



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:00 PM UTC

PDB ID : 3W78 / pdb_00003w78
Title : Crystal Structure of azoreductase AzrC in complex with NAD(P)-inhibitor Cibacron Blue
Authors : Yu, J.; Ogata, D.; Ooi, T.; Yao, M.
Deposited on : 2013-02-27
Resolution : 2.62 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

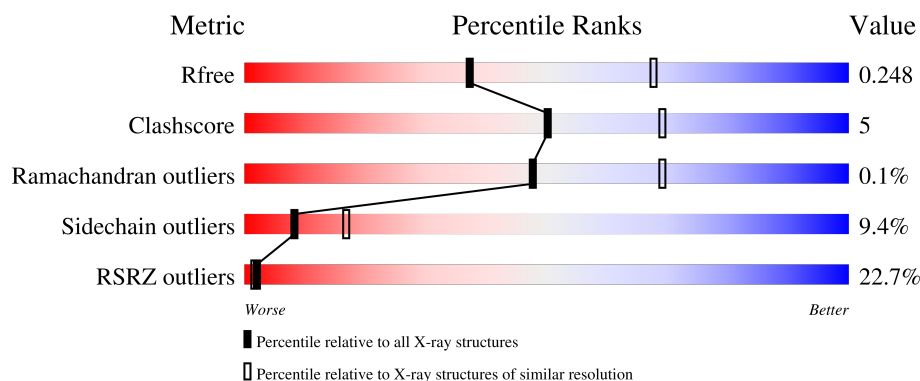
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	211	2% 86% 11% .
1	B	211	10% 85% 13% .
1	C	211	69% 73% 22% .
1	D	211	9% 88% 9% .

2 Entry composition [i](#)

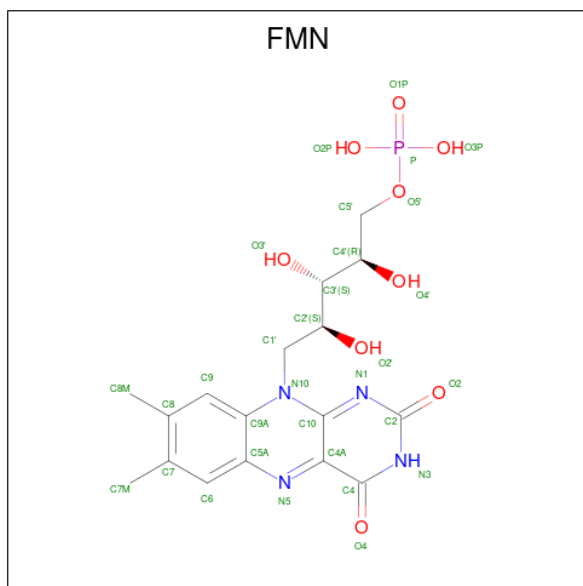
There are 4 unique types of molecules in this entry. The entry contains 6789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FMN-dependent NADH-azoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1610	1032	264	309	5			
1	D	210	Total	C	N	O	S	0	0	0
			1610	1032	264	309	5			
1	B	210	Total	C	N	O	S	0	0	0
			1610	1032	264	309	5			
1	C	210	Total	C	N	O	S	0	0	0
			1610	1032	264	309	5			

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



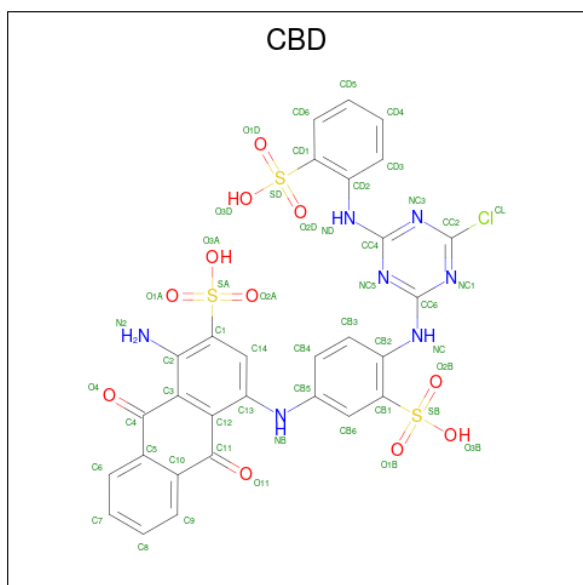
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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

- Molecule 3 is CIBACRON BLUE (CCD ID: CBD) (formula: $C_{29}H_{20}ClN_7O_{11}S_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			51	29	1	7	11	3		
3	D	1	Total	C	Cl	N	O	S	0	0
			51	29	1	7	11	3		
3	B	1	Total	C	Cl	N	O	S	0	0
			51	29	1	7	11	3		
3	C	1	Total	C	Cl	N	O	S	0	0
			51	29	1	7	11	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	D	6	Total	O	0	0
			6	6		
4	B	4	Total	O	0	0
			4	4		

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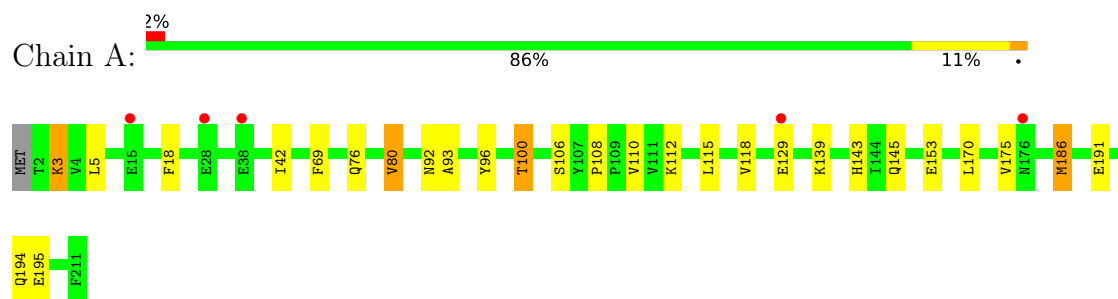
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	5	Total	O	0	0
			5	5		

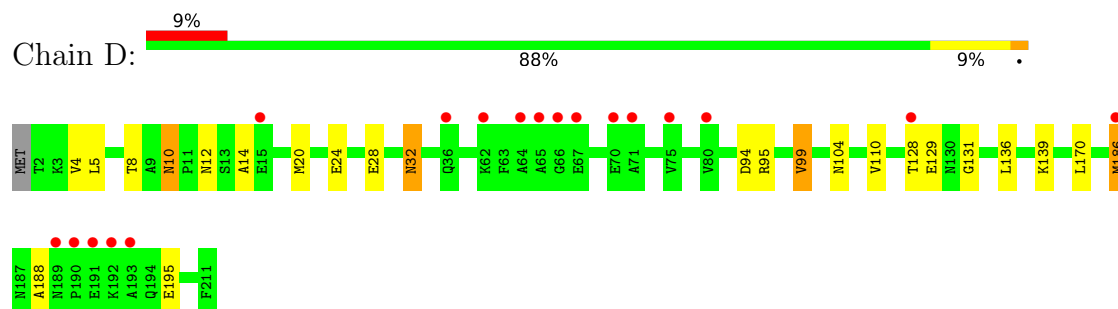
3 Residue-property plots [i](#)

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.

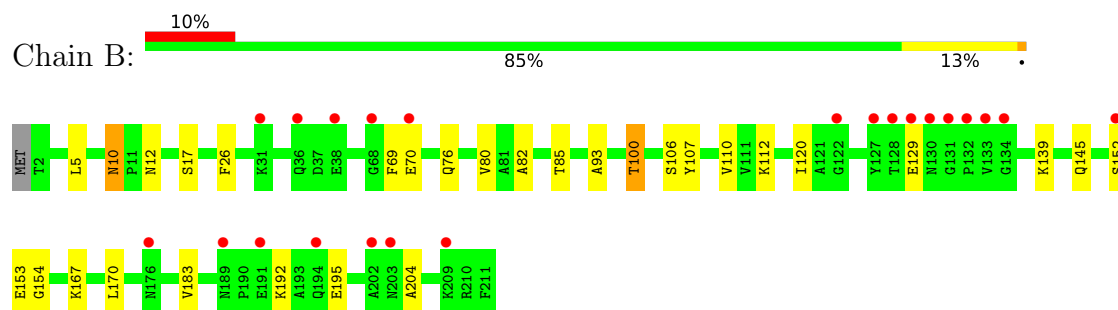
- Molecule 1: FMN-dependent NADH-azoreductase



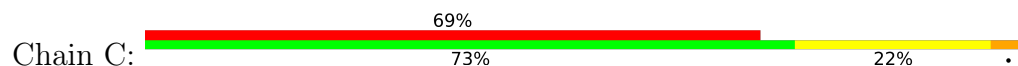
- Molecule 1: FMN-dependent NADH-azoreductase

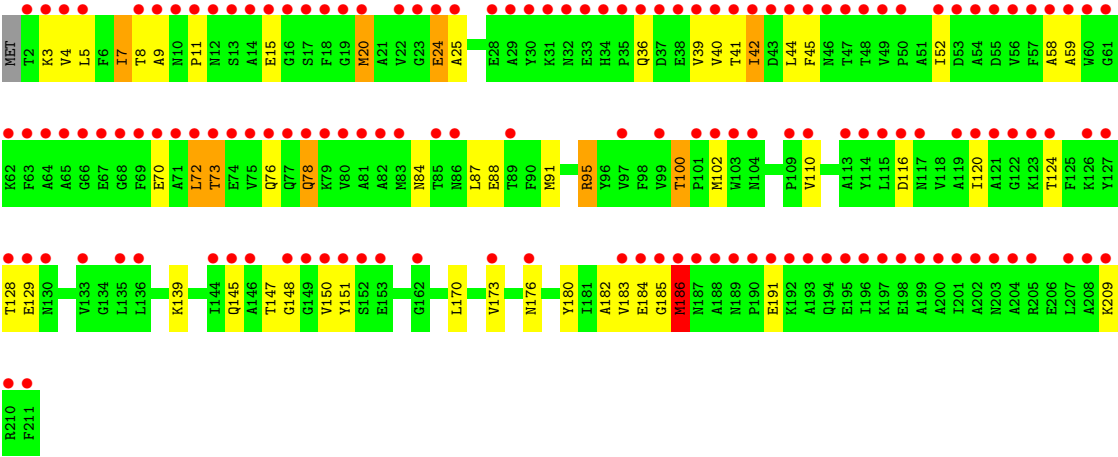


- Molecule 1: FMN-dependent NADH-azoreductase



- Molecule 1: FMN-dependent NADH-azoreductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.37Å 146.37Å 116.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.62 50.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.62) 99.3 (50.00-2.62)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.253 , 0.285 (Not available) , 0.248	Depositor DCC
R_{free} test set	3079 reflections (7.10%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6789	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

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	0.53	0/1646	0.81	3/2236 (0.1%)
1	B	0.53	0/1646	0.80	0/2236
1	C	0.54	0/1646	0.87	0/2236
1	D	0.52	0/1646	0.79	0/2236
All	All	0.53	0/6584	0.82	3/8944 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	VAL	N-CA-C	6.09	112.73	106.21
1	A	108	PRO	CA-C-N	5.19	126.33	119.84
1	A	108	PRO	C-N-CA	5.19	126.33	119.84

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	1610	0	1562	15	0
1	B	1610	0	1562	10	0
1	C	1610	0	1562	34	0
1	D	1610	0	1562	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	1	0
2	D	31	0	19	0	0
3	A	51	0	20	0	0
3	B	51	0	20	0	0
3	C	51	0	20	0	0
3	D	51	0	20	2	0
4	A	6	0	0	0	0
4	B	4	0	0	0	0
4	C	5	0	0	0	0
4	D	6	0	0	0	0
All	All	6789	0	6404	70	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 5.

All (70) 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:95:ARG:HG3	1:C:95:ARG:HH11	1.15	1.09
1:C:95:ARG:HH11	1:C:95:ARG:CG	1.87	0.87
1:C:185:GLY:HA2	1:C:186:MET:CB	2.10	0.81
1:C:185:GLY:HA2	1:C:186:MET:CG	2.10	0.81
1:C:95:ARG:HG3	1:C:95:ARG:NH1	1.90	0.78
1:B:10:ASN:HD22	1:B:12:ASN:H	1.35	0.75
1:D:10:ASN:HD22	1:D:12:ASN:H	1.35	0.73
1:C:185:GLY:HA2	1:C:186:MET:HG2	1.72	0.70
1:C:102:MET:HE1	1:C:151:TYR:CE1	2.29	0.68
1:A:100:THR:HB	1:A:143:HIS:HE1	1.62	0.65
1:A:5:LEU:HD13	1:A:93:ALA:HB2	1.79	0.64
1:A:112:LYS:HE3	1:B:106:SER:HB3	1.81	0.62
1:C:58:ALA:HB3	1:C:76:GLN:HE22	1.64	0.61
1:C:148:GLY:O	1:C:185:GLY:HA3	2.01	0.60
1:B:100:THR:HG22	1:B:145:GLN:HG3	1.84	0.59
1:C:11:PRO:HA	1:C:45:PHE:CE2	2.37	0.59
1:C:102:MET:HE3	2:C:301:FMN:N3	2.17	0.59
1:C:185:GLY:HA2	1:C:186:MET:HB3	1.84	0.59
1:C:59:ALA:HA	1:C:72:LEU:HD11	1.85	0.58
1:D:104:ASN:HD22	3:D:302:CBD:H8	1.68	0.58
1:B:82:ALA:HA	1:B:85:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ILE:HD11	1:C:116:ASP:HB3	1.87	0.55
1:C:102:MET:HE1	1:C:151:TYR:CZ	2.42	0.54
1:C:8:THR:HB	1:C:20:MET:HE1	1.89	0.54
1:C:124:THR:HG22	1:C:173:VAL:HB	1.91	0.52
1:C:40:VAL:HB	1:C:41:THR:HB	1.92	0.52
1:B:93:ALA:O	1:B:139:LYS:HE3	2.11	0.51
1:A:3:LYS:HE3	1:A:92:ASN:HD22	1.76	0.51
1:C:84:ASN:O	1:C:88:GLU:HG2	2.11	0.51
1:A:106:SER:HB3	1:B:112:LYS:HE3	1.94	0.50
1:D:4:VAL:HG22	1:D:95:ARG:HB2	1.94	0.49
1:C:150:VAL:HG12	1:C:184:GLU:HB3	1.94	0.49
1:D:128:THR:HG22	1:D:129:GLU:N	2.27	0.49
1:D:14:ALA:HA	1:D:20:MET:HB3	1.95	0.48
1:C:52:ILE:CD1	1:C:116:ASP:HB3	2.43	0.48
1:C:73:THR:HB	1:C:76:GLN:HG3	1.96	0.47
1:A:5:LEU:HG	1:A:42:ILE:CD1	2.45	0.47
1:B:26:PHE:HB2	1:B:204:ALA:HB1	1.97	0.47
1:C:95:ARG:CG	1:C:95:ARG:NH1	2.57	0.47
1:A:3:LYS:CE	1:A:92:ASN:HD22	2.28	0.46
1:A:100:THR:HG22	1:A:145:GLN:HG3	1.98	0.45
1:D:14:ALA:HB2	1:D:24:GLU:HG3	1.99	0.45
1:A:186:MET:HE3	1:A:186:MET:HB3	1.73	0.45
1:C:100:THR:HG22	1:C:145:GLN:HG3	1.99	0.45
1:B:100:THR:O	1:B:145:GLN:HA	2.17	0.45
1:C:58:ALA:HB3	1:C:76:GLN:NE2	2.32	0.45
1:D:94:ASP:C	1:D:95:ARG:HD3	2.42	0.44
1:A:76:GLN:O	1:A:80:VAL:HG13	2.17	0.44
1:D:136:LEU:HB3	1:D:139:LYS:HD3	2.00	0.44
1:C:4:VAL:HG13	1:C:39:VAL:HA	2.00	0.44
1:C:9:ALA:HB2	1:C:44:LEU:HD12	1.99	0.44
1:D:188:ALA:HA	3:D:302:CBD:CC6	2.48	0.44
1:A:18:PHE:CD2	1:A:186:MET:HE2	2.53	0.43
1:A:69:PHE:HE1	1:A:80:VAL:CG2	2.30	0.43
1:C:102:MET:HE2	1:C:147:THR:HB	2.00	0.43
1:D:32:ASN:C	1:D:32:ASN:HD22	2.26	0.43
1:A:93:ALA:O	1:A:139:LYS:HE2	2.19	0.43
1:B:153:GLU:HG2	1:B:154:GLY:N	2.33	0.43
1:C:87:LEU:O	1:C:91:MET:HB2	2.19	0.43
1:C:78:GLN:H	1:C:78:GLN:HG3	1.72	0.43
1:C:100:THR:O	1:C:145:GLN:HA	2.20	0.42
1:C:180:TYR:CE2	1:C:182:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TYR:CE2	1:A:139:LYS:HG2	2.55	0.41
1:A:115:LEU:HA	1:A:118:VAL:HG22	2.01	0.41
1:D:8:THR:HG22	1:D:99:VAL:CG1	2.50	0.41
1:C:24:GLU:HG3	1:C:25:ALA:N	2.36	0.41
1:C:7:ILE:HA	1:C:42:ILE:HG23	2.02	0.41
1:D:128:THR:HB	1:D:131:GLY:O	2.20	0.40
1:D:186:MET:HE2	1:D:186:MET:HB3	1.83	0.40
1:B:76:GLN:O	1:B:80:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
1	B	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
1	C	208/211 (99%)	199 (96%)	8 (4%)	1 (0%)	24	44
1	D	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
All	All	832/844 (99%)	806 (97%)	25 (3%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	186	MET

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	162/163 (99%)	151 (93%)	11 (7%)	14	30
1	B	162/163 (99%)	146 (90%)	16 (10%)	7	15
1	C	162/163 (99%)	137 (85%)	25 (15%)	2	4
1	D	162/163 (99%)	153 (94%)	9 (6%)	19	39
All	All	648/652 (99%)	587 (91%)	61 (9%)	8	17

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	80	VAL
1	A	100	THR
1	A	110	VAL
1	A	129	GLU
1	A	153	GLU
1	A	170	LEU
1	A	186	MET
1	A	191	GLU
1	A	194	GLN
1	A	195	GLU
1	D	5	LEU
1	D	10	ASN
1	D	28	GLU
1	D	32	ASN
1	D	99	VAL
1	D	110	VAL
1	D	170	LEU
1	D	186	MET
1	D	195	GLU
1	B	5	LEU
1	B	10	ASN
1	B	17	SER
1	B	69	PHE
1	B	70	GLU
1	B	100	THR
1	B	107	TYR
1	B	110	VAL
1	B	120	ILE
1	B	129	GLU

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Mol	Chain	Res	Type
1	B	152	SER
1	B	167	LYS
1	B	170	LEU
1	B	183	VAL
1	B	192	LYS
1	B	195	GLU
1	C	3	LYS
1	C	5	LEU
1	C	7	ILE
1	C	15	GLU
1	C	20	MET
1	C	24	GLU
1	C	36	GLN
1	C	42	ILE
1	C	70	GLU
1	C	72	LEU
1	C	73	THR
1	C	78	GLN
1	C	95	ARG
1	C	100	THR
1	C	110	VAL
1	C	120	ILE
1	C	128	THR
1	C	129	GLU
1	C	139	LYS
1	C	170	LEU
1	C	176	ASN
1	C	183	VAL
1	C	186	MET
1	C	191	GLU
1	C	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	84	ASN
1	A	92	ASN
1	A	143	HIS
1	A	145	GLN
1	A	194	GLN
1	D	10	ASN

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Mol	Chain	Res	Type
1	D	32	ASN
1	D	77	GLN
1	D	84	ASN
1	D	104	ASN
1	D	176	ASN
1	D	189	ASN
1	B	10	ASN
1	B	32	ASN
1	B	34	HIS
1	B	84	ASN
1	B	145	GLN
1	C	46	ASN
1	C	84	ASN
1	C	86	ASN
1	C	194	GLN

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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CBD	C	302	-	56,56,56	2.74	15 (26%)	81,87,87	1.91	11 (13%)
3	CBD	A	302	-	56,56,56	2.73	15 (26%)	81,87,87	2.02	13 (16%)
2	FMN	B	301	-	33,33,33	1.52	4 (12%)	48,50,50	1.31	9 (18%)
3	CBD	D	302	-	56,56,56	2.69	14 (25%)	81,87,87	1.99	13 (16%)
2	FMN	C	301	-	33,33,33	1.61	5 (15%)	48,50,50	1.27	6 (12%)
3	CBD	B	302	-	56,56,56	2.71	15 (26%)	81,87,87	1.93	12 (14%)
2	FMN	A	301	-	33,33,33	1.50	5 (15%)	48,50,50	1.29	9 (18%)
2	FMN	D	301	-	33,33,33	1.53	4 (12%)	48,50,50	1.28	9 (18%)

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
3	CBD	C	302	-	-	12/30/46/46	0/6/6/6
3	CBD	A	302	-	-	10/30/46/46	0/6/6/6
2	FMN	B	301	-	-	2/18/18/18	0/3/3/3
3	CBD	D	302	-	-	3/30/46/46	0/6/6/6
2	FMN	C	301	-	-	7/18/18/18	0/3/3/3
3	CBD	B	302	-	-	12/30/46/46	0/6/6/6
2	FMN	A	301	-	-	1/18/18/18	0/3/3/3
2	FMN	D	301	-	-	1/18/18/18	0/3/3/3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	CBD	C2-C1	7.07	1.50	1.42
3	B	302	CBD	C2-C1	6.87	1.49	1.42
3	C	302	CBD	C2-C1	6.83	1.49	1.42
3	C	302	CBD	C1-SA	-6.73	1.60	1.77
3	D	302	CBD	CB1-SB	-6.72	1.60	1.77
3	D	302	CBD	C1-SA	-6.70	1.60	1.77
3	B	302	CBD	CB1-SB	-6.70	1.60	1.77
3	C	302	CBD	CB1-SB	-6.64	1.60	1.77
3	D	302	CBD	CD1-SD	-6.64	1.60	1.77
3	A	302	CBD	CB1-SB	-6.64	1.60	1.77
3	B	302	CBD	CD1-SD	-6.62	1.60	1.77
3	C	302	CBD	CD1-SD	-6.53	1.60	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	CBD	C2-C1	6.48	1.49	1.42
3	A	302	CBD	C1-SA	-6.47	1.60	1.77
3	A	302	CBD	CD1-SD	-6.46	1.60	1.77
3	B	302	CBD	C1-SA	-6.41	1.61	1.77
3	A	302	CBD	CD2-CD1	6.29	1.50	1.40
3	C	302	CBD	CD2-CD1	6.23	1.50	1.40
3	D	302	CBD	CB2-CB1	5.98	1.50	1.40
3	B	302	CBD	CD2-CD1	5.94	1.49	1.40
3	A	302	CBD	CB2-CB1	5.91	1.49	1.40
3	D	302	CBD	CD2-CD1	5.84	1.49	1.40
3	B	302	CBD	CB2-CB1	5.82	1.49	1.40
3	C	302	CBD	CB2-CB1	5.78	1.49	1.40
2	C	301	FMN	C9A-C5A	5.67	1.50	1.41
3	D	302	CBD	C10-C5	5.66	1.49	1.40
3	C	302	CBD	C10-C5	5.66	1.49	1.40
3	B	302	CBD	C10-C5	5.65	1.49	1.40
2	B	301	FMN	C9A-C5A	5.61	1.50	1.41
3	A	302	CBD	C10-C5	5.59	1.49	1.40
3	C	302	CBD	C3-C2	5.51	1.49	1.42
2	D	301	FMN	C9A-C5A	5.48	1.50	1.41
3	A	302	CBD	C3-C2	5.40	1.49	1.42
2	A	301	FMN	C9A-C5A	5.36	1.49	1.41
3	B	302	CBD	C3-C2	5.31	1.49	1.42
3	D	302	CBD	C3-C2	4.83	1.48	1.42
3	A	302	CBD	C12-C13	4.52	1.50	1.41
3	D	302	CBD	C12-C13	4.47	1.50	1.41
3	C	302	CBD	C12-C13	4.42	1.50	1.41
3	B	302	CBD	C12-C13	4.34	1.49	1.41
2	C	301	FMN	C8-C7	3.81	1.50	1.40
2	B	301	FMN	C8-C7	3.74	1.50	1.40
2	D	301	FMN	C8-C7	3.69	1.49	1.40
3	B	302	CBD	O3A-SA	3.63	1.64	1.45
3	B	302	CBD	O3B-SB	3.62	1.64	1.45
3	C	302	CBD	O3B-SB	3.60	1.64	1.45
3	D	302	CBD	O3B-SB	3.60	1.64	1.45
3	D	302	CBD	O3A-SA	3.60	1.64	1.45
3	C	302	CBD	O3D-SD	3.57	1.64	1.45
3	C	302	CBD	O3A-SA	3.56	1.64	1.45
3	A	302	CBD	O3B-SB	3.56	1.64	1.45
3	A	302	CBD	O3D-SD	3.53	1.63	1.45
3	A	302	CBD	O3A-SA	3.52	1.63	1.45
2	A	301	FMN	C8-C7	3.52	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	CBD	C12-C3	3.51	1.49	1.41
3	B	302	CBD	O3D-SD	3.50	1.63	1.45
3	D	302	CBD	O3D-SD	3.50	1.63	1.45
3	D	302	CBD	C12-C3	3.43	1.49	1.41
3	A	302	CBD	C12-C3	3.38	1.49	1.41
3	B	302	CBD	C12-C3	3.34	1.49	1.41
2	D	301	FMN	C4A-N5	2.59	1.36	1.30
2	B	301	FMN	C4A-N5	2.47	1.36	1.30
2	D	301	FMN	C4-N3	-2.43	1.34	1.38
2	C	301	FMN	C4-N3	-2.33	1.34	1.38
2	C	301	FMN	C4A-N5	2.32	1.35	1.30
2	A	301	FMN	C4-N3	-2.26	1.34	1.38
2	A	301	FMN	C4A-N5	2.25	1.35	1.30
2	C	301	FMN	C10-N10	2.25	1.42	1.37
3	A	302	CBD	CC2-CL	2.24	1.80	1.73
2	A	301	FMN	C10-N10	2.21	1.42	1.37
3	B	302	CBD	CB5-NB	-2.18	1.36	1.40
2	B	301	FMN	C4-N3	-2.14	1.34	1.38
3	C	302	CBD	CB5-NB	-2.13	1.36	1.40
3	C	302	CBD	CC2-CL	2.09	1.80	1.73
3	D	302	CBD	CC2-CL	2.08	1.80	1.73
3	B	302	CBD	CC2-CL	2.04	1.80	1.73
3	A	302	CBD	CC2-NC3	2.04	1.36	1.32

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	CBD	CC6-NC1-CC2	8.26	121.11	112.41
3	A	302	CBD	CC6-NC1-CC2	8.23	121.08	112.41
3	A	302	CBD	CC4-NC3-CC2	7.90	120.73	112.41
3	D	302	CBD	CC4-NC3-CC2	7.83	120.66	112.41
3	B	302	CBD	CC6-NC1-CC2	7.73	120.55	112.41
3	C	302	CBD	CC6-NC1-CC2	7.57	120.38	112.41
3	B	302	CBD	CC4-NC3-CC2	7.51	120.32	112.41
3	C	302	CBD	CC4-NC3-CC2	7.44	120.25	112.41
3	A	302	CBD	NC3-CC2-NC1	-5.63	119.23	129.52
3	D	302	CBD	NC3-CC2-NC1	-5.44	119.57	129.52
3	C	302	CBD	NC3-CC2-NC1	-5.28	119.87	129.52
3	B	302	CBD	NC3-CC2-NC1	-5.25	119.93	129.52
3	D	302	CBD	NC5-CC6-NC1	-4.52	118.86	126.26
3	A	302	CBD	NC5-CC6-NC1	-4.27	119.27	126.26
3	A	302	CBD	NC5-CC4-NC3	-4.25	119.30	126.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	CBD	NC5-CC6-NC1	-4.25	119.30	126.26
3	B	302	CBD	NC5-CC4-NC3	-4.22	119.34	126.26
3	C	302	CBD	NC5-CC4-NC3	-4.21	119.36	126.26
3	D	302	CBD	CL-CC2-NC1	4.18	121.05	115.17
3	C	302	CBD	NC5-CC6-NC1	-4.15	119.46	126.26
3	A	302	CBD	CL-CC2-NC3	4.12	120.98	115.17
3	D	302	CBD	NC5-CC4-NC3	-4.07	119.59	126.26
3	B	302	CBD	CL-CC2-NC3	3.88	120.63	115.17
3	C	302	CBD	CC6-NC5-CC4	3.81	120.68	113.85
3	C	302	CBD	CL-CC2-NC3	3.79	120.51	115.17
3	B	302	CBD	CC6-NC5-CC4	3.74	120.56	113.85
2	B	301	FMN	C4-C4A-N5	3.73	123.36	118.21
2	D	301	FMN	C4-C4A-N5	3.68	123.30	118.21
3	A	302	CBD	CC6-NC5-CC4	3.65	120.39	113.85
3	D	302	CBD	CC6-NC5-CC4	3.55	120.21	113.85
3	C	302	CBD	C12-C3-C2	-3.35	118.05	119.88
3	A	302	CBD	CL-CC2-NC1	3.28	119.79	115.17
3	C	302	CBD	CL-CC2-NC1	3.16	119.62	115.17
3	B	302	CBD	CB1-CB2-NC	-3.13	118.61	121.50
3	A	302	CBD	C12-C3-C2	-3.11	118.18	119.88
3	B	302	CBD	CL-CC2-NC1	3.03	119.44	115.17
3	D	302	CBD	C12-C3-C2	-3.03	118.23	119.88
3	D	302	CBD	CL-CC2-NC3	2.99	119.38	115.17
2	A	301	FMN	C4-C4A-N5	2.88	122.18	118.21
3	D	302	CBD	C2-C1-SA	-2.83	118.19	121.58
2	A	301	FMN	C4A-C10-N1	-2.77	117.80	124.59
2	C	301	FMN	C4-C4A-N5	2.76	122.02	118.21
2	C	301	FMN	C4A-C10-N1	-2.71	117.95	124.59
3	A	302	CBD	CB1-CB2-NC	-2.69	119.02	121.50
2	A	301	FMN	C10-N1-C2	2.54	122.35	116.85
2	B	301	FMN	C4A-C10-N10	2.42	119.94	116.48
2	D	301	FMN	C4A-C10-N1	-2.39	118.74	124.59
2	B	301	FMN	C4A-C10-N1	-2.34	118.84	124.59
2	B	301	FMN	C10-N1-C2	2.33	121.89	116.85
2	B	301	FMN	O2-C2-N1	-2.31	117.96	121.80
2	A	301	FMN	O4-C4-C4A	-2.31	120.43	126.53
2	C	301	FMN	C4A-C10-N10	2.29	119.76	116.48
2	C	301	FMN	C10-N1-C2	2.29	121.80	116.85
3	C	302	CBD	O3B-SB-CB1	2.28	110.55	106.12
3	A	302	CBD	O3D-SD-CD1	2.24	110.47	106.12
2	A	301	FMN	C4A-C4-N3	2.23	118.93	113.25
3	A	302	CBD	CD6-CD1-CD2	-2.22	118.47	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	CBD	O3A-SA-C1	2.21	110.42	106.12
2	D	301	FMN	C10-N1-C2	2.20	121.61	116.85
3	D	302	CBD	ND-CC4-NC5	2.16	124.31	116.90
3	B	302	CBD	C12-C3-C2	-2.15	118.71	119.88
2	D	301	FMN	C9A-C5A-N5	-2.15	120.17	122.45
2	D	301	FMN	C5A-N5-C4A	2.15	121.56	118.09
2	D	301	FMN	C4A-C4-N3	2.13	118.68	113.25
2	A	301	FMN	C4A-C10-N10	2.12	119.51	116.48
3	D	302	CBD	NC-CC6-NC5	2.11	124.15	116.90
2	A	301	FMN	C5A-N5-C4A	2.11	121.50	118.09
2	C	301	FMN	O4-C4-C4A	-2.10	120.99	126.53
3	B	302	CBD	C3-C2-N2	-2.10	119.74	122.59
2	B	301	FMN	O3P-P-O2P	2.10	115.67	107.80
2	B	301	FMN	C10-C4A-N5	-2.08	120.57	124.81
2	B	301	FMN	C4A-C4-N3	2.07	118.52	113.25
2	B	301	FMN	C5A-N5-C4A	2.06	121.42	118.09
3	C	302	CBD	C1-C2-N2	-2.06	120.56	122.64
2	D	301	FMN	C4A-C10-N10	2.06	119.43	116.48
2	A	301	FMN	C4-N3-C2	-2.05	122.00	125.64
2	D	301	FMN	C10-C4A-N5	-2.04	120.64	124.81
3	D	302	CBD	CB1-CB2-NC	-2.04	119.61	121.50
2	C	301	FMN	C4A-C4-N3	2.02	118.41	113.25
2	D	301	FMN	O3P-P-O2P	2.02	115.39	107.80
2	A	301	FMN	C9A-C5A-N5	-2.02	120.31	122.45
3	A	302	CBD	NC-CC6-NC5	2.01	123.81	116.90

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	FMN	N10-C1'-C2'-O2'
2	C	301	FMN	O3'-C3'-C4'-C5'
3	A	302	CBD	CB6-CB1-SB-O3B
3	A	302	CBD	CD2-CD1-SD-O3D
3	A	302	CBD	CD6-CD1-SD-O1D
3	A	302	CBD	CD6-CD1-SD-O2D
3	A	302	CBD	CD6-CD1-SD-O3D
3	D	302	CBD	CD1-CD2-ND-CC4
3	B	302	CBD	C14-C1-SA-O2A
3	B	302	CBD	C14-C1-SA-O3A
3	B	302	CBD	CB2-CB1-SB-O3B
3	C	302	CBD	CD1-CD2-ND-CC4

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Mol	Chain	Res	Type	Atoms
3	C	302	CBD	CD2-CD1-SD-O3D
3	C	302	CBD	CD6-CD1-SD-O1D
3	C	302	CBD	CD6-CD1-SD-O2D
3	C	302	CBD	CD6-CD1-SD-O3D
2	C	301	FMN	O3'-C3'-C4'-O4'
2	C	301	FMN	C2'-C3'-C4'-C5'
3	B	302	CBD	C2-C1-SA-O1A
2	C	301	FMN	C2'-C3'-C4'-O4'
3	C	302	CBD	CB2-CB1-SB-O1B
3	B	302	CBD	CD1-CD2-ND-CC4
3	A	302	CBD	CB6-CB1-SB-O1B
3	B	302	CBD	CB6-CB1-SB-O2B
3	C	302	CBD	CB6-CB1-SB-O1B
3	C	302	CBD	CB6-CB1-SB-O2B
2	C	301	FMN	N10-C1'-C2'-C3'
3	A	302	CBD	CB2-CB1-SB-O3B
3	D	302	CBD	CB2-CB1-SB-O3B
3	B	302	CBD	C2-C1-SA-O3A
3	C	302	CBD	CB2-CB1-SB-O3B
3	D	302	CBD	CB6-CB1-SB-O3B
3	B	302	CBD	CB6-CB1-SB-O3B
3	C	302	CBD	CB6-CB1-SB-O3B
3	C	302	CBD	CB2-CB1-SB-O2B
2	A	301	FMN	C4'-C5'-O5'-P
2	D	301	FMN	C4'-C5'-O5'-P
3	A	302	CBD	CD2-CD1-SD-O1D
3	B	302	CBD	C2-C1-SA-O2A
3	B	302	CBD	CB2-CB1-SB-O1B
3	C	302	CBD	CD2-CD1-SD-O1D
2	B	301	FMN	C4'-C5'-O5'-P
3	B	302	CBD	CD3-CD2-ND-CC4
2	C	301	FMN	C3'-C4'-C5'-O5'
3	A	302	CBD	CB6-CB1-SB-O2B
3	B	302	CBD	C14-C1-SA-O1A
2	B	301	FMN	C2'-C3'-C4'-C5'
3	A	302	CBD	CD1-CD2-ND-CC4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

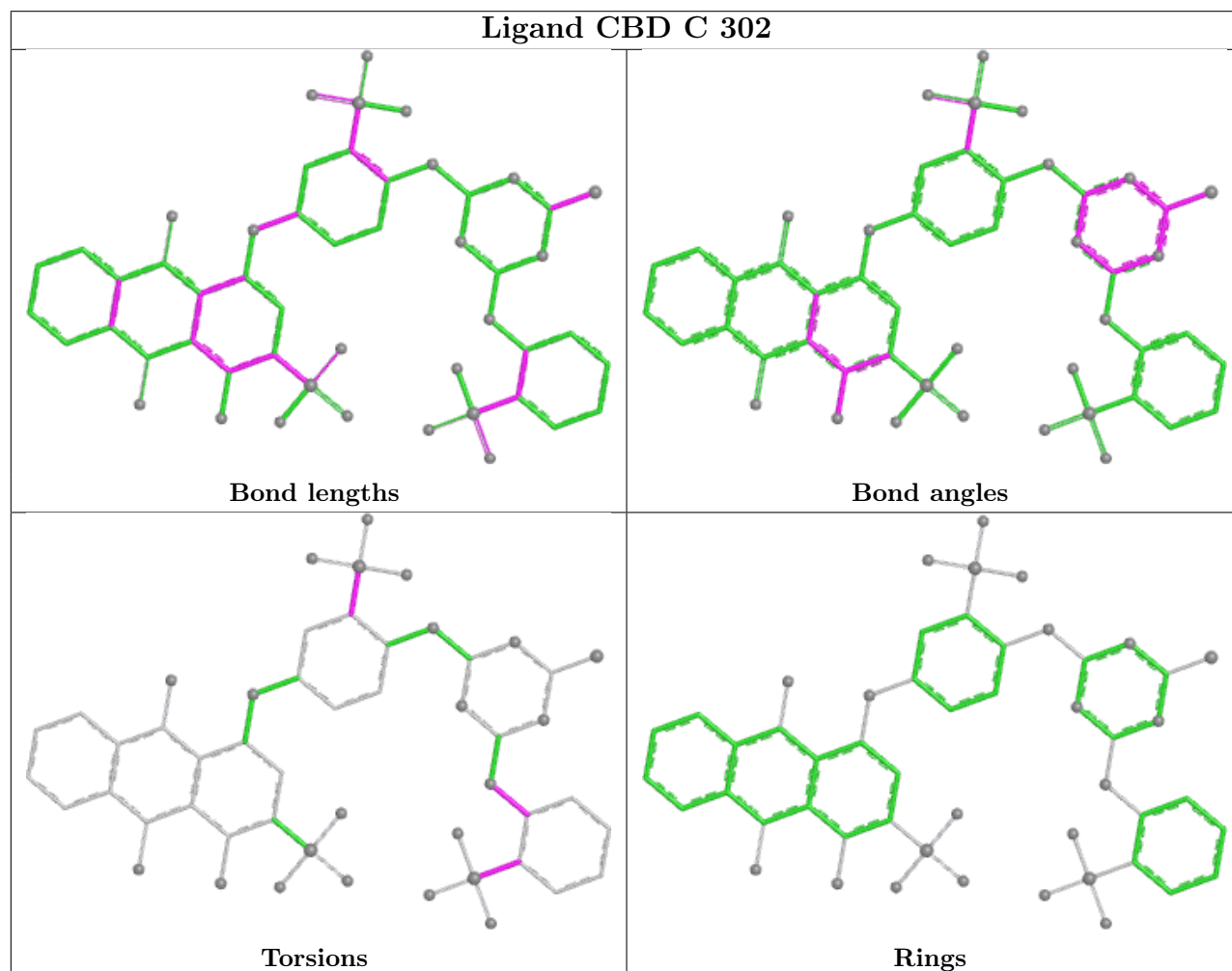
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	CBD	2	0

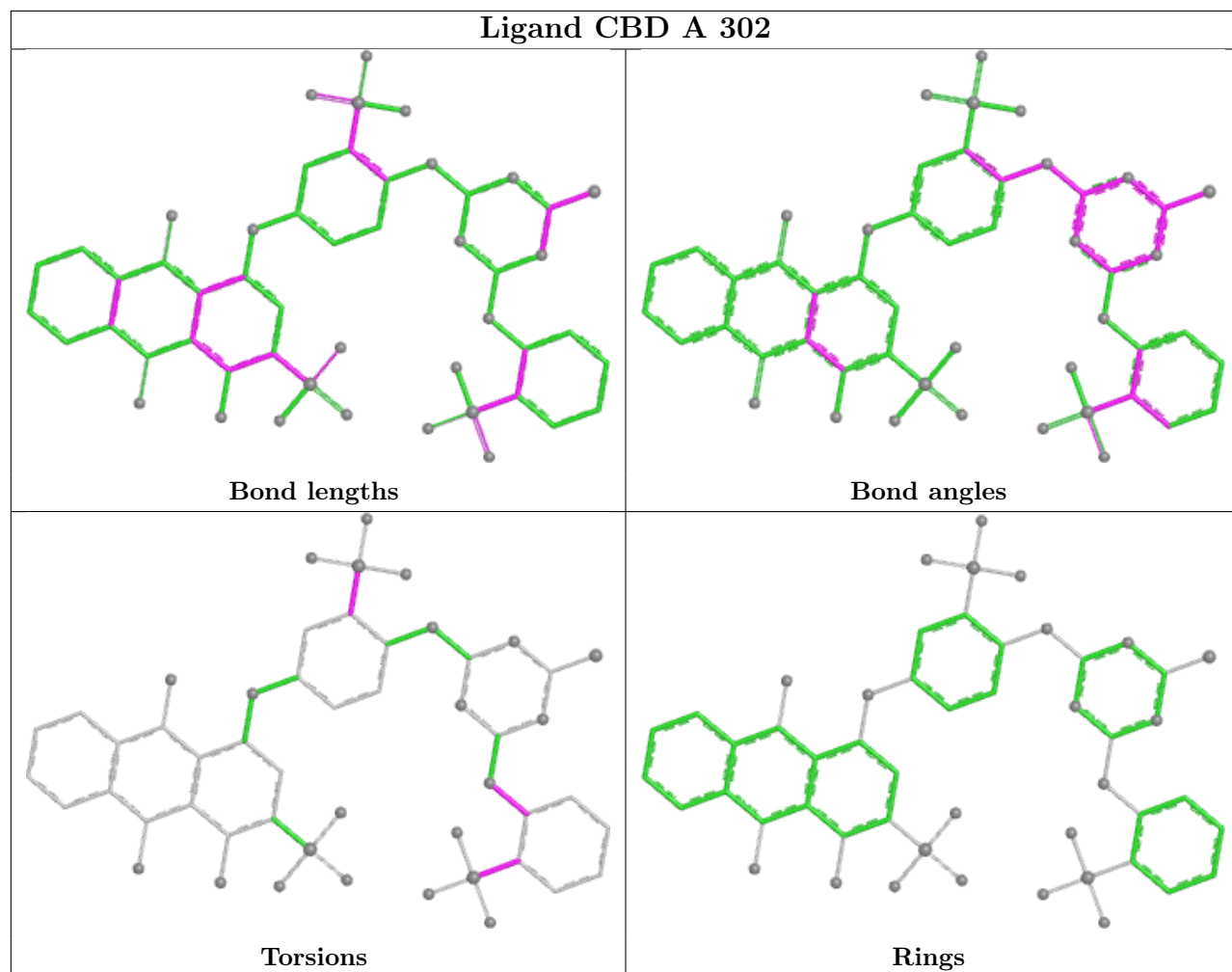
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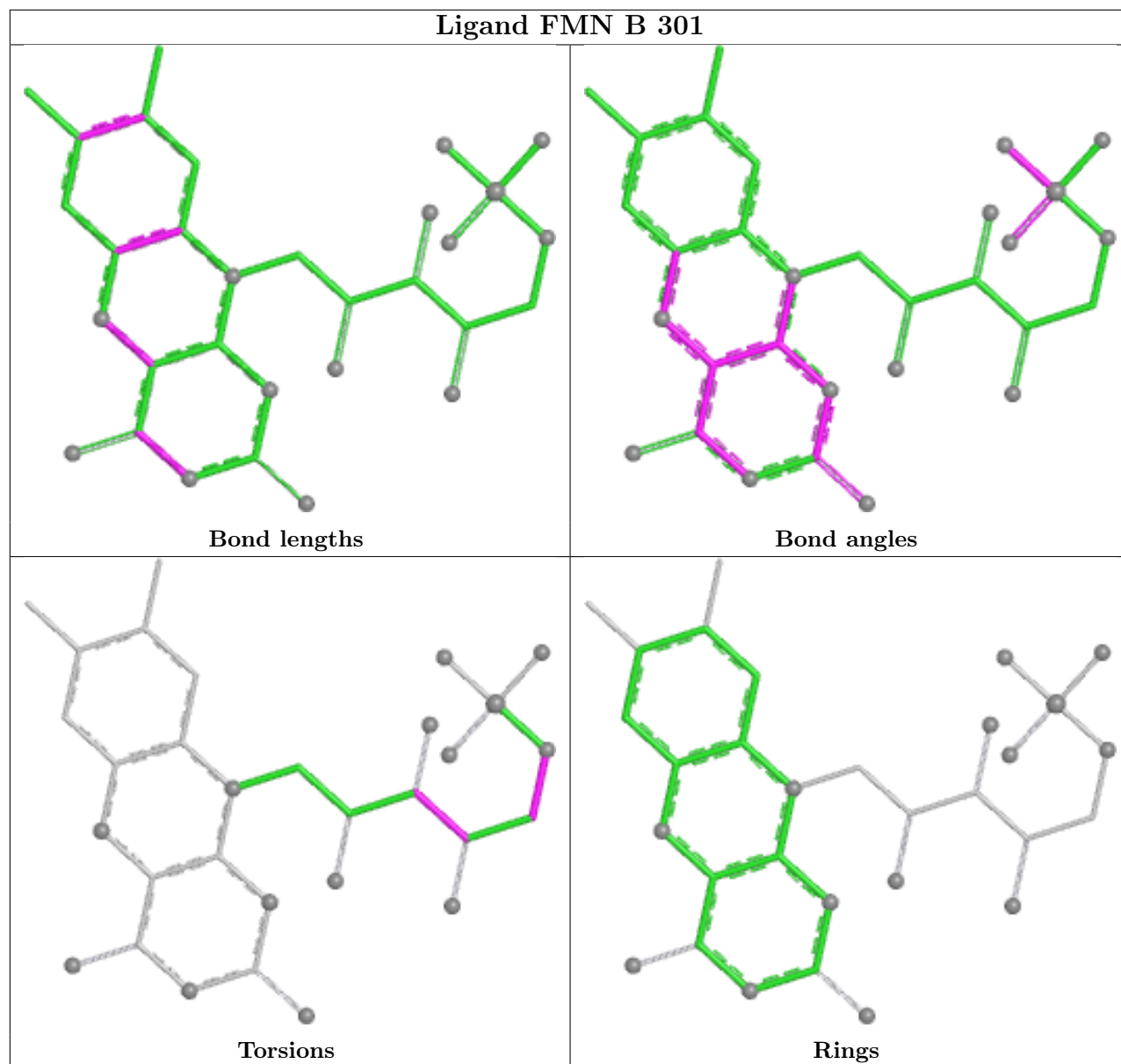
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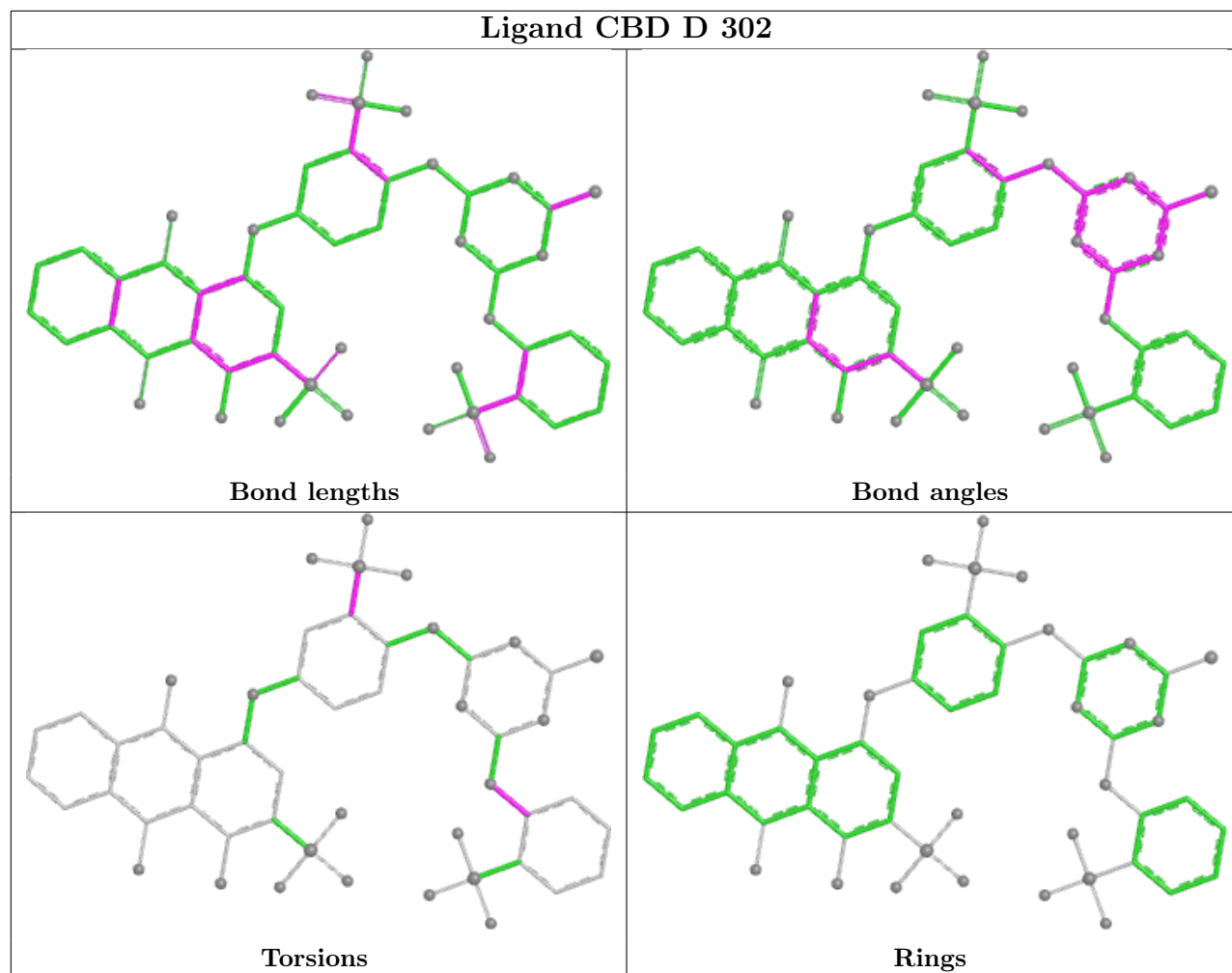
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	FMN	1	0

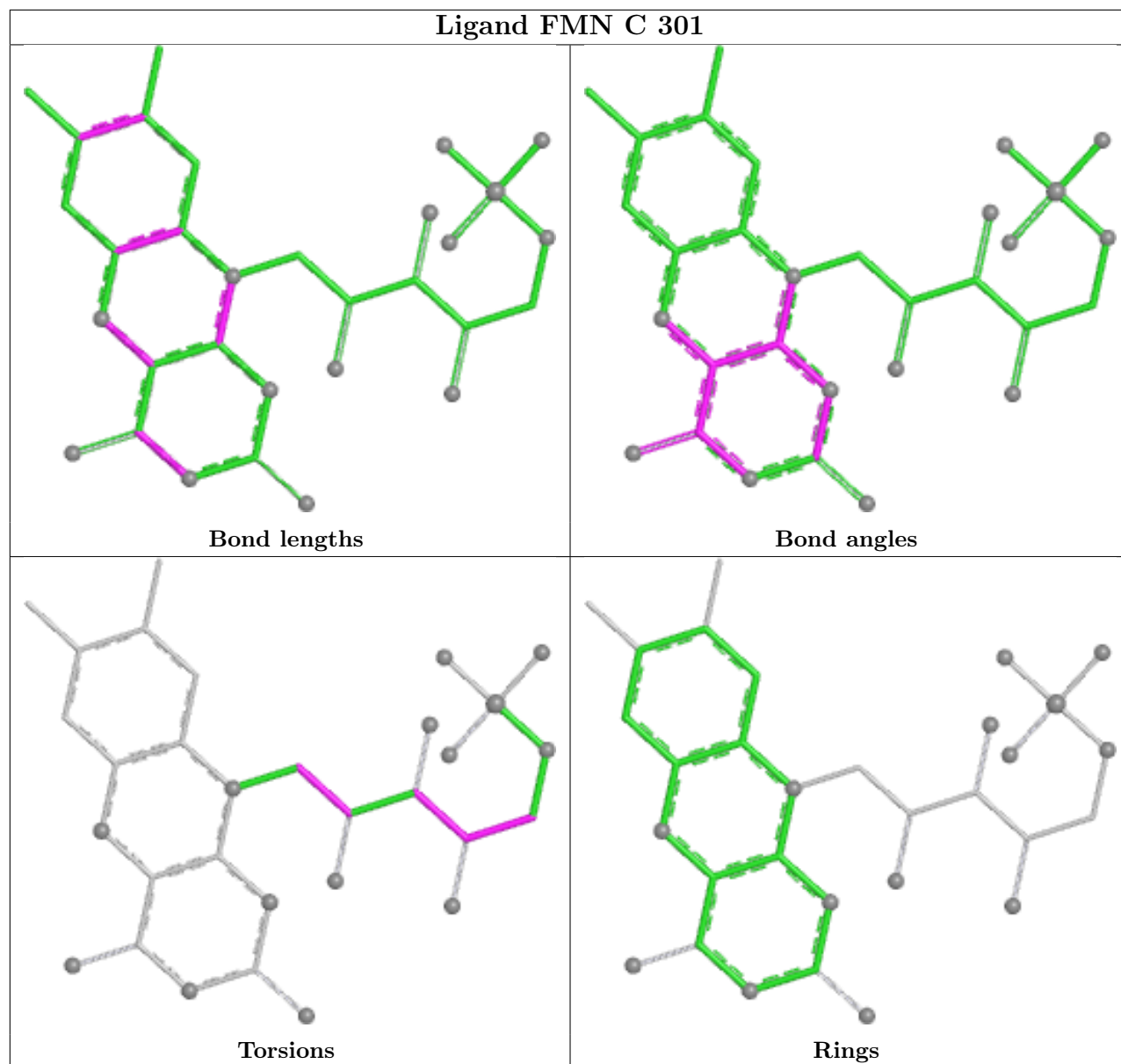
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

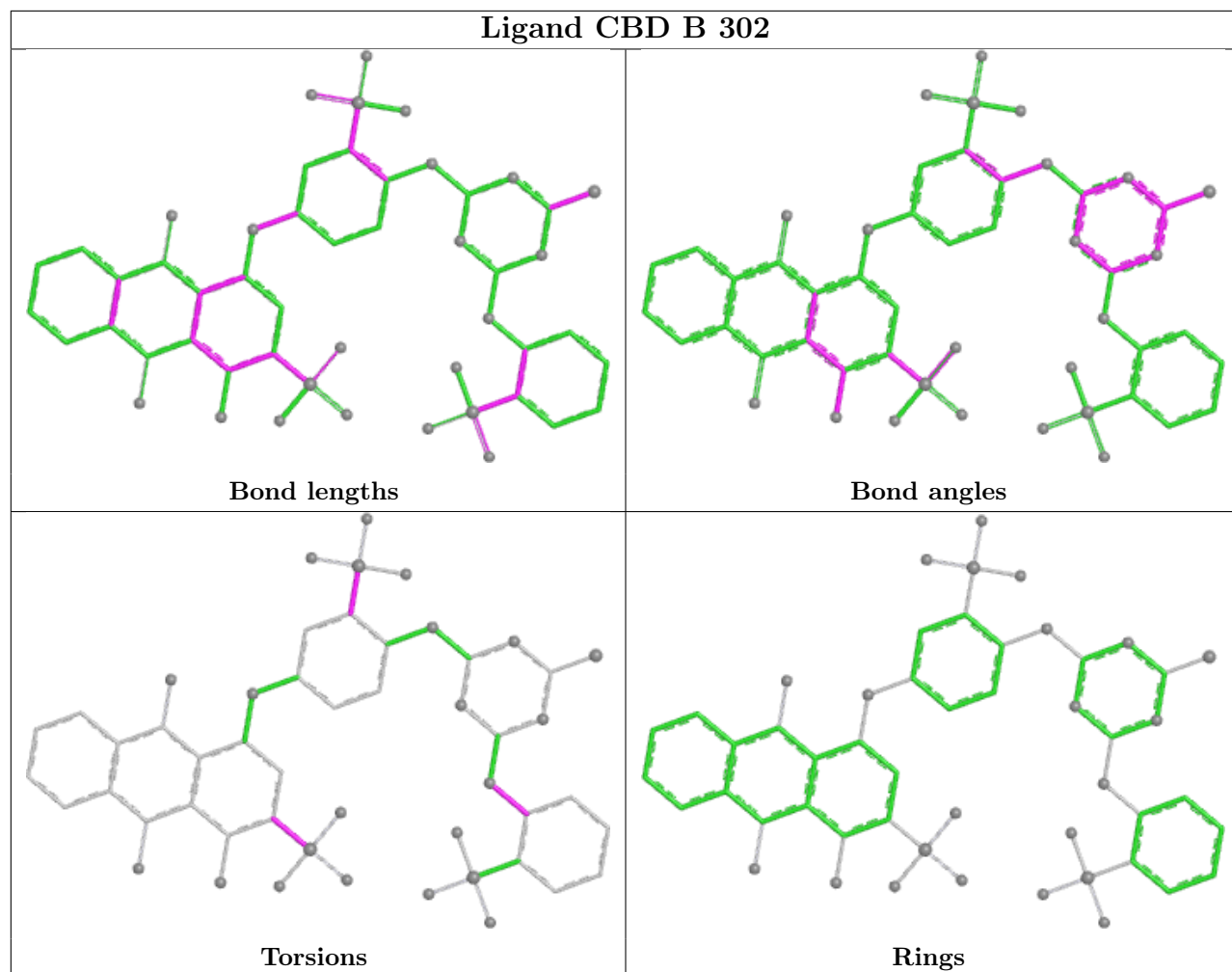


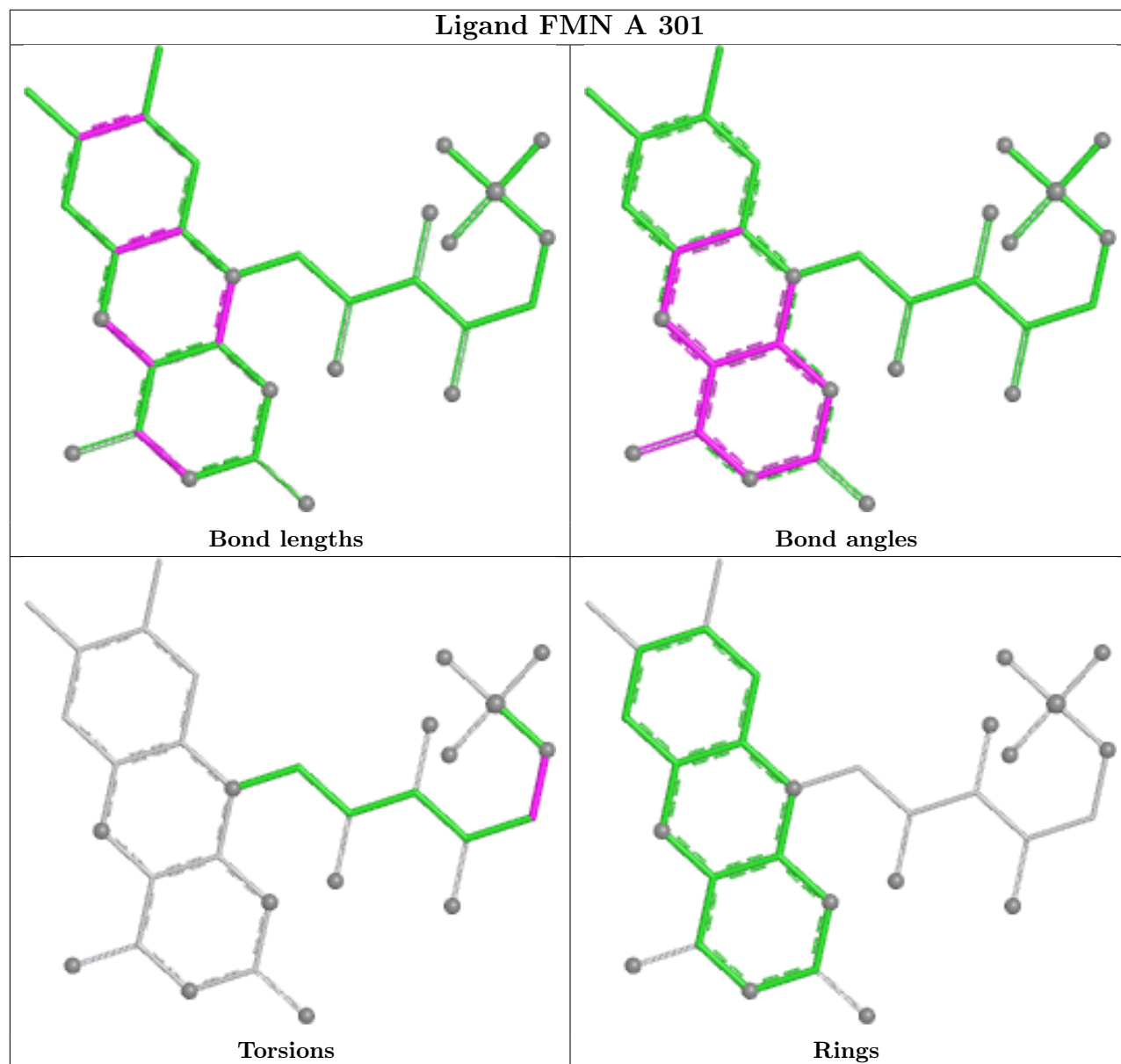


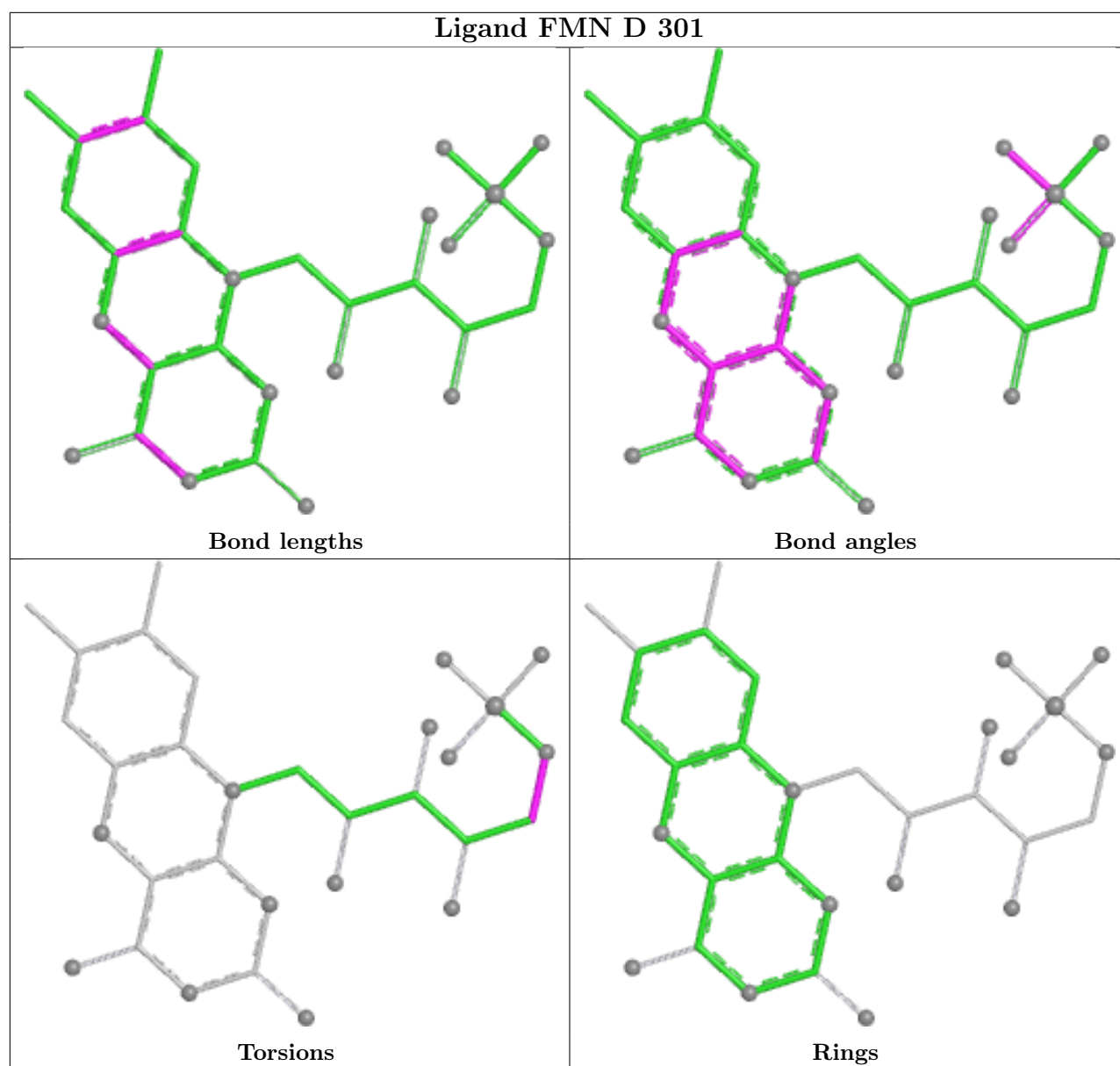












5.7 Other polymers [i](#)

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	210/211 (99%)	0.18	5 (2%) 59 54	30, 41, 59, 73	0
1	B	210/211 (99%)	0.69	22 (10%) 11 9	35, 62, 89, 107	0
1	C	210/211 (99%)	2.94	146 (69%) 0 0	70, 110, 175, 202	0
1	D	210/211 (99%)	0.56	18 (8%) 16 13	35, 54, 101, 129	0
All	All	840/844 (99%)	1.09	191 (22%) 2 1	30, 59, 135, 202	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	ALA	12.3
1	C	40	VAL	7.5
1	C	75	VAL	6.3
1	C	37	ASP	6.2
1	C	81	ALA	6.2
1	C	64	ALA	6.0
1	C	192	LYS	5.9
1	C	41	THR	5.8
1	C	188	ALA	5.8
1	C	187	ASN	5.7
1	B	129	GLU	5.6
1	C	68	GLY	5.6
1	C	58	ALA	5.4
1	C	70	GLU	5.4
1	C	77	GLN	5.3
1	C	72	LEU	5.2
1	C	65	ALA	5.2
1	C	36	GLN	5.1
1	C	186	MET	5.1
1	C	127	TYR	5.1
1	C	190	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	73	THR	5.0
1	C	9	ALA	4.9
1	C	117	ASN	4.9
1	C	2	THR	4.8
1	C	193	ALA	4.8
1	C	149	GLY	4.8
1	C	83	MET	4.8
1	C	80	VAL	4.8
1	C	16	GLY	4.7
1	D	189	ASN	4.7
1	C	60	TRP	4.7
1	C	45	PHE	4.6
1	C	15	GLU	4.5
1	C	196	ILE	4.5
1	C	121	ALA	4.5
1	C	11	PRO	4.4
1	C	128	THR	4.4
1	C	209	LYS	4.4
1	C	39	VAL	4.4
1	C	189	ASN	4.4
1	C	54	ALA	4.3
1	C	194	GLN	4.3
1	B	36	GLN	4.2
1	C	69	PHE	4.2
1	C	74	GLU	4.2
1	C	208	ALA	4.2
1	C	79	LYS	4.2
1	C	197	LYS	4.2
1	C	185	GLY	4.1
1	C	123	LYS	4.1
1	C	67	GLU	4.0
1	B	131	GLY	4.0
1	D	192	LYS	4.0
1	C	191	GLU	4.0
1	D	65	ALA	4.0
1	C	210	ARG	4.0
1	C	76	GLN	3.9
1	C	57	PHE	3.9
1	C	110	VAL	3.9
1	C	184	GLU	3.9
1	C	199	ALA	3.9
1	B	130	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	176	ASN	3.8
1	A	15	GLU	3.8
1	C	52	ILE	3.8
1	C	44	LEU	3.7
1	C	211	PHE	3.7
1	C	85	THR	3.7
1	C	48	THR	3.6
1	C	113	ALA	3.6
1	C	62	LYS	3.6
1	C	203	ASN	3.6
1	B	128	THR	3.5
1	C	31	LYS	3.5
1	B	191	GLU	3.5
1	C	101	PRO	3.5
1	C	78	GLN	3.5
1	C	35	PRO	3.4
1	D	71	ALA	3.4
1	C	198	GLU	3.4
1	C	56	VAL	3.4
1	C	126	LYS	3.4
1	B	70	GLU	3.4
1	C	122	GLY	3.4
1	C	86	ASN	3.4
1	C	66	GLY	3.3
1	C	116	ASP	3.3
1	D	191	GLU	3.3
1	C	13	SER	3.3
1	C	10	ASN	3.2
1	C	8	THR	3.2
1	C	17	SER	3.2
1	D	64	ALA	3.2
1	A	129	GLU	3.2
1	C	4	VAL	3.2
1	C	201	ILE	3.1
1	C	22	VAL	3.1
1	C	146	ALA	3.1
1	C	205	ARG	3.1
1	C	18	PHE	3.1
1	D	67	GLU	3.0
1	B	38	GLU	3.0
1	C	14	ALA	3.0
1	C	195	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	61	GLY	3.0
1	A	28	GLU	3.0
1	C	50	PRO	2.9
1	C	200	ALA	2.9
1	D	15	GLU	2.9
1	C	19	GLY	2.9
1	B	133	VAL	2.9
1	A	176	ASN	2.9
1	B	134	GLY	2.9
1	C	162	GLY	2.9
1	C	55	ASP	2.9
1	C	135	LEU	2.9
1	C	202	ALA	2.9
1	C	3	LYS	2.8
1	C	103	TRP	2.8
1	D	193	ALA	2.8
1	B	122	GLY	2.8
1	C	148	GLY	2.8
1	C	53	ASP	2.8
1	C	34	HIS	2.8
1	C	183	VAL	2.8
1	B	176	ASN	2.7
1	C	150	VAL	2.7
1	C	120	ILE	2.7
1	C	29	ALA	2.7
1	C	63	PHE	2.7
1	C	82	ALA	2.7
1	C	114	TYR	2.7
1	C	42	ILE	2.6
1	C	25	ALA	2.6
1	C	12	ASN	2.6
1	C	49	VAL	2.6
1	B	132	PRO	2.5
1	C	59	ALA	2.5
1	C	43	ASP	2.5
1	C	33	GLU	2.5
1	B	127	TYR	2.5
1	C	97	VAL	2.5
1	D	70	GLU	2.4
1	C	102	MET	2.4
1	C	136	LEU	2.4
1	C	207	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	38	GLU	2.4
1	C	5	LEU	2.4
1	B	68	GLY	2.4
1	C	151	TYR	2.3
1	C	104	ASN	2.3
1	B	189	ASN	2.3
1	B	203	ASN	2.3
1	C	46	ASN	2.3
1	C	130	ASN	2.3
1	C	28	GLU	2.3
1	C	38	GLU	2.3
1	C	99	VAL	2.3
1	C	124	THR	2.3
1	D	66	GLY	2.3
1	B	31	LYS	2.3
1	D	128	THR	2.2
1	C	153	GLU	2.2
1	C	30	TYR	2.2
1	C	133	VAL	2.2
1	C	145	GLN	2.2
1	C	152	SER	2.2
1	C	173	VAL	2.2
1	D	75	VAL	2.2
1	C	24	GLU	2.2
1	C	119	ALA	2.1
1	C	20	MET	2.1
1	C	204	ALA	2.1
1	C	129	GLU	2.1
1	C	47	THR	2.1
1	D	186	MET	2.1
1	C	32	ASN	2.1
1	B	202	ALA	2.1
1	D	190	PRO	2.1
1	C	109	PRO	2.1
1	C	115	LEU	2.1
1	D	80	VAL	2.1
1	C	89	THR	2.1
1	D	36	GLN	2.1
1	B	194	GLN	2.1
1	D	62	LYS	2.0
1	B	209	LYS	2.0
1	C	23	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	152	SER	2.0
1	C	144	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](#)

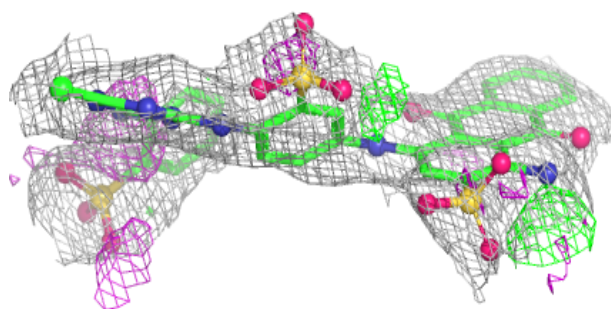
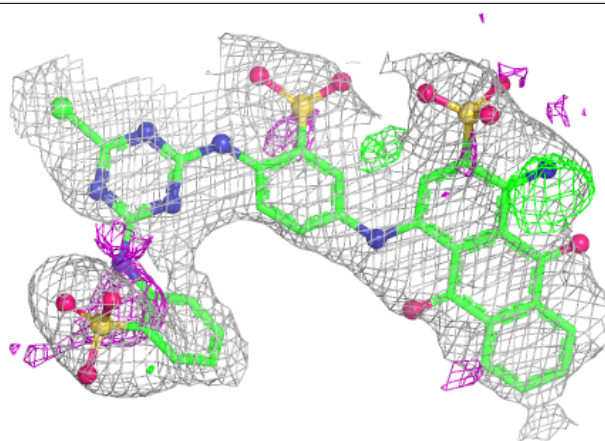
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CBD	C	302	51/51	0.70	0.20	93,101,112,114	0
2	FMN	C	301	31/31	0.74	0.20	71,78,84,85	0
3	CBD	B	302	51/51	0.83	0.16	60,76,88,99	0
3	CBD	D	302	51/51	0.91	0.12	57,59,64,74	0
3	CBD	A	302	51/51	0.92	0.12	54,63,72,81	0
2	FMN	B	301	31/31	0.94	0.10	46,47,48,49	0
2	FMN	D	301	31/31	0.95	0.09	40,43,45,47	0
2	FMN	A	301	31/31	0.96	0.09	32,34,35,37	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.

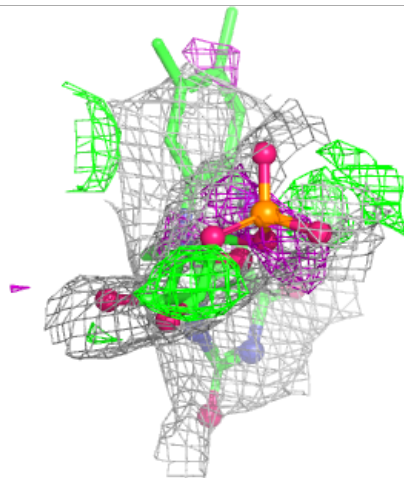
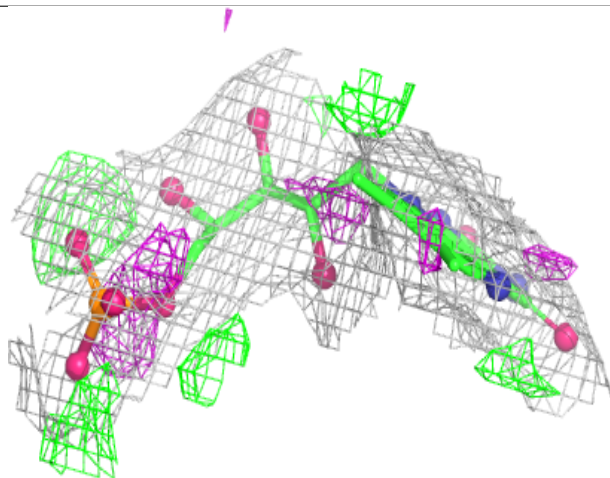
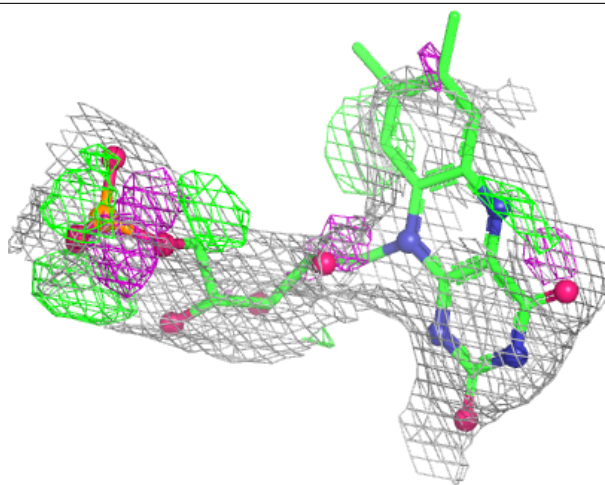
Electron density around CBD C 302:

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



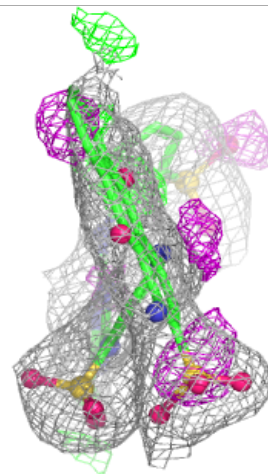
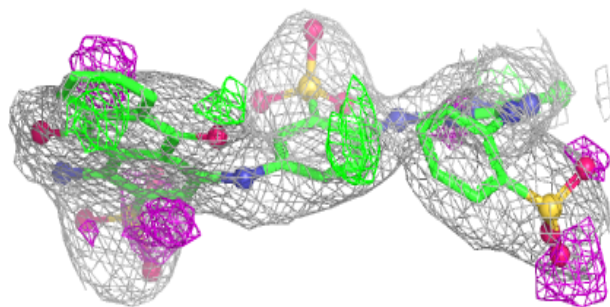
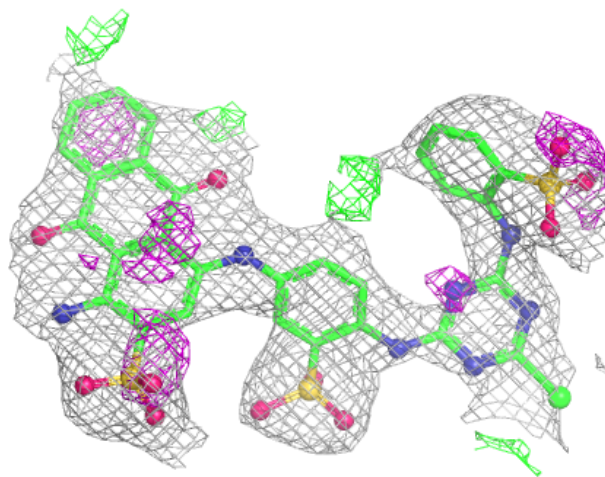
Electron density around FMN C 301:

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



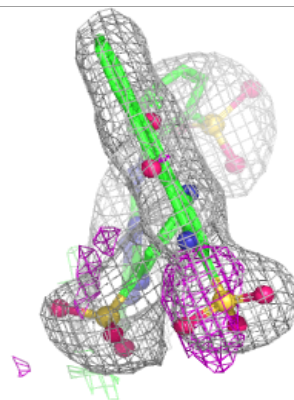
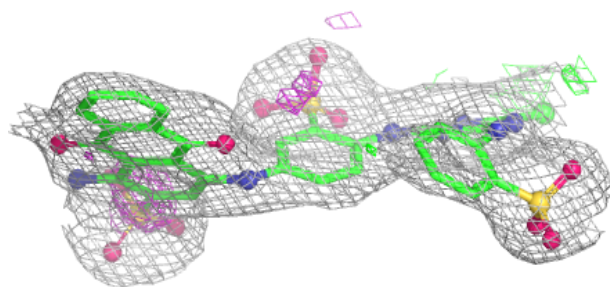
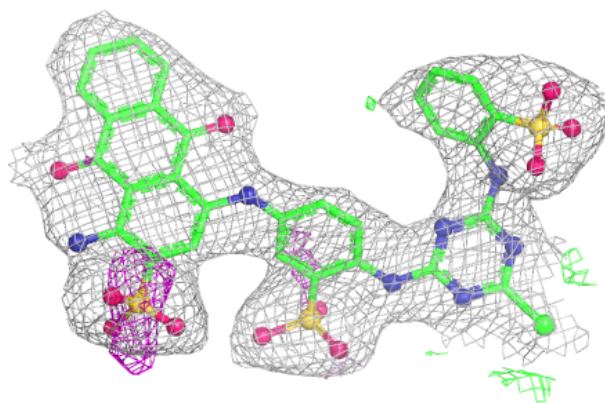
Electron density around CBD B 302:

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

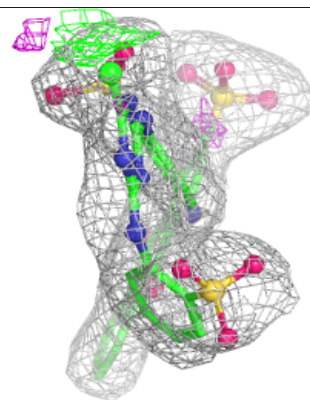
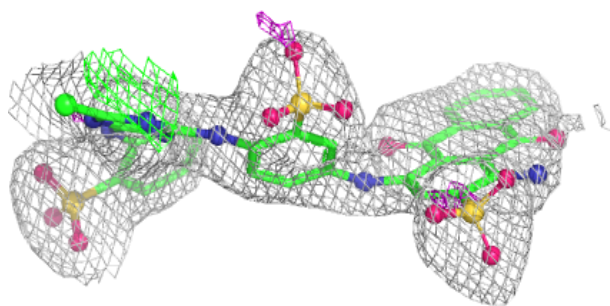
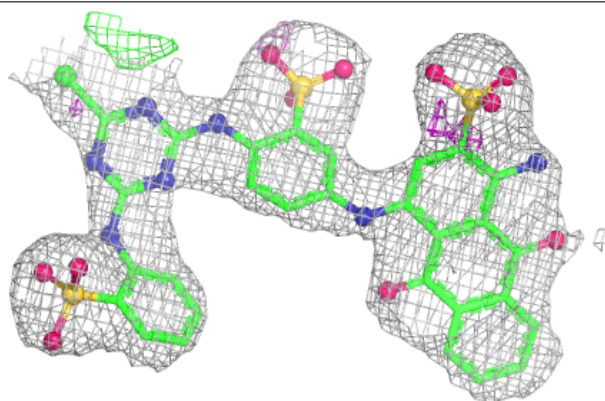


Electron density around CBD D 302:

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

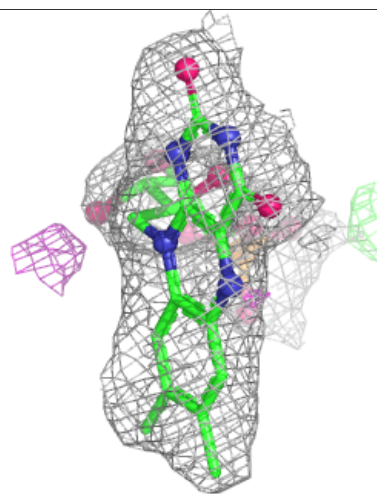
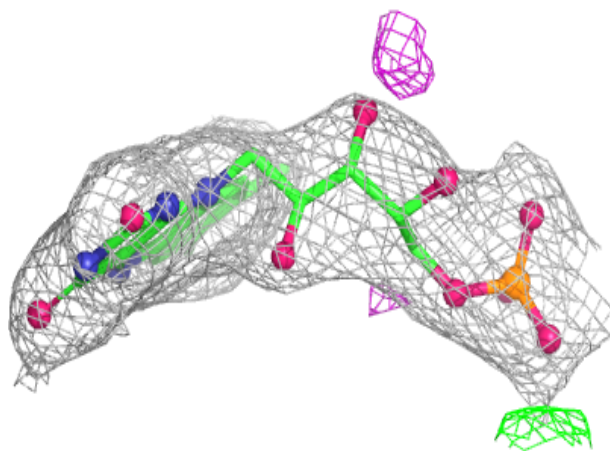
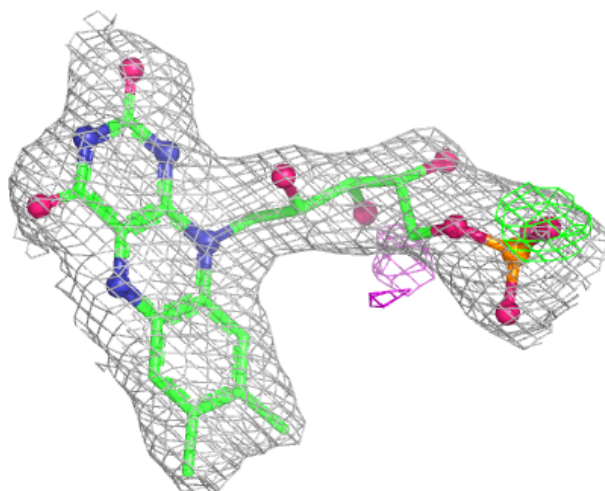
**Electron density around CBD A 302:**

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



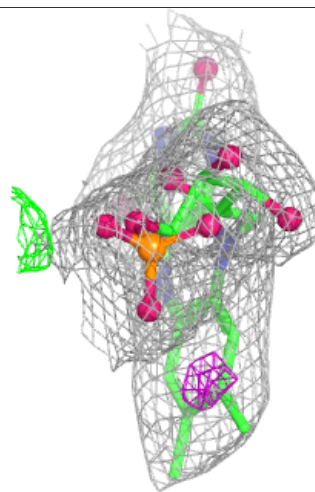
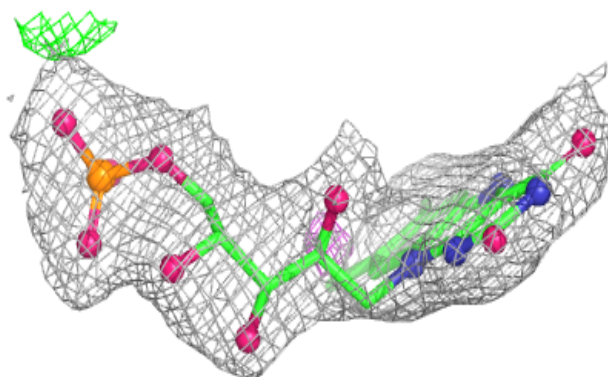
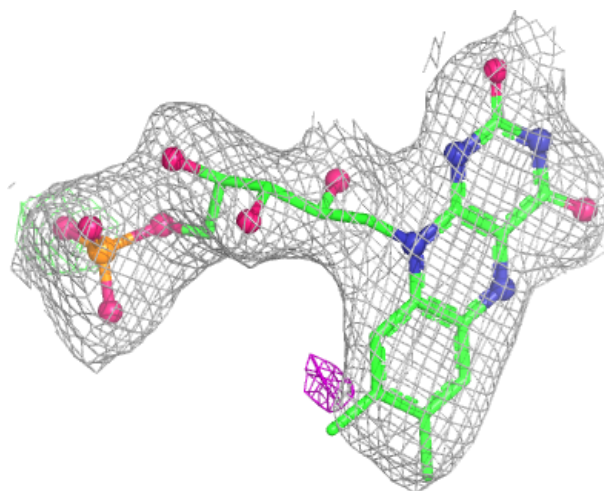
Electron density around FMN B 301:

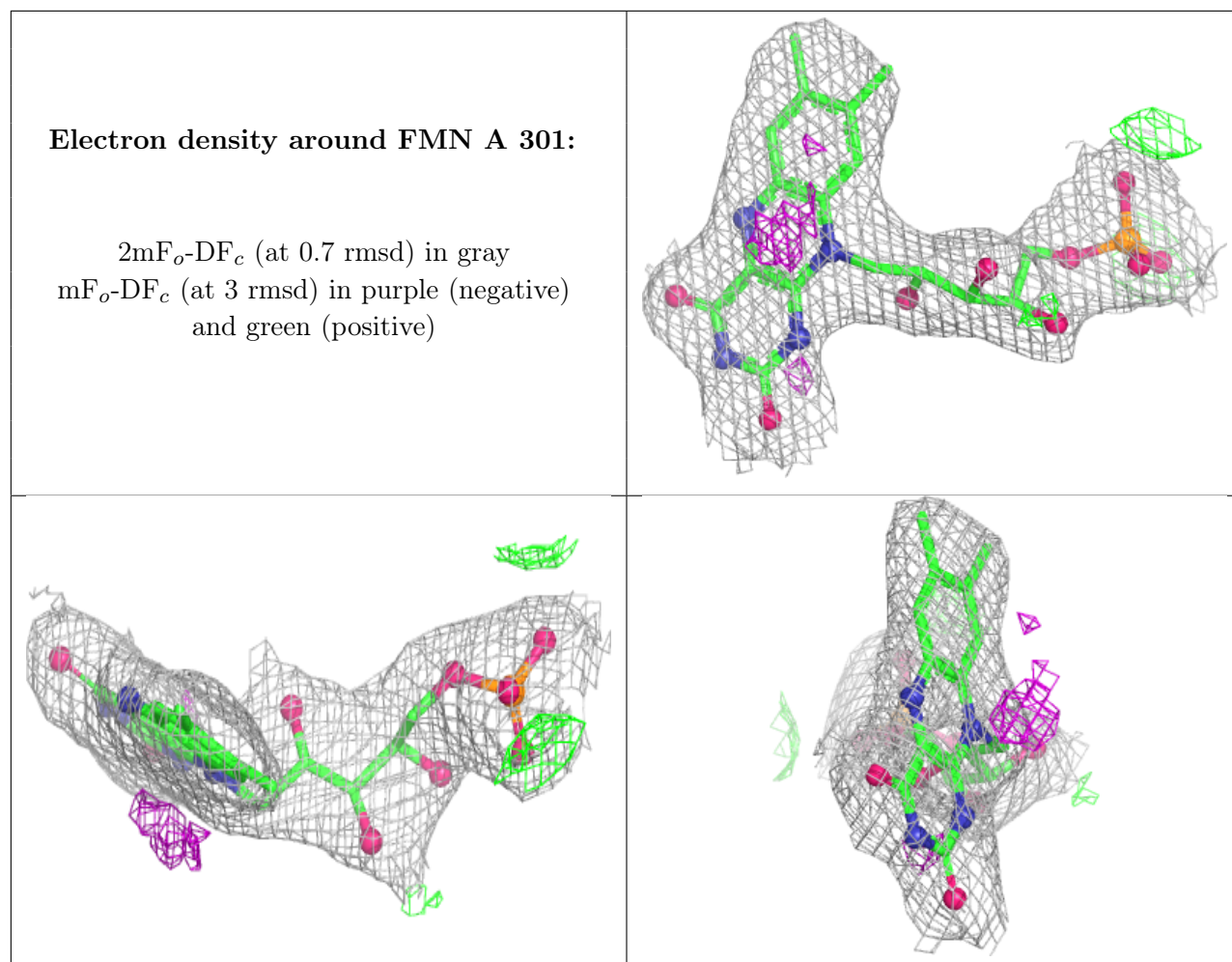
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN D 301:

$2mF_o-DF_c$ (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.