



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:54 PM UTC

PDB ID : 8A52 / pdb_00008a52
Title : Crystal structure of a chimeric LOV-Histidine kinase SB2F1 (asymmetrical variant, trigonal form with long c-axis)
Authors : Batra-Safferling, R.; Arinkin, V.; Granzin, J.
Deposited on : 2022-06-14
Resolution : 2.46 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

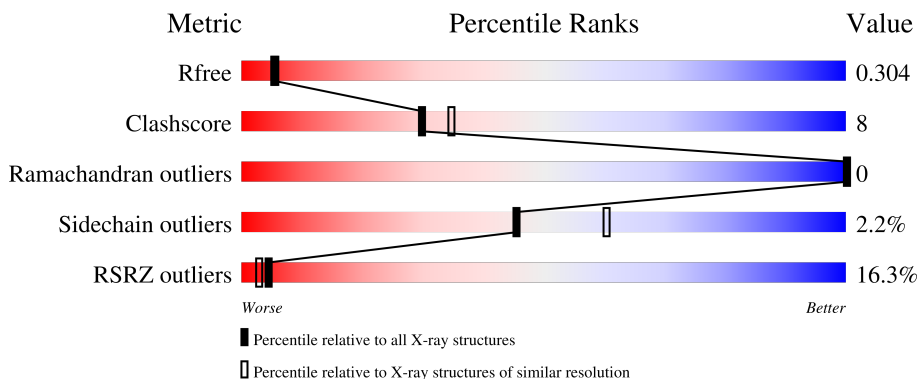
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	388	 14% 77% 15% • 6%
1	B	388	 16% 76% 17% • 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5784 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 Putative Sensory box protein,Putative Sensory box protein,Sensor protein FixL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	364	2830	1751	514	552	4	9	65	0	0
1	B	364	2830	1751	514	552	4	9	62	0	0

There are 40 discrepancies between the modelled and reference sequences:

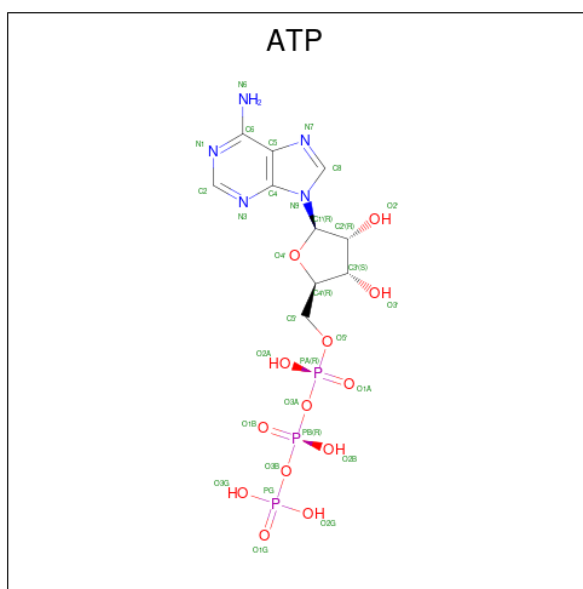
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	initiating methionine	UNP Q88JB0
A	-18	GLY	-	expression tag	UNP Q88JB0
A	-17	SER	-	expression tag	UNP Q88JB0
A	-16	SER	-	expression tag	UNP Q88JB0
A	-15	HIS	-	expression tag	UNP Q88JB0
A	-14	HIS	-	expression tag	UNP Q88JB0
A	-13	HIS	-	expression tag	UNP Q88JB0
A	-12	HIS	-	expression tag	UNP Q88JB0
A	-11	HIS	-	expression tag	UNP Q88JB0
A	-10	HIS	-	expression tag	UNP Q88JB0
A	-9	SER	-	expression tag	UNP Q88JB0
A	-8	SER	-	expression tag	UNP Q88JB0
A	-7	GLY	-	expression tag	UNP Q88JB0
A	-6	LEU	-	expression tag	UNP Q88JB0
A	-5	VAL	-	expression tag	UNP Q88JB0
A	-4	PRO	-	expression tag	UNP Q88JB0
A	-3	ARG	-	expression tag	UNP Q88JB0
A	-2	GLY	-	expression tag	UNP Q88JB0
A	-1	SER	-	expression tag	UNP Q88JB0
A	0	HIS	-	expression tag	UNP Q88JB0
B	-19	MSE	-	initiating methionine	UNP Q88JB0
B	-18	GLY	-	expression tag	UNP Q88JB0
B	-17	SER	-	expression tag	UNP Q88JB0
B	-16	SER	-	expression tag	UNP Q88JB0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q88JB0
B	-14	HIS	-	expression tag	UNP Q88JB0
B	-13	HIS	-	expression tag	UNP Q88JB0
B	-12	HIS	-	expression tag	UNP Q88JB0
B	-11	HIS	-	expression tag	UNP Q88JB0
B	-10	HIS	-	expression tag	UNP Q88JB0
B	-9	SER	-	expression tag	UNP Q88JB0
B	-8	SER	-	expression tag	UNP Q88JB0
B	-7	GLY	-	expression tag	UNP Q88JB0
B	-6	LEU	-	expression tag	UNP Q88JB0
B	-5	VAL	-	expression tag	UNP Q88JB0
B	-4	PRO	-	expression tag	UNP Q88JB0
B	-3	ARG	-	expression tag	UNP Q88JB0
B	-2	GLY	-	expression tag	UNP Q88JB0
B	-1	SER	-	expression tag	UNP Q88JB0
B	0	HIS	-	expression tag	UNP Q88JB0

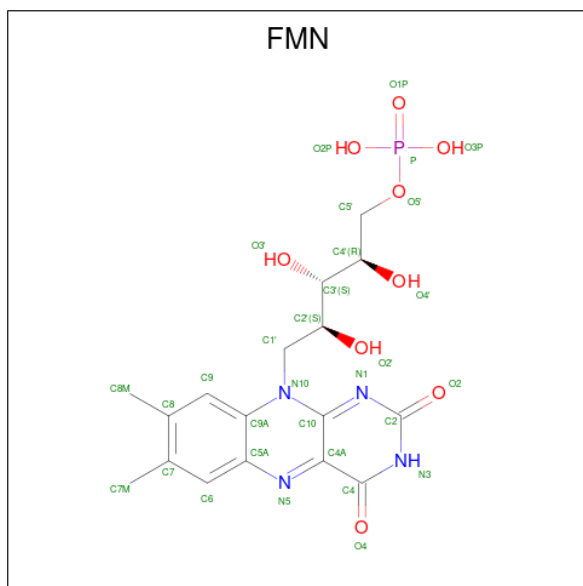
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$)

(labeled as "Ligand of Interest" by depositor).

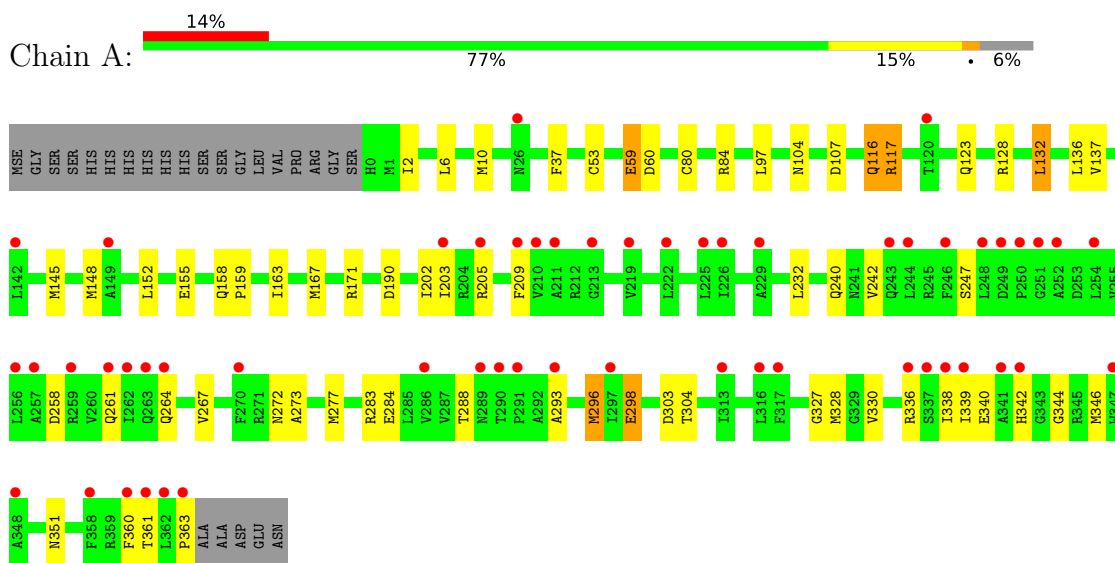


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

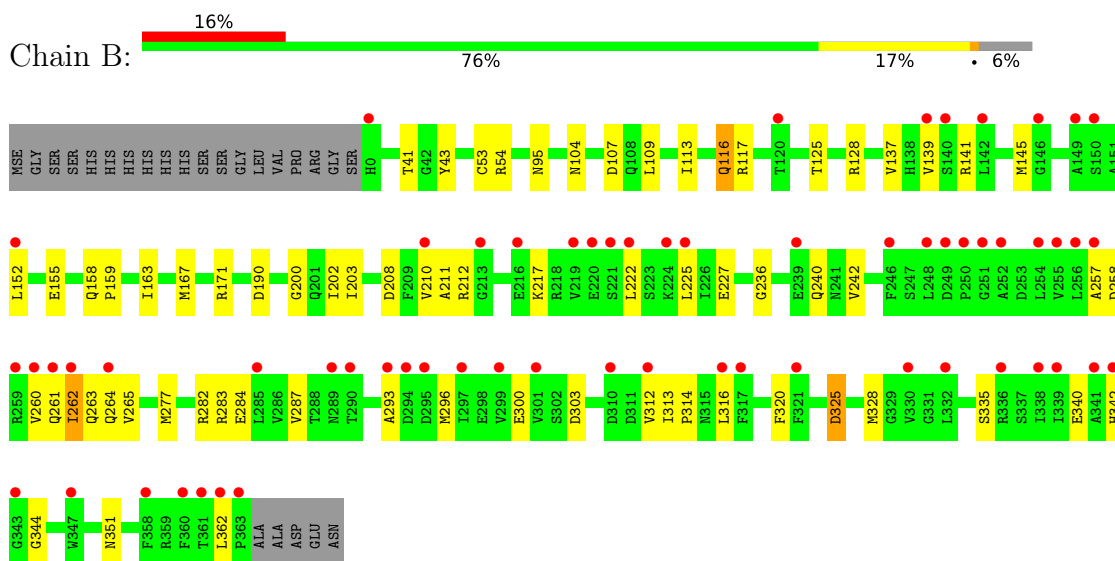
3 Residue-property plots [i](#)

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: Putative Sensory box protein,Putative Sensory box protein,Sensor protein FixL



- Molecule 1: Putative Sensory box protein,Putative Sensory box protein,Sensor protein FixL



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.25Å 138.25Å 94.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.25 – 2.46 45.25 – 2.46	Depositor EDS
% Data completeness (in resolution range)	71.3 (45.25-2.46) 71.3 (45.25-2.46)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.19rc6_4061	Depositor
R, R_{free}	0.243 , 0.295 0.251 , 0.304	Depositor DCC
R_{free} test set	1394 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5784	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: FMN, ATP

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	0.18	0/2862	0.43	0/3854
1	B	0.21	0/2862	0.46	0/3854
All	All	0.19	0/5724	0.44	0/7708

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2830	0	2791	56	0
1	B	2830	0	2791	54	0
2	A	31	0	12	2	0
2	B	31	0	12	0	0
3	A	31	0	19	0	0
3	B	31	0	19	1	0
All	All	5784	0	5644	94	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 8.

All (94) 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:148:MSE:HE2	1:B:145:MSE:HE2	1.62	0.81
1:A:277:MSE:HE1	1:A:284:GLU:H	1.52	0.73
1:A:277:MSE:HE3	1:A:304:THR:H	1.53	0.73
1:A:258:ASP:H	1:A:342:HIS:HE1	1.36	0.70
1:A:152:LEU:HD23	1:B:152:LEU:HD23	1.73	0.70
1:B:277:MSE:O	1:B:283:ARG:NH1	2.25	0.70
1:A:117:ARG:HE	1:B:117:ARG:CZ	2.06	0.68
1:A:136:LEU:HD21	1:A:267:VAL:HG11	1.77	0.66
1:A:171:ARG:NH1	1:A:190:ASP:OD1	2.30	0.65
1:B:171:ARG:NH1	1:B:190:ASP:OD1	2.31	0.64
1:A:298:GLU:HB2	1:A:361:THR:HG22	1.78	0.64
1:A:258:ASP:OD2	1:A:261:GLN:NE2	2.31	0.64
2:A:401:ATP:O1G	1:B:141:ARG:NH2	2.31	0.63
1:A:336:ARG:HD3	1:A:346:MSE:HB3	1.81	0.63
1:A:167:MSE:HE1	1:B:167:MSE:SE	2.50	0.62
1:B:41:THR:HG23	1:B:43:TYR:H	1.66	0.61
1:A:339:ILE:HG21	1:A:360:PHE:HB2	1.81	0.60
1:B:261:GLN:OE1	1:B:261:GLN:N	2.34	0.60
1:A:104:ASN:ND2	1:A:107:ASP:OD2	2.35	0.59
1:A:303:ASP:O	1:A:351:ASN:ND2	2.28	0.58
1:A:327:GLY:O	1:B:212:ARG:NH2	2.36	0.58
1:A:203:ILE:HG22	1:B:152:LEU:HD21	1.85	0.57
1:A:117:ARG:HH21	1:B:117:ARG:NH2	2.02	0.57
1:A:145:MSE:HE1	1:B:328:MSE:SE	2.54	0.57
1:B:208:ASP:HA	1:B:211:ALA:HB3	1.85	0.56
1:A:296:MSE:HE2	1:A:363:PRO:HB3	1.89	0.55
1:A:273:ALA:O	1:A:277:MSE:HG3	2.06	0.55
1:A:60:ASP:OD2	1:A:84:ARG:NE	2.32	0.55
1:A:136:LEU:HD22	1:A:232:LEU:HD13	1.88	0.54
1:A:258:ASP:H	1:A:342:HIS:CE1	2.23	0.54
1:A:128:ARG:O	1:A:132:LEU:HD23	2.08	0.54
1:B:240:GLN:HG3	1:B:242:VAL:HG23	1.88	0.54
1:B:303:ASP:O	1:B:351:ASN:ND2	2.37	0.54
1:A:2:ILE:HD11	1:A:6:LEU:HD23	1.90	0.53
1:A:117:ARG:HH21	1:B:117:ARG:HH21	1.57	0.53
1:B:225:LEU:HD11	1:B:263:GLN:HB2	1.92	0.52
1:A:240:GLN:HG3	1:A:242:VAL:HG23	1.91	0.52
1:A:202:ILE:HD13	1:B:155:GLU:HG2	1.91	0.51
1:A:137:VAL:HG22	1:B:137:VAL:HG22	1.92	0.51
1:B:261:GLN:O	1:B:264:GLN:HG2	2.11	0.51
1:B:163:ILE:O	1:B:167:MSE:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD21	1:B:362:LEU:HD12	1.93	0.50
1:B:293:ALA:HB3	1:B:296:MSE:HB2	1.94	0.50
1:B:236:GLY:O	1:B:240:GLN:HG2	2.12	0.49
1:B:217:LYS:HD3	1:B:258:ASP:HB2	1.95	0.49
1:B:312:VAL:C	1:B:314:PRO:HD2	2.37	0.49
1:A:37:PHE:HE1	1:A:116:GLN:HE21	1.60	0.49
1:A:261:GLN:OE1	1:A:261:GLN:N	2.44	0.48
1:A:328:MSE:HE1	1:B:210:VAL:HA	1.95	0.48
1:B:313:ILE:HA	1:B:316:LEU:HD12	1.96	0.48
1:A:59:GLU:H	1:A:59:GLU:CD	2.20	0.48
1:B:139:VAL:HG11	1:B:260:VAL:HG11	1.95	0.48
1:B:257:ALA:HA	1:B:342:HIS:HD2	1.79	0.47
1:A:155:GLU:HG2	1:B:202:ILE:HD13	1.96	0.47
1:B:258:ASP:H	1:B:342:HIS:CD2	2.33	0.47
1:A:293:ALA:HB3	1:A:296:MSE:HB2	1.96	0.47
1:B:258:ASP:O	1:B:262:ILE:HG22	2.14	0.47
1:A:117:ARG:HE	1:B:117:ARG:NH2	2.13	0.46
1:B:158:GLN:HB3	1:B:159:PRO:HD3	1.97	0.46
1:A:330:VAL:HG11	1:B:145:MSE:HE1	1.97	0.46
1:A:277:MSE:HE3	1:A:304:THR:N	2.26	0.46
1:A:205:ARG:O	1:A:205:ARG:NH1	2.49	0.45
1:A:158:GLN:HB3	1:A:159:PRO:HD3	1.98	0.45
1:A:277:MSE:HE2	1:A:283:ARG:HA	1.98	0.45
1:A:247:SER:O	1:A:288:THR:HA	2.17	0.45
1:B:139:VAL:HG11	1:B:260:VAL:CG1	2.47	0.45
1:A:277:MSE:CE	1:A:304:THR:H	2.25	0.45
1:A:298:GLU:HA	1:A:361:THR:HA	1.99	0.44
1:A:338:ILE:O	1:A:342:HIS:HD2	2.01	0.44
1:A:80:CYS:HA	1:A:97:LEU:O	2.18	0.44
1:B:296:MSE:HE2	1:B:344:GLY:HA2	1.99	0.44
1:B:325:ASP:OD1	1:B:325:ASP:N	2.44	0.44
1:A:205:ARG:HH22	1:A:209:PHE:HD1	1.66	0.43
1:A:261:GLN:O	1:A:264:GLN:HG2	2.18	0.43
1:B:225:LEU:HD21	1:B:263:GLN:N	2.33	0.43
1:B:287:VAL:HA	1:B:300:GLU:O	2.17	0.43
1:B:265:VAL:HG13	1:B:335:SER:OG	2.18	0.43
1:B:107:ASP:HB3	1:B:109:LEU:HB2	2.01	0.43
1:A:272:ASN:HB3	2:A:401:ATP:N7	2.34	0.43
1:B:104:ASN:ND2	1:B:107:ASP:OD2	2.52	0.42
1:B:54:ARG:NH2	3:B:402:FMN:O2P	2.45	0.42
1:B:282:ARG:HE	1:B:284:GLU:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:CG	1:A:84:ARG:HH21	2.26	0.42
1:B:125:THR:HG22	1:B:128:ARG:NH2	2.34	0.42
1:B:261:GLN:O	1:B:265:VAL:HG23	2.19	0.41
1:A:336:ARG:NE	1:A:346:MSE:O	2.54	0.41
1:A:340:GLU:HA	1:A:344:GLY:O	2.20	0.41
1:B:340:GLU:HA	1:B:344:GLY:O	2.21	0.41
1:B:200:GLY:O	1:B:203:ILE:HG13	2.21	0.41
1:A:10:MSE:HB3	1:B:113:ILE:HB	2.03	0.40
1:A:240:GLN:O	1:A:283:ARG:NH1	2.54	0.40
1:B:95:ASN:HD21	1:B:116:GLN:HE21	1.69	0.40
1:B:320:PHE:HA	1:B:328:MSE:O	2.21	0.40
1:A:163:ILE:O	1:A:167:MSE:HG2	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	362/388 (93%)	354 (98%)	8 (2%)	0	100	100
1	B	362/388 (93%)	351 (97%)	11 (3%)	0	100	100
All	All	724/776 (93%)	705 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	302/311 (97%)	294 (97%)	8 (3%)	40	55
1	B	302/311 (97%)	297 (98%)	5 (2%)	53	67
All	All	604/622 (97%)	591 (98%)	13 (2%)	45	60

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	59	GLU
1	A	116	GLN
1	A	117	ARG
1	A	123	GLN
1	A	132	LEU
1	A	296	MSE
1	A	298	GLU
1	B	53	CYS
1	B	116	GLN
1	B	227	GLU
1	B	262	ILE
1	B	325	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	116	GLN
1	A	157	ASN
1	A	158	GLN
1	A	342	HIS
1	B	116	GLN
1	B	130	GLN
1	B	157	ASN
1	B	158	GLN
1	B	263	GLN
1	B	268	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	FMN	A	402	-	33,33,33	0.82	0	48,50,50	0.65	0
2	ATP	B	401	-	32,33,33	0.61	1 (3%)	48,52,52	0.37	0
2	ATP	A	401	-	32,33,33	0.46	0	48,52,52	0.34	0
3	FMN	B	402	-	33,33,33	0.79	0	48,50,50	0.67	1 (2%)

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	FMN	A	402	-	-	3/18/18/18	0/3/3/3
2	ATP	B	401	-	-	1/22/38/38	0/3/3/3
2	ATP	A	401	-	-	1/22/38/38	0/3/3/3
3	FMN	B	402	-	-	3/18/18/18	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ATP	PB-O3B	-3.08	1.56	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	FMN	C4-N3-C2	-2.05	122.00	125.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

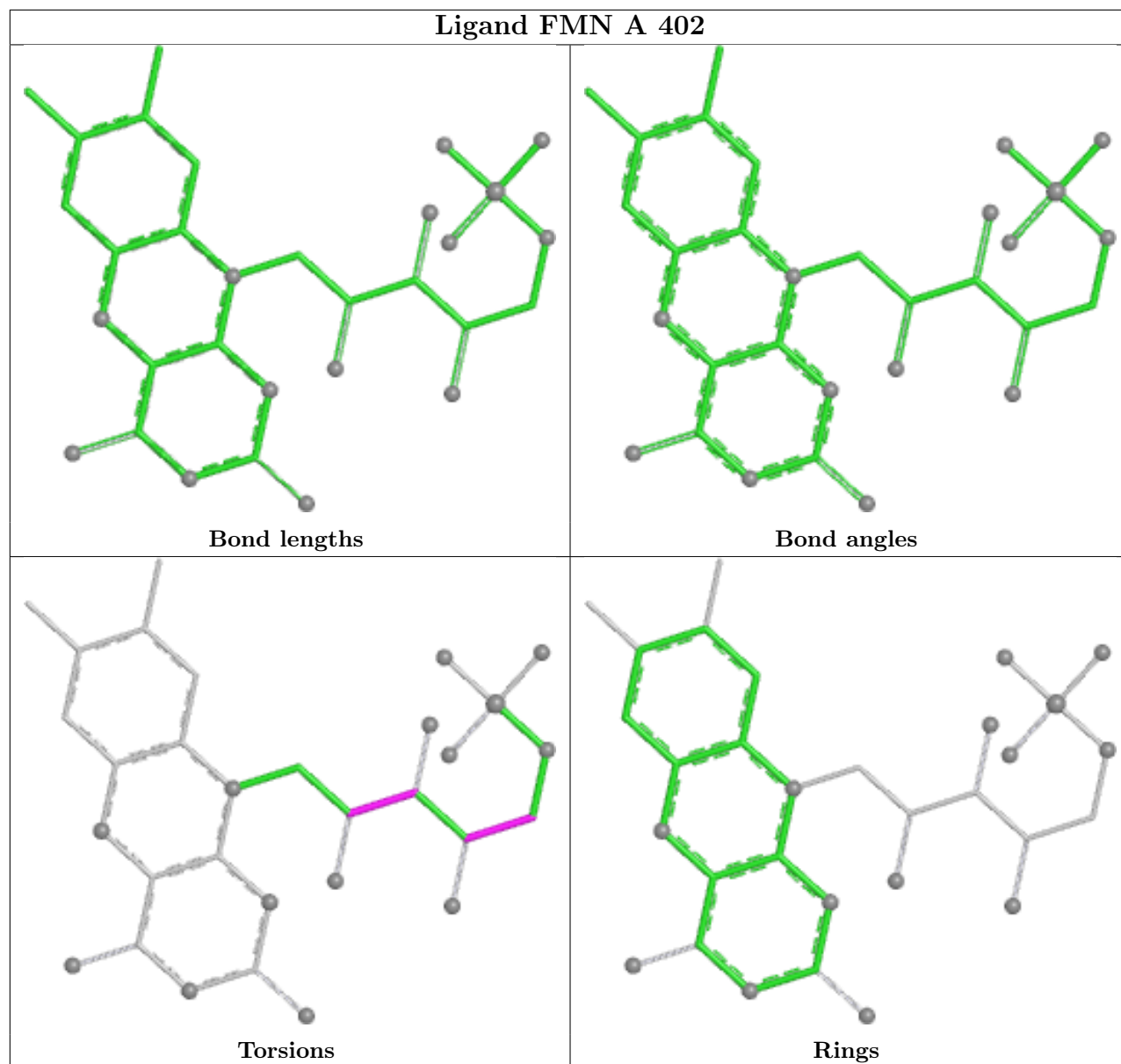
Mol	Chain	Res	Type	Atoms
3	A	402	FMN	C3'-C4'-C5'-O5'
3	A	402	FMN	O4'-C4'-C5'-O5'
3	B	402	FMN	C3'-C4'-C5'-O5'
2	A	401	ATP	PB-O3A-PA-O5'
2	B	401	ATP	PB-O3A-PA-O5'
3	B	402	FMN	O4'-C4'-C5'-O5'
3	B	402	FMN	C4'-C5'-O5'-P
3	A	402	FMN	C1'-C2'-C3'-C4'

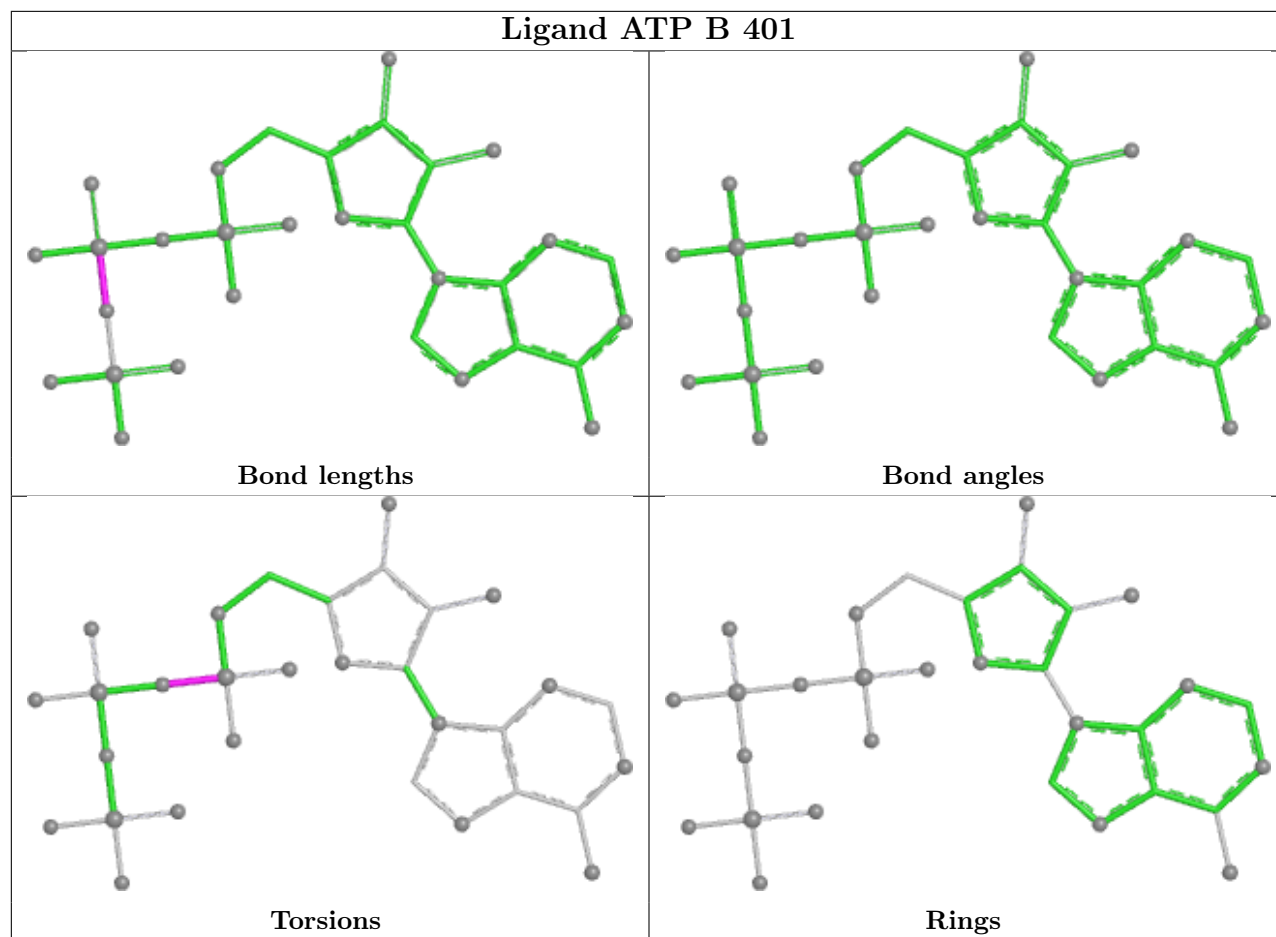
There are no ring outliers.

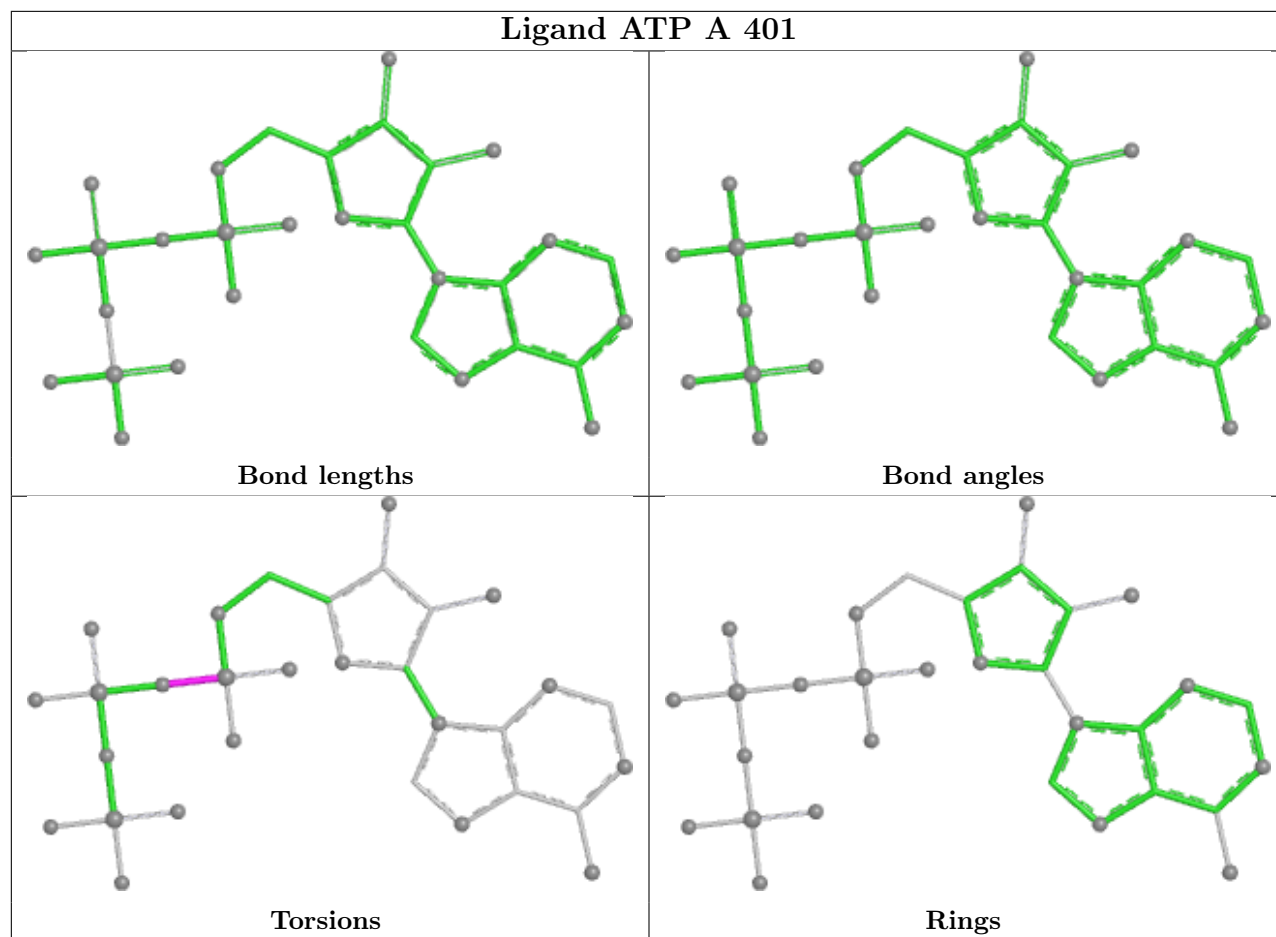
2 monomers are involved in 3 short contacts:

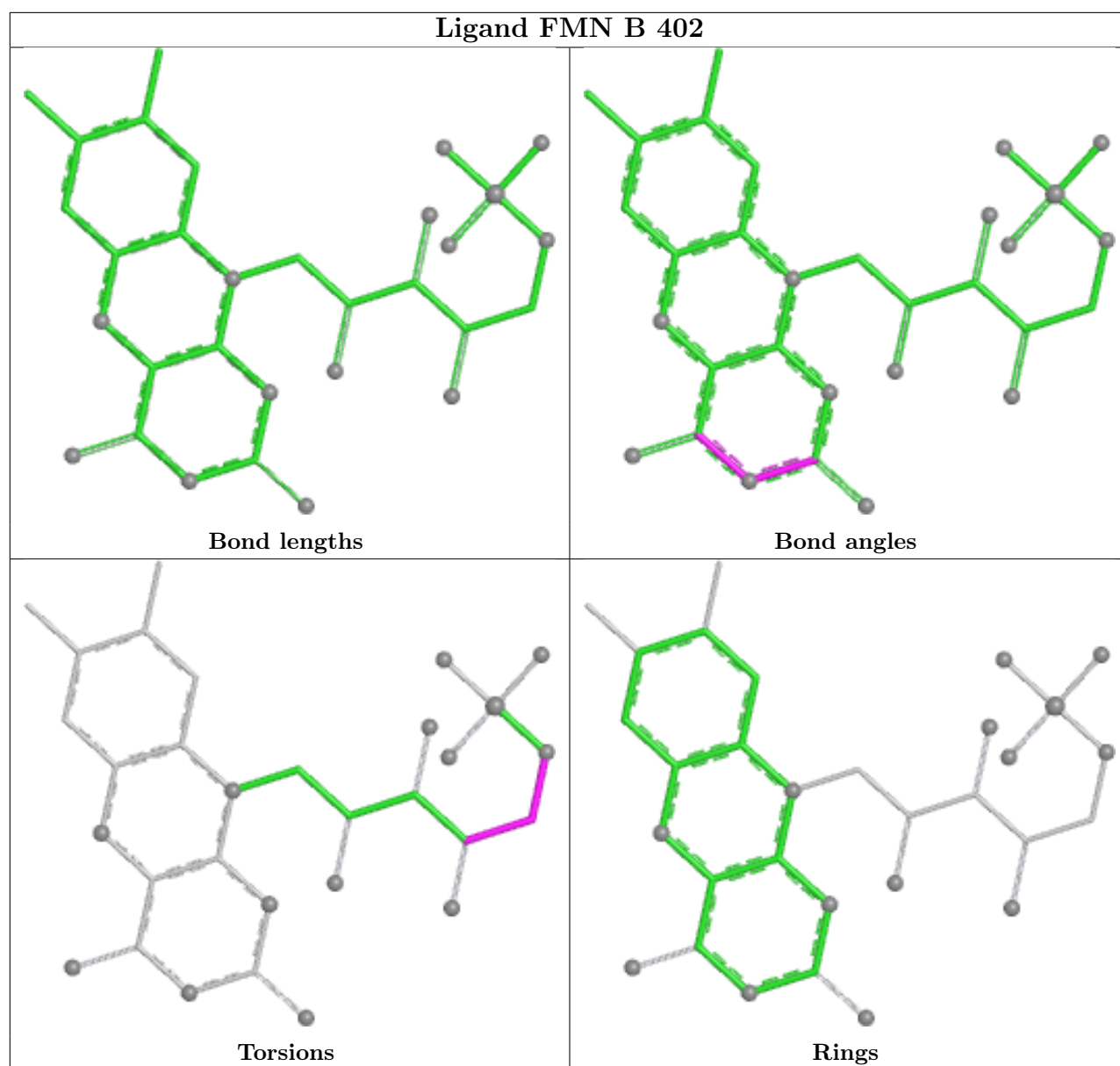
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ATP	2	0
3	B	402	FMN	1	0

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	355/388 (91%)	0.79	54 (15%) 5 4	34, 85, 174, 237	13 (3%)
1	B	355/388 (91%)	0.84	62 (17%) 4 3	31, 80, 139, 189	13 (3%)
All	All	710/776 (91%)	0.82	116 (16%) 4 3	31, 82, 162, 237	26 (3%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	VAL	6.7
1	B	339	ILE	6.1
1	A	203	ILE	5.9
1	B	255	VAL	5.4
1	A	362	LEU	4.9
1	B	257	ALA	4.8
1	B	262	ILE	4.6
1	B	222	LEU	4.4
1	A	210	VAL	4.4
1	A	219	VAL	4.3
1	B	360	PHE	4.2
1	A	252	ALA	4.2
1	B	342	HIS	4.2
1	A	262	ILE	4.1
1	B	256	LEU	4.1
1	B	149	ALA	4.0
1	B	362	LEU	4.0
1	B	250	PRO	3.8
1	A	254	LEU	3.8
1	A	317	PHE	3.8
1	A	251	GLY	3.6
1	A	289	ASN	3.6
1	B	140	SER	3.5
1	B	142	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	256	LEU	3.4
1	A	264	GLN	3.4
1	A	360	PHE	3.3
1	B	220	GLU	3.3
1	A	213	GLY	3.3
1	B	252	ALA	3.3
1	A	222	LEU	3.2
1	B	332	LEU	3.2
1	A	263	GLN	3.2
1	B	285	LEU	3.2
1	B	330	VAL	3.2
1	B	0	HIS	3.1
1	A	259	ARG	3.1
1	A	297	ILE	3.1
1	A	248	LEU	3.1
1	B	310	ASP	3.1
1	B	289	ASN	3.0
1	A	339	ILE	3.0
1	B	248	LEU	3.0
1	B	221	SER	3.0
1	B	338	ILE	3.0
1	A	211	ALA	3.0
1	A	291	PRO	3.0
1	B	317	PHE	3.0
1	A	361	THR	2.9
1	B	254	LEU	2.9
1	B	210	VAL	2.9
1	B	290	THR	2.9
1	A	209	PHE	2.9
1	B	297	ILE	2.9
1	B	336	ARG	2.9
1	A	257	ALA	2.9
1	A	341	ALA	2.8
1	A	290	THR	2.8
1	B	293	ALA	2.8
1	B	341	ALA	2.8
1	B	259	ARG	2.8
1	B	213	GLY	2.8
1	B	225	LEU	2.8
1	B	239	GLU	2.7
1	B	299	VAL	2.7
1	B	361	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	139	VAL	2.6
1	B	260	VAL	2.6
1	B	246	PHE	2.5
1	A	342	HIS	2.5
1	A	250	PRO	2.5
1	A	363	PRO	2.5
1	B	363	PRO	2.5
1	A	225	LEU	2.5
1	A	347	TRP	2.5
1	B	347	TRP	2.5
1	A	313	ILE	2.4
1	B	152	LEU	2.4
1	B	216	GLU	2.4
1	A	244	LEU	2.4
1	B	224	LYS	2.4
1	A	142	LEU	2.4
1	B	358	PHE	2.4
1	B	294	ASP	2.4
1	A	246	PHE	2.4
1	B	321	PHE	2.4
1	B	146	GLY	2.3
1	B	150	SER	2.3
1	B	251	GLY	2.3
1	B	249	ASP	2.3
1	A	120	THR	2.3
1	B	261	GLN	2.3
1	B	264	GLN	2.2
1	A	226	ILE	2.2
1	B	312	VAL	2.2
1	A	26	ASN	2.2
1	A	293	ALA	2.2
1	B	316	LEU	2.2
1	A	270	PHE	2.2
1	B	301	VAL	2.2
1	A	229	ALA	2.2
1	B	343	GLY	2.2
1	B	295	ASP	2.2
1	A	286	VAL	2.1
1	A	336	ARG	2.1
1	A	149	ALA	2.1
1	A	338	ILE	2.1
1	A	261	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	358	PHE	2.1
1	A	348	ALA	2.1
1	A	205	ARG	2.1
1	A	249	ASP	2.1
1	A	243	GLN	2.0
1	B	120	THR	2.0
1	A	337	SER	2.0
1	A	316	LEU	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](#)

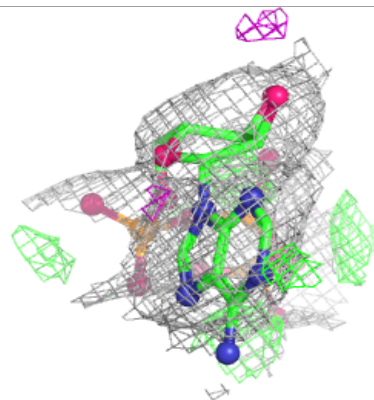
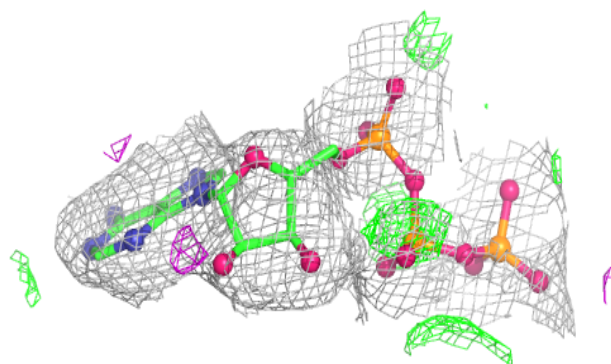
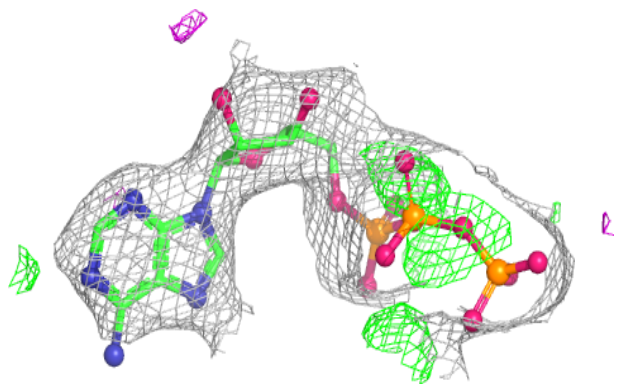
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ATP	B	401	31/31	0.91	0.11	93,96,114,116	0
2	ATP	A	401	31/31	0.95	0.08	76,90,104,119	0
3	FMN	A	402	31/31	0.96	0.07	57,58,67,74	0
3	FMN	B	402	31/31	0.96	0.06	47,51,67,73	0

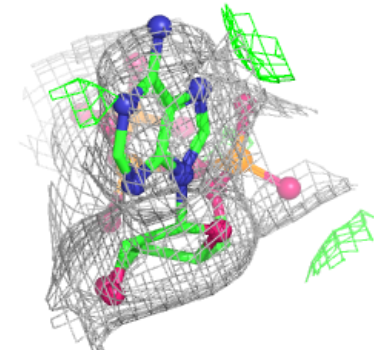
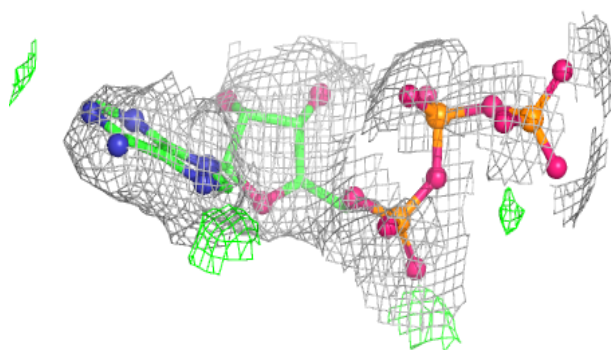
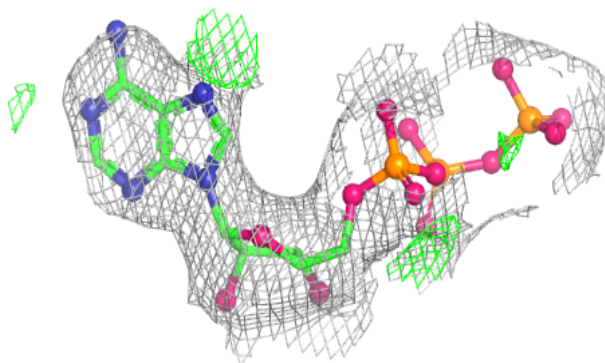
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 401:

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

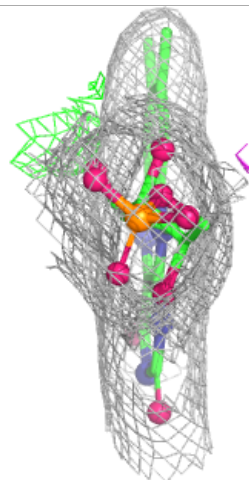
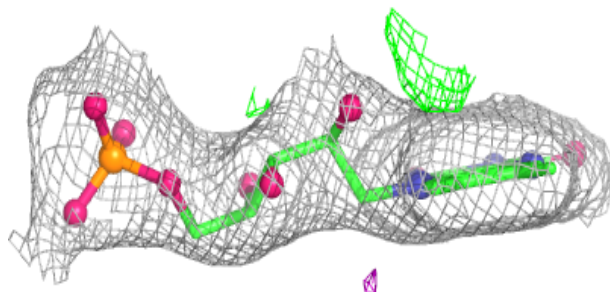
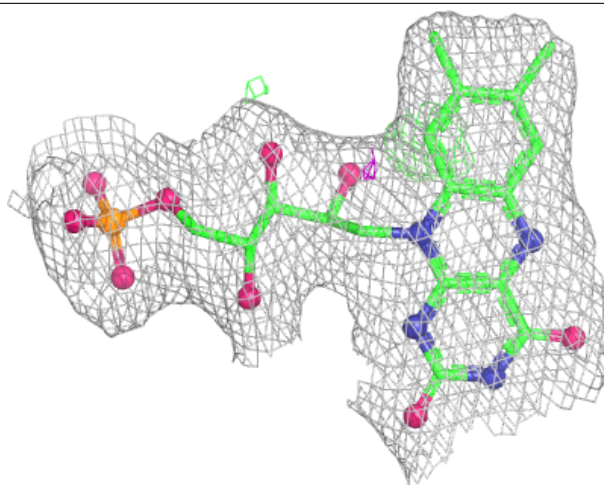
**Electron density around ATP A 401:**

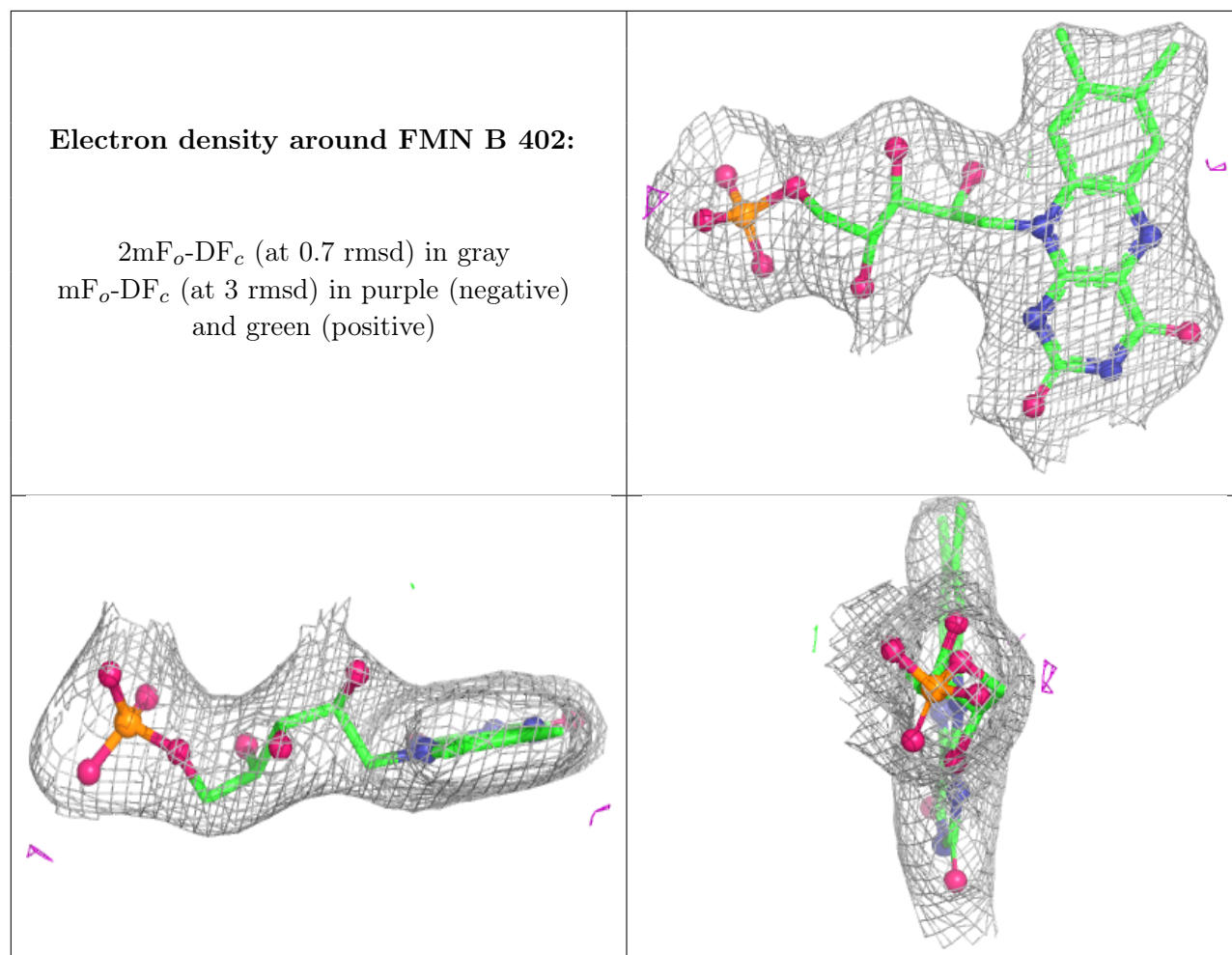
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN A 402:

$2mF_o-DF_c$ (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.