Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:04 am BST

PDB ID	:	6GRG
Title	:	E. coli Microcin synthetase McbBCD complex with pro-MccB17, ADP and phosphate bound
Authors	:	Ghilarov, D.; Stevenson, C.E.M.; Travin, D.Y.; Piskunova, J.; Serebryakova, M.; Maxwell, A.; Lawson, D.M.; Severinov, K.
Deposited on	:	2018-06-11
Resolution	:	2.35 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

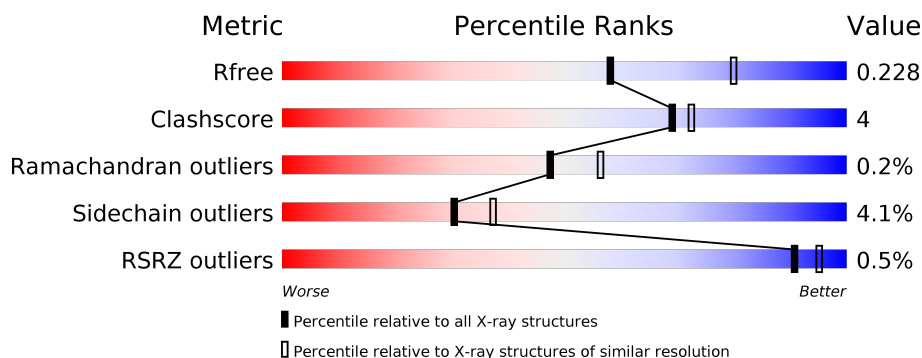|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	Percentile Ranks	Value
Rfree		0.228
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		4.1%
RSRZ outliers		0.5%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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 <=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	68	3% / 28% · 69%
2	1	295	83% 12% · ·
2	2	295	% 84% 11% · ·
3	C	272	90% 7% ·
4	D	396	84% 15% ·

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 10322 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 Bacteriocin microcin B17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	0	0	0
			149	93	26	30			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P05834
A	-6	GLY	-	expression tag	UNP P05834
A	-5	HIS	-	expression tag	UNP P05834
A	-4	HIS	-	expression tag	UNP P05834
A	-3	HIS	-	expression tag	UNP P05834
A	-2	HIS	-	expression tag	UNP P05834
A	-1	HIS	-	expression tag	UNP P05834
A	0	HIS	-	expression tag	UNP P05834
A	39	OTZ	GLY	modified residue	UNP P05834
A	39	OTZ	SER	modified residue	UNP P05834
A	39	OTZ	CYS	modified residue	UNP P05834
A	45	F75	GLY	modified residue	UNP P05834
A	45	F75	CYS	modified residue	UNP P05834
A	47	TOZ	GLY	modified residue	UNP P05834
A	47	TOZ	CYS	modified residue	UNP P05834
A	47	TOZ	SER	modified residue	UNP P05834
A	49	TOZ	GLY	modified residue	UNP P05834
A	49	TOZ	CYS	modified residue	UNP P05834
A	49	TOZ	SER	modified residue	UNP P05834
A	54	F6N	GLY	modified residue	UNP P05834
A	54	F6N	SER	modified residue	UNP P05834
A	56	F6N	GLY	modified residue	UNP P05834
A	56	F6N	SER	modified residue	UNP P05834

- Molecule 2 is a protein called Microcin B17-processing protein McbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	284	Total 2312	C 1482	N 390	O 428	S 12	0	4	0
2	2	282	Total 2247	C 1442	N 372	O 422	S 11	0	0	0

- Molecule 3 is a protein called Microcin B17-processing protein McbC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total 2110	C 1352	N 362	O 388	S 8	0	1	0

- Molecule 4 is a protein called Microcin B17-processing protein McbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	396	Total 3156	C 2015	N 520	O 603	S 18	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	171	ARG	THR	conflict	UNP P23186

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).
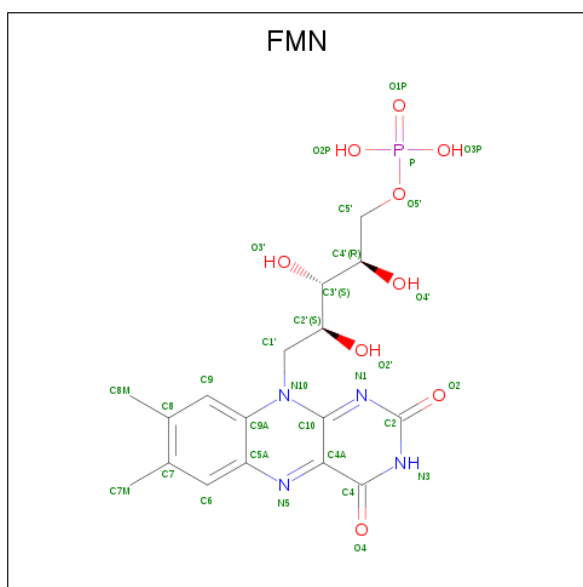
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 17	N 4	O 9	P 1	0	0

• Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	2	1	Total 1	Zn 1	0	0
6	1	1	Total 1	Zn 1	0	0

• Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O$_4$S).
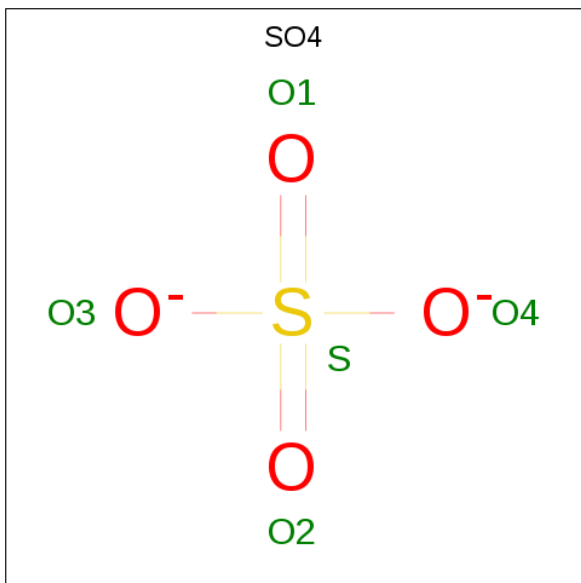
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	1	1	Total 5	O 4	S 1	0	0

• Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C$_3$H$_8$O$_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	1	1	Total 6	C 3	O 3	0	0

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

ATP
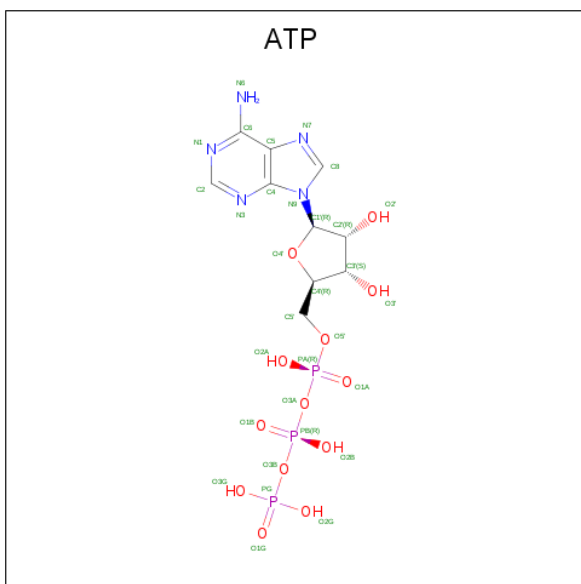
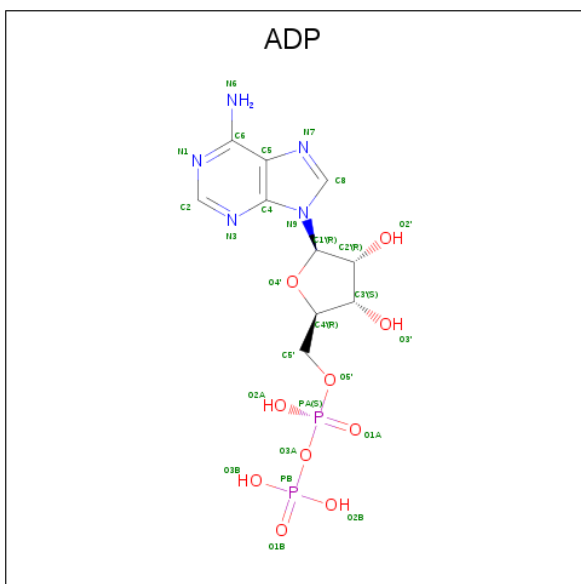| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	2	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1
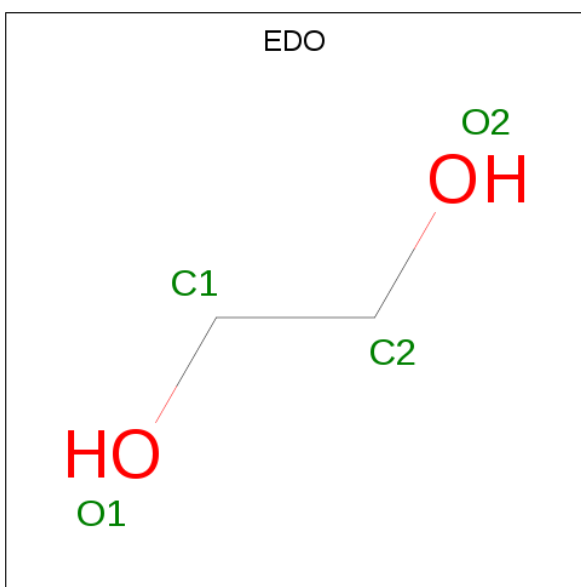
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	2	1	Total C O 4 2 2		0	0
10	D	1	Total C O 4 2 2		0	0

- Molecule 11 is A D E N O S I N E - 5 ' - D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
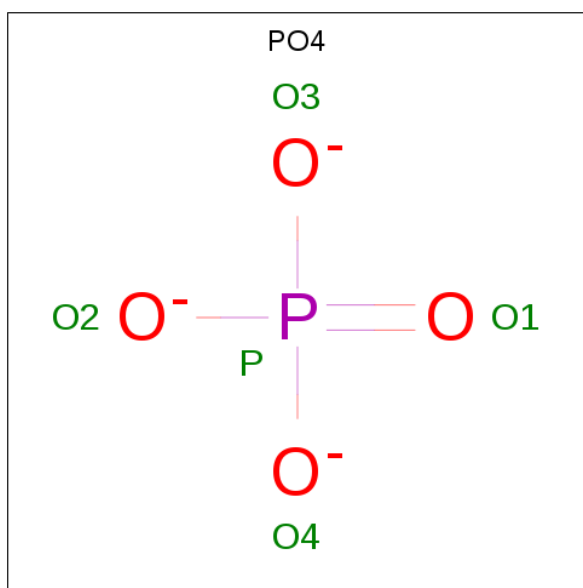
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	D	1	Total 5	O 4	P 1	0	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	3	Total 3	Mg 3	0	0

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	D	1	Total 1	Cl 1	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total 2	O 2	0	0
15	1	57	Total 58	O 58	0	1
15	2	56	Total 57	O 57	0	1
15	C	48	Total 49	O 49	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	63	Total O 63 63	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
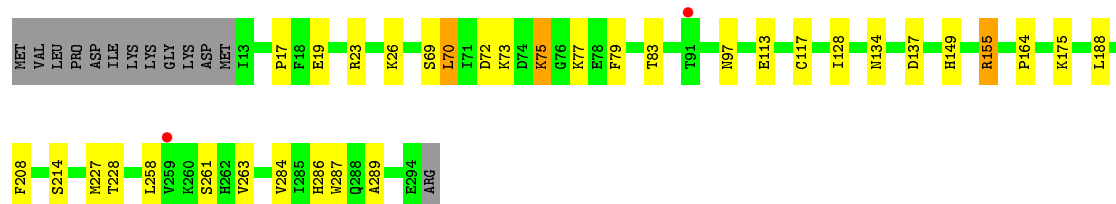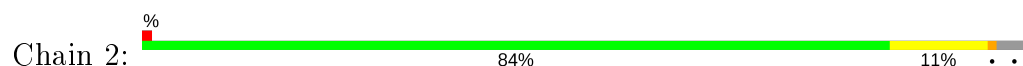
- Molecule 1: Bacteriocin microcin B17
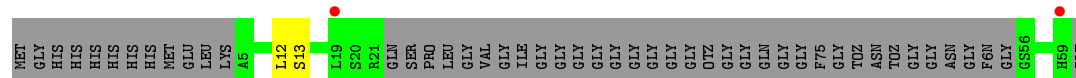
Chain A:

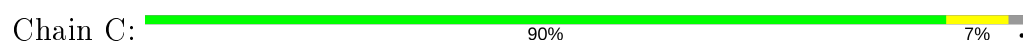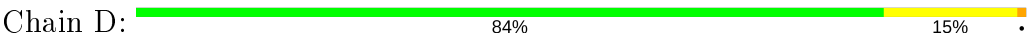- Molecule 2: Microcin B17-processing protein McbB

Chain 1:

- Molecule 2: Microcin B17-processing protein McbB

Chain 2:
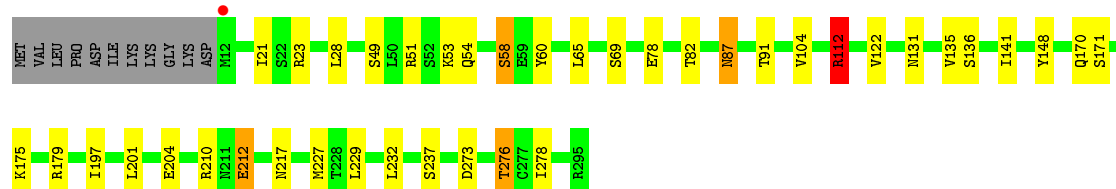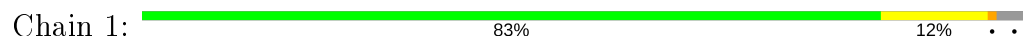
- Molecule 3: Microcin B17-processing protein McbC

Chain C:

- Molecule 4: Microcin B17-processing protein McbD

Chain D:

84% 15%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	180.64Å 83.28Å 86.79Å 90.00° 91.43° 90.00°	Depositor
Resolution (Å)	86.76 – 2.35 86.76 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (86.76-2.35) 99.9 (86.76-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.23 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.226 0.175 , 0.228	Depositor DCC
R_{free} test set	2683 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.0	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10322	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: GOL, MG, ADP, CL, PO4, ZN, F6N, FMN, SO4, ATP, EDO

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	0.57	0/139	0.73	0/184
2	1	0.56	0/2361	0.73	0/3194
2	2	0.55	0/2296	0.74	0/3116
3	C	0.54	0/2163	0.73	0/2935
4	D	0.53	0/3226	0.71	1/4373 (0.0%)
All	All	0.54	0/10185	0.73	1/13802 (0.0%)

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
2	1	0	3
3	C	0	1
4	D	0	3
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	346	ARG	NE-CZ-NH2	-5.76	117.42	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	112	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	1	23	ARG	Sidechain
2	1	51	ARG	Sidechain
3	C	205	ARG	Sidechain
4	D	100	ARG	Sidechain
4	D	206	ARG	Sidechain
4	D	72	GLY	Peptide

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	149	0	142	2	0
2	1	2312	0	2305	24	1
2	2	2247	0	2210	16	0
3	C	2110	0	2069	11	0
4	D	3156	0	3084	28	0
5	A	31	0	19	1	0
6	1	1	0	0	0	0
6	2	1	0	0	0	0
7	1	5	0	0	0	0
8	1	6	0	8	1	0
9	2	31	0	12	0	0
10	2	4	0	6	0	0
10	D	4	0	6	0	0
11	D	27	0	12	0	0
12	D	5	0	0	0	0
13	D	3	0	0	0	0
14	D	1	0	0	0	0
15	1	58	0	0	0	0
15	2	57	0	0	0	0
15	A	2	0	0	0	0
15	C	49	0	0	0	0
15	D	63	0	0	1	0
All	All	10322	0	9873	73	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (73) 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)
2:1:87:ASN:C	2:1:87:ASN:HD22	1.68	0.93
2:1:197:ILE:HD11	2:1:229:LEU:HD21	1.55	0.89
4:D:169:MET:CE	4:D:331:LEU:HD21	2.13	0.79
4:D:169:MET:HE2	4:D:331:LEU:HD21	1.68	0.75
2:1:87:ASN:C	2:1:87:ASN:ND2	2.44	0.68
2:2:149:HIS:HB2	2:2:228:THR:HG22	1.77	0.67
4:D:70:THR:HG21	4:D:109:LYS:HB3	1.79	0.63
2:1:78:GLU:O	2:1:82:THR:HG23	1.99	0.62
2:1:49:SER:HB3	2:1:65:LEU:HD21	1.84	0.60
2:1:53[B]:LYS:O	2:1:54[B]:GLN:HB2	2.04	0.57
2:2:69:SER:C	2:2:70:LEU:HD12	2.26	0.56
4:D:215:ASP:OD1	4:D:217:THR:OG1	2.20	0.55
4:D:284:ASP:C	4:D:284:ASP:OD1	2.46	0.54
2:2:79:PHE:CE1	2:2:83:THR:HG21	2.44	0.53
2:2:17:PRO:HB2	4:D:351:LEU:HG	1.91	0.53
4:D:169:MET:HE1	4:D:331:LEU:HD21	1.90	0.53
2:1:112:ARG:HG3	2:1:122:VAL:O	2.09	0.52
4:D:212:ARG:HG3	4:D:303:CYS:SG	2.50	0.51
3:C:117[A]:ARG:HB3	3:C:117[A]:ARG:CZ	2.41	0.50
2:1:273:ASP:HB3	2:1:276:THR:HG22	1.94	0.49
4:D:169:MET:HE3	4:D:331:LEU:HD11	1.94	0.49
4:D:231:GLY:HA2	4:D:240:LYS:O	2.12	0.49
2:1:212:GLU:O	2:1:217:ASN:ND2	2.46	0.49
2:1:276:THR:HG22	2:1:278:ILE:H	1.77	0.48
2:2:128:ILE:O	2:2:155:ARG:NH2	2.46	0.48
2:1:104:VAL:HG23	2:1:104:VAL:O	2.14	0.47
2:2:137:ASP:OD1	2:2:164:PRO:HD2	2.14	0.47
4:D:95:ILE:O	4:D:371:ALA:HB1	2.15	0.47
3:C:88:ASN:HA	3:C:182:LEU:O	2.15	0.47
2:2:286:HIS:HD2	4:D:346:ARG:HB3	1.79	0.46
2:2:19:GLU:HG3	4:D:353:TRP:CZ2	2.50	0.46
4:D:175:LEU:HD11	4:D:366:MET:HA	1.97	0.46
4:D:224:HIS:O	4:D:247:TYR:HA	2.14	0.46
3:C:88:ASN:HA	3:C:182:LEU:C	2.36	0.46
2:2:287:TRP:CE2	2:2:289:ALA:HB3	2.51	0.46
2:1:197:ILE:HD11	2:1:229:LEU:HD11	1.98	0.46
2:2:72:ASP:OD2	2:2:75:LYS:HB2	2.16	0.45
1:A:13:SER:HB3	2:2:214:SER:O	2.16	0.45
3:C:35:LEU:HD12	3:C:38:PHE:CE2	2.52	0.45
2:2:23:ARG:O	2:2:26:LYS:HB2	2.17	0.44
3:C:190:VAL:HG22	3:C:259:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:ASP:OD2	4:D:21:LYS:HE2	2.17	0.43
5:A:401:FMN:P	3:C:117[B]:ARG:HH21	2.41	0.43
2:1:171:SER:HA	2:1:179:ARG:O	2.17	0.43
2:1:197:ILE:HD11	2:1:229:LEU:CD2	2.39	0.43
2:1:197:ILE:CD1	2:1:229:LEU:HD11	2.49	0.43
2:1:175:LYS:HD2	2:1:204:GLU:OE1	2.18	0.43
4:D:264:GLN:NE2	15:D:805:HOH:O	2.52	0.43
2:1:135:VAL:HG11	2:1:141:ILE:HD11	2.00	0.42
4:D:272:PHE:CE2	4:D:282:ILE:HD11	2.53	0.42
4:D:131:LEU:CD2	4:D:148:THR:HG22	2.49	0.42
2:2:188:LEU:HD22	2:2:258:LEU:HD11	2.01	0.42
3:C:232:ASN:HA	3:C:261:PHE:O	2.20	0.42
2:1:21:ILE:HG13	2:2:227:MET:HE1	2.02	0.42
2:1:197:ILE:O	2:1:201:LEU:HG	2.20	0.42
2:2:73:LYS:O	2:2:77:LYS:HB2	2.20	0.42
2:1:210:ARG:HH22	8:1:403:GOL:HO2	1.61	0.42
4:D:234:ASN:HD21	4:D:236:ILE:HG12	1.84	0.42
4:D:316:THR:OG1	4:D:318:GLU:HG3	2.21	0.41
2:1:148:TYR:CD2	2:1:229:LEU:HG	2.55	0.41
3:C:116:VAL:HA	3:C:155:LEU:HD22	2.02	0.41
4:D:332:GLN:HA	4:D:335:SER:O	2.20	0.41
2:1:276:THR:CG2	2:1:278:ILE:H	2.33	0.41
3:C:19:VAL:O	3:C:23:VAL:HG23	2.20	0.41
4:D:345:GLU:OE1	4:D:354:TYR:OH	2.24	0.41
3:C:193:ILE:HB	3:C:257:LEU:HD11	2.02	0.41
2:2:208:PHE:HE2	4:D:284:ASP:HB2	1.85	0.41
4:D:164:SER:HB3	4:D:357:ILE:HG13	2.03	0.41
4:D:113:ALA:HA	4:D:340:VAL:O	2.21	0.41
2:1:58:SER:OG	2:1:60:TYR:HB2	2.21	0.40
4:D:368:ASN:ND2	4:D:391:LYS:O	2.55	0.40
4:D:211:ILE:HA	4:D:229:LEU:O	2.21	0.40
1:A:12:LEU:HD11	2:1:28:LEU:CD2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:131:ASN:ND2	2:1:131:ASN:ND2[2_757]	2.15	0.05

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	17/68 (25%)	17 (100%)	0	0	100	100
2	1	286/295 (97%)	271 (95%)	15 (5%)	0	100	100
2	2	280/295 (95%)	265 (95%)	15 (5%)	0	100	100
3	C	264/272 (97%)	255 (97%)	8 (3%)	1 (0%)	34	38
4	D	395/396 (100%)	384 (97%)	10 (2%)	1 (0%)	41	47
All	All	1242/1326 (94%)	1192 (96%)	48 (4%)	2 (0%)	47	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	88	ASN
4	D	311	ASP

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	15/37 (40%)	15 (100%)	0	100	100
2	1	261/276 (95%)	249 (95%)	12 (5%)	27	32
2	2	253/276 (92%)	242 (96%)	11 (4%)	29	35
3	C	229/239 (96%)	226 (99%)	3 (1%)	69	80
4	D	347/351 (99%)	328 (94%)	19 (6%)	21	24
All	All	1105/1179 (94%)	1060 (96%)	45 (4%)	30	37

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	58	SER
2	1	69	SER
2	1	87	ASN
2	1	91	THR
2	1	112	ARG
2	1	136	SER
2	1	170	GLN
2	1	212	GLU
2	1	227	MET
2	1	232	LEU
2	1	237	SER
2	1	276	THR
2	2	70	LEU
2	2	75	LYS
2	2	97	ASN
2	2	113	GLU
2	2	117	CYS
2	2	134	ASN
2	2	155	ARG
2	2	175	LYS
2	2	261	SER
2	2	263	VAL
2	2	284	VAL
3	C	53	GLU
3	C	167	THR
3	C	218	TYR
4	D	8	LEU
4	D	16	MET
4	D	75	THR
4	D	131	LEU
4	D	146	ARG
4	D	152	SER
4	D	156	SER
4	D	158	ASN
4	D	185	THR
4	D	203	LEU
4	D	260	VAL
4	D	312	ASP
4	D	314	LYS
4	D	315	LEU
4	D	318	GLU
4	D	323	SER

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Mol	Chain	Res	Type
4	D	336	ASP
4	D	344	ARG
4	D	368	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	14	ASN
2	1	87	ASN
2	1	97	ASN
2	1	163	ASN
2	1	217	ASN
2	2	286	HIS
3	C	71	ASN
4	D	73	GLN
4	D	234	ASN
4	D	264	GLN
4	D	333	GLN
4	D	368	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)

1 non-standard protein/DNA/RNA residue is 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	#$|Z| > 2$
1	F6N	A	56	1	5,9,10	2.60	1 (20%)	1,11,13	4.44	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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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
1	F6N	A	56	1	-	0/0/4/6	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	F6N	CA2-C	5.61	1.54	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	F6N	O-C-CA2	-4.44	120.02	124.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\#|Z| > 2$
9	ATP	2	402	-	26,33,33	1.05	3 (11%)	31,52,52	1.37	4 (12%)
8	GOL	1	403	-	5,5,5	0.54	0	5,5,5	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
10	EDO	D	701	-	3,3,3	0.59	0	2,2,2	0.33	0
5	FMN	A	401	-	31,33,33	2.26	6 (19%)	40,50,50	2.33	10 (25%)
10	EDO	2	403	-	3,3,3	0.44	0	2,2,2	0.36	0
11	ADP	D	702	13	24,29,29	1.05	2 (8%)	29,45,45	1.26	4 (13%)
12	PO4	D	703	13	4,4,4	0.45	0	6,6,6	0.62	0
7	SO4	1	402	-	4,4,4	0.33	0	6,6,6	0.17	0

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
9	ATP	2	402	-	-	8/18/38/38	0/3/3/3
8	GOL	1	403	-	-	0/4/4/4	-
10	EDO	D	701	-	-	1/1/1/1	-
5	FMN	A	401	-	-	0/18/18/18	0/3/3/3
10	EDO	2	403	-	-	0/1/1/1	-
11	ADP	D	702	13	-	1/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	FMN	C4A-C10	9.53	1.48	1.38
5	A	401	FMN	C9A-C5A	4.00	1.50	1.42
5	A	401	FMN	C4-C4A	3.69	1.47	1.41
5	A	401	FMN	C9A-N10	3.34	1.43	1.38
5	A	401	FMN	C8-C7	3.02	1.48	1.40
11	D	702	ADP	C2-N3	2.92	1.36	1.32
9	2	402	ATP	C5-C4	2.72	1.48	1.40
11	D	702	ADP	C5-C4	2.43	1.47	1.40
9	2	402	ATP	C2-N3	2.14	1.35	1.32
9	2	402	ATP	O4'-C1'	2.09	1.44	1.41
5	A	401	FMN	C10-N1	2.04	1.35	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	FMN	C4-N3-C2	8.96	122.70	115.14
5	A	401	FMN	C4-C4A-C10	-6.43	115.69	119.95
5	A	401	FMN	C1'-N10-C9A	5.06	122.28	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	402	ATP	N3-C2-N1	-3.94	122.52	128.68
5	A	401	FMN	C4A-N5-C5A	3.64	120.41	116.77
11	D	702	ADP	N3-C2-N1	-3.39	123.37	128.68
5	A	401	FMN	C4A-C4-N3	-3.25	118.99	123.43
9	2	402	ATP	PA-O3A-PB	-3.04	122.39	132.83
9	2	402	ATP	C3'-C2'-C1'	3.01	105.51	100.98
5	A	401	FMN	C4-C4A-N5	2.97	121.99	118.60
11	D	702	ADP	C4-C5-N7	-2.76	106.52	109.40
5	A	401	FMN	O2'-C2'-C3'	2.74	115.75	109.10
9	2	402	ATP	C4-C5-N7	-2.51	106.78	109.40
11	D	702	ADP	O4'-C1'-C2'	-2.38	103.45	106.93
5	A	401	FMN	O3P-P-O2P	2.36	116.67	107.64
11	D	702	ADP	O2A-PA-O1A	2.23	123.27	112.24
5	A	401	FMN	C9A-N10-C10	-2.14	119.10	121.91
5	A	401	FMN	O2P-P-O5'	-2.13	101.07	106.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	2	402	ATP	C5'-O5'-PA-O1A
11	D	702	ADP	PA-O3A-PB-O3B
9	2	402	ATP	O4'-C4'-C5'-O5'
9	2	402	ATP	C3'-C4'-C5'-O5'
9	2	402	ATP	C5'-O5'-PA-O2A
9	2	402	ATP	PB-O3B-PG-O1G
10	D	701	EDO	O1-C1-C2-O2
9	2	402	ATP	PB-O3B-PG-O2G
9	2	402	ATP	PB-O3B-PG-O3G
9	2	402	ATP	C5'-O5'-PA-O3A

There are no ring outliers.
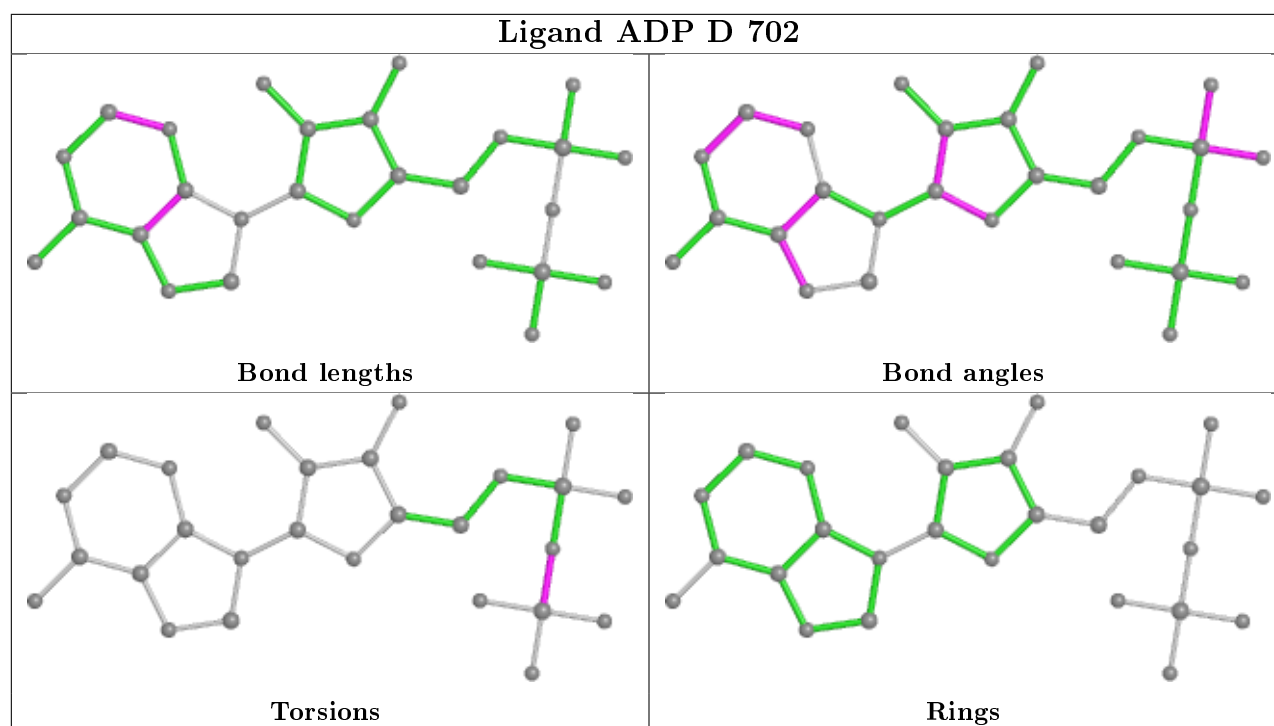
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	1	403	GOL	1	0
5	A	401	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 then 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 ATP 2 402

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 702
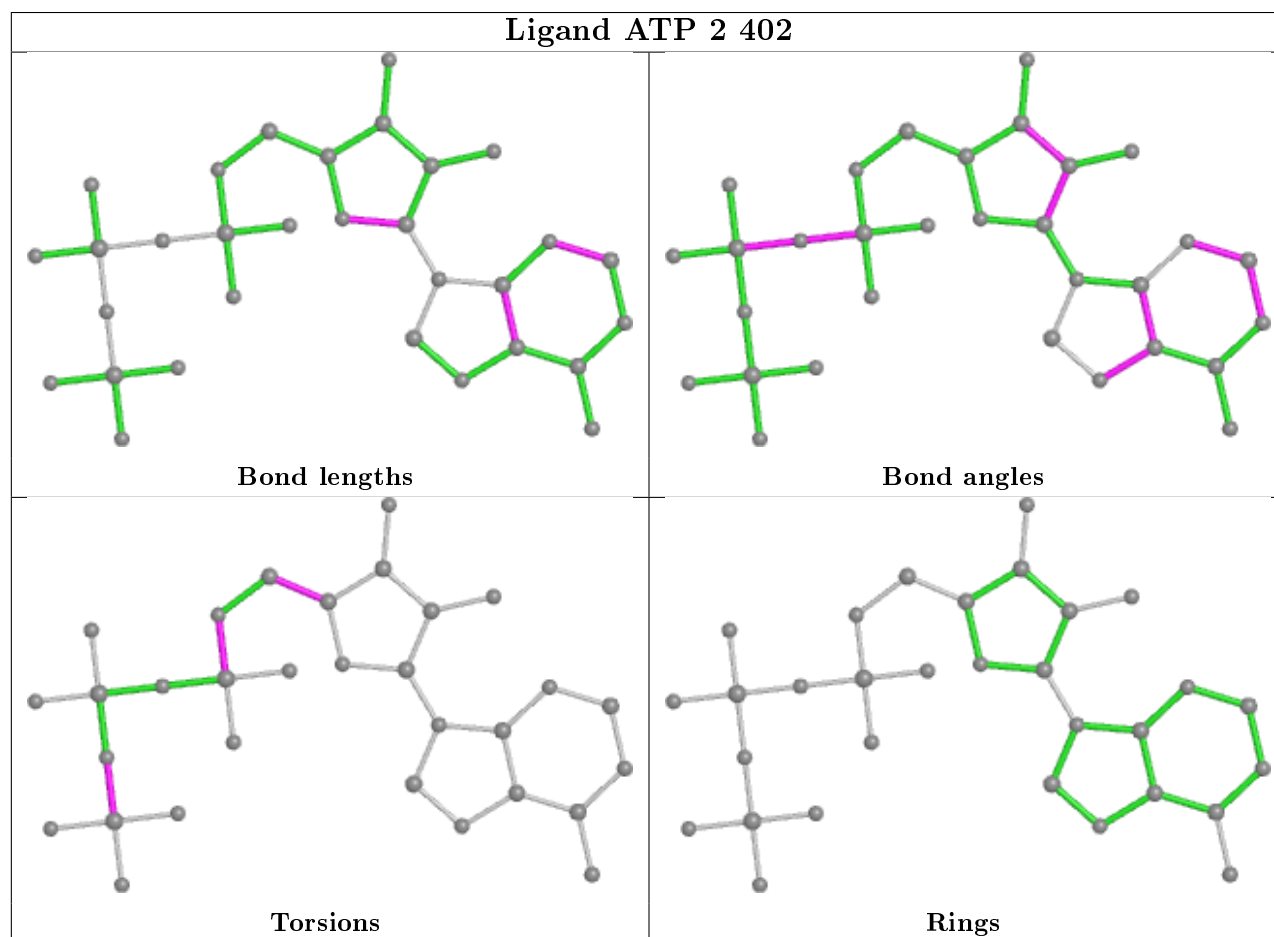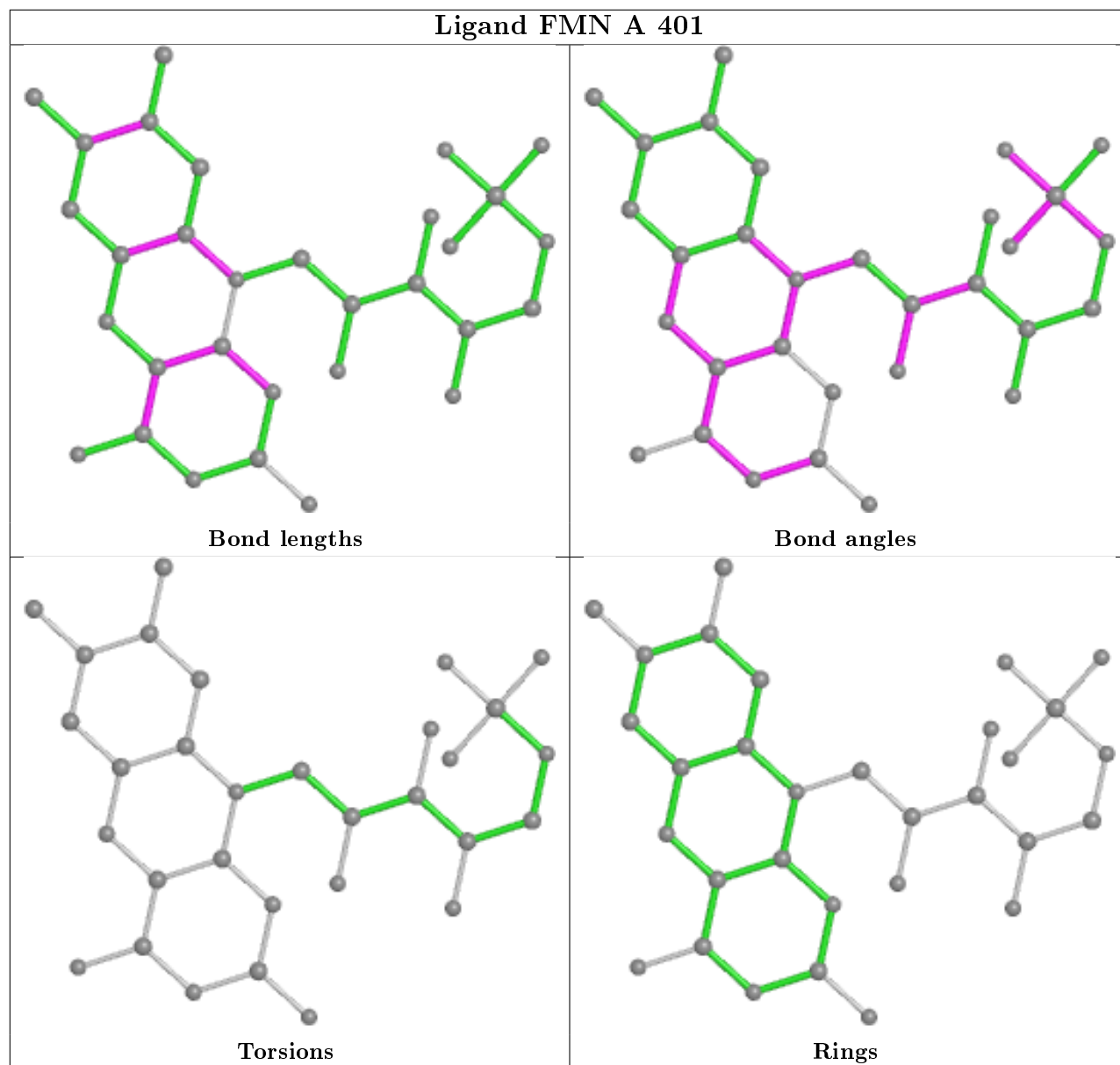
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	20/68 (29%)	0.61	2 (10%)	7	11	62, 73, 85, 86	0
2	1	284/295 (96%)	-0.30	1 (0%)	92	96	35, 51, 79, 96	0
2	2	282/295 (95%)	-0.20	2 (0%)	87	92	35, 53, 89, 103	0
3	C	265/272 (97%)	-0.34	0	100	100	34, 50, 67, 82	0
4	D	396/396 (100%)	-0.29	1 (0%)	94	97	36, 55, 76, 93	0
All	All	1247/1326 (94%)	-0.27	6 (0%)	91	95	34, 53, 81, 103	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	2	259	VAL	4.0
1	A	19	LEU	3.6
2	1	12	MET	2.7
4	D	315	LEU	2.4
1	A	59	HIS	2.3
2	2	91	THR	2.2

## 6.2 Non-standard residues in protein, DNA, RNA chains (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(Å²)	Q<0.9
1	F6N	A	56	9/10	0.80	0.29	76,86,87,88	0

6.3 Carbohydrates (i)

There are no carbohydrates 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
14	CL	D	707	1/1	0.83	0.13	71,71,71,71	0
13	MG	D	704	1/1	0.86	0.10	45,45,45,45	0
9	ATP	2	402	31/31	0.87	0.19	81,112,129,144	0
8	GOL	1	403	6/6	0.92	0.27	51,56,59,72	0
10	EDO	2	403	4/4	0.94	0.15	54,55,55,61	0
13	MG	D	706	1/1	0.94	0.11	42,42,42,42	0
10	EDO	D	701	4/4	0.96	0.10	44,44,46,49	0
5	FMN	A	401	31/31	0.97	0.11	31,40,47,50	0
13	MG	D	705	1/1	0.97	0.13	39,39,39,39	0
11	ADP	D	702	27/27	0.98	0.11	34,40,45,52	0
12	PO4	D	703	5/5	0.99	0.10	36,36,44,47	0
6	ZN	2	401	1/1	0.99	0.12	44,44,44,44	0
7	SO4	1	402	5/5	0.99	0.07	61,62,71,74	0
6	ZN	1	401	1/1	1.00	0.11	45,45,45,45	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.
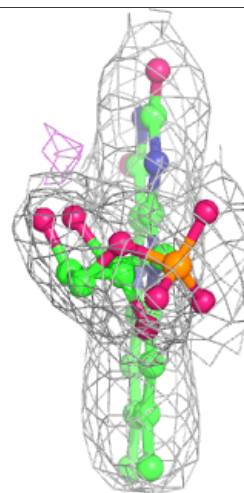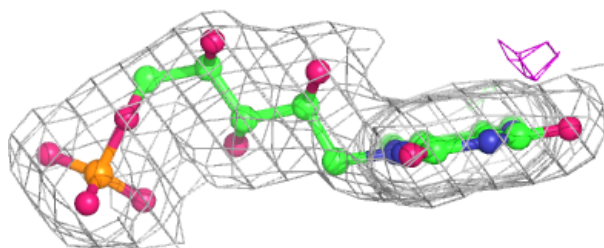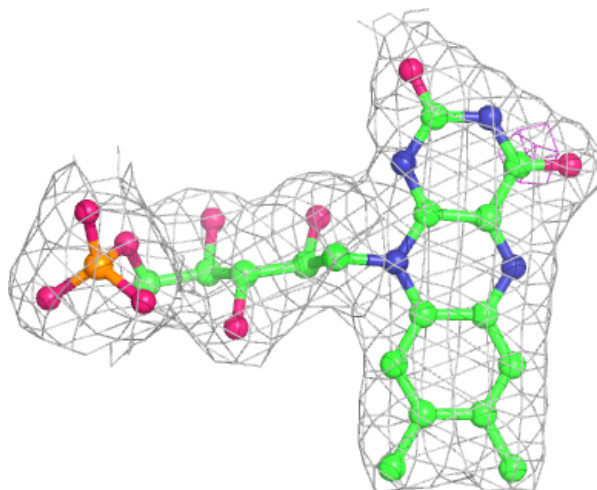
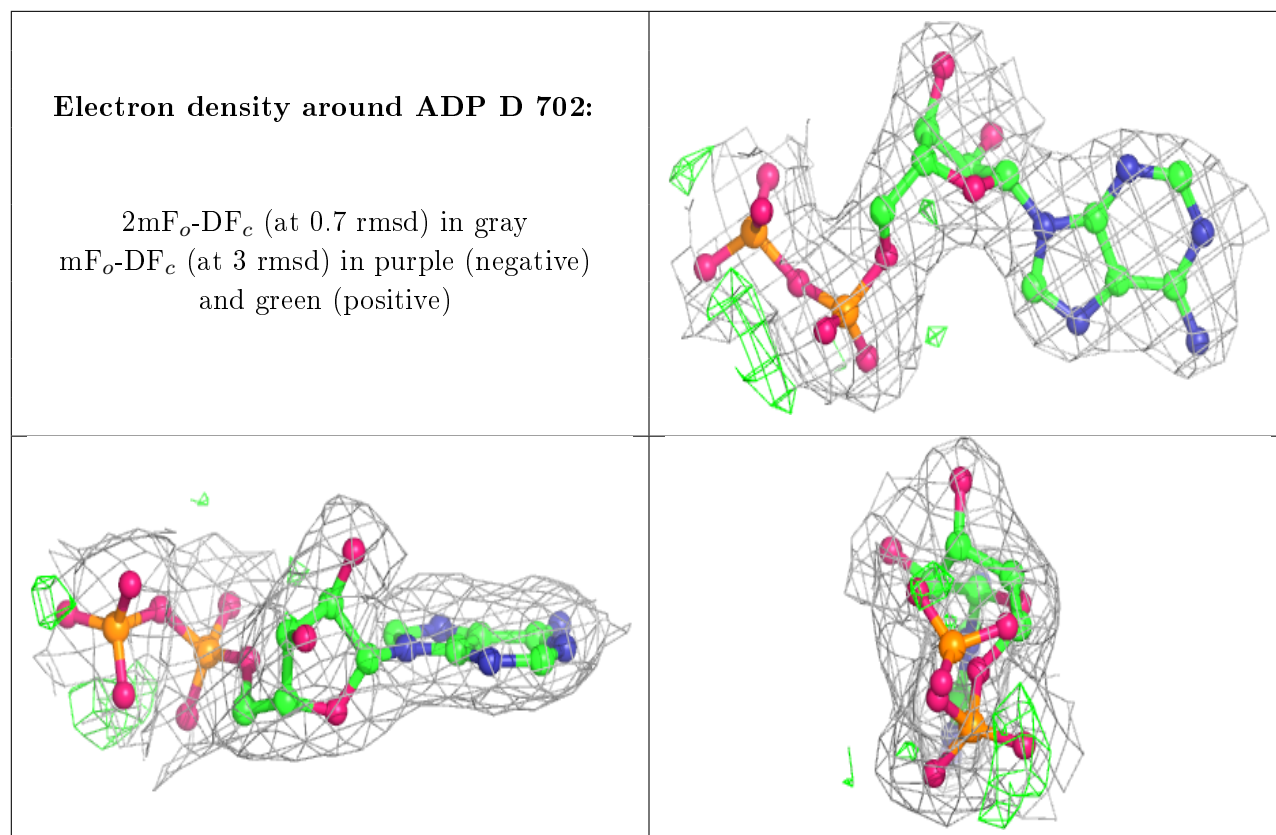**Electron density around ATP 2 402:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
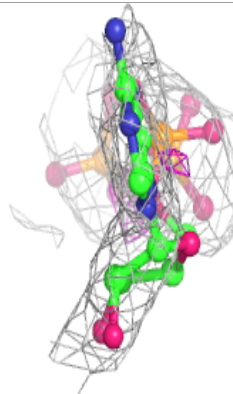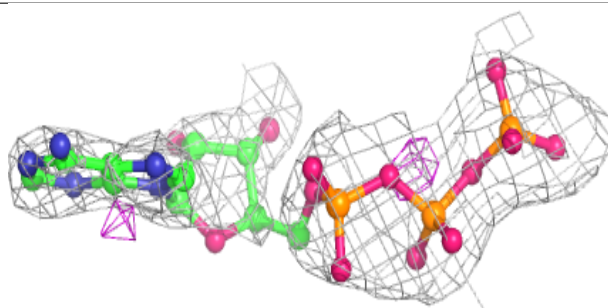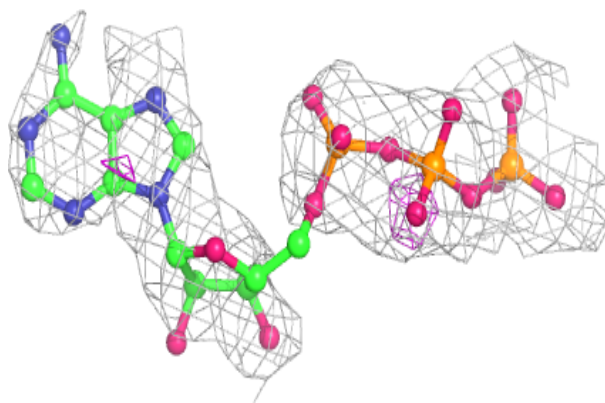
Electron density around FMN A 401:

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

Electron density around ADP D 702:

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

6.5 Other polymers (i)

There are no such residues in this entry.