Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 12:15 AM EDT

PDB ID	:	4GXQ
Title	:	Crystal Structure of ATP bound RpMatB-BxBclM chimera B1
Authors	:	Rank, K.C.; Crosby, H.A.; Escalante-Semerena, J.C.; Rayment, I.
Deposited on	:	2012-09-04
Resolution	:	2.00 Å(reported)

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

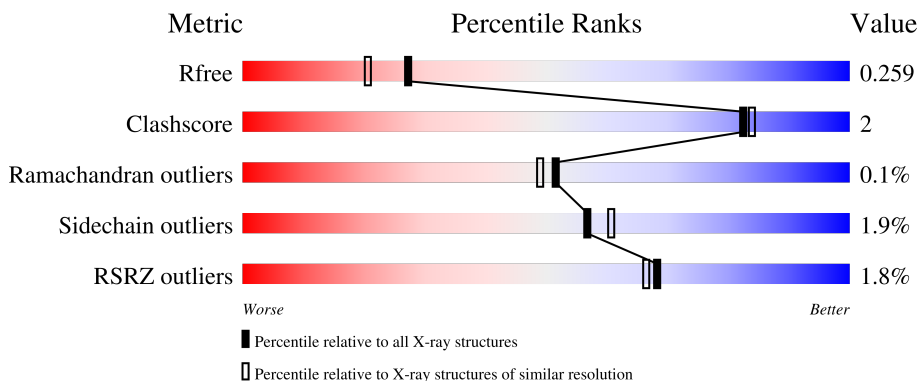|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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		0.259
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		1.9%
RSRZ outliers		1.8%

Worse ... *Better*

■ 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	506	% 94% 5% •
1	B	506	94% 5% •
1	C	506	3% 94% 6%

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:

WORLDWIDE wwPDB PROTEIN DATA BANK

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	62	-	-	X	-
1	MLY	C	62	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13557 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 Malonyl CoA synthetase, Benzoate-CoA ligase Chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	1	0
			3944	2532	669	729	14			
1	B	506	Total	C	N	O	S	0	6	0
			3972	2550	673	735	14			
1	C	506	Total	C	N	O	S	0	2	0
			3947	2534	669	730	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	491	ALA	LYS	engineered mutation	UNP Q6ND88
B	491	ALA	LYS	engineered mutation	UNP Q6ND88
C	491	ALA	LYS	engineered mutation	UNP Q6ND88

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
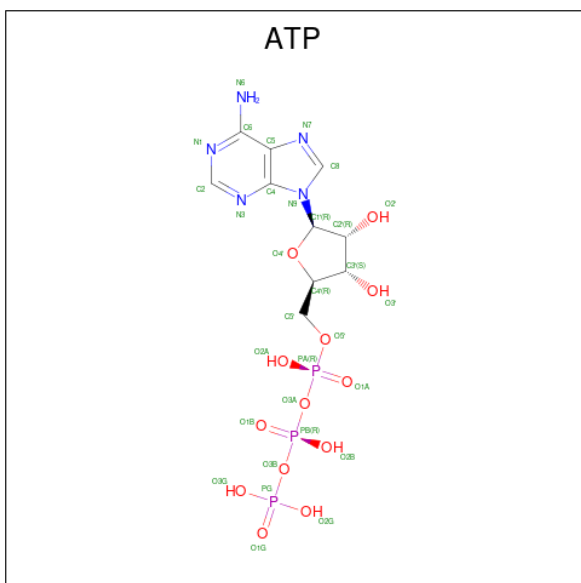
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).
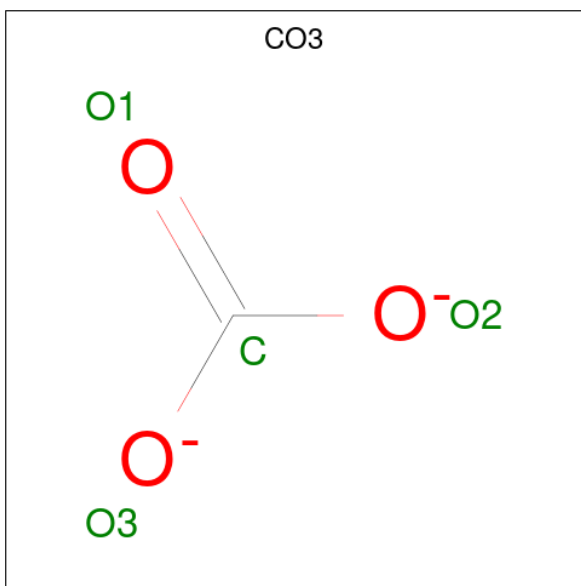
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		
4	C	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	476	Total 476	O 476	0	0
5	B	668	Total 668	O 668	0	0
5	C	442	Total 442	O 442	0	0

3 Residue-property plots ⓘ

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.

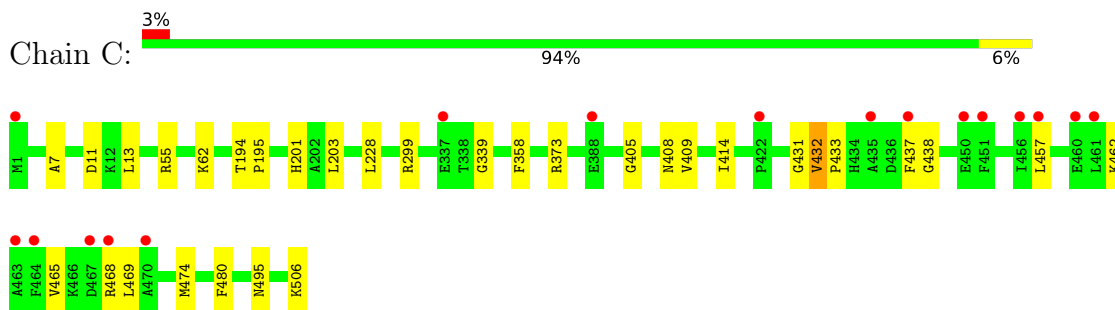• Molecule 1: Malonyl CoA synthetase, Benzoate-CoA ligase Chimeric protein
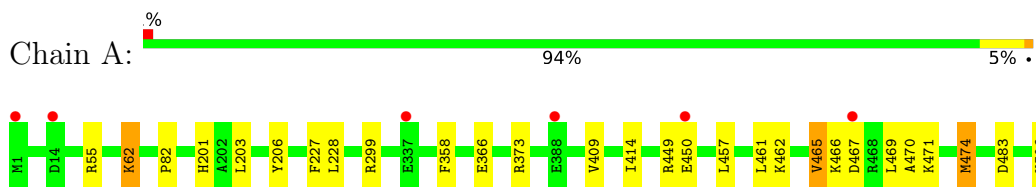
Chain A:

• Molecule 1: Malonyl CoA synthetase, Benzoate-CoA ligase Chimeric protein

Chain B:

• Molecule 1: Malonyl CoA synthetase, Benzoate-CoA ligase Chimeric protein

Chain C:
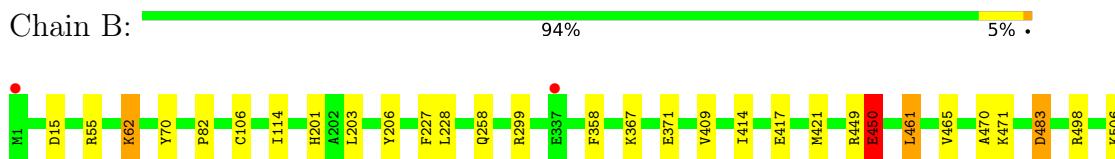
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	299.31Å 299.31Å 47.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.95 – 2.00 24.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.95-2.00) 99.6 (24.94-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.219 , 0.254 0.225 , 0.259	Depositor DCC
R_{free} test set	8364 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.1	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13557	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2680e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, MG, CO3, 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	0.39	0/3696	0.59	0/5048
1	B	0.49	0/3739	0.66	1/5105 (0.0%)
1	C	0.39	0/3702	0.59	0/5056
All	All	0.43	0/11137	0.61	1/15209 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	498	ARG	NE-CZ-NH1	5.13	122.87	120.30

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	3944	0	3994	17	0
1	B	3972	0	4032	18	0
1	C	3947	0	4000	24	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
5	A	476	0	0	1	0
5	B	668	0	0	3	0
5	C	442	0	0	3	0
All	All	13557	0	12062	59	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 2.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:GLY:HA2	5:C:1112:HOH:O	1.75	0.85
1:A:62:MLY:HH23	1:A:203:LEU:O	1.83	0.78
1:A:461:LEU:O	1:A:465:VAL:HG23	1.84	0.78
1:C:495:ASN:HB2	5:C:1046:HOH:O	1.86	0.74
1:A:465:VAL:CG1	1:A:469:LEU:HD12	2.18	0.73
1:A:465:VAL:HG11	1:A:469:LEU:HD12	1.72	0.71
1:C:431:GLY:O	5:C:992:HOH:O	2.09	0.70
1:C:339:GLY:O	1:C:373[A]:ARG:NH1	2.26	0.69
1:B:62:MLY:HH23	1:B:203:LEU:O	1.93	0.68
1:A:62:MLY:NZ	1:A:228:LEU:O	2.29	0.66
1:C:62:MLY:CH1	1:C:228:LEU:O	2.44	0.64
1:A:62:MLY:HH11	1:A:201:HIS:ND1	2.12	0.63
1:C:62:MLY:HH23	1:C:203:LEU:O	1.99	0.62
1:C:432:VAL:HG23	1:C:433:PRO:HD2	1.82	0.62
1:B:421:MET:SD	1:B:461:LEU:HD23	2.40	0.62
1:B:62:MLY:HH21	1:B:201:HIS:O	1.99	0.61
1:B:15:ASP:OD1	5:B:1052:HOH:O	2.16	0.61
1:B:62:MLY:HH22	1:B:228:LEU:O	2.00	0.61
1:C:405:GLY:N	1:C:437:PHE:O	2.35	0.59
1:B:62:MLY:HH13	1:B:227:PHE:CZ	2.40	0.57
1:B:62:MLY:CH2	1:B:228:LEU:O	2.53	0.57
1:C:7:ALA:O	1:C:11:ASP:HB2	2.05	0.55
1:C:62:MLY:NZ	1:C:228:LEU:O	2.39	0.55
1:C:62:MLY:HH11	1:C:228:LEU:O	2.07	0.55
1:B:62:MLY:HH12	1:B:201:HIS:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ARG:O	1:B:450:GLU:CG	2.55	0.54
1:C:432:VAL:HG23	1:C:433:PRO:CD	2.37	0.54
1:B:417:GLU:HB3	1:B:465:VAL:HG23	1.90	0.53
1:C:457:LEU:HD12	1:C:480:PHE:CZ	2.44	0.53
1:B:449:ARG:O	1:B:450:GLU:CB	2.58	0.52
1:A:62:MLY:CH2	1:A:228:LEU:O	2.58	0.51
1:A:462:MLY:O	1:A:474:MET:HE1	2.09	0.51
1:A:62:MLY:CE	1:A:228:LEU:O	2.59	0.51
1:B:483:ASP:OD1	5:B:1294:HOH:O	2.20	0.50
1:C:62:MLY:HH13	1:C:201:HIS:O	2.11	0.50
1:A:462:MLY:O	1:A:466:MLY:HB3	2.12	0.50
1:A:62:MLY:HH22	1:A:228:LEU:O	2.13	0.49
1:B:106:CYS:HB2	1:B:114:ILE:HD12	1.94	0.48
1:C:409:VAL:HG13	1:C:414:ILE:HD11	1.96	0.48
1:A:62:MLY:HH13	1:A:227:PHE:CZ	2.49	0.47
1:C:409:VAL:CG1	1:C:414:ILE:HD11	2.44	0.47
1:A:470:ALA:O	1:A:471:MLY:C	2.63	0.47
1:A:82:PRO:HB2	1:A:206:TYR:HA	1.97	0.46
1:B:258[B]:GLN:NE2	5:B:1273:HOH:O	2.49	0.46
1:C:462:MLY:HG3	1:C:474:MET:HE1	1.99	0.45
1:C:465:VAL:CG1	1:C:469:LEU:HD22	2.47	0.45
1:B:470:ALA:O	1:B:471:MLY:C	2.63	0.44
1:C:62:MLY:HH12	1:C:203:LEU:O	2.18	0.44
1:A:373:ARG:NH1	5:A:981:HOH:O	2.51	0.44
1:B:367:MLY:HH13	1:B:371:GLU:OE1	2.18	0.43
1:B:409:VAL:CG1	1:B:414:ILE:HD11	2.49	0.43
1:C:62:MLY:CB	1:C:62:MLY:HH22	2.50	0.42
1:B:82:PRO:HB2	1:B:206:TYR:HA	2.02	0.42
1:C:194:THR:HB	1:C:195:PRO:CD	2.50	0.41
1:A:409:VAL:CG1	1:A:414:ILE:HD11	2.49	0.41
1:C:468:ARG:HD2	1:C:468:ARG:N	2.35	0.41
1:A:62:MLY:HD3	1:A:62:MLY:HH12	1.60	0.41
1:C:465:VAL:HG13	1:C:469:LEU:HD13	2.03	0.41
1:C:408:ASN:HD22	1:C:408:ASN:HA	1.74	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	476/506 (94%)	472 (99%)	3 (1%)	1 (0%)	47	44
1	B	481/506 (95%)	478 (99%)	2 (0%)	1 (0%)	47	44
1	C	477/506 (94%)	473 (99%)	4 (1%)	0	100	100
All	All	1434/1518 (94%)	1423 (99%)	9 (1%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	VAL
1	B	450	GLU

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	378/377 (100%)	368 (97%)	10 (3%)	46	48
1	B	383/377 (102%)	376 (98%)	7 (2%)	59	63
1	C	379/377 (100%)	374 (99%)	5 (1%)	69	74
All	All	1140/1131 (101%)	1118 (98%)	22 (2%)	57	61

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG

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Mol	Chain	Res	Type
1	A	299	ARG
1	A	358	PHE
1	A	366	GLU
1	A	449	ARG
1	A	450	GLU
1	A	457	LEU
1	A	467	ASP
1	A	474	MET
1	A	483	ASP
1	B	55	ARG
1	B	70	TYR
1	B	299	ARG
1	B	358	PHE
1	B	450	GLU
1	B	461	LEU
1	B	483	ASP
1	C	13	LEU
1	C	55	ARG
1	C	299	ARG
1	C	358	PHE
1	C	432	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	ASN
1	C	216	ASN
1	C	408	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

90 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	MLY	A	462	1	9,10,11	0.46	0	6,11,13	0.66	0
1	MLY	A	473	1	9,10,11	0.52	0	6,11,13	0.73	0
1	MLY	B	12	1	9,10,11	0.56	0	6,11,13	0.54	0
1	MLY	C	506	1	10,11,11	0.79	1 (10%)	12,13,13	1.17	2 (16%)
1	MLY	A	476	1	9,10,11	0.53	0	6,11,13	0.54	0
1	MLY	B	235	1	9,10,11	0.51	0	6,11,13	0.53	0
1	MLY	C	471	1	9,10,11	0.53	0	6,11,13	0.29	0
1	MLY	A	466	1	9,10,11	0.57	0	6,11,13	0.71	0
1	MLY	B	462	1	9,10,11	0.48	0	6,11,13	0.65	0
1	MLY	B	359	1	9,10,11	0.51	0	6,11,13	0.49	0
1	MLY	C	473	1	9,10,11	0.49	0	6,11,13	0.90	0
1	MLY	B	494	1	9,10,11	0.64	0	6,11,13	0.61	0
1	MLY	A	230	1	9,10,11	0.48	0	6,11,13	0.56	0
1	MLY	B	506	1	10,11,11	0.76	1 (10%)	12,13,13	1.28	2 (16%)
1	MLY	A	264	1	9,10,11	0.67	0	6,11,13	0.50	0
1	MLY	C	412	1	9,10,11	0.58	0	6,11,13	0.44	0
1	MLY	A	399	1	9,10,11	0.46	0	6,11,13	0.52	0
1	MLY	C	235	1	9,10,11	0.48	0	6,11,13	0.45	0
1	MLY	B	353	1	9,10,11	0.58	0	6,11,13	0.66	0
1	MLY	C	230	1	9,10,11	0.48	0	6,11,13	0.61	0
1	MLY	A	353	1	9,10,11	0.56	0	6,11,13	0.59	0
1	MLY	C	110	1	9,10,11	0.49	0	6,11,13	0.48	0
1	MLY	C	476	1	9,10,11	0.56	0	6,11,13	0.50	0
1	MLY	B	264	1	9,10,11	0.63	0	6,11,13	0.60	0
1	MLY	A	385	1	9,10,11	0.56	0	6,11,13	0.52	0
1	MLY	C	462	1	9,10,11	0.51	0	6,11,13	0.72	0
1	MLY	C	448	1	9,10,11	0.52	0	6,11,13	0.34	0
1	MLY	C	359	1	9,10,11	0.57	0	6,11,13	0.45	0
1	MLY	A	502	1	9,10,11	0.47	0	6,11,13	0.94	0
1	MLY	C	62	1	9,10,11	0.54	0	6,11,13	0.85	0
1	MLY	B	369	1	9,10,11	0.46	0	6,11,13	0.65	0
1	MLY	A	235	1	9,10,11	0.42	0	6,11,13	0.45	0
1	MLY	C	477	1	9,10,11	0.57	0	6,11,13	0.57	0
1	MLY	C	502	1	9,10,11	0.37	0	6,11,13	0.81	0
1	MLY	C	367	1	9,10,11	0.59	0	6,11,13	0.53	0
1	MLY	B	466	1	9,10,11	0.47	0	6,11,13	0.60	0
1	MLY	A	369	1	9,10,11	0.51	0	6,11,13	0.35	0
1	MLY	B	120	1	9,10,11	0.49	0	6,11,13	0.53	0
1	MLY	B	28	1	9,10,11	0.65	0	6,11,13	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MLY	A	494	1	9,10,11	0.62	0	6,11,13	0.61	0
1	MLY	B	476	1	9,10,11	0.49	0	6,11,13	0.53	0
1	MLY	B	412	1	9,10,11	0.56	0	6,11,13	0.52	0
1	MLY	B	448	1	9,10,11	0.55	0	6,11,13	0.73	0
1	MLY	A	367	1	9,10,11	0.56	0	6,11,13	0.37	0
1	MLY	A	28	1	9,10,11	0.59	0	6,11,13	0.67	0
1	MLY	C	353	1	9,10,11	0.63	0	6,11,13	0.60	0
1	MLY	C	264	1	9,10,11	0.55	0	6,11,13	0.63	0
1	MLY	C	28	1	9,10,11	0.65	0	6,11,13	0.53	0
1	MLY	B	62	1	9,10,11	1.12	1 (11%)	6,11,13	1.70	2 (33%)
1	MLY	A	291	1	9,10,11	0.57	0	6,11,13	0.55	0
1	MLY	A	171	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	C	120	1	9,10,11	0.43	0	6,11,13	0.85	0
1	MLY	B	399	1	9,10,11	0.54	0	6,11,13	0.35	0
1	MLY	B	102	1	9,10,11	0.68	0	6,11,13	0.73	0
1	MLY	A	340	1	9,10,11	0.62	0	6,11,13	0.71	0
1	MLY	C	291	1	9,10,11	0.58	0	6,11,13	0.41	0
1	MLY	B	367	1	9,10,11	0.59	0	6,11,13	0.43	0
1	MLY	C	385	1	9,10,11	0.47	0	6,11,13	0.76	0
1	MLY	A	448	1	9,10,11	0.59	0	6,11,13	0.64	0
1	MLY	A	18	1	9,10,11	0.58	0	6,11,13	0.56	0
1	MLY	C	369	1	9,10,11	0.42	0	6,11,13	0.67	0
1	MLY	B	502	1	9,10,11	0.46	0	6,11,13	0.44	0
1	MLY	B	291	1	9,10,11	0.58	0	6,11,13	0.46	0
1	MLY	C	102	1	9,10,11	0.63	0	6,11,13	0.43	0
1	MLY	C	494	1	9,10,11	0.54	0	6,11,13	0.55	0
1	MLY	B	385	1	9,10,11	0.63	0	6,11,13	0.34	0
1	MLY	A	110	1	9,10,11	0.50	0	6,11,13	0.54	0
1	MLY	B	340	1	9,10,11	0.52	0	6,11,13	0.64	0
1	MLY	A	120	1	9,10,11	0.46	0	6,11,13	0.59	0
1	MLY	A	359	1	9,10,11	0.49	0	6,11,13	0.39	0
1	MLY	A	506	1	10,11,11	0.81	1 (10%)	12,13,13	1.13	1 (8%)
1	MLY	B	110	1	9,10,11	0.78	0	6,11,13	0.46	0
1	MLY	A	477	1	9,10,11	0.47	0	6,11,13	0.57	0
1	MLY	C	399	1	9,10,11	0.42	0	6,11,13	0.58	0
1	MLY	A	471	1	9,10,11	0.52	0	6,11,13	0.41	0
1	MLY	C	18	1	9,10,11	0.51	0	6,11,13	0.54	0
1	MLY	B	477	1	9,10,11	0.58	0	6,11,13	0.63	0
1	MLY	B	473	1	9,10,11	0.49	0	6,11,13	0.69	0
1	MLY	C	340	1	9,10,11	0.55	0	6,11,13	0.85	0
1	MLY	C	171	1	9,10,11	0.57	0	6,11,13	0.64	0
1	MLY	A	12	1	9,10,11	0.53	0	6,11,13	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MLY	A	102	1	9,10,11	0.55	0	6,11,13	0.46	0
1	MLY	B	18	1	9,10,11	0.53	0	6,11,13	0.46	0
1	MLY	C	12	1	9,10,11	0.53	0	6,11,13	0.44	0
1	MLY	A	412	1	9,10,11	0.42	0	6,11,13	0.58	0
1	MLY	B	171	1	9,10,11	0.54	0	6,11,13	0.48	0
1	MLY	B	471	1	9,10,11	0.50	0	6,11,13	0.43	0
1	MLY	C	466	1	9,10,11	0.48	0	6,11,13	0.50	0
1	MLY	A	62	1	9,10,11	1.00	1 (11%)	6,11,13	1.26	1 (16%)
1	MLY	B	230	1	9,10,11	0.47	0	6,11,13	0.46	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
1	MLY	A	462	1	-	0/8/9/11	-
1	MLY	A	473	1	-	0/8/9/11	-
1	MLY	B	12	1	-	3/8/9/11	-
1	MLY	C	506	1	-	3/11/11/11	-
1	MLY	A	476	1	-	1/8/9/11	-
1	MLY	B	235	1	-	0/8/9/11	-
1	MLY	C	471	1	-	3/8/9/11	-
1	MLY	A	466	1	-	1/8/9/11	-
1	MLY	B	462	1	-	3/8/9/11	-
1	MLY	B	359	1	-	1/8/9/11	-
1	MLY	C	473	1	-	4/8/9/11	-
1	MLY	B	494	1	-	2/8/9/11	-
1	MLY	A	230	1	-	2/8/9/11	-
1	MLY	B	506	1	-	3/11/11/11	-
1	MLY	A	264	1	-	1/8/9/11	-
1	MLY	C	412	1	-	0/8/9/11	-
1	MLY	A	399	1	-	2/8/9/11	-
1	MLY	C	235	1	-	2/8/9/11	-
1	MLY	B	353	1	-	0/8/9/11	-
1	MLY	C	230	1	-	1/8/9/11	-
1	MLY	A	353	1	-	1/8/9/11	-
1	MLY	C	110	1	-	0/8/9/11	-
1	MLY	C	476	1	-	2/8/9/11	-
1	MLY	B	264	1	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	385	1	-	1/8/9/11	-
1	MLY	C	462	1	-	2/8/9/11	-
1	MLY	C	448	1	-	2/8/9/11	-
1	MLY	C	359	1	-	2/8/9/11	-
1	MLY	A	502	1	-	0/8/9/11	-
1	MLY	C	62	1	-	3/8/9/11	-
1	MLY	B	369	1	-	5/8/9/11	-
1	MLY	A	235	1	-	0/8/9/11	-
1	MLY	C	477	1	-	1/8/9/11	-
1	MLY	C	502	1	-	0/8/9/11	-
1	MLY	C	367	1	-	0/8/9/11	-
1	MLY	B	466	1	-	5/8/9/11	-
1	MLY	A	369	1	-	4/8/9/11	-
1	MLY	B	120	1	-	0/8/9/11	-
1	MLY	B	28	1	-	2/8/9/11	-
1	MLY	A	494	1	-	3/8/9/11	-
1	MLY	B	476	1	-	0/8/9/11	-
1	MLY	B	412	1	-	0/8/9/11	-
1	MLY	B	448	1	-	5/8/9/11	-
1	MLY	A	367	1	-	0/8/9/11	-
1	MLY	A	28	1	-	1/8/9/11	-
1	MLY	C	353	1	-	0/8/9/11	-
1	MLY	C	264	1	-	0/8/9/11	-
1	MLY	C	28	1	-	0/8/9/11	-
1	MLY	B	62	1	-	5/8/9/11	-
1	MLY	A	291	1	-	2/8/9/11	-
1	MLY	A	171	1	-	1/8/9/11	-
1	MLY	C	120	1	-	4/8/9/11	-
1	MLY	B	399	1	-	1/8/9/11	-
1	MLY	B	102	1	-	1/8/9/11	-
1	MLY	A	340	1	-	1/8/9/11	-
1	MLY	C	291	1	-	2/8/9/11	-
1	MLY	B	367	1	-	1/8/9/11	-
1	MLY	C	385	1	-	1/8/9/11	-
1	MLY	A	448	1	-	1/8/9/11	-
1	MLY	A	18	1	-	6/8/9/11	-
1	MLY	C	369	1	-	1/8/9/11	-
1	MLY	B	502	1	-	0/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	291	1	-	3/8/9/11	-
1	MLY	C	102	1	-	3/8/9/11	-
1	MLY	C	494	1	-	2/8/9/11	-
1	MLY	B	385	1	-	1/8/9/11	-
1	MLY	A	110	1	-	0/8/9/11	-
1	MLY	B	340	1	-	2/8/9/11	-
1	MLY	A	120	1	-	0/8/9/11	-
1	MLY	A	359	1	-	1/8/9/11	-
1	MLY	A	506	1	-	2/11/11/11	-
1	MLY	B	110	1	-	0/8/9/11	-
1	MLY	A	477	1	-	1/8/9/11	-
1	MLY	C	399	1	-	2/8/9/11	-
1	MLY	A	471	1	-	3/8/9/11	-
1	MLY	C	18	1	-	2/8/9/11	-
1	MLY	B	477	1	-	0/8/9/11	-
1	MLY	B	473	1	-	0/8/9/11	-
1	MLY	C	340	1	-	2/8/9/11	-
1	MLY	C	171	1	-	3/8/9/11	-
1	MLY	A	12	1	-	3/8/9/11	-
1	MLY	A	102	1	-	3/8/9/11	-
1	MLY	B	18	1	-	4/8/9/11	-
1	MLY	C	12	1	-	3/8/9/11	-
1	MLY	A	412	1	-	0/8/9/11	-
1	MLY	B	171	1	-	0/8/9/11	-
1	MLY	B	471	1	-	3/8/9/11	-
1	MLY	C	466	1	-	1/8/9/11	-
1	MLY	A	62	1	-	3/8/9/11	-
1	MLY	B	230	1	-	0/8/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	MLY	CB-CA	-2.80	1.49	1.53
1	A	62	MLY	CB-CA	-2.48	1.50	1.53
1	A	506	MLY	OXT-C	-2.29	1.23	1.30
1	C	506	MLY	OXT-C	-2.14	1.23	1.30
1	B	506	MLY	OXT-C	-2.10	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	506	MLY	OXT-C-O	-3.15	116.93	124.09
1	C	506	MLY	OXT-C-O	-3.00	117.28	124.09
1	A	506	MLY	OXT-C-O	-2.61	118.16	124.09
1	B	62	MLY	CD-CG-CB	-2.57	104.53	113.62
1	A	62	MLY	CD-CG-CB	-2.38	105.22	113.62
1	B	62	MLY	CG-CD-CE	-2.08	103.61	113.21
1	B	506	MLY	OXT-C-CA	2.03	120.31	113.38
1	C	506	MLY	OXT-C-CA	2.01	120.22	113.38

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	12	MLY	O-C-CA-CB
1	A	18	MLY	O-C-CA-CB
1	A	102	MLY	O-C-CA-CB
1	A	171	MLY	O-C-CA-CB
1	A	340	MLY	O-C-CA-CB
1	A	369	MLY	C-CA-CB-CG
1	A	477	MLY	O-C-CA-CB
1	A	494	MLY	C-CA-CB-CG
1	A	494	MLY	O-C-CA-CB
1	A	506	MLY	C-CA-CB-CG
1	B	18	MLY	O-C-CA-CB
1	B	102	MLY	O-C-CA-CB
1	B	369	MLY	N-CA-CB-CG
1	B	369	MLY	C-CA-CB-CG
1	B	466	MLY	N-CA-CB-CG
1	B	466	MLY	C-CA-CB-CG
1	B	506	MLY	C-CA-CB-CG
1	C	18	MLY	O-C-CA-CB
1	C	102	MLY	O-C-CA-CB
1	C	171	MLY	O-C-CA-CB
1	C	399	MLY	N-CA-CB-CG
1	C	399	MLY	C-CA-CB-CG
1	C	494	MLY	C-CA-CB-CG
1	A	12	MLY	CD-CE-NZ-CH1
1	A	12	MLY	CD-CE-NZ-CH2
1	B	18	MLY	CD-CE-NZ-CH1
1	B	18	MLY	CD-CE-NZ-CH2
1	B	369	MLY	CD-CE-NZ-CH1
1	B	369	MLY	CD-CE-NZ-CH2
1	B	448	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	B	448	MLY	CD-CE-NZ-CH2
1	B	462	MLY	CD-CE-NZ-CH1
1	B	462	MLY	CD-CE-NZ-CH2
1	C	473	MLY	CD-CE-NZ-CH1
1	A	291	MLY	CG-CD-CE-NZ
1	C	473	MLY	CG-CD-CE-NZ
1	A	62	MLY	CG-CD-CE-NZ
1	C	477	MLY	CG-CD-CE-NZ
1	B	291	MLY	CG-CD-CE-NZ
1	C	291	MLY	CG-CD-CE-NZ
1	C	385	MLY	CG-CD-CE-NZ
1	A	62	MLY	CD-CE-NZ-CH1
1	B	62	MLY	CD-CE-NZ-CH1
1	C	473	MLY	CD-CE-NZ-CH2
1	C	476	MLY	CA-CB-CG-CD
1	A	399	MLY	CG-CD-CE-NZ
1	B	12	MLY	CG-CD-CE-NZ
1	A	476	MLY	CA-CB-CG-CD
1	C	120	MLY	CG-CD-CE-NZ
1	C	171	MLY	CG-CD-CE-NZ
1	B	367	MLY	CD-CE-NZ-CH1
1	B	494	MLY	CD-CE-NZ-CH2
1	C	12	MLY	CG-CD-CE-NZ
1	C	235	MLY	CG-CD-CE-NZ
1	A	230	MLY	CG-CD-CE-NZ
1	C	62	MLY	CA-CB-CG-CD
1	A	18	MLY	CG-CD-CE-NZ
1	B	385	MLY	CG-CD-CE-NZ
1	A	471	MLY	CG-CD-CE-NZ
1	C	171	MLY	CD-CE-NZ-CH2
1	C	462	MLY	CD-CE-NZ-CH2
1	C	476	MLY	CG-CD-CE-NZ
1	B	471	MLY	CA-CB-CG-CD
1	C	235	MLY	CE-CD-CG-CB
1	B	506	MLY	CA-CB-CG-CD
1	A	369	MLY	CE-CD-CG-CB
1	C	12	MLY	CE-CD-CG-CB
1	C	506	MLY	CE-CD-CG-CB
1	A	466	MLY	CA-CB-CG-CD
1	A	471	MLY	CA-CB-CG-CD
1	C	12	MLY	CA-CB-CG-CD
1	C	18	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	C	62	MLY	CE-CD-CG-CB
1	C	506	MLY	CA-CB-CG-CD
1	C	120	MLY	CE-CD-CG-CB
1	C	471	MLY	CE-CD-CG-CB
1	C	230	MLY	CE-CD-CG-CB
1	A	399	MLY	CA-CB-CG-CD
1	A	506	MLY	CA-CB-CG-CD
1	B	28	MLY	CD-CE-NZ-CH1
1	A	18	MLY	CA-CB-CG-CD
1	B	62	MLY	CA-CB-CG-CD
1	B	359	MLY	CA-CB-CG-CD
1	B	448	MLY	CA-CB-CG-CD
1	C	359	MLY	CA-CB-CG-CD
1	B	28	MLY	CD-CE-NZ-CH2
1	C	340	MLY	CD-CE-NZ-CH1
1	B	291	MLY	CA-CB-CG-CD
1	A	494	MLY	CD-CE-NZ-CH2
1	C	340	MLY	CD-CE-NZ-CH2
1	A	230	MLY	CA-CB-CG-CD
1	C	62	MLY	CD-CE-NZ-CH2
1	A	18	MLY	CE-CD-CG-CB
1	A	359	MLY	CA-CB-CG-CD
1	A	291	MLY	CA-CB-CG-CD
1	B	462	MLY	CA-CB-CG-CD
1	C	102	MLY	CG-CD-CE-NZ
1	A	369	MLY	CG-CD-CE-NZ
1	A	353	MLY	CG-CD-CE-NZ
1	A	385	MLY	CE-CD-CG-CB
1	A	264	MLY	CD-CE-NZ-CH1
1	B	340	MLY	CD-CE-NZ-CH1
1	B	62	MLY	CG-CD-CE-NZ
1	B	18	MLY	CG-CD-CE-NZ
1	C	506	MLY	N-CA-CB-CG
1	B	264	MLY	CD-CE-NZ-CH1
1	B	340	MLY	CD-CE-NZ-CH2
1	B	291	MLY	CE-CD-CG-CB
1	B	471	MLY	CE-CD-CG-CB
1	B	471	MLY	N-CA-CB-CG
1	C	466	MLY	N-CA-CB-CG
1	C	471	MLY	N-CA-CB-CG
1	B	466	MLY	CG-CD-CE-NZ
1	B	399	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	B	494	MLY	C-CA-CB-CG
1	C	369	MLY	C-CA-CB-CG
1	C	291	MLY	CA-CB-CG-CD
1	C	102	MLY	CE-CD-CG-CB
1	A	448	MLY	CE-CD-CG-CB
1	A	62	MLY	CD-CE-NZ-CH2
1	B	466	MLY	CA-CB-CG-CD
1	C	359	MLY	CE-CD-CG-CB
1	B	466	MLY	CE-CD-CG-CB
1	A	18	MLY	CD-CE-NZ-CH2
1	B	12	MLY	CD-CE-NZ-CH2
1	B	448	MLY	CE-CD-CG-CB
1	A	102	MLY	CG-CD-CE-NZ
1	C	120	MLY	CD-CE-NZ-CH1
1	A	102	MLY	CE-CD-CG-CB
1	B	62	MLY	CE-CD-CG-CB
1	C	462	MLY	CA-CB-CG-CD
1	A	28	MLY	C-CA-CB-CG
1	C	448	MLY	C-CA-CB-CG
1	C	471	MLY	C-CA-CB-CG
1	C	494	MLY	CG-CD-CE-NZ
1	C	473	MLY	CE-CD-CG-CB
1	B	12	MLY	CD-CE-NZ-CH1
1	B	62	MLY	CD-CE-NZ-CH2
1	C	120	MLY	CD-CE-NZ-CH2
1	C	448	MLY	CE-CD-CG-CB
1	A	18	MLY	CD-CE-NZ-CH1
1	B	448	MLY	CG-CD-CE-NZ
1	B	506	MLY	N-CA-CB-CG
1	A	369	MLY	N-CA-CB-CG
1	B	369	MLY	CE-CD-CG-CB
1	A	471	MLY	CE-CD-CG-CB

There are no ring outliers.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	462	MLY	2	0
1	A	466	MLY	1	0
1	C	462	MLY	1	0
1	C	62	MLY	7	0
1	B	62	MLY	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	367	MLY	1	0
1	A	471	MLY	1	0
1	B	471	MLY	1	0
1	A	62	MLY	8	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	#$|Z| > 2$
2	ATP	A	601	3	26,33,33	0.86	1 (3%)	31,52,52	1.34	5 (16%)
4	CO3	B	603	-	2,3,3	1.12	0	2,3,3	0.09	0
4	CO3	A	603	-	2,3,3	1.21	0	2,3,3	0.28	0
4	CO3	C	603	-	2,3,3	1.21	0	2,3,3	0.31	0
2	ATP	B	601	3	26,33,33	1.06	2 (7%)	31,52,52	1.33	3 (9%)
2	ATP	C	601	3	26,33,33	0.91	1 (3%)	31,52,52	1.29	3 (9%)

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
2	ATP	A	601	3	-	7/18/38/38	0/3/3/3
2	ATP	C	601	3	-	6/18/38/38	0/3/3/3
2	ATP	B	601	3	-	6/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ATP	C5-C4	2.61	1.47	1.40
2	B	601	ATP	C5-C4	2.53	1.47	1.40
2	C	601	ATP	C5-C4	2.14	1.46	1.40
2	B	601	ATP	C2-N3	2.03	1.35	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	ATP	N3-C2-N1	-3.66	122.96	128.68
2	A	601	ATP	N3-C2-N1	-3.62	123.02	128.68
2	C	601	ATP	N3-C2-N1	-3.61	123.03	128.68
2	C	601	ATP	PA-O3A-PB	-2.67	123.67	132.83
2	A	601	ATP	PA-O3A-PB	-2.60	123.90	132.83
2	B	601	ATP	C2-N1-C6	2.43	122.91	118.75
2	A	601	ATP	C2-N1-C6	2.31	122.70	118.75
2	B	601	ATP	C1'-N9-C4	-2.25	122.69	126.64
2	A	601	ATP	C4-C5-N7	-2.21	107.09	109.40
2	A	601	ATP	PB-O3B-PG	-2.03	125.87	132.83
2	C	601	ATP	O3G-PG-O2G	2.00	115.29	107.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	PB-O3A-PA-O5'
2	B	601	ATP	C5'-O5'-PA-O1A
2	C	601	ATP	PB-O3A-PA-O5'
2	C	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	PG-O3B-PB-O1B
2	C	601	ATP	PG-O3B-PB-O1B
2	A	601	ATP	PB-O3A-PA-O5'
2	A	601	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	C5'-O5'-PA-O3A
2	C	601	ATP	C5'-O5'-PA-O3A
2	A	601	ATP	C5'-O5'-PA-O2A
2	B	601	ATP	C5'-O5'-PA-O2A
2	C	601	ATP	C5'-O5'-PA-O2A
2	B	601	ATP	PG-O3B-PB-O2B
2	A	601	ATP	PG-O3B-PB-O1B
2	A	601	ATP	PG-O3B-PB-O2B

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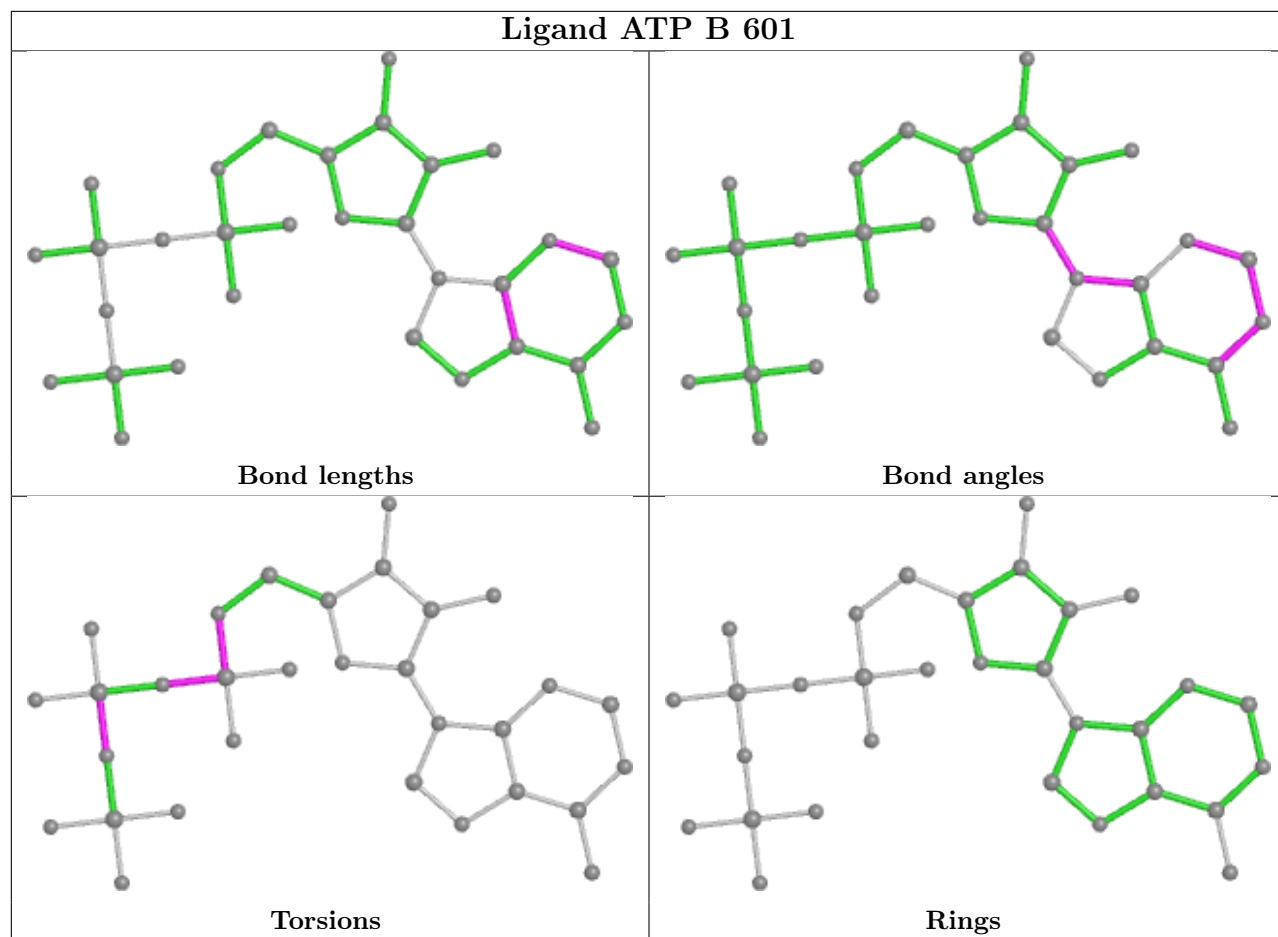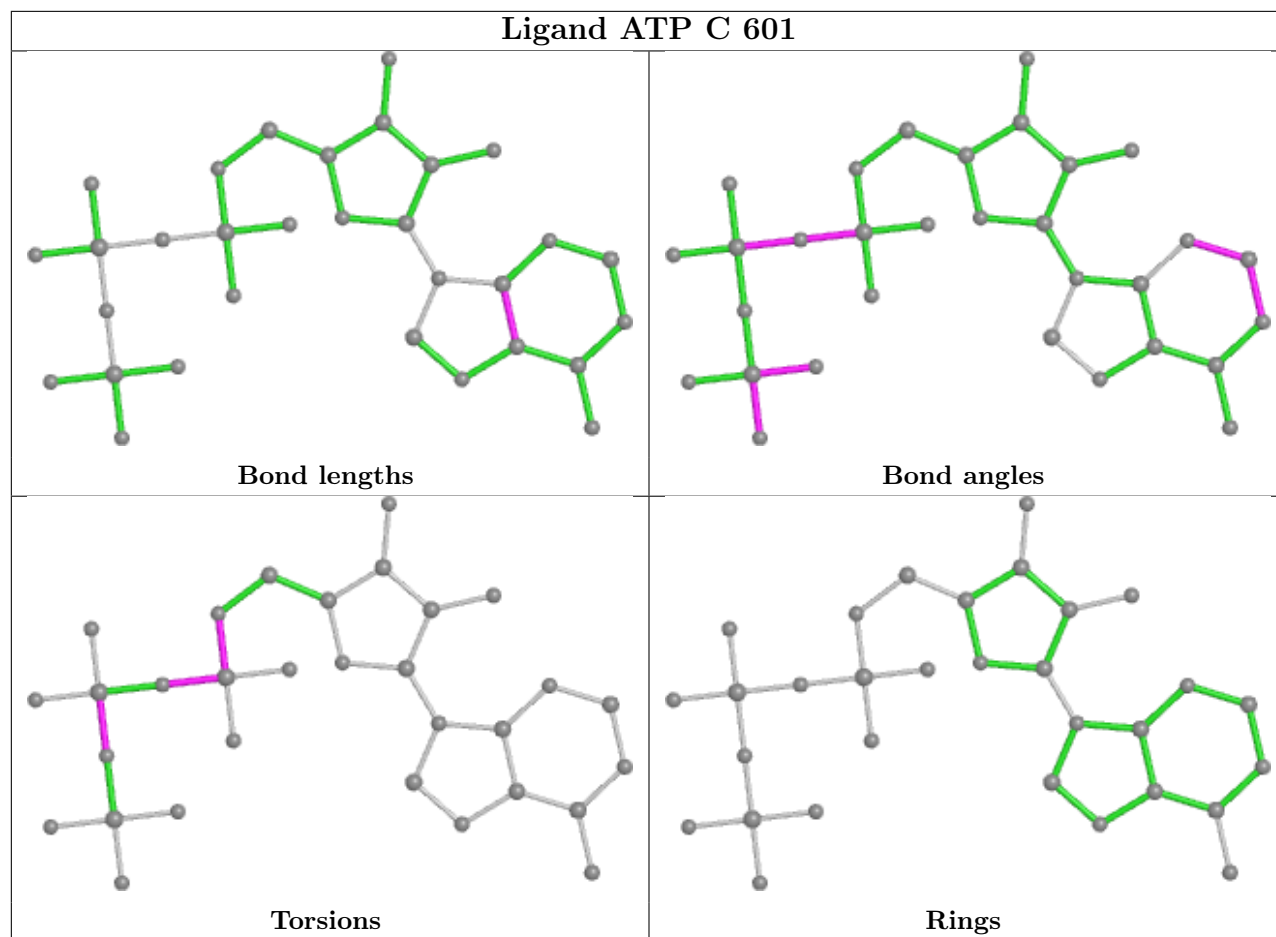| Mol	Chain	Res	Type	Atoms
2	A	601	ATP	PB-O3A-PA-O1A
2	C	601	ATP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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 A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 601

Bond lengths

Bond angles

Torsions

Rings
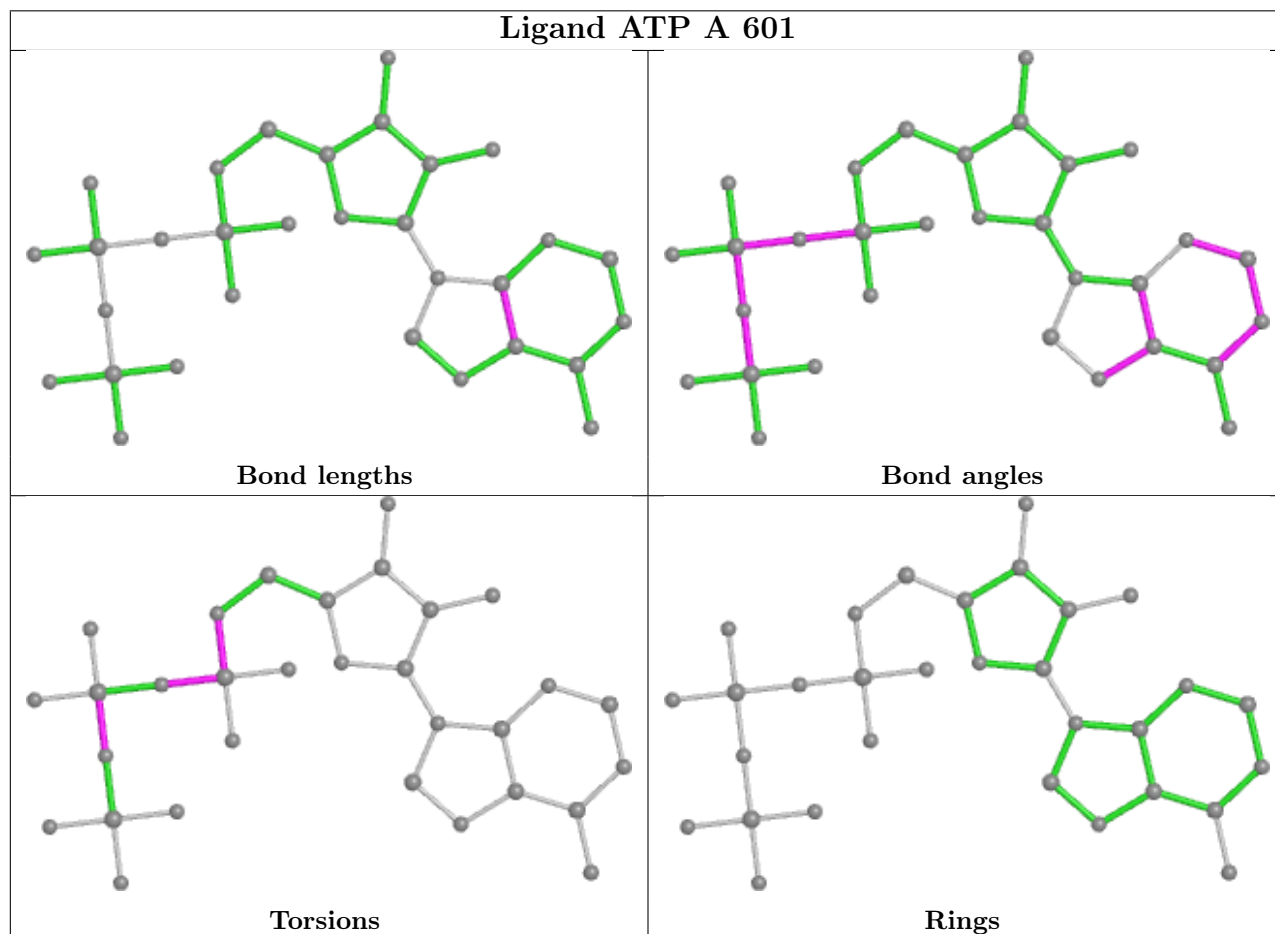
5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

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	476/506 (94%)	-0.21	6 (1%)	77	76	21, 29, 49, 79	0
1	B	476/506 (94%)	-0.27	2 (0%)	92	92	13, 19, 43, 82	0
1	C	476/506 (94%)	0.03	17 (3%)	42	42	19, 30, 70, 107	0
All	All	1428/1518 (94%)	-0.15	25 (1%)	68	66	13, 27, 61, 107	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	456	ILE	4.4
1	C	450	GLU	4.2
1	C	422	PRO	3.8
1	B	1	MET	3.6
1	C	464	PHE	3.5
1	C	435	ALA	3.5
1	C	1	MET	3.5
1	C	337	GLU	3.3
1	C	467	ASP	3.2
1	B	337	GLU	3.1
1	C	451	PHE	3.1
1	C	468	ARG	2.9
1	C	437	PHE	2.8
1	C	457	LEU	2.8
1	A	1	MET	2.6
1	C	463	ALA	2.5
1	C	460	GLU	2.5
1	A	388	GLU	2.4
1	C	470	ALA	2.4
1	C	388	GLU	2.4
1	A	14	ASP	2.4
1	A	337	GLU	2.3
1	C	461	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	450	GLU	2.2
1	A	467	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	MLY	C	473	11/12	0.80	0.20	61,65,82,89	0
1	MLY	C	476	11/12	0.81	0.20	55,68,84,94	0
1	MLY	C	477	11/12	0.82	0.17	51,54,77,90	0
1	MLY	C	506	12/12	0.84	0.30	72,85,104,107	0
1	MLY	A	466	11/12	0.85	0.22	38,55,90,98	0
1	MLY	C	494	11/12	0.86	0.16	52,56,63,63	0
1	MLY	C	359	11/12	0.86	0.17	28,40,64,69	0
1	MLY	C	448	11/12	0.87	0.24	53,61,78,79	0
1	MLY	A	473	11/12	0.88	0.14	29,33,42,44	0
1	MLY	C	412	11/12	0.88	0.17	53,59,70,74	0
1	MLY	C	466	11/12	0.89	0.41	61,84,139,141	0
1	MLY	B	473	11/12	0.89	0.16	29,31,50,61	0
1	MLY	C	291	11/12	0.89	0.20	38,44,99,103	0
1	MLY	A	12	11/12	0.89	0.29	37,47,91,100	0
1	MLY	A	506	12/12	0.89	0.24	29,56,90,91	0
1	MLY	B	462	11/12	0.89	0.13	37,45,53,59	0
1	MLY	A	359	11/12	0.90	0.15	29,43,68,70	0
1	MLY	A	62	11/12	0.90	0.13	30,32,50,52	0
1	MLY	C	462	11/12	0.90	0.15	71,81,93,106	0
1	MLY	B	506	12/12	0.91	0.27	33,53,74,81	0
1	MLY	C	62	11/12	0.91	0.16	26,31,63,93	0
1	MLY	A	340	11/12	0.91	0.23	35,55,84,94	0
1	MLY	A	471	11/12	0.91	0.23	33,65,103,113	0
1	MLY	C	471	11/12	0.91	0.34	65,99,124,128	0
1	MLY	A	18	11/12	0.92	0.17	23,32,64,69	0
1	MLY	B	12	11/12	0.92	0.28	33,46,112,123	0
1	MLY	C	171	11/12	0.92	0.15	31,37,54,72	0
1	MLY	C	264	11/12	0.92	0.11	27,30,35,41	0
1	MLY	B	359	11/12	0.92	0.13	18,34,53,55	0
1	MLY	A	291	11/12	0.92	0.16	29,41,82,84	0
1	MLY	B	466	11/12	0.92	0.33	42,54,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	MLY	A	462	11/12	0.92	0.12	32,37,42,48	0
1	MLY	C	110	11/12	0.93	0.14	31,40,56,59	0
1	MLY	A	448	11/12	0.93	0.18	32,40,92,95	0
1	MLY	C	230	11/12	0.93	0.18	32,43,72,77	0
1	MLY	B	230	11/12	0.93	0.15	26,38,80,90	0
1	MLY	B	494	11/12	0.93	0.13	19,21,31,32	0
1	MLY	A	235	11/12	0.93	0.24	29,41,120,122	0
1	MLY	C	367	11/12	0.93	0.16	36,42,69,75	0
1	MLY	C	399	11/12	0.93	0.23	38,62,100,102	0
1	MLY	C	502	11/12	0.93	0.23	54,58,92,96	0
1	MLY	A	369	11/12	0.93	0.31	40,59,93,101	0
1	MLY	B	340	11/12	0.94	0.17	28,41,74,78	0
1	MLY	A	385	11/12	0.94	0.11	29,35,60,66	0
1	MLY	C	340	11/12	0.94	0.26	39,63,93,97	0
1	MLY	B	367	11/12	0.94	0.14	25,30,60,73	0
1	MLY	B	385	11/12	0.94	0.11	17,20,48,54	0
1	MLY	C	369	11/12	0.94	0.28	39,57,105,112	0
1	MLY	C	385	11/12	0.94	0.14	35,40,64,67	0
1	MLY	B	399	11/12	0.94	0.17	22,32,81,82	0
1	MLY	A	399	11/12	0.94	0.24	31,54,117,123	0
1	MLY	A	494	11/12	0.94	0.10	25,27,32,32	0
1	MLY	B	471	11/12	0.94	0.19	37,59,89,94	0
1	MLY	A	110	11/12	0.94	0.16	33,38,53,55	0
1	MLY	A	264	11/12	0.94	0.11	25,35,39,39	0
1	MLY	B	102	11/12	0.94	0.14	16,18,36,44	0
1	MLY	C	12	11/12	0.94	0.26	36,56,93,99	0
1	MLY	A	230	11/12	0.94	0.21	33,49,96,102	0
1	MLY	B	235	11/12	0.94	0.20	18,30,86,96	0
1	MLY	B	264	11/12	0.94	0.11	18,19,23,24	0
1	MLY	B	291	11/12	0.94	0.15	21,30,69,74	0
1	MLY	A	28	11/12	0.95	0.13	27,38,54,54	0
1	MLY	C	353	11/12	0.95	0.11	25,28,56,58	0
1	MLY	A	120	11/12	0.95	0.26	38,56,75,79	0
1	MLY	B	476	11/12	0.95	0.12	23,28,48,59	0
1	MLY	B	18	11/12	0.95	0.14	19,26,58,62	0
1	MLY	B	502	11/12	0.95	0.16	21,29,58,61	0
1	MLY	A	171	11/12	0.95	0.12	30,32,48,51	0
1	MLY	B	369	11/12	0.95	0.21	24,35,98,109	0
1	MLY	C	18	11/12	0.95	0.17	20,29,66,74	0
1	MLY	B	171	11/12	0.95	0.11	16,19,33,35	0
1	MLY	C	102	11/12	0.95	0.14	26,30,57,64	0
1	MLY	A	102	11/12	0.95	0.13	27,33,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
1	MLY	C	120	11/12	0.95	0.23	35,47,82,83	0
1	MLY	B	412	11/12	0.95	0.10	21,24,30,32	0
1	MLY	B	448	11/12	0.95	0.15	28,35,77,82	0
1	MLY	C	235	11/12	0.95	0.22	27,42,89,97	0
1	MLY	A	476	11/12	0.95	0.12	20,24,55,70	0
1	MLY	A	353	11/12	0.95	0.09	25,30,58,60	0
1	MLY	A	477	11/12	0.96	0.15	20,23,31,31	0
1	MLY	B	28	11/12	0.96	0.11	23,29,55,64	0
1	MLY	B	62	11/12	0.96	0.14	17,19,33,49	0
1	MLY	B	477	11/12	0.96	0.15	20,22,32,33	0
1	MLY	A	367	11/12	0.96	0.19	34,39,54,57	0
1	MLY	B	120	11/12	0.96	0.12	29,35,50,53	0
1	MLY	A	502	11/12	0.97	0.16	24,32,72,72	0
1	MLY	B	110	11/12	0.97	0.08	19,22,35,43	0
1	MLY	C	28	11/12	0.97	0.12	27,35,48,54	0
1	MLY	A	412	11/12	0.97	0.09	22,27,43,45	0
1	MLY	B	353	11/12	0.97	0.09	16,18,40,45	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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($\mathring{A}^2$)	Q<0.9
4	CO3	B	603	4/4	0.93	0.15	9,28,32,43	0
3	MG	C	602	1/1	0.94	0.06	27,27,27,27	0
4	CO3	A	603	4/4	0.95	0.15	21,38,45,48	0
3	MG	B	602	1/1	0.96	0.11	16,16,16,16	0
4	CO3	C	603	4/4	0.96	0.10	23,39,45,50	0
3	MG	A	602	1/1	0.97	0.10	29,29,29,29	0
2	ATP	C	601	31/31	0.97	0.10	22,30,37,43	0
2	ATP	B	601	31/31	0.98	0.10	10,16,23,27	0
2	ATP	A	601	31/31	0.98	0.08	22,27,32,36	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.
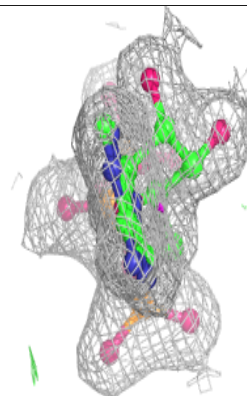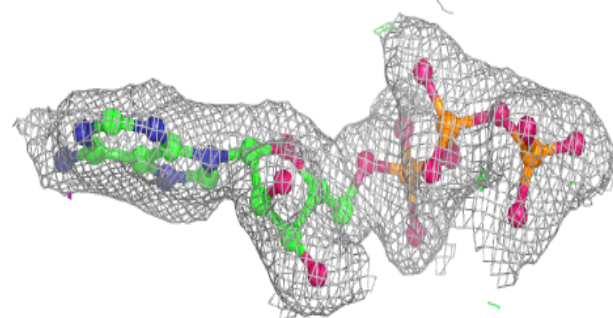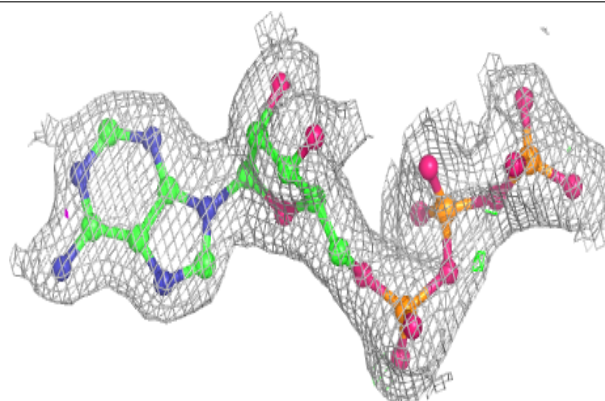
Electron density around ATP C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
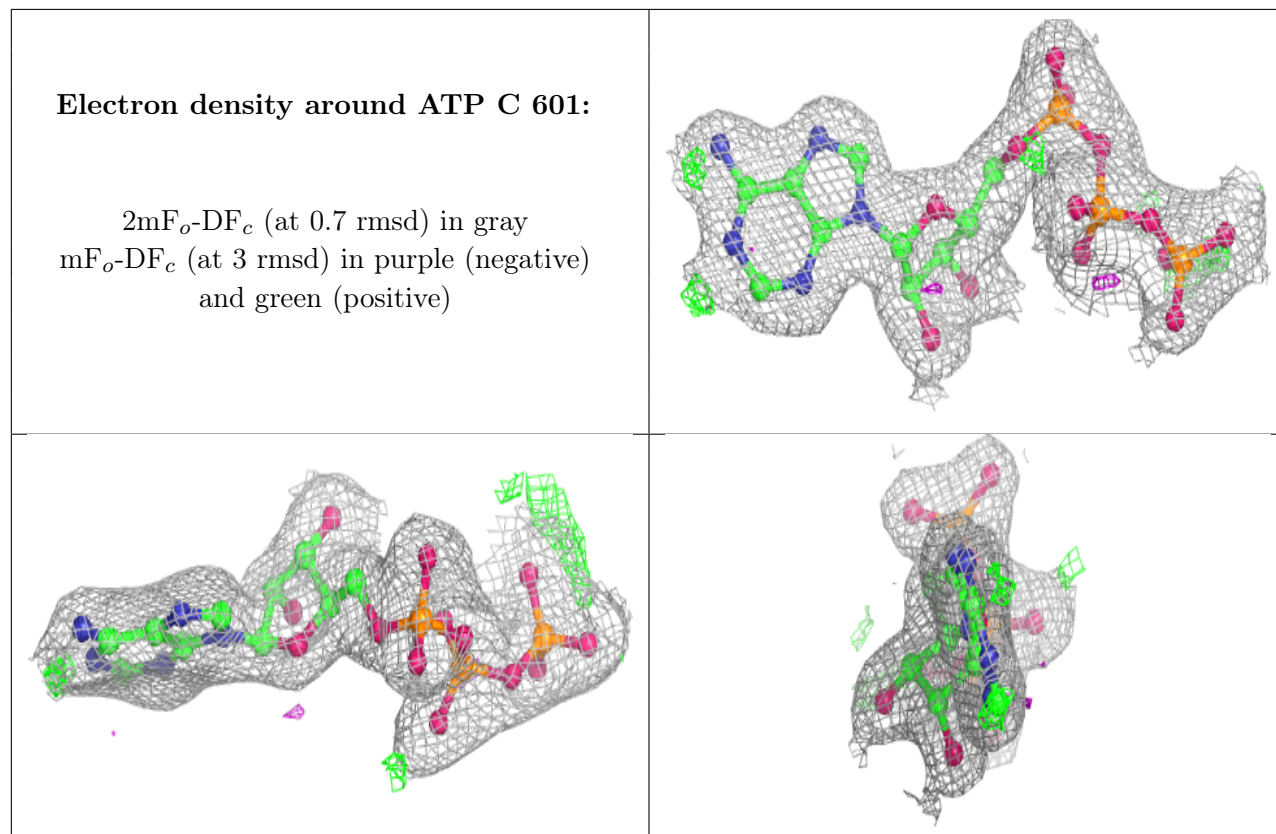
Electron density around ATP B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
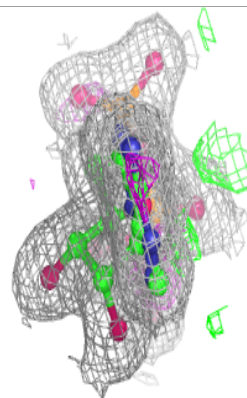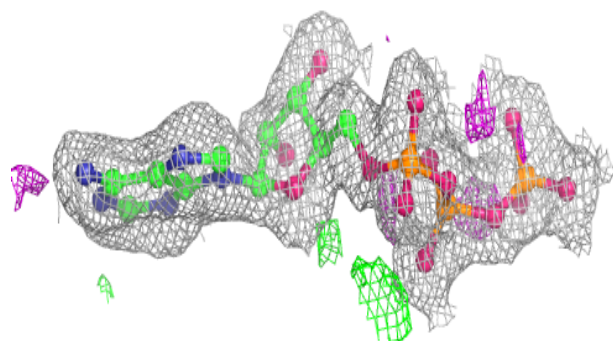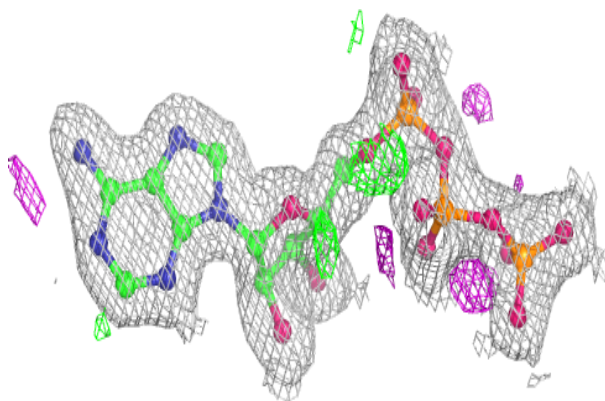
Electron density around ATP A 601:

$2mF_o$-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.