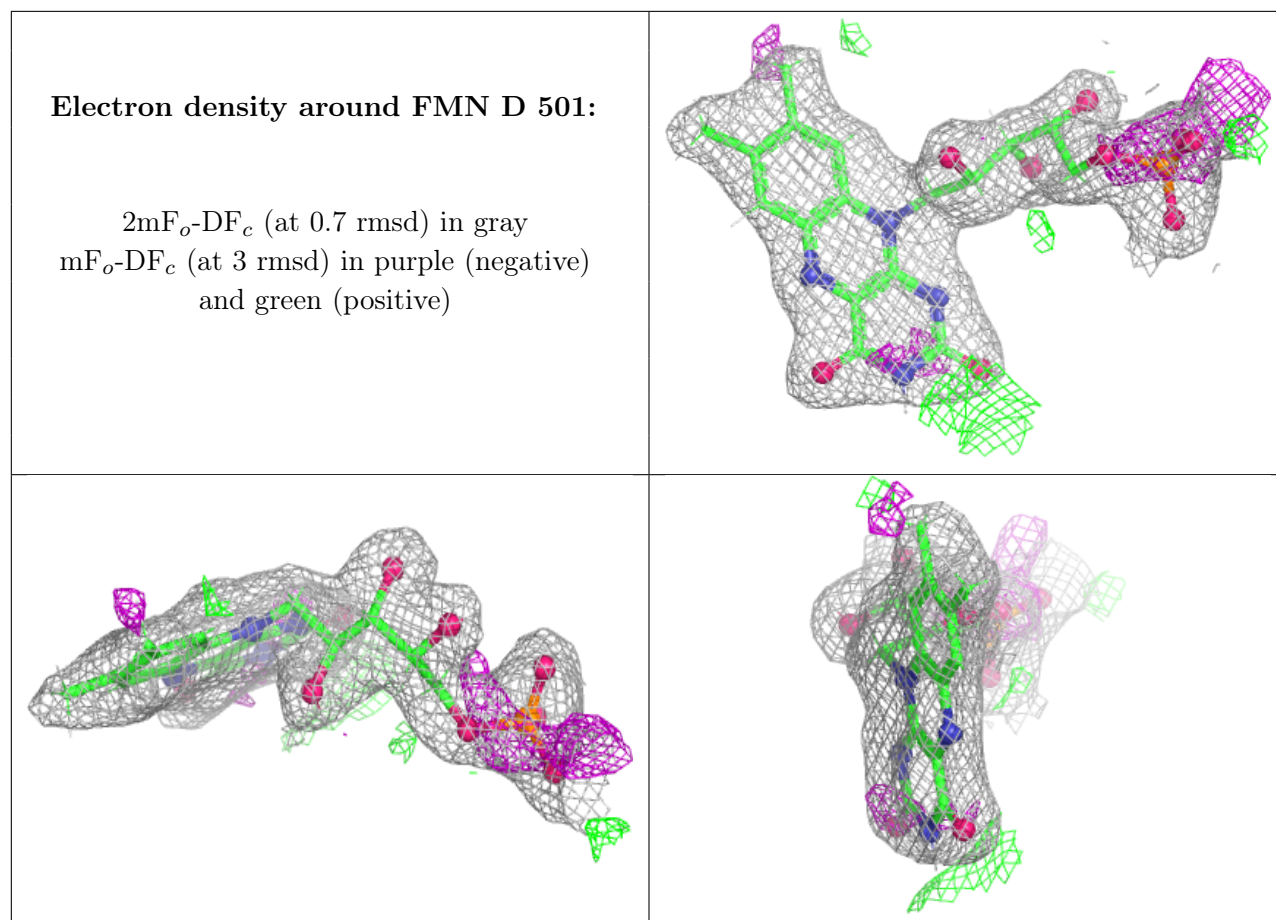
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.