



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:29 AM UTC

PDB ID : 3GG1 / pdb_00003gg1
Title : Klebsiella pneumoniae BlrP1 pH 8.0 calcium/cy-diGMP complex
Authors : Barends, T.; Hartmann, E.; Griesse, J.; Beitlich, T.; Kirienko, N.; Ryjenkov, D.; Reinstein, J.; Shoeman, R.; Gomelsky, M.; Schlichting, I.
Deposited on : 2009-02-27
Resolution : 2.30 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

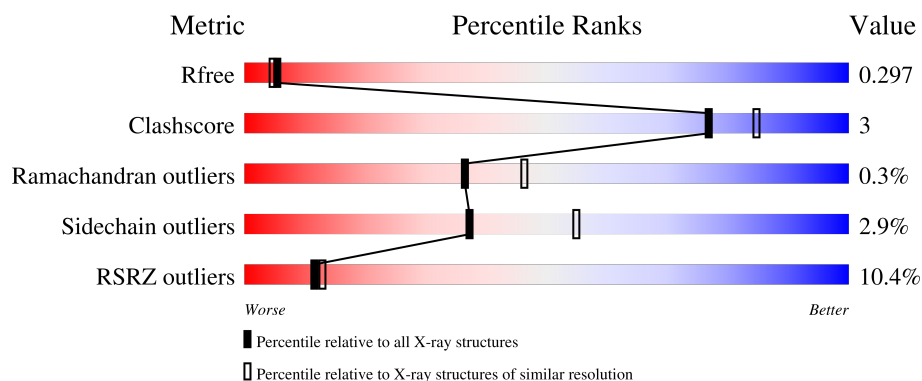
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	413	9% 88% 6% 5%
1	B	413	11% 86% 9% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C2E	A	501	X	-	-	-
2	C2E	B	501	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6500 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.

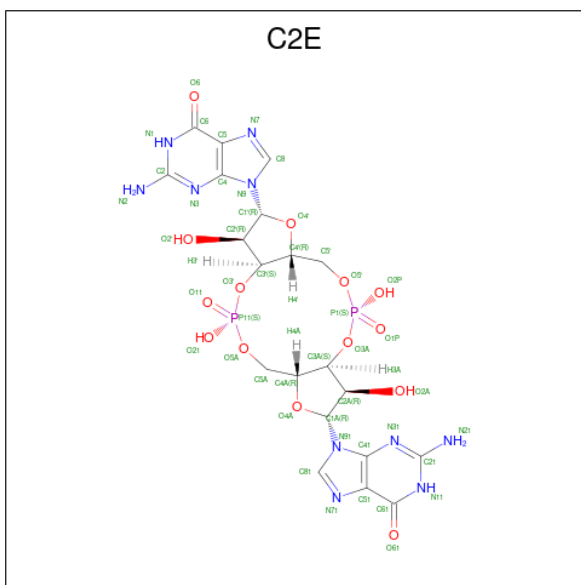
- Molecule 1 is a protein called *Klebsiella pneumoniae* Blrp1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3069	1967	529	555	18			
1	B	394	Total	C	N	O	S	0	0	0
			3094	1983	534	559	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ILE	-	expression tag	UNP A6T8V8
A	-6	SER	-	expression tag	UNP A6T8V8
A	-5	GLU	-	expression tag	UNP A6T8V8
A	-4	PHE	-	expression tag	UNP A6T8V8
A	-3	GLY	-	expression tag	UNP A6T8V8
A	-2	SER	-	expression tag	UNP A6T8V8
A	-1	SER	-	expression tag	UNP A6T8V8
A	0	ARG	-	expression tag	UNP A6T8V8
B	-7	ILE	-	expression tag	UNP A6T8V8
B	-6	SER	-	expression tag	UNP A6T8V8
B	-5	GLU	-	expression tag	UNP A6T8V8
B	-4	PHE	-	expression tag	UNP A6T8V8
B	-3	GLY	-	expression tag	UNP A6T8V8
B	-2	SER	-	expression tag	UNP A6T8V8
B	-1	SER	-	expression tag	UNP A6T8V8
B	0	ARG	-	expression tag	UNP A6T8V8

- Molecule 2 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).

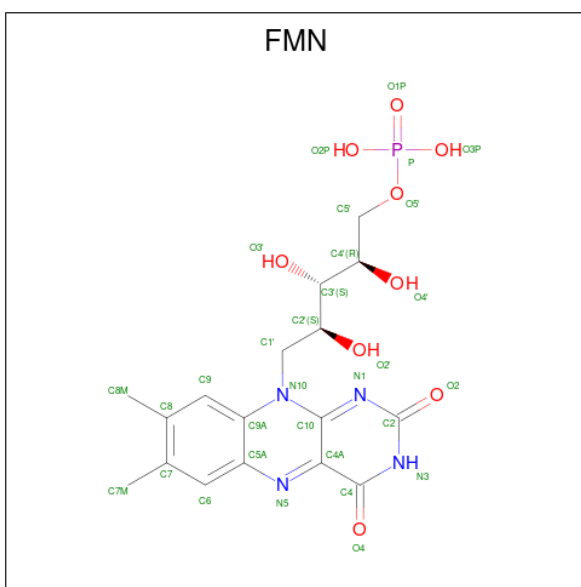


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	B	1	Total 46	C 20	N 10	O 14	P 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

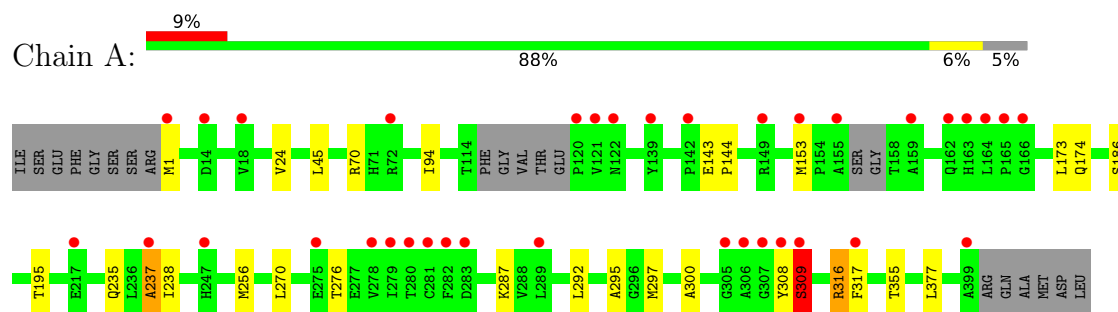
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	93	Total O 93 93	0	0
5	B	86	Total O 86 86	0	0

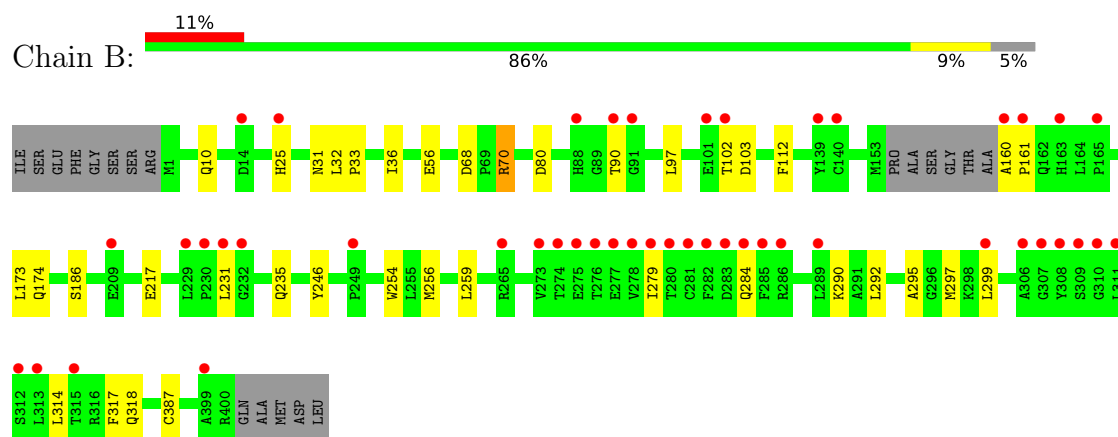
3 Residue-property plots [i](#)

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: *Klebsiella pneumoniae* Blrp1



• Molecule 1: *Klebsiella pneumoniae* Blrp1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.85Å 96.69Å 127.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 99.8 (20.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.90 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.244 , 0.296 0.248 , 0.297	Depositor DCC
R_{free} test set	1947 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6500	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C2E, CA, 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	0.44	0/3137	0.79	7/4252 (0.2%)
1	B	0.42	0/3163	0.68	0/4287
All	All	0.43	0/6300	0.74	7/8539 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	238	ILE	N-CA-C	13.79	131.57	109.78
1	A	317	PHE	N-CA-C	10.95	125.71	109.95
1	A	316	ARG	N-CA-C	8.06	123.04	112.72
1	A	237	ALA	N-CA-C	-6.57	99.20	109.25
1	A	237	ALA	CA-C-N	5.98	128.66	120.35
1	A	237	ALA	C-N-CA	5.98	128.66	120.35
1	A	317	PHE	N-CA-CB	-5.32	102.51	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	309	SER	Peptide
1	A	316	ARG	Peptide

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	3069	0	3087	21	0
1	B	3094	0	3110	16	0
2	A	46	0	18	1	0
2	B	46	0	18	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	31	0	19	0	0
4	B	31	0	19	0	0
5	A	93	0	0	0	0
5	B	86	0	0	0	0
All	All	6500	0	6271	36	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 3.

All (36) 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:A:24:VAL:HG21	1:A:94:ILE:HB	1.83	0.60
1:A:292:LEU:HD23	1:A:297:MET:HE3	1.83	0.60
1:B:161:PRO:HG3	1:B:387:CYS:SG	2.43	0.59
1:A:308:TYR:N	1:A:309:SER:HB3	2.18	0.58
1:B:246:TYR:CE2	1:B:284:GLN:HB2	2.39	0.56
1:A:292:LEU:CD2	1:A:297:MET:HE3	2.36	0.56
1:A:256:MET:CE	1:A:297:MET:HE2	2.36	0.55
1:B:68:ASP:OD1	1:B:70:ARG:HD3	2.09	0.53
1:A:355:THR:HG23	1:A:377:LEU:HD12	1.92	0.51
1:B:314:LEU:O	1:B:318:GLN:NE2	2.41	0.51
1:B:174:GLN:OE1	2:B:501:C2E:H8	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:MET:HE3	1:B:259:LEU:HD21	1.95	0.49
1:A:308:TYR:CA	1:A:309:SER:HB3	2.43	0.49
1:A:270:LEU:HD21	1:A:300:ALA:HB2	1.95	0.48
1:A:270:LEU:HD21	1:A:300:ALA:CB	2.44	0.48
1:A:1:MET:HE1	1:B:290:LYS:NZ	2.29	0.48
1:A:256:MET:HE1	1:A:297:MET:HG3	1.96	0.47
1:A:186:SER:HB3	1:A:235:GLN:HB2	1.96	0.47
1:A:308:TYR:HA	1:A:309:SER:CB	2.46	0.46
1:B:32:LEU:HD13	1:B:90:THR:HB	1.99	0.45
1:B:32:LEU:HB3	1:B:33:PRO:HD3	1.99	0.45
1:A:308:TYR:HA	1:A:309:SER:HB3	1.98	0.44
1:A:308:TYR:CA	1:A:309:SER:CB	2.95	0.44
1:A:256:MET:HE3	1:A:295:ALA:HB1	2.01	0.43
1:B:217:GLU:HA	1:B:254:TRP:CH2	2.52	0.43
1:B:256:MET:SD	1:B:295:ALA:HB1	2.59	0.43
1:B:160:ALA:N	1:B:161:PRO:CD	2.81	0.43
1:A:355:THR:CG2	1:A:377:LEU:HD12	2.49	0.42
1:A:256:MET:HE1	1:A:297:MET:HE2	2.01	0.42
1:B:186:SER:HB3	1:B:235:GLN:HB3	2.03	0.41
1:B:292:LEU:HD23	1:B:297:MET:HE3	2.02	0.41
1:A:174:GLN:OE1	2:A:501:C2E:H8	2.20	0.41
1:A:195:THR:HG22	1:A:195:THR:O	2.21	0.40
1:B:256:MET:HE3	1:B:256:MET:HA	2.02	0.40
1:A:143:GLU:N	1:A:144:PRO:CD	2.84	0.40
1:B:31:ASN:HB3	1:B:36:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/413 (94%)	378 (98%)	7 (2%)	1 (0%)	36	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	390/413 (94%)	378 (97%)	11 (3%)	1 (0%)	36	46
All	All	776/826 (94%)	756 (97%)	18 (2%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	SER
1	B	102	THR

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	329/346 (95%)	323 (98%)	6 (2%)	51	70
1	B	332/346 (96%)	319 (96%)	13 (4%)	28	43
All	All	661/692 (96%)	642 (97%)	19 (3%)	37	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	70	ARG
1	A	153	MET
1	A	173	LEU
1	A	276	THR
1	A	287	LYS
1	B	10	GLN
1	B	25	HIS
1	B	56	GLU
1	B	70	ARG
1	B	80	ASP
1	B	97	LEU
1	B	103	ASP
1	B	112	PHE

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Mol	Chain	Res	Type
1	B	173	LEU
1	B	231	LEU
1	B	279	ILE
1	B	299	LEU
1	B	317	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	GLN
1	B	12	HIS
1	B	25	HIS
1	B	49	GLN
1	B	88	HIS
1	B	167	GLN
1	B	248	HIS
1	B	268	GLN
1	B	339	GLN
1	B	371	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](#)

Of 8 ligands modelled in this entry, 4 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
4	FMN	A	504	-	33,33,33	0.99	2 (6%)	48,50,50	1.29	7 (14%)
2	C2E	B	501	3	52,52,52	2.02	9 (17%)	78,82,82	2.41	32 (41%)
4	FMN	B	504	-	33,33,33	1.01	2 (6%)	48,50,50	1.27	7 (14%)
2	C2E	A	501	3	52,52,52	2.03	9 (17%)	78,82,82	2.40	30 (38%)

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
4	FMN	A	504	-	-	1/18/18/18	0/3/3/3
2	C2E	B	501	3	1/1/10/10	6/30/62/62	0/6/7/7
4	FMN	B	504	-	-	1/18/18/18	0/3/3/3
2	C2E	A	501	3	1/1/10/10	8/30/62/62	0/6/7/7

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	C2E	C2A-C1A	-6.46	1.33	1.53
2	A	501	C2E	C2'-C1'	-6.44	1.33	1.53
2	A	501	C2E	C2A-C1A	-6.40	1.33	1.53
2	B	501	C2E	C2'-C1'	-6.23	1.33	1.53
2	A	501	C2E	C8-N9	-3.95	1.28	1.37
2	A	501	C2E	O2'-C2'	-3.95	1.33	1.43
2	B	501	C2E	O2'-C2'	-3.95	1.33	1.43
2	B	501	C2E	C8-N9	-3.91	1.28	1.37
2	B	501	C2E	C1A-N91	-3.83	1.36	1.47
2	A	501	C2E	C1'-N9	-3.82	1.36	1.47
2	B	501	C2E	O2A-C2A	-3.73	1.33	1.43
2	A	501	C2E	C1A-N91	-3.71	1.37	1.47
4	A	504	FMN	C4A-N5	3.67	1.38	1.30
2	B	501	C2E	C1'-N9	-3.62	1.37	1.47
2	A	501	C2E	O2A-C2A	-3.61	1.34	1.43
4	B	504	FMN	C4A-N5	3.52	1.38	1.30
2	B	501	C2E	P11-O11	2.79	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	C2E	P11-O11	2.72	1.60	1.50
4	B	504	FMN	C10-N1	2.70	1.38	1.33
4	A	504	FMN	C10-N1	2.31	1.37	1.33
2	B	501	C2E	C41-N91	-2.07	1.32	1.38
2	A	501	C2E	C41-N91	-2.01	1.32	1.38

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	C2E	O4A-C1A-N91	7.47	125.28	108.36
2	B	501	C2E	O4A-C1A-N91	7.32	124.94	108.36
2	B	501	C2E	C5-C4-N3	-5.20	120.11	128.39
2	A	501	C2E	C5-C4-N3	-5.09	120.30	128.39
2	B	501	C2E	N91-C41-N31	4.94	135.82	125.95
2	A	501	C2E	C51-C41-N31	-4.86	120.66	128.39
2	A	501	C2E	N9-C4-N3	4.85	135.64	125.95
2	B	501	C2E	C51-C41-N31	-4.78	120.79	128.39
2	B	501	C2E	N9-C4-N3	4.73	135.42	125.95
2	A	501	C2E	N91-C41-N31	4.73	135.41	125.95
2	B	501	C2E	C81-N91-C41	4.39	114.26	106.03
2	A	501	C2E	N91-C81-N71	-4.34	105.36	113.40
2	B	501	C2E	N91-C81-N71	-4.29	105.44	113.40
2	A	501	C2E	C81-N91-C41	4.19	113.87	106.03
2	A	501	C2E	C21-N31-C41	4.13	119.42	112.30
2	B	501	C2E	C2-N3-C4	4.10	119.35	112.30
2	B	501	C2E	C21-N31-C41	3.96	119.12	112.30
2	A	501	C2E	C2-N3-C4	3.89	119.00	112.30
2	B	501	C2E	C2'-C1'-N9	3.81	123.86	113.25
2	B	501	C2E	C3'-C2'-C1'	3.80	108.24	99.89
2	A	501	C2E	O4'-C1'-N9	3.80	116.96	108.36
2	A	501	C2E	C3'-C2'-C1'	3.77	108.19	99.89
2	B	501	C2E	C8-N7-C5	3.73	110.90	104.26
2	B	501	C2E	C4-C5-N7	-3.72	104.77	110.67
2	A	501	C2E	C8-N7-C5	3.63	110.73	104.26
2	B	501	C2E	O2'-C2'-C1'	3.55	122.32	110.10
2	A	501	C2E	O2'-C2'-C1'	3.52	122.22	110.10
2	A	501	C2E	C4-C5-N7	-3.50	105.12	110.67
2	B	501	C2E	O4A-C1A-C2A	3.49	114.08	106.62
2	A	501	C2E	C8-N9-C4	3.42	112.43	106.03
4	B	504	FMN	C4-N3-C2	-3.38	119.64	125.64
4	A	504	FMN	C4-N3-C2	-3.37	119.65	125.64
2	B	501	C2E	C8-N9-C4	3.25	112.11	106.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	C2E	O4'-C1'-N9	3.23	115.67	108.36
4	A	504	FMN	C4A-C10-N10	3.20	121.06	116.48
2	B	501	C2E	O5A-C5A-C4A	-3.12	98.38	108.99
2	A	501	C2E	O21-P11-O5A	3.11	121.65	107.57
2	A	501	C2E	N9-C8-N7	-3.10	107.66	113.40
2	A	501	C2E	C2'-C1'-N9	3.09	121.85	113.25
2	A	501	C2E	C4A-O4A-C1A	-3.07	102.69	109.47
2	B	501	C2E	N9-C8-N7	-3.05	107.74	113.40
2	A	501	C2E	O4A-C1A-C2A	3.01	113.05	106.62
2	B	501	C2E	C4A-O4A-C1A	-2.98	102.89	109.47
2	B	501	C2E	C6-C5-N7	2.97	135.69	130.29
4	B	504	FMN	C4A-C10-N10	2.86	120.58	116.48
2	A	501	C2E	C2A-C1A-N91	2.85	121.19	113.25
2	A	501	C2E	O2'-C2'-C3'	2.84	119.14	111.19
2	A	501	C2E	C6-C5-N7	2.82	135.43	130.29
4	A	504	FMN	C4A-C4-N3	2.76	120.27	113.25
2	B	501	C2E	O2'-C2'-C3'	2.69	118.70	111.19
2	A	501	C2E	O5A-C5A-C4A	-2.65	99.99	108.99
4	A	504	FMN	C10-C4A-N5	-2.64	119.42	124.81
2	B	501	C2E	C2A-C1A-N91	2.62	120.54	113.25
4	B	504	FMN	C4A-C4-N3	2.62	119.92	113.25
4	B	504	FMN	C10-C4A-N5	-2.57	119.56	124.81
2	A	501	C2E	C81-N71-C51	2.53	108.77	104.26
2	B	501	C2E	O61-C61-C51	-2.42	120.14	126.53
2	B	501	C2E	O21-P11-O5A	2.37	118.29	107.57
2	B	501	C2E	C81-N71-C51	2.30	108.36	104.26
2	B	501	C2E	C51-C61-N11	2.29	119.09	113.25
2	B	501	C2E	C1A-N91-C81	-2.25	120.34	126.73
2	B	501	C2E	C21-N11-C61	-2.22	121.08	125.11
2	A	501	C2E	C51-C61-N11	2.22	118.90	113.25
4	A	504	FMN	C4-C4A-N5	2.19	121.23	118.21
2	A	501	C2E	O61-C61-C51	-2.17	120.81	126.53
2	A	501	C2E	C21-N11-C61	-2.16	121.20	125.11
4	B	504	FMN	O4-C4-C4A	-2.14	120.88	126.53
4	B	504	FMN	C4A-C10-N1	-2.12	119.39	124.59
4	A	504	FMN	O4-C4-C4A	-2.09	121.02	126.53
2	A	501	C2E	C5-C6-N1	2.09	118.57	113.25
2	B	501	C2E	O5A-P11-O11	-2.08	100.68	108.94
2	A	501	C2E	C1A-N91-C81	-2.08	120.83	126.73
2	B	501	C2E	C2-N1-C6	-2.07	121.36	125.11
2	B	501	C2E	C5-C6-N1	2.05	118.47	113.25
4	A	504	FMN	C4A-C10-N1	-2.04	119.59	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	FMN	C9A-C5A-N5	-2.02	120.31	122.45

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	C2E	C1A
2	B	501	C2E	C1A

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	C2E	C5'-O5'-P1-O1P
2	B	501	C2E	C5'-O5'-P1-O1P
2	B	501	C2E	C5'-O5'-P1-O3A
4	B	504	FMN	C5'-O5'-P-O2P
2	A	501	C2E	C2A-C3A-O3A-P1
2	A	501	C2E	C4A-C3A-O3A-P1
2	A	501	C2E	C4'-C5'-O5'-P1
2	A	501	C2E	C5'-O5'-P1-O3A
2	B	501	C2E	C5'-O5'-P1-O2P
2	B	501	C2E	C4'-C5'-O5'-P1
2	A	501	C2E	O4'-C4'-C5'-O5'
2	B	501	C2E	O4'-C4'-C5'-O5'
4	A	504	FMN	C4'-C5'-O5'-P
2	B	501	C2E	C3'-C4'-C5'-O5'
2	A	501	C2E	C3'-C4'-C5'-O5'
2	A	501	C2E	O4A-C4A-C5A-O5A

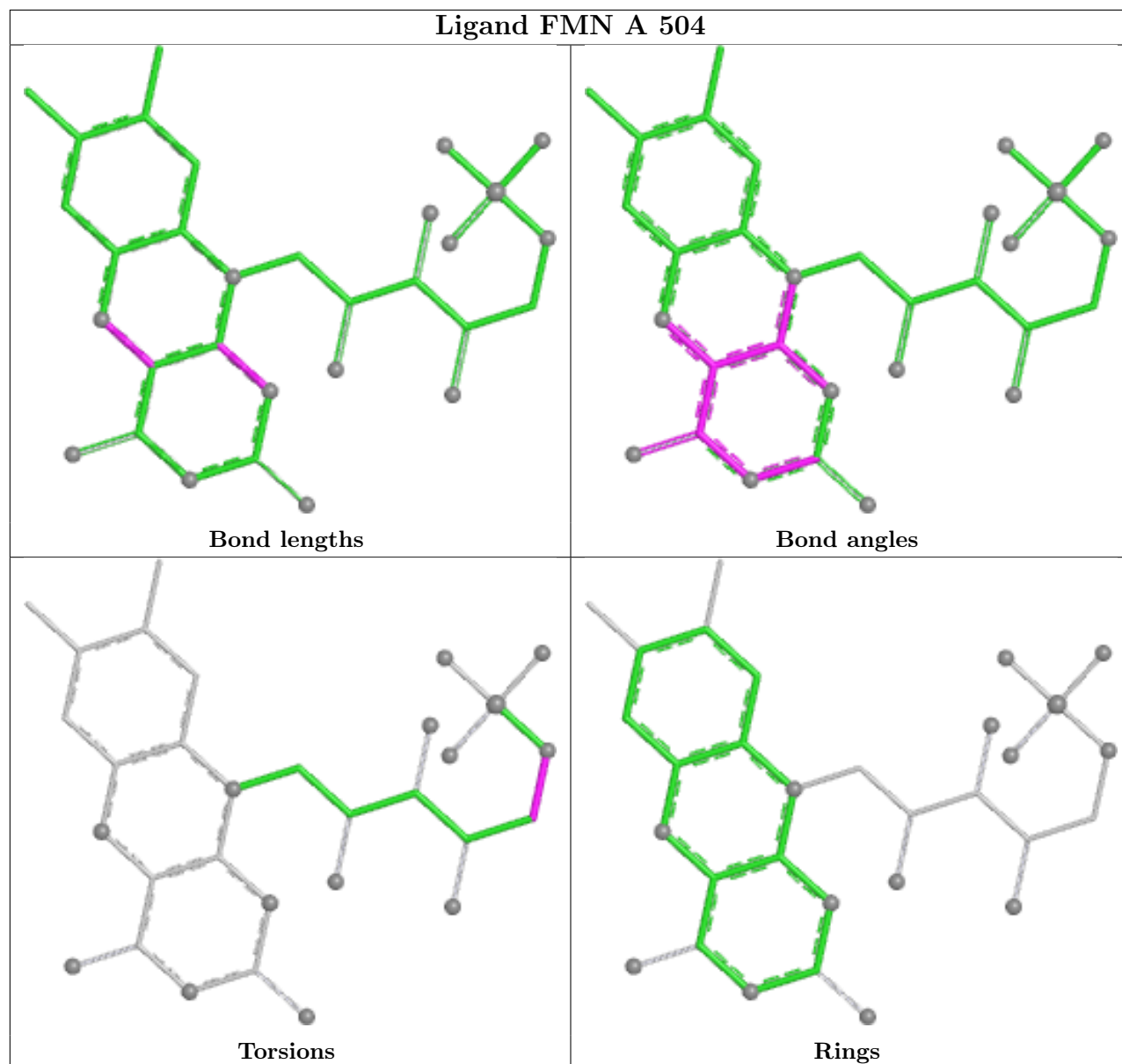
There are no ring outliers.

2 monomers are involved in 2 short contacts:

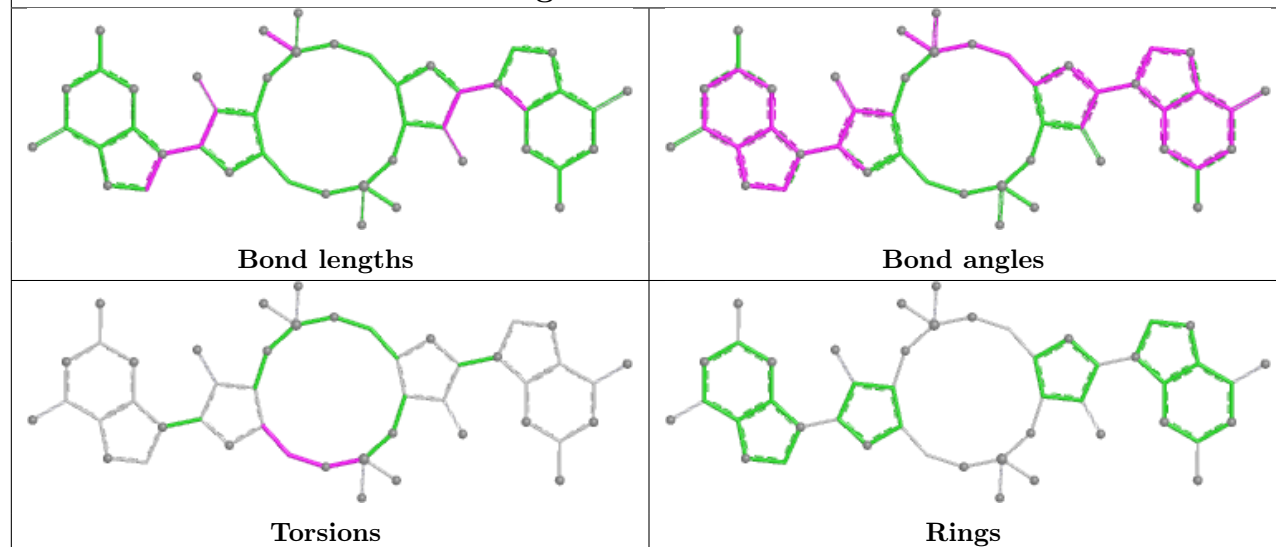
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	C2E	1	0
2	A	501	C2E	1	0

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

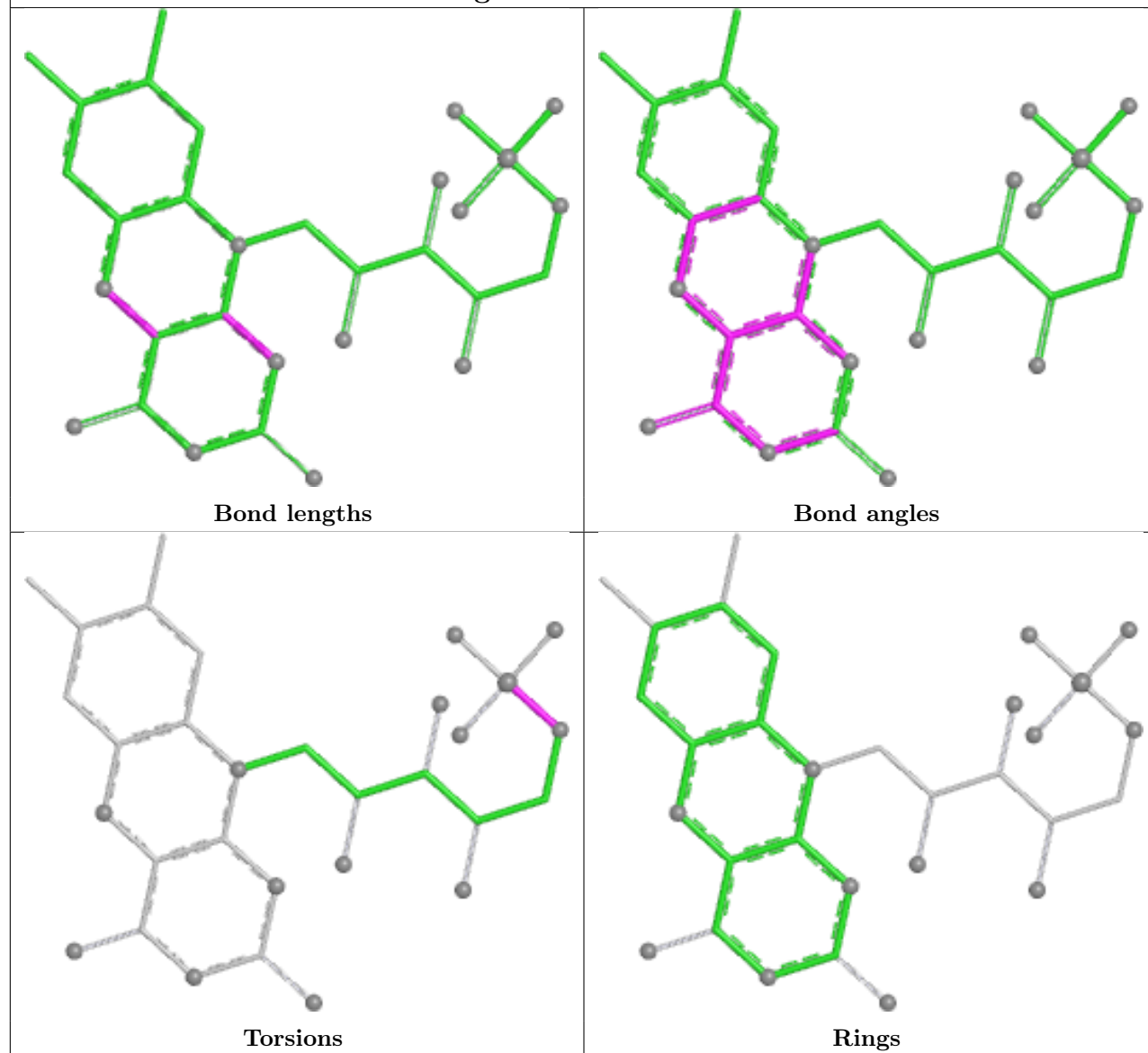
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

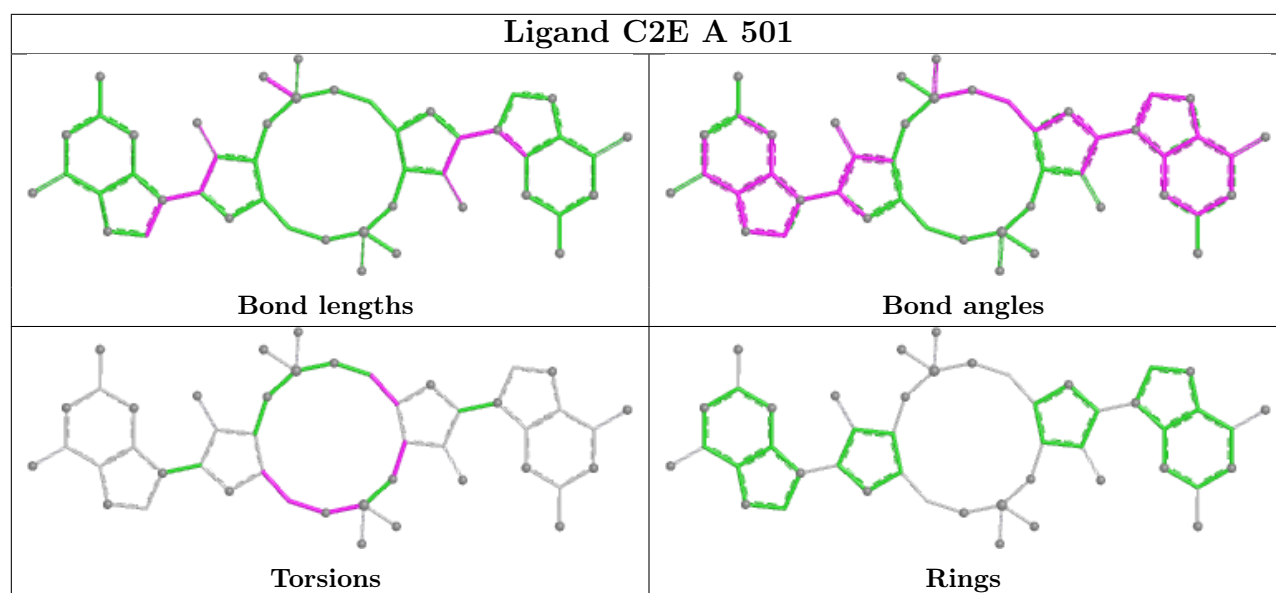


Ligand C2E B 501



Ligand FMN B 504





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	392/413 (94%)	0.65	36 (9%) 14 16	20, 29, 40, 47	0
1	B	394/413 (95%)	0.74	46 (11%) 9 10	20, 29, 40, 47	0
All	All	786/826 (95%)	0.70	82 (10%) 11 13	20, 29, 40, 47	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	TYR	8.5
1	A	309	SER	6.1
1	B	285	PHE	6.0
1	B	308	TYR	5.6
1	B	282	PHE	5.4
1	B	284	GLN	5.4
1	A	281	CYS	5.1
1	A	165	PRO	5.0
1	A	282	PHE	4.9
1	B	90	THR	4.8
1	B	280	THR	4.8
1	B	278	VAL	4.8
1	B	102	THR	4.3
1	B	279	ILE	4.0
1	B	232	GLY	3.9
1	B	283	ASP	3.8
1	B	14	ASP	3.8
1	B	276	THR	3.7
1	A	307	GLY	3.7
1	A	14	ASP	3.7
1	B	309	SER	3.7
1	B	307	GLY	3.4
1	A	121	VAL	3.4
1	B	91	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLY	3.2
1	A	279	ILE	3.2
1	A	139	TYR	3.1
1	B	312	SER	3.1
1	A	162	GLN	3.1
1	A	120	PRO	3.1
1	B	313	LEU	3.1
1	A	283	ASP	3.0
1	B	306	ALA	3.0
1	B	231	LEU	3.0
1	B	160	ALA	3.0
1	B	275	GLU	2.9
1	B	289	LEU	2.8
1	A	155	ALA	2.8
1	A	159	ALA	2.8
1	A	317	PHE	2.8
1	B	299	LEU	2.8
1	B	165	PRO	2.8
1	B	311	LEU	2.7
1	B	277	GLU	2.7
1	A	153	MET	2.7
1	B	399	ALA	2.6
1	B	101	GLU	2.6
1	A	163	HIS	2.6
1	A	247	HIS	2.6
1	B	25	HIS	2.6
1	A	278	VAL	2.5
1	A	305	GLY	2.5
1	B	274	THR	2.4
1	A	306	ALA	2.4
1	B	139	TYR	2.4
1	A	237	ALA	2.4
1	B	229	LEU	2.3
1	A	142	PRO	2.3
1	A	289	LEU	2.3
1	B	230	PRO	2.3
1	B	286	ARG	2.3
1	B	273	VAL	2.3
1	B	88	HIS	2.2
1	A	280	THR	2.2
1	A	149	ARG	2.2
1	A	217	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	275	GLU	2.2
1	B	265	ARG	2.2
1	A	1	MET	2.2
1	B	161	PRO	2.2
1	B	209	GLU	2.2
1	A	164	LEU	2.1
1	A	72	ARG	2.1
1	B	281	CYS	2.1
1	A	122	ASN	2.1
1	B	163	HIS	2.1
1	B	310	GLY	2.1
1	A	18	VAL	2.0
1	B	315	THR	2.0
1	A	399	ALA	2.0
1	B	140	CYS	2.0
1	B	249	PRO	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.

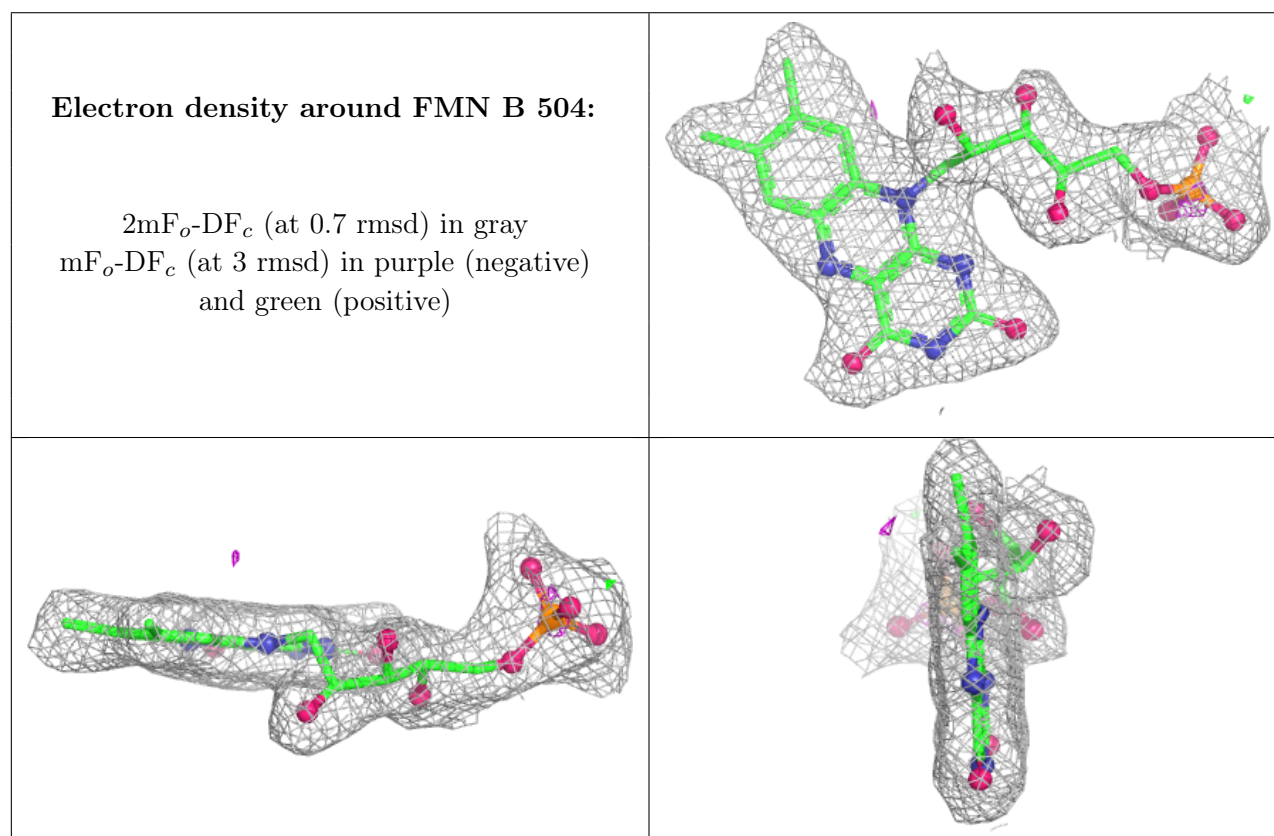
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	B	503	1/1	0.90	0.05	34,34,34,34	0
4	FMN	B	504	31/31	0.90	0.08	22,23,38,38	0
4	FMN	A	504	31/31	0.91	0.09	22,23,37,37	0
2	C2E	B	501	46/46	0.94	0.08	22,23,24,24	0
2	C2E	A	501	46/46	0.95	0.08	21,22,23,24	0
3	CA	A	503	1/1	0.97	0.08	30,30,30,30	0
3	CA	B	502	1/1	0.99	0.03	18,18,18,18	0

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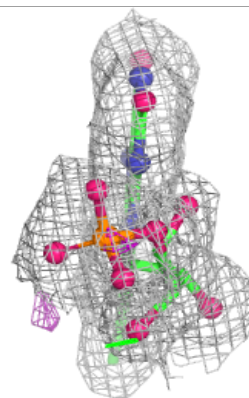
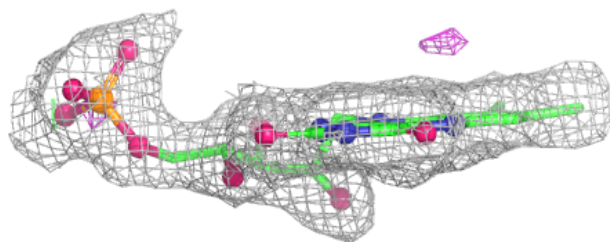
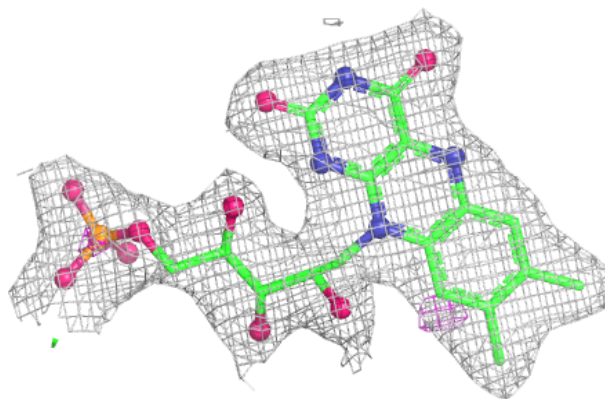
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	502	1/1	1.00	0.01	17,17,17,17	0

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.

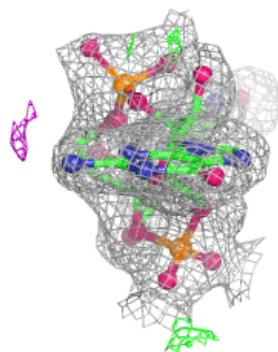
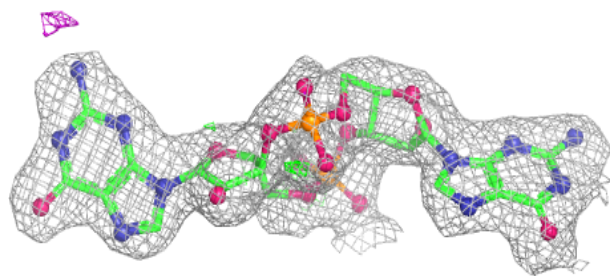
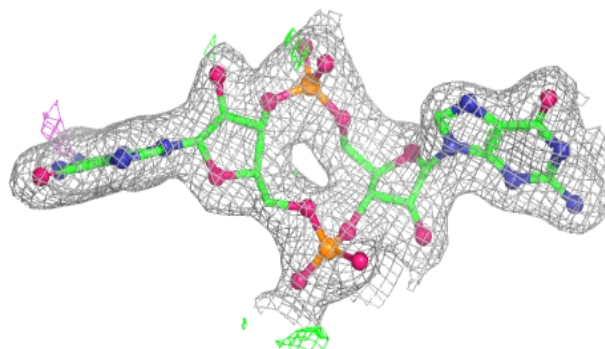


Electron density around FMN A 504:

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

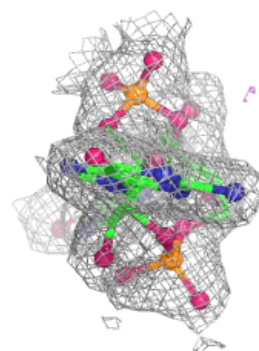
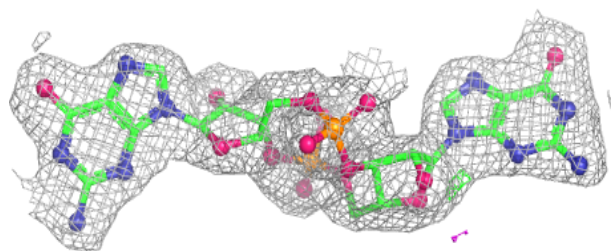
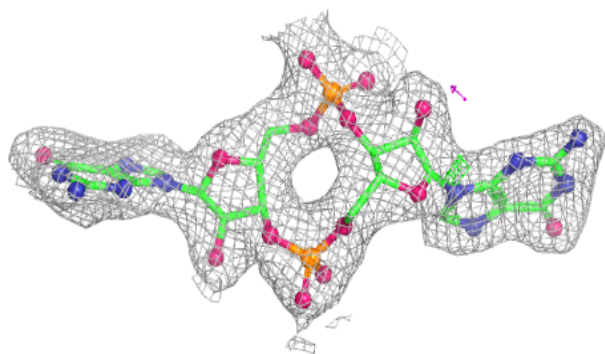
**Electron density around C2E B 501:**

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



Electron density around C2E 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.