



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:53 AM UTC

PDB ID : 3EYW / pdb_00003eyw
Title : Crystal structure of the C-terminal domain of E. coli KefC in complex with KefF
Authors : Roosild, T.P.
Deposited on : 2008-10-22
Resolution : 2.40 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

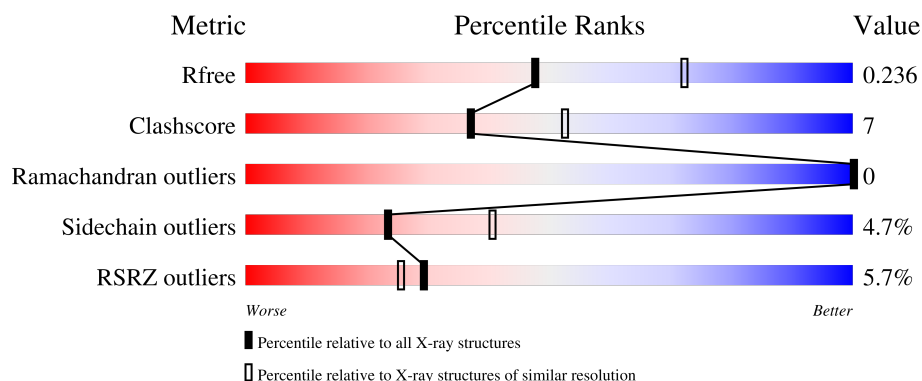
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	5% 69% 12% • 18%
1	B	413	4% 69% 14% • 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5823 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 C-terminal domain of Glutathione-regulated potassium-efflux system protein kefC fused to full length Glutathione-regulated potassium-efflux system ancillary protein kefF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2708	1733	479	481	15			
1	B	352	Total	C	N	O	S	0	0	0
			2823	1802	503	503	15			

There are 34 discrepancies between the modelled and reference sequences:

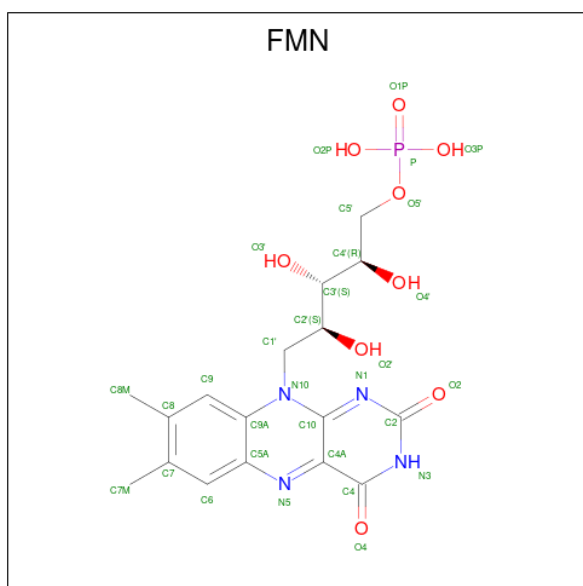
Chain	Residue	Modelled	Actual	Comment	Reference
A	396	GLY	-	expression tag	UNP P03819
A	397	SER	-	expression tag	UNP P03819
A	398	HIS	-	expression tag	UNP P03819
A	399	GLY	-	expression tag	UNP P03819
A	400	MET	-	expression tag	UNP P03819
A	621	THR	-	linker	UNP P03819
A	622	SER	-	linker	UNP P03819
A	623	GLY	-	linker	UNP P03819
A	624	GLY	-	linker	UNP P03819
A	625	LEU	-	linker	UNP P03819
A	626	VAL	-	linker	UNP P03819
A	627	PRO	-	linker	UNP P03819
A	628	ARG	-	linker	UNP P03819
A	629	GLY	-	linker	UNP P03819
A	630	SER	-	linker	UNP P03819
A	631	SER	-	linker	UNP P03819
A	632	GLY	-	linker	UNP P03819
B	396	GLY	-	expression tag	UNP P03819
B	397	SER	-	expression tag	UNP P03819
B	398	HIS	-	expression tag	UNP P03819
B	399	GLY	-	expression tag	UNP P03819
B	400	MET	-	expression tag	UNP P03819
B	621	THR	-	linker	UNP P03819

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Chain	Residue	Modelled	Actual	Comment	Reference
B	622	SER	-	linker	UNP P03819
B	623	GLY	-	linker	UNP P03819
B	624	GLY	-	linker	UNP P03819
B	625	LEU	-	linker	UNP P03819
B	626	VAL	-	linker	UNP P03819
B	627	PRO	-	linker	UNP P03819
B	628	ARG	-	linker	UNP P03819
B	629	GLY	-	linker	UNP P03819
B	630	SER	-	linker	UNP P03819
B	631	SER	-	linker	UNP P03819
B	632	GLY	-	linker	UNP P03819

- 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	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

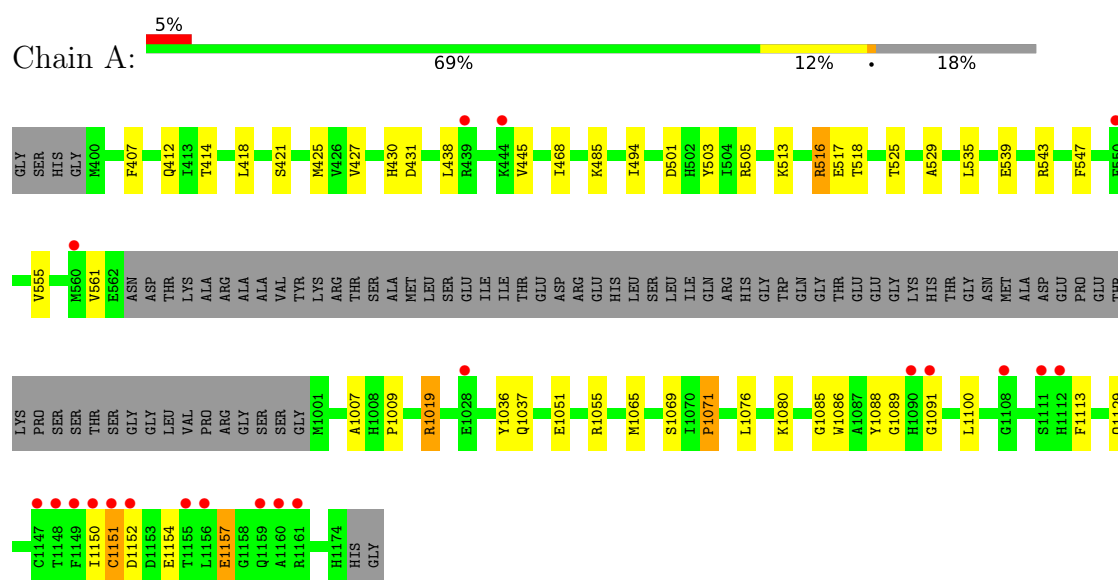
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total	O	0	0
			90	90		
6	B	91	Total	O	0	0
			91	91		

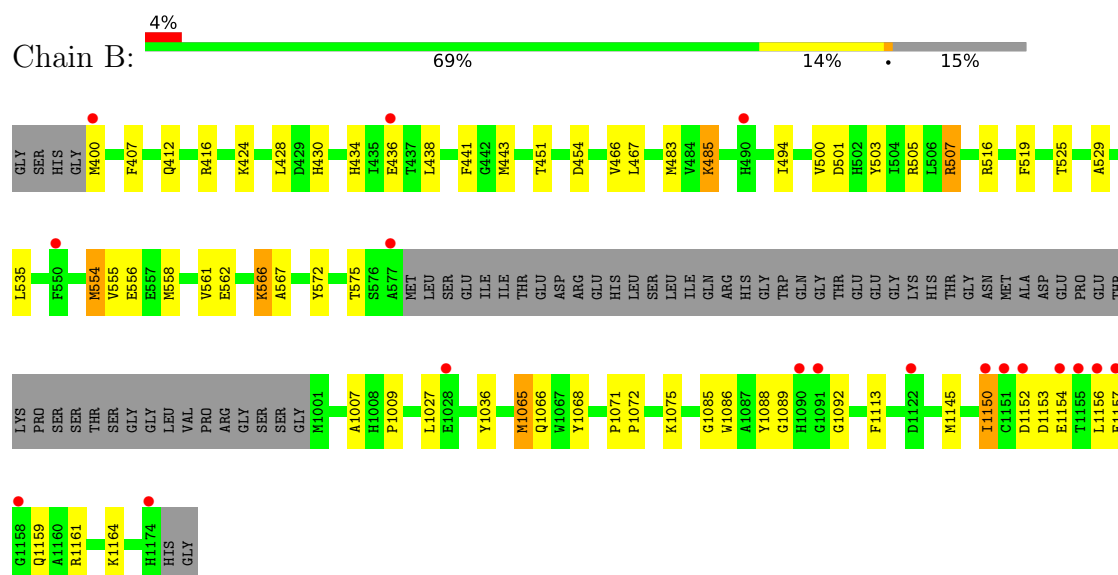
3 Residue-property plots [i](#)

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: C-terminal domain of Glutathione-regulated potassium-efflux system protein kefC fused to full length Glutathione-regulated potassium-efflux system ancillary protein kefF



- Molecule 1: C-terminal domain of Glutathione-regulated potassium-efflux system protein kefC fused to full length Glutathione-regulated potassium-efflux system ancillary protein kefF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.47Å 85.02Å 188.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.40) 99.6 (50.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.97 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.239 0.196 , 0.236	Depositor DCC
R_{free} test set	2074 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	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	0.94	EDS
Total number of atoms	5823	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 4.19% 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: ZN, NAD, MG, 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	0.77	1/2779 (0.0%)	0.95	4/3763 (0.1%)
1	B	0.75	0/2895	0.97	2/3919 (0.1%)
All	All	0.76	1/5674 (0.0%)	0.96	6/7682 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	ASP	C-O	-5.03	1.20	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1151	CYS	N-CA-C	7.40	118.36	108.38
1	B	1086	TRP	N-CA-C	-6.97	104.76	113.55
1	A	1071	PRO	CA-C-N	5.53	125.63	119.32
1	A	1071	PRO	C-N-CA	5.53	125.63	119.32
1	B	519	PHE	N-CA-C	5.34	116.79	110.97
1	A	1086	TRP	N-CA-C	-5.23	106.02	112.72

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	2708	0	2659	33	0
1	B	2823	0	2778	53	0
2	A	31	0	19	1	0
2	B	31	0	19	1	0
3	A	23	0	12	0	0
3	B	23	0	12	1	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	90	0	0	4	0
6	B	91	0	0	3	0
All	All	5823	0	5499	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (79) 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:B:441:PHE:HB2	1:B:443:MET:HE2	1.27	1.08
1:A:1065:MET:HE1	1:A:1113:PHE:HE2	1.18	1.06
1:A:1065:MET:HE1	1:A:1113:PHE:CE2	1.99	0.97
1:B:1065:MET:HE1	1:B:1113:PHE:HE2	1.32	0.93
1:B:1065:MET:HE1	1:B:1113:PHE:CE2	2.02	0.93
1:A:1037:GLN:HG3	6:A:82:HOH:O	1.67	0.91
1:B:558:MET:HE2	1:B:572:TYR:HB2	1.55	0.88
1:B:1065:MET:CE	1:B:1113:PHE:HE2	1.89	0.86
1:B:1065:MET:HE3	1:B:1068:TYR:HA	1.59	0.85
1:B:554:MET:SD	1:B:572:TYR:CD1	2.76	0.78
1:B:554:MET:SD	1:B:572:TYR:HD1	2.07	0.78
1:B:558:MET:CE	1:B:572:TYR:HB2	2.15	0.75
1:B:1027:LEU:HD11	1:B:1164:LYS:HG3	1.68	0.74
1:A:1129:GLN:NE2	6:A:179:HOH:O	2.24	0.71
1:B:501:ASP:O	1:B:505:ARG:HG3	1.92	0.70
1:B:1157:GLU:O	1:B:1161:ARG:HG3	1.92	0.69
1:B:1065:MET:CE	1:B:1113:PHE:CE2	2.68	0.67
1:B:441:PHE:CB	1:B:443:MET:HE2	2.14	0.66
1:B:566:LYS:H	1:B:566:LYS:HE2	1.63	0.64
1:A:438:LEU:HD13	1:A:445:VAL:HG21	1.81	0.62
1:A:418:LEU:HB2	1:A:425:MET:HE1	1.81	0.61
1:B:1150:ILE:O	1:B:1150:ILE:HD12	2.01	0.61
1:B:451:THR:HB	1:B:483:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:MET:HE2	1:B:575:THR:HB	1.87	0.56
1:B:1085:GLY:HA2	1:B:1088:TYR:O	2.07	0.55
1:A:1065:MET:HE2	2:A:2400:FMN:N3	2.21	0.55
1:A:516:ARG:HD3	6:A:134:HOH:O	2.05	0.55
1:B:428:LEU:HD12	1:B:428:LEU:N	2.22	0.55
1:A:407:PHE:CG	1:A:427:VAL:HG11	2.42	0.54
1:B:1009:PRO:HA	1:B:1036:TYR:CG	2.42	0.54
1:B:438:LEU:HD23	1:B:443:MET:HE3	1.90	0.54
1:A:494:ILE:HG22	1:B:525:THR:HG23	1.90	0.53
1:A:414:THR:HG21	1:A:468:ILE:HD13	1.91	0.53
1:B:407:PHE:CE1	1:B:412:GLN:HG2	2.44	0.53
1:B:466:VAL:HG13	1:B:494:ILE:HD12	1.91	0.52
1:B:1152:ASP:HB3	1:B:1154:GLU:HG2	1.91	0.52
1:A:414:THR:CG2	1:A:468:ILE:HD13	2.40	0.51
1:B:507:ARG:HD3	1:B:556:GLU:OE2	2.10	0.51
1:B:1065:MET:CE	1:B:1068:TYR:HA	2.34	0.51
1:B:561:VAL:HG12	1:B:562:GLU:N	2.26	0.51
1:A:1085:GLY:HA2	1:A:1088:TYR:O	2.11	0.50
1:A:1051:GLU:OE1	1:A:1055:ARG:NH1	2.45	0.50
1:A:1069:SER:HB3	1:B:1075:LYS:HE3	1.94	0.48
1:B:1089:GLY:O	1:B:1092:GLY:HA3	2.13	0.48
1:B:500:VAL:HG23	6:B:10:HOH:O	2.13	0.47
1:A:529:ALA:HA	1:B:494:ILE:HD13	1.97	0.47
1:A:1152:ASP:C	1:A:1154:GLU:H	2.23	0.47
1:A:525:THR:HG23	1:B:494:ILE:HG22	1.98	0.46
1:A:1037:GLN:CG	6:A:82:HOH:O	2.43	0.46
1:A:1007:ALA:O	1:A:1071:PRO:HG2	2.16	0.46
1:B:1071:PRO:HA	1:B:1072:PRO:HD3	1.91	0.46
1:A:547:PHE:CE1	1:B:416:ARG:HG3	2.51	0.45
1:A:1009:PRO:HA	1:A:1036:TYR:CG	2.52	0.45
1:B:500:VAL:CG2	6:B:25:HOH:O	2.65	0.45
1:A:1089:GLY:O	1:A:1091:GLY:HA2	2.17	0.45
1:B:485:LYS:HD2	6:B:188:HOH:O	2.17	0.44
1:B:1145:MET:HE2	1:B:1159:GLN:CB	2.47	0.44
1:A:501:ASP:O	1:A:505:ARG:HG3	2.18	0.44
1:B:503:TYR:CE1	1:B:555:VAL:HG12	2.52	0.44
1:B:554:MET:CE	1:B:575:THR:HB	2.47	0.44
1:A:517:GLU:HG3	1:A:518:THR:HG23	2.00	0.43
1:B:483:MET:HE3	1:B:483:MET:HB2	1.89	0.43
1:A:1076:LEU:O	1:A:1080:LYS:HG2	2.18	0.43
1:B:434:HIS:HE1	3:B:2401:NAD:O3B	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:MET:HE3	1:B:443:MET:HB2	1.93	0.43
1:A:1019:ARG:NH1	1:A:1157:GLU:HG3	2.34	0.42
1:B:554:MET:HE3	1:B:554:MET:HB2	1.85	0.42
1:B:561:VAL:CG1	1:B:567:ALA:HB1	2.49	0.42
1:A:539:GLU:O	1:A:543:ARG:HG3	2.21	0.41
1:A:494:ILE:CG2	1:B:525:THR:HG23	2.50	0.41
1:A:503:TYR:CE1	1:A:555:VAL:HG12	2.55	0.41
1:A:494:ILE:CD1	1:B:529:ALA:HA	2.51	0.41
1:B:1066:GLN:HA	2:B:2400:FMN:C5A	2.51	0.41
1:B:1145:MET:HE2	1:B:1159:GLN:HB3	2.03	0.41
1:A:412:GLN:HG2	1:A:438:LEU:HD21	2.03	0.41
1:B:561:VAL:CG1	1:B:562:GLU:N	2.84	0.40
1:A:513:LYS:HB3	1:A:513:LYS:HE3	1.69	0.40
1:B:503:TYR:CE1	1:B:555:VAL:CG1	3.04	0.40
1:B:1007:ALA:O	1:B:1071:PRO:HG2	2.21	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	333/413 (81%)	323 (97%)	10 (3%)	0	100	100
1	B	348/413 (84%)	339 (97%)	9 (3%)	0	100	100
All	All	681/826 (82%)	662 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	280/340 (82%)	269 (96%)	11 (4%)	28	48
1	B	291/340 (86%)	275 (94%)	16 (6%)	19	34
All	All	571/680 (84%)	544 (95%)	27 (5%)	23	41

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	421	SER
1	A	430	HIS
1	A	485	LYS
1	A	516	ARG
1	A	535	LEU
1	A	561	VAL
1	A	1019	ARG
1	A	1100	LEU
1	A	1150	ILE
1	A	1151	CYS
1	A	1157	GLU
1	B	400	MET
1	B	424	LYS
1	B	430	HIS
1	B	436	GLU
1	B	454	ASP
1	B	467	LEU
1	B	485	LYS
1	B	507	ARG
1	B	516	ARG
1	B	535	LEU
1	B	554	MET
1	B	566	LYS
1	B	1065	MET
1	B	1150	ILE
1	B	1153	ASP
1	B	1156	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1062	GLN
1	A	1084	HIS
1	A	1138	ASN
1	B	1017	ASN
1	B	1062	GLN
1	B	1066	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 7 ligands modelled in this entry, 3 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	$\# Z > 2$
3	NAD	B	2401	-	25,25,48	1.26	4 (16%)	37,38,73	1.98	9 (24%)
3	NAD	A	2401	-	25,25,48	1.28	4 (16%)	37,38,73	1.98	8 (21%)
2	FMN	B	2400	-	33,33,33	1.06	2 (6%)	48,50,50	1.33	7 (14%)
2	FMN	A	2400	-	33,33,33	1.11	2 (6%)	48,50,50	1.36	8 (16%)

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	NAD	B	2401	-	-	1/10/26/62	0/3/3/5
3	NAD	A	2401	-	-	0/10/26/62	0/3/3/5
2	FMN	B	2400	-	-	0/18/18/18	0/3/3/3
2	FMN	A	2400	-	-	0/18/18/18	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2400	FMN	C4A-N5	3.93	1.39	1.30
2	A	2400	FMN	C4A-N5	3.70	1.38	1.30
3	A	2401	NAD	C2A-N3A	3.18	1.39	1.33
3	A	2401	NAD	C2A-N1A	3.18	1.39	1.33
3	B	2401	NAD	C2A-N1A	3.01	1.39	1.33
2	B	2400	FMN	C10-N1	2.83	1.38	1.33
2	A	2400	FMN	C10-N1	2.79	1.38	1.33
3	B	2401	NAD	C2A-N3A	2.53	1.38	1.33
3	A	2401	NAD	C8A-N7A	2.50	1.36	1.31
3	B	2401	NAD	PA-O2A	-2.07	1.47	1.54
3	B	2401	NAD	C8A-N7A	2.05	1.35	1.31
3	A	2401	NAD	PA-O2A	-2.02	1.47	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2401	NAD	N3A-C2A-N1A	-6.59	118.60	128.58
3	B	2401	NAD	N3A-C2A-N1A	-6.12	119.32	128.58
3	A	2401	NAD	N9A-C8A-N7A	-4.54	107.50	113.94
3	B	2401	NAD	N9A-C8A-N7A	-4.18	108.01	113.94
3	A	2401	NAD	C5A-C4A-N3A	-3.87	121.38	126.72
3	B	2401	NAD	C5A-C4A-N3A	-3.82	121.46	126.72
2	A	2400	FMN	C4A-C10-N10	3.62	121.66	116.48
3	B	2401	NAD	C5A-N7A-C8A	3.60	109.11	103.45
3	A	2401	NAD	C2A-N3A-C4A	3.42	120.17	111.83
3	B	2401	NAD	C2A-N3A-C4A	3.34	119.99	111.83
2	B	2400	FMN	C4A-C10-N10	3.17	121.01	116.48
2	B	2400	FMN	C4-C4A-N5	3.14	122.54	118.21
3	A	2401	NAD	C4A-N9A-C8A	3.08	108.98	105.74
2	A	2400	FMN	C4-N3-C2	-3.05	120.22	125.64
3	A	2401	NAD	C5A-N7A-C8A	3.01	108.18	103.45
2	B	2400	FMN	C10-C4A-N5	-2.88	118.93	124.81
3	B	2401	NAD	N3A-C4A-N9A	2.86	132.02	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2401	NAD	N3A-C4A-N9A	2.79	131.92	127.17
2	A	2400	FMN	C4A-C4-N3	2.77	120.30	113.25
3	B	2401	NAD	O2A-PA-O5B	2.73	113.78	106.67
2	B	2400	FMN	C4-N3-C2	-2.71	120.84	125.64
2	A	2400	FMN	C10-C4A-N5	-2.55	119.61	124.81
2	B	2400	FMN	C4A-C4-N3	2.49	119.60	113.25
3	B	2401	NAD	C4A-N9A-C8A	2.40	108.26	105.74
2	B	2400	FMN	C9A-C5A-N5	-2.36	119.95	122.45
2	B	2400	FMN	O2P-P-O5'	2.33	112.73	106.67
2	A	2400	FMN	O4-C4-C4A	-2.25	120.59	126.53
3	B	2401	NAD	C4A-C5A-N7A	-2.17	108.10	110.58
2	A	2400	FMN	C8M-C8-C9	-2.14	115.81	119.57
2	A	2400	FMN	C4-C4A-N5	2.05	121.04	118.21
2	A	2400	FMN	C4A-C10-N1	-2.04	119.60	124.59
3	A	2401	NAD	O5B-PA-O1A	2.02	111.90	106.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

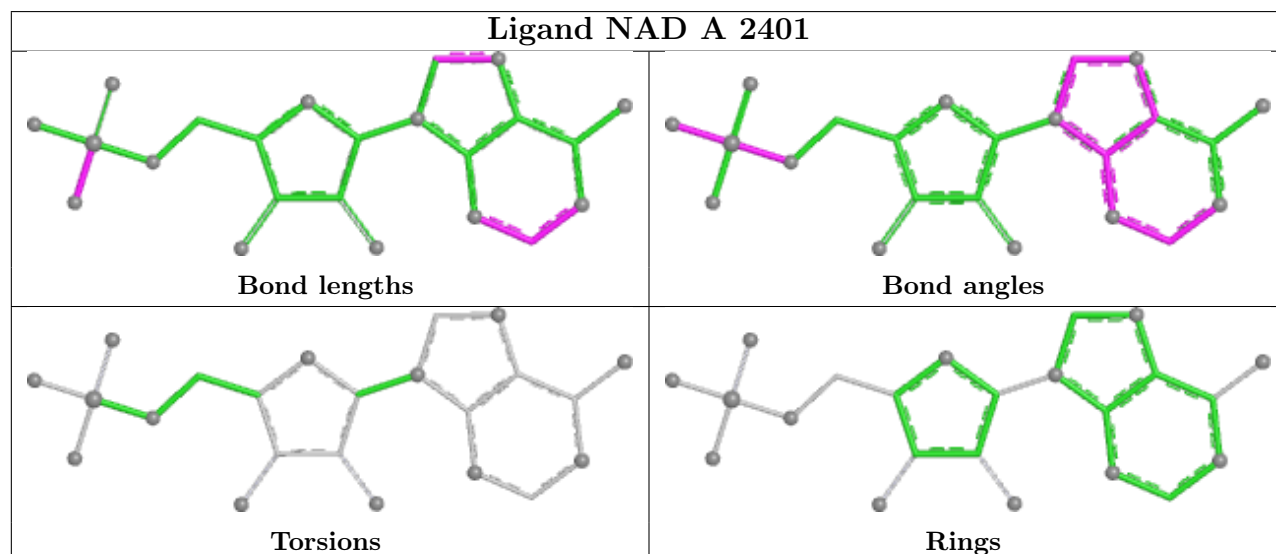
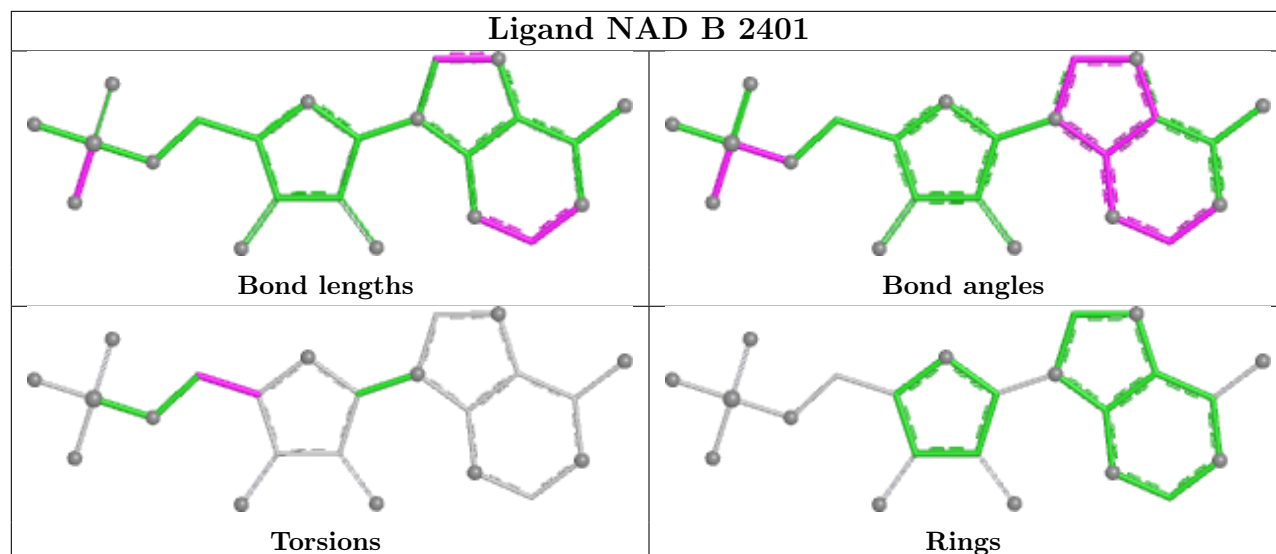
Mol	Chain	Res	Type	Atoms
3	B	2401	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

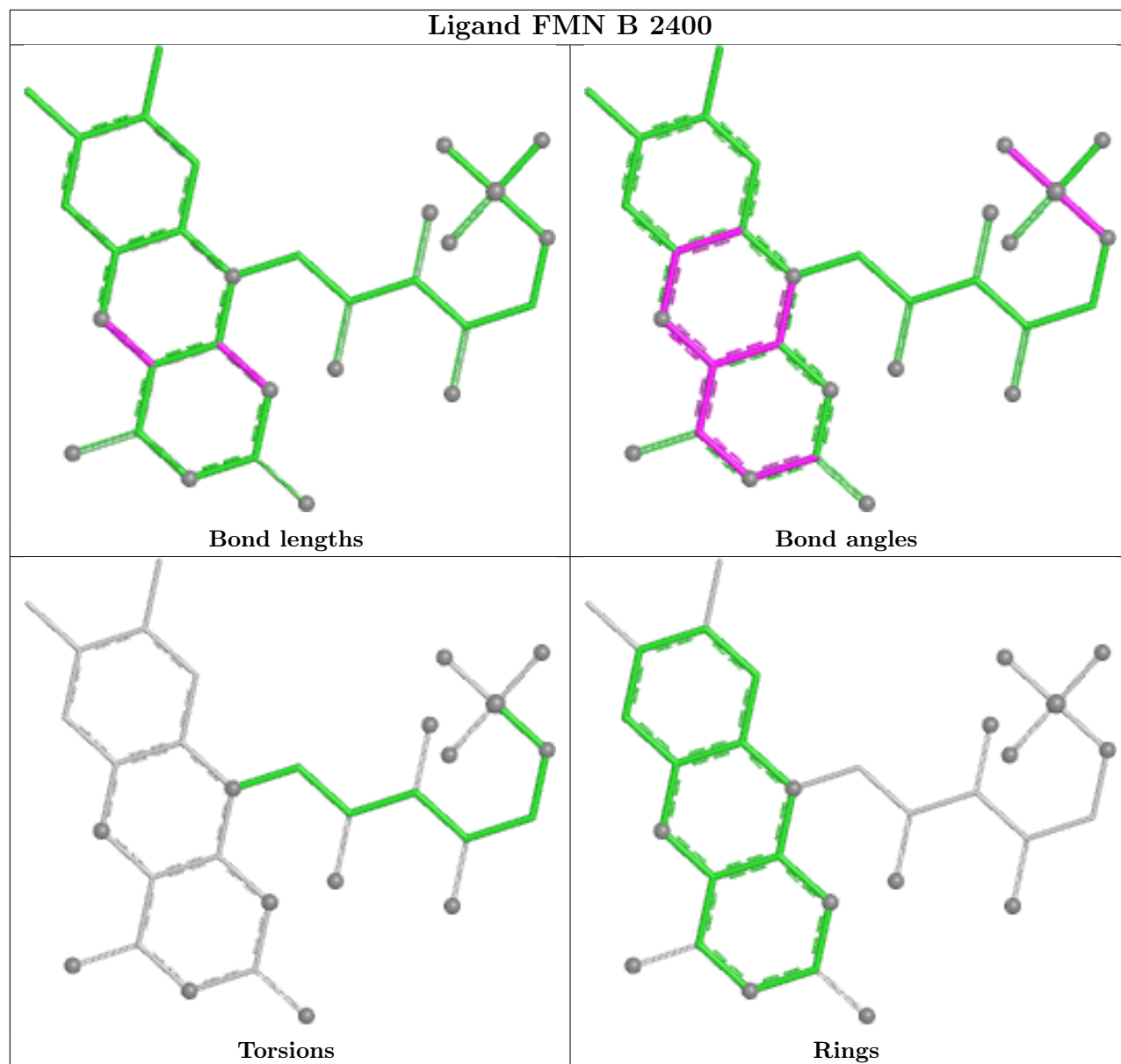
3 monomers are involved in 3 short contacts:

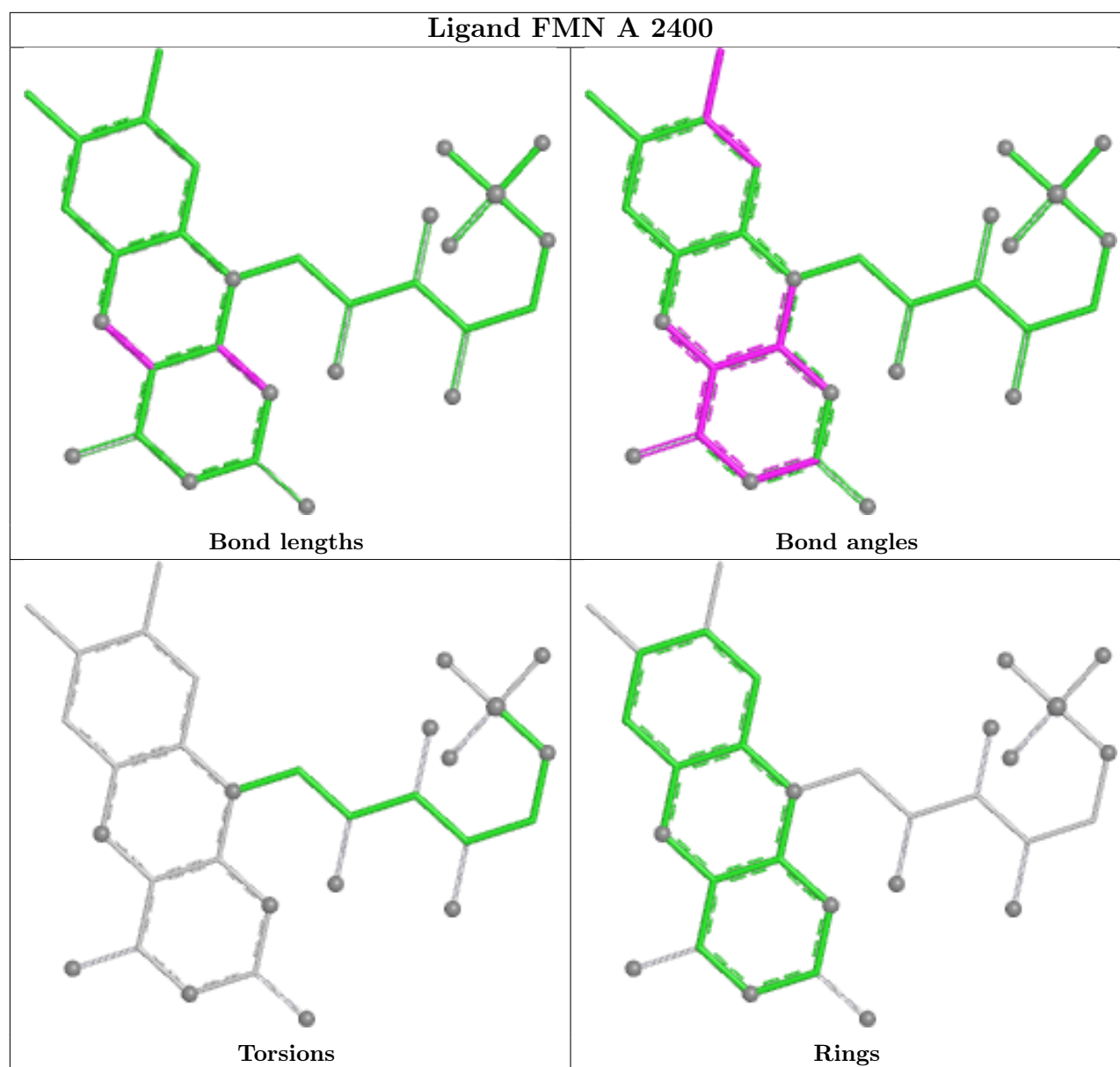
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2401	NAD	1	0
2	B	2400	FMN	1	0
2	A	2400	FMN	1	0

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.



Ligand FMN B 2400





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	337/413 (81%)	0.11	21 (6%) 26 23	14, 27, 56, 81	0
1	B	352/413 (85%)	-0.01	18 (5%) 33 30	12, 27, 54, 69	0
All	All	689/826 (83%)	0.05	39 (5%) 29 25	12, 27, 56, 81	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1151	CYS	5.5
1	A	1150	ILE	5.3
1	B	1151	CYS	4.8
1	A	1156	LEU	4.3
1	B	436	GLU	4.1
1	A	550	PHE	4.1
1	A	1147	CYS	3.3
1	A	1090	HIS	3.2
1	B	490	HIS	3.2
1	B	400	MET	3.2
1	A	1149	PHE	3.2
1	A	1028	GLU	3.2
1	B	1090	HIS	3.1
1	A	1155	THR	3.1
1	A	560	MET	3.0
1	A	1161	ARG	3.0
1	B	1122	ASP	3.0
1	A	444	LYS	3.0
1	A	1091	GLY	3.0
1	B	1174	HIS	3.0
1	A	1152	ASP	3.0
1	B	550	PHE	2.9
1	B	1155	THR	2.9
1	A	1159	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	439	ARG	2.7
1	B	1158	GLY	2.6
1	B	1156	LEU	2.5
1	B	1150	ILE	2.5
1	B	1028	GLU	2.5
1	B	1154	GLU	2.5
1	B	1157	GLU	2.5
1	B	1091	GLY	2.4
1	B	577	ALA	2.4
1	A	1112	HIS	2.3
1	A	1108	GLY	2.3
1	B	1152	ASP	2.2
1	A	1148	THR	2.1
1	A	1160	ALA	2.0
1	A	1111	SER	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](#)

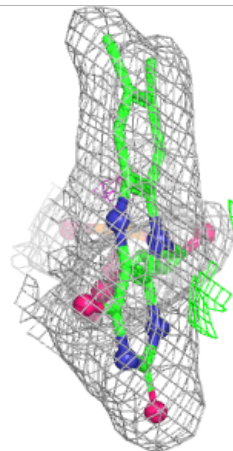
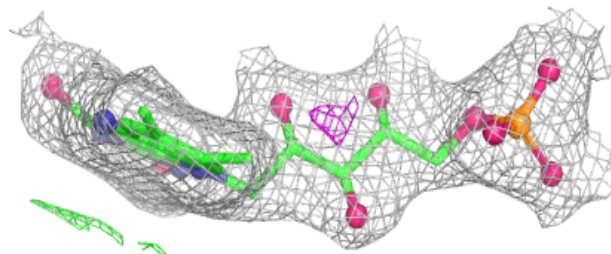
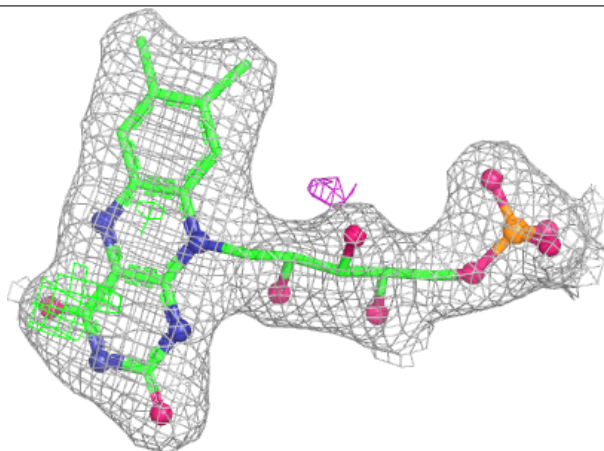
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	A	2400	31/31	0.97	0.06	19,22,25,27	0
3	NAD	A	2401	23/44	0.98	0.05	14,18,19,21	0
4	MG	A	2403	1/1	0.98	0.09	20,20,20,20	0
5	ZN	B	2402	1/1	0.98	0.25	52,52,52,52	0
2	FMN	B	2400	31/31	0.99	0.04	14,18,21,22	0
5	ZN	A	2402	1/1	0.99	0.19	52,52,52,52	0
3	NAD	B	2401	23/44	0.99	0.04	14,18,23,28	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.

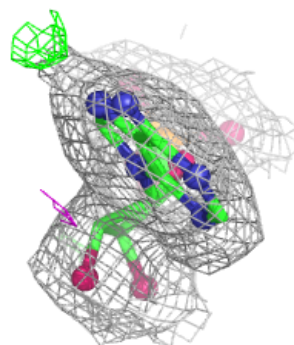
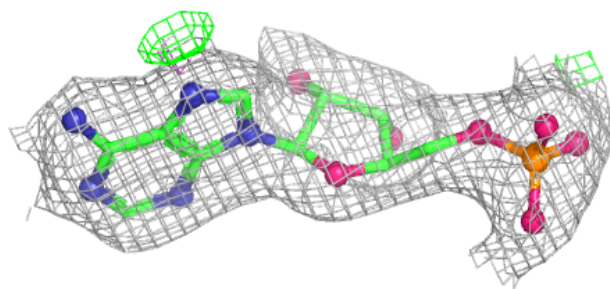
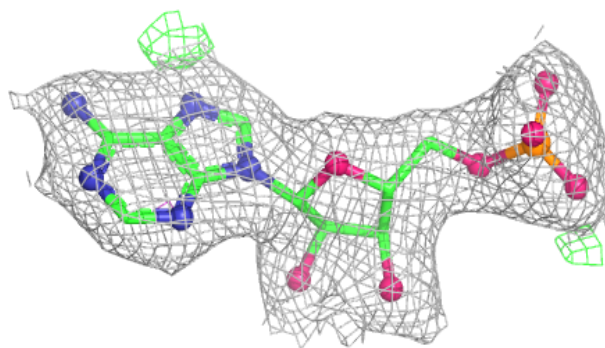
Electron density around FMN A 2400:

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



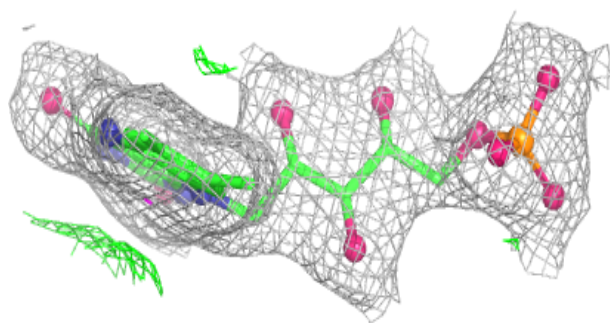
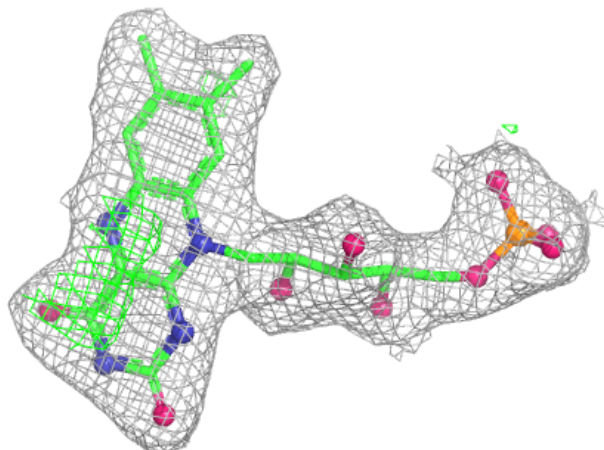
Electron density around NAD A 2401:

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



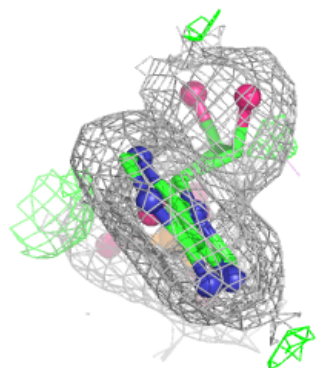
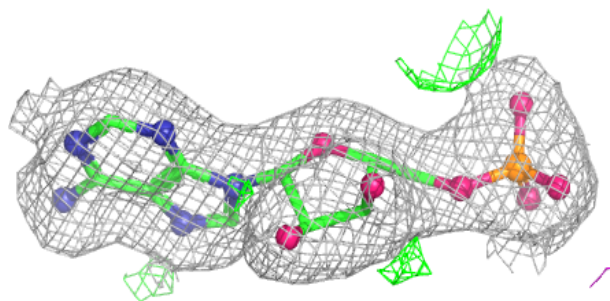
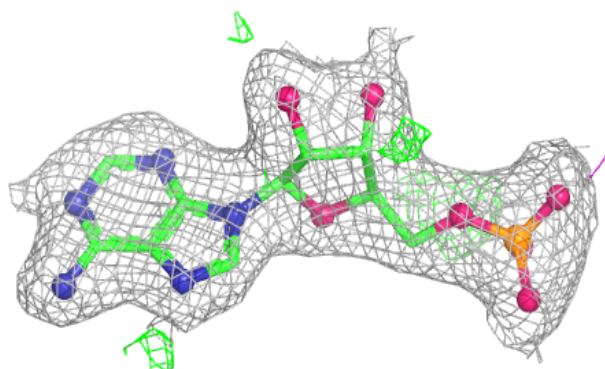
Electron density around FMN B 2400:

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



Electron density around NAD B 2401:

$2mF_o-DF_c$ (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.