



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:33 PM UTC

PDB ID : 4BGB / pdb_00004bgb
Title : Nucleotide-bound closed form of a putative sugar kinase MK0840 from
Methanopyrus kandleri
Authors : Schacherl, M.; Baumann, U.
Deposited on : 2013-03-24
Resolution : 1.34 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

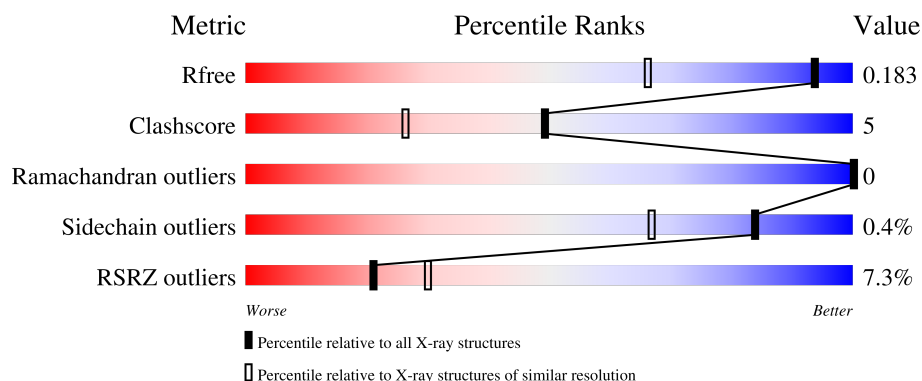
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

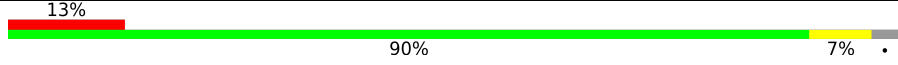
The reported resolution of this entry is 1.34 Å.

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	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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	325	
1	B	325	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	1356	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5714 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.

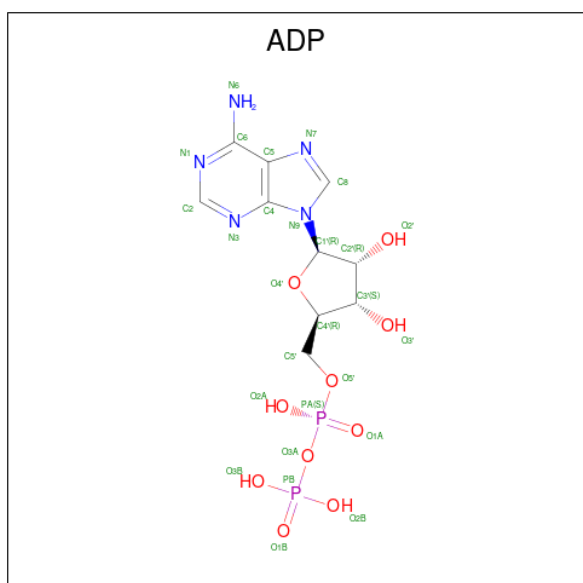
- Molecule 1 is a protein called PUTATIVE SUGAR KINASE MK0840.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	13	0
			2514	1570	441	490	13			
1	B	315	Total	C	N	O	S	0	18	0
			2548	1596	451	490	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP Q8TX37
A	35	SER	-	expression tag	UNP Q8TX37
A	36	HIS	-	expression tag	UNP Q8TX37
B	34	GLY	-	expression tag	UNP Q8TX37
B	35	SER	-	expression tag	UNP Q8TX37
B	36	HIS	-	expression tag	UNP Q8TX37

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	1
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total K 2 2	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0

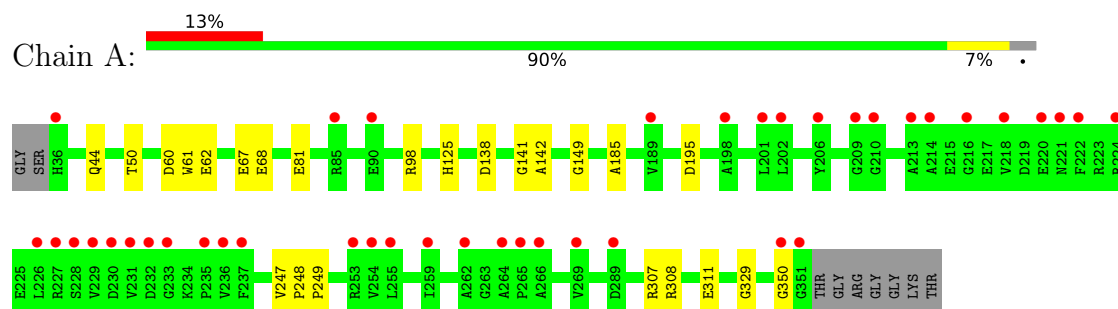
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	225	Total O 225 225	0	0
7	B	294	Total O 294 294	0	0

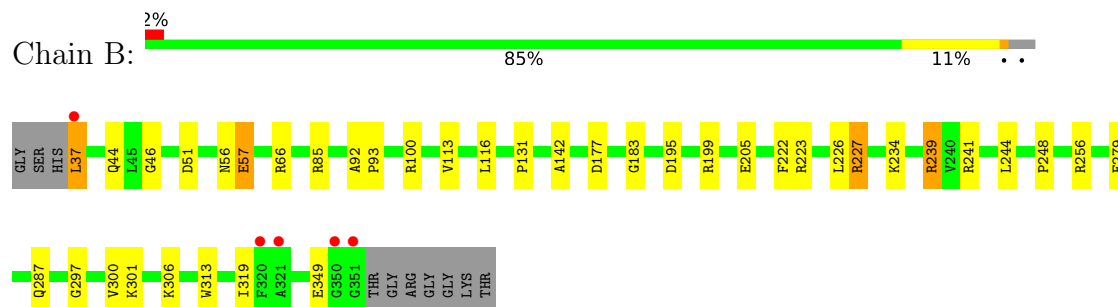
3 Residue-property plots

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: PUTATIVE SUGAR KINASE MK0840



• Molecule 1: PUTATIVE SUGAR KINASE MK0840



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.79Å 108.54Å 117.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.15 – 1.34 45.15 – 1.34	Depositor EDS
% Data completeness (in resolution range)	98.3 (45.15-1.34) 98.3 (45.15-1.34)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.34Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.158 , 0.183 0.159 , 0.183	Depositor DCC
R_{free} test set	7732 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5714	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: ADP, CA, MG, K, GOL

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	0.62	7/2559 (0.3%)	0.76	3/3475 (0.1%)
1	B	0.73	7/2595 (0.3%)	0.73	1/3520 (0.0%)
All	All	0.68	14/5154 (0.3%)	0.75	4/6995 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	ASN	C-N	-15.64	1.12	1.33
1	A	142	ALA	C-O	-6.34	1.17	1.24
1	B	205	GLU	C-O	-6.12	1.16	1.24
1	B	57	GLU	C-N	-6.02	1.24	1.33
1	A	60	ASP	C-O	-5.92	1.16	1.23
1	A	185	ALA	C-O	-5.78	1.16	1.23
1	A	141	GLY	C-O	-5.77	1.16	1.23
1	A	138	ASP	C-O	-5.75	1.17	1.24
1	B	183	GLY	C-O	-5.74	1.16	1.23
1	A	81	GLU	C-O	-5.72	1.17	1.24
1	B	239	ARG	C-O	-5.40	1.17	1.23
1	B	142	ALA	C-O	-5.29	1.18	1.24
1	A	307	ARG	C-O	-5.24	1.18	1.24
1	B	85	ARG	C-O	-5.05	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ASP	CA-C-N	-7.82	111.74	119.87
1	A	138	ASP	C-N-CA	-7.82	111.74	119.87
1	B	248	PRO	N-CA-C	5.79	117.77	110.70
1	A	248	PRO	N-CA-C	5.71	117.66	110.70

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	2514	0	2477	20	0
1	B	2548	0	2539	40	0
2	A	54	0	24	3	0
2	B	27	0	12	0	0
3	A	18	0	23	3	0
3	B	24	0	31	5	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0
6	A	1	0	0	0	0
7	A	225	0	0	4	0
7	B	294	0	0	4	1
All	All	5714	0	5106	56	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 5.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44[A]:GLN:CG	3:B:1356:GOL:O1	2.03	1.06
1:B:44[A]:GLN:OE1	3:B:1356:GOL:O1	1.78	1.01
1:B:66[B]:ARG:HH11	1:B:66[B]:ARG:HG3	1.39	0.87
1:B:44[A]:GLN:HG3	3:B:1356:GOL:O1	1.70	0.85
1:B:223[B]:ARG:NH1	1:B:227:ARG:NH2	2.28	0.81
1:B:66[B]:ARG:HG3	1:B:66[B]:ARG:NH1	1.99	0.78
1:B:66[B]:ARG:HH11	1:B:66[B]:ARG:CG	1.94	0.77
1:B:223[B]:ARG:HH11	1:B:227:ARG:NH2	1.86	0.74
1:A:67[B]:GLU:OE1	3:A:1354:GOL:O3	2.06	0.73
1:B:223[B]:ARG:NH1	1:B:227:ARG:CZ	2.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASP:CG	3:B:1356:GOL:O3	2.35	0.70
1:A:67[B]:GLU:CD	1:A:98:ARG:NH1	2.53	0.66
1:A:308:ARG:NH1	1:A:311:GLU:OE1	2.28	0.66
1:A:62:GLU:OE1	7:A:2029:HOH:O	2.14	0.66
1:B:313:TRP:O	7:B:2249:HOH:O	2.13	0.65
1:A:62:GLU:HG2	7:A:2030:HOH:O	1.97	0.64
1:B:234:LYS:NZ	1:B:241:ARG:O	2.33	0.61
1:A:68[B]:GLU:H	1:A:68[B]:GLU:CD	2.08	0.61
1:A:67[B]:GLU:OE1	1:A:98:ARG:NH1	2.35	0.60
1:B:223[A]:ARG:NE	1:B:227:ARG:HH21	2.01	0.59
1:B:195:ASP:O	1:B:199[A]:ARG:HG3	2.03	0.58
1:A:62:GLU:CG	1:B:301[B]:LYS:HZ3	2.16	0.57
1:A:62:GLU:HG2	1:B:301[B]:LYS:NZ	2.19	0.57
1:A:195:ASP:OD1	2:A:1352[A]:ADP:O2'	2.24	0.55
1:A:62:GLU:CG	1:B:301[B]:LYS:NZ	2.70	0.55
3:A:1353:GOL:H32	7:A:2225:HOH:O	2.06	0.55
1:B:37:LEU:HA	1:B:57:GLU:OE2	2.07	0.54
1:A:149:GLY:O	1:A:329:GLY:HA3	2.08	0.53
1:B:223[B]:ARG:HH11	1:B:227:ARG:CZ	2.20	0.53
1:B:223[B]:ARG:HH11	1:B:227:ARG:HH21	1.56	0.51
1:B:223[A]:ARG:HE	1:B:227:ARG:HH21	1.57	0.51
1:B:234:LYS:HE2	1:B:244:LEU:O	2.11	0.50
1:B:66[B]:ARG:NH1	1:B:66[B]:ARG:CG	2.52	0.50
1:B:239:ARG:NE	1:B:287:GLN:OE1	2.31	0.50
1:B:256[A]:ARG:NH1	7:B:2214:HOH:O	2.45	0.49
3:A:1353:GOL:C3	7:A:2225:HOH:O	2.60	0.48
1:B:177:ASP:OD2	7:B:2138:HOH:O	2.20	0.48
1:B:306:LYS:HD2	1:B:319:ILE:HD13	1.96	0.47
1:A:195:ASP:OD2	2:A:1352[A]:ADP:O3'	2.28	0.47
1:B:113[A]:VAL:HG21	1:B:116:LEU:HD12	1.97	0.47
1:A:247:VAL:HG23	1:A:249:PRO:HD2	1.97	0.47
1:B:223[A]:ARG:NH2	1:B:279:GLU:OE2	2.49	0.45
1:A:44:GLN:O	1:A:50:THR:HA	2.17	0.45
1:B:46:GLY:HA3	3:B:1356:GOL:H12	1.98	0.45
1:B:297:GLY:O	1:B:300[B]:VAL:HG22	2.16	0.44
1:A:62:GLU:HG3	1:B:301[B]:LYS:HZ3	1.81	0.44
1:A:125:HIS:HE1	1:A:350:GLY:O	2.01	0.43
1:A:61:TRP:O	1:B:301[A]:LYS:NZ	2.52	0.42
1:A:62:GLU:HG2	1:B:301[B]:LYS:HZ3	1.78	0.42
1:B:100:ARG:NH1	7:B:2070:HOH:O	2.50	0.42
1:B:222:PHE:CE2	1:B:226:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223[A]:ARG:NE	1:B:227:ARG:NH2	2.66	0.41
1:B:131:PRO:HB3	1:B:349:GLU:HG2	2.02	0.41
1:A:195:ASP:OD2	2:A:1352[B]:ADP:O3'	2.36	0.41
1:B:113[A]:VAL:CG2	1:B:116:LEU:HD12	2.49	0.41
1:B:92:ALA:HB3	1:B:93:PRO:HD3	2.02	0.41

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)
7:B:2226:HOH:O	7:B:2249:HOH:O[4_445]	2.11	0.09

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	327/325 (101%)	325 (99%)	2 (1%)	0	100	100
1	B	331/325 (102%)	329 (99%)	2 (1%)	0	100	100
All	All	658/650 (101%)	654 (99%)	4 (1%)	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	267/259 (103%)	267 (100%)	0	100	100
1	B	271/259 (105%)	269 (99%)	2 (1%)	76	51
All	All	538/518 (104%)	536 (100%)	2 (0%)	84	67

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	LEU
1	B	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	B	47	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	ADP	A	1352[A]	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
3	GOL	A	1354	-	5,5,5	0.39	0	5,5,5	0.27	0
3	GOL	A	1353	-	5,5,5	0.47	0	5,5,5	0.53	0
3	GOL	B	1356	5	5,5,5	2.06	1 (20%)	5,5,5	2.94	1 (20%)
3	GOL	B	1355	5	5,5,5	0.33	0	5,5,5	0.42	0
2	ADP	A	1352[B]	-	28,29,29	2.09	9 (32%)	43,45,45	2.28	12 (27%)
3	GOL	B	1353	-	5,5,5	0.31	0	5,5,5	0.94	1 (20%)
3	GOL	B	1354	-	5,5,5	0.31	0	5,5,5	0.31	0
2	ADP	B	1352	5	28,29,29	1.46	6 (21%)	43,45,45	1.68	12 (27%)
3	GOL	A	1355	6	5,5,5	0.28	0	5,5,5	0.59	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
2	ADP	A	1352[A]	-	-	0/16/32/32	0/3/3/3
3	GOL	A	1354	-	-	2/4/4/4	-
3	GOL	A	1353	-	-	3/4/4/4	-
3	GOL	B	1356	5	-	3/4/4/4	-
3	GOL	B	1355	5	-	1/4/4/4	-
2	ADP	A	1352[B]	-	-	0/16/32/32	0/3/3/3
3	GOL	B	1353	-	-	0/4/4/4	-
3	GOL	B	1354	-	-	0/4/4/4	-
2	ADP	B	1352	5	-	0/16/32/32	0/3/3/3
3	GOL	A	1355	6	-	0/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1352[B]	ADP	PB-O2B	-5.14	1.35	1.54
2	A	1352[A]	ADP	C5-C4	4.74	1.47	1.39
3	B	1356	GOL	O1-C1	-4.51	1.23	1.42
2	B	1352	ADP	C5-C4	4.11	1.46	1.39
2	A	1352[B]	ADP	C5-C4	3.75	1.45	1.39
2	A	1352[B]	ADP	C5-N7	-3.64	1.32	1.39
2	A	1352[B]	ADP	O4'-C4'	-3.22	1.37	1.45
2	A	1352[B]	ADP	C4-N9	-2.83	1.31	1.37
2	B	1352	ADP	C8-N7	2.82	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1352[B]	ADP	C8-N9	-2.78	1.32	1.37
2	A	1352[A]	ADP	C5-C6	2.76	1.48	1.41
2	A	1352[B]	ADP	PA-O2A	-2.73	1.42	1.55
2	B	1352	ADP	C5-C6	2.40	1.47	1.41
2	A	1352[A]	ADP	C8-N7	2.38	1.36	1.31
2	B	1352	ADP	C5-N7	-2.30	1.34	1.39
2	A	1352[B]	ADP	C5-C6	2.28	1.47	1.41
2	A	1352[A]	ADP	C5-N7	-2.25	1.35	1.39
2	B	1352	ADP	PB-O3B	-2.19	1.46	1.54
2	A	1352[B]	ADP	C2'-C1'	-2.05	1.47	1.53
2	B	1352	ADP	C4-N9	-2.01	1.33	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1352[B]	ADP	O3A-PB-O1B	-6.61	76.25	111.04
3	B	1356	GOL	O1-C1-C2	6.02	137.49	110.38
2	A	1352[A]	ADP	C5-C4-N3	-5.84	118.68	126.72
2	A	1352[B]	ADP	C5-C4-N3	-5.23	119.51	126.72
2	A	1352[B]	ADP	N3-C4-N9	4.62	135.03	127.17
2	A	1352[A]	ADP	N3-C4-N9	4.60	134.99	127.17
2	A	1352[B]	ADP	O3B-PB-O1B	-4.39	93.74	110.83
2	B	1352	ADP	C4-N9-C8	4.08	110.02	105.74
2	A	1352[B]	ADP	O3B-PB-O3A	3.92	117.77	104.64
2	A	1352[A]	ADP	C2-N3-C4	3.70	120.87	111.83
2	A	1352[B]	ADP	C2-N3-C4	3.68	120.81	111.83
2	A	1352[B]	ADP	N3-C2-N1	-3.66	123.04	128.58
2	A	1352[B]	ADP	O3B-PB-O2B	3.55	121.12	107.80
2	A	1352[A]	ADP	C4-C5-N7	-3.49	106.59	110.58
2	A	1352[B]	ADP	O2B-PB-O3A	3.33	115.81	104.64
2	A	1352[A]	ADP	N3-C2-N1	-3.21	123.72	128.58
2	A	1352[B]	ADP	C2-N1-C6	3.20	123.99	118.73
2	B	1352	ADP	C5-C4-N3	-3.13	122.41	126.72
2	B	1352	ADP	N3-C4-N9	3.03	132.31	127.17
2	B	1352	ADP	C2-N1-C6	2.85	123.41	118.73
2	B	1352	ADP	N9-C8-N7	-2.81	109.95	113.94
2	B	1352	ADP	N3-C2-N1	-2.78	124.38	128.58
2	A	1352[B]	ADP	O2B-PB-O1B	2.68	121.29	110.83
2	A	1352[B]	ADP	N6-C6-N1	2.67	124.32	118.38
2	A	1352[A]	ADP	C4-N9-C8	2.59	108.46	105.74
2	A	1352[A]	ADP	C5-N7-C8	2.55	107.46	103.45
2	A	1352[A]	ADP	C3'-C2'-C1'	2.54	106.27	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1352	ADP	O3A-PA-O1A	-2.51	103.16	110.70
2	B	1352	ADP	C4-C5-N7	-2.48	107.75	110.58
2	B	1352	ADP	O3B-PB-O3A	2.32	112.43	104.64
2	B	1352	ADP	C5-N7-C8	2.27	107.02	103.45
2	B	1352	ADP	O2A-PA-O1A	2.15	122.46	112.44
2	A	1352[A]	ADP	C6-C5-N7	2.08	136.11	132.09
3	B	1353	GOL	C3-C2-C1	-2.06	104.24	111.80
2	B	1352	ADP	C2-N3-C4	2.05	116.83	111.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1353	GOL	C1-C2-C3-O3
3	A	1353	GOL	O2-C2-C3-O3
3	A	1354	GOL	O1-C1-C2-C3
3	B	1356	GOL	O1-C1-C2-O2
3	B	1356	GOL	O1-C1-C2-C3
3	B	1356	GOL	C1-C2-C3-O3
3	A	1354	GOL	O1-C1-C2-O2
3	B	1355	GOL	O1-C1-C2-O2
3	A	1353	GOL	O1-C1-C2-O2

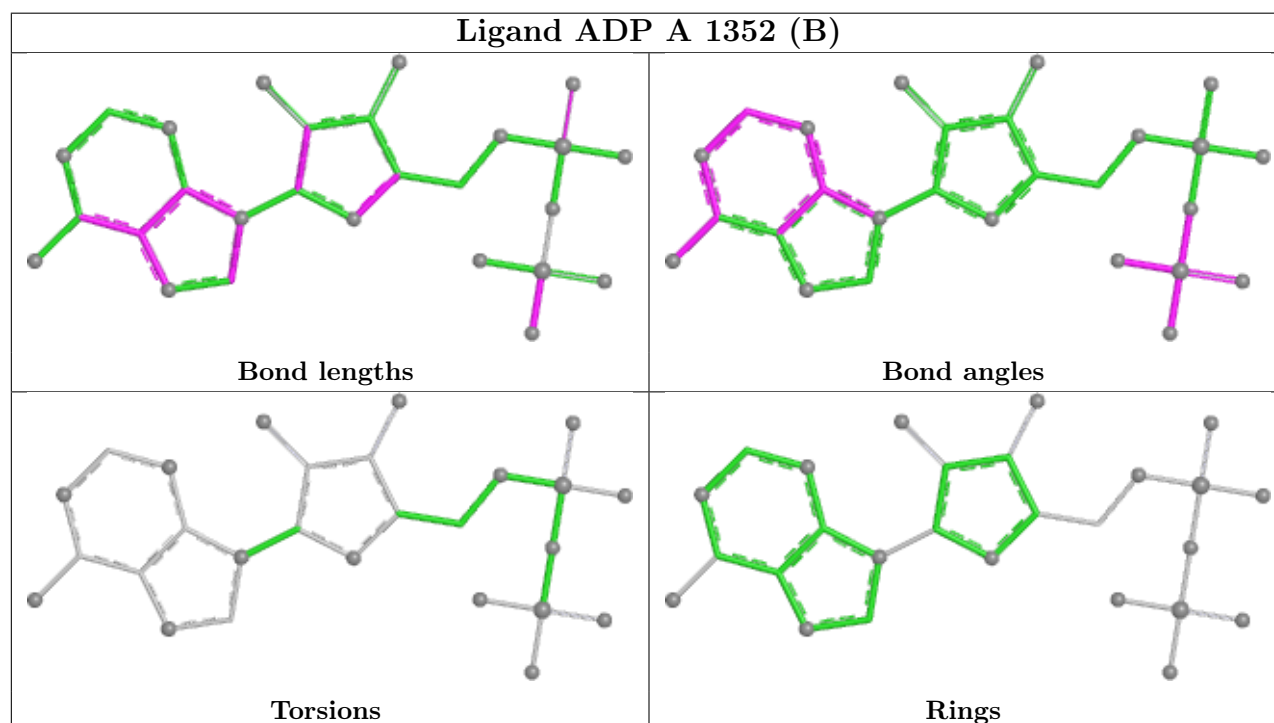
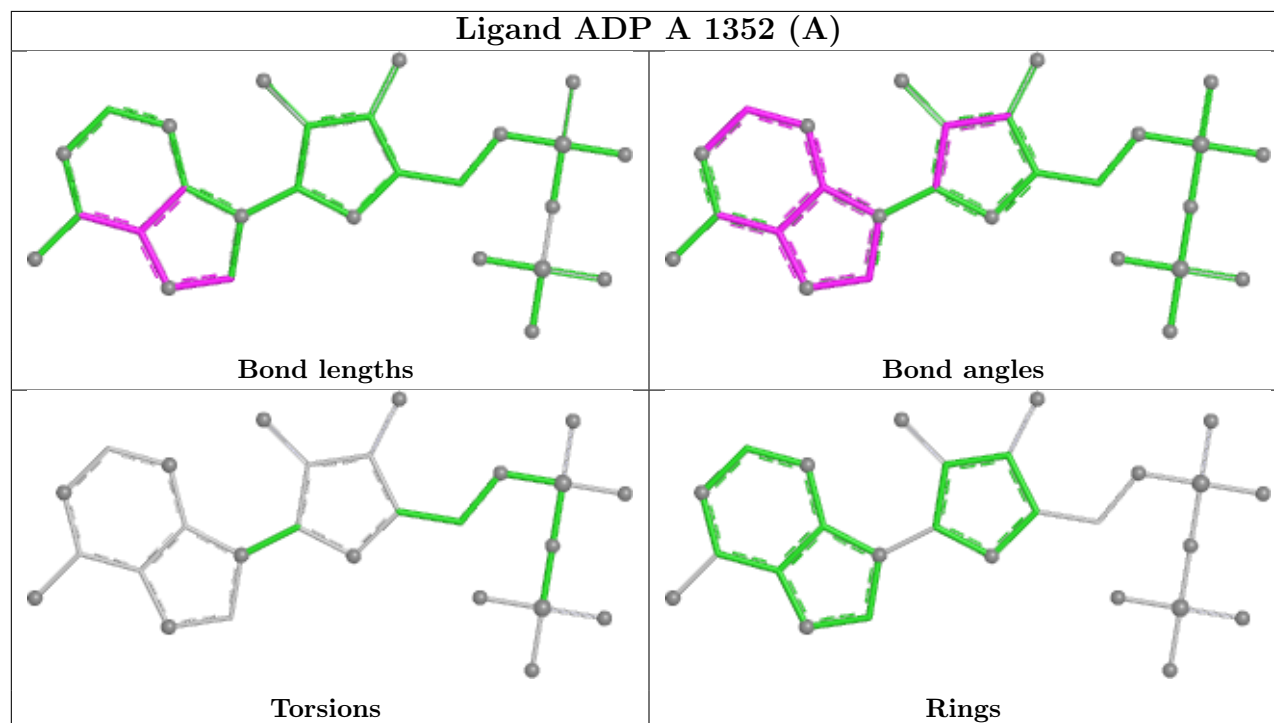
There are no ring outliers.

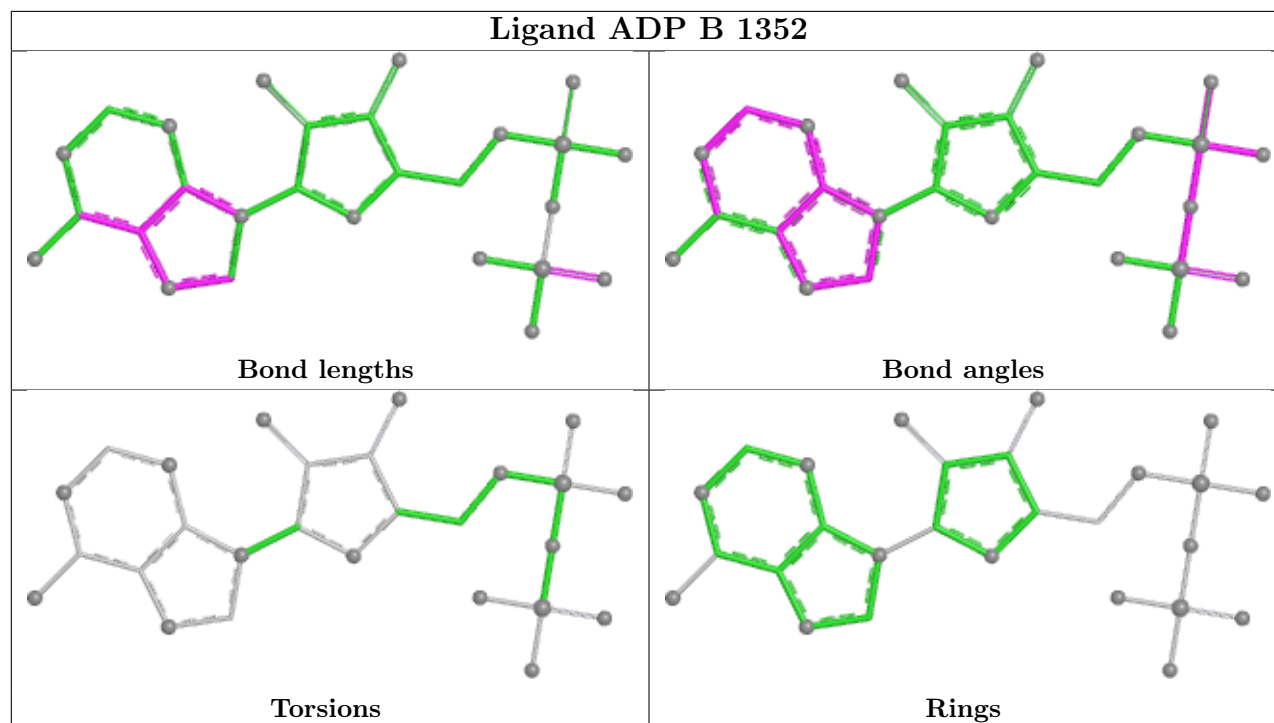
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1352[A]	ADP	2	0
3	A	1354	GOL	1	0
3	A	1353	GOL	2	0
3	B	1356	GOL	5	0
2	A	1352[B]	ADP	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	56:ASN	C	57:GLU	N	1.12

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	316/325 (97%)	0.53	41 (12%) 7 13	8, 23, 63, 85	14 (4%)
1	B	315/325 (96%)	-0.03	5 (1%) 70 80	6, 17, 32, 55	18 (5%)
All	All	631/650 (97%)	0.25	46 (7%) 21 30	6, 20, 57, 85	32 (5%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	LEU	5.9
1	A	202	LEU	4.8
1	A	351	GLY	4.7
1	B	351	GLY	4.3
1	A	36	HIS	4.0
1	A	201	LEU	3.9
1	A	222	PHE	3.8
1	A	226	LEU	3.7
1	A	259	ILE	3.7
1	A	266	ALA	3.5
1	A	231	VAL	3.4
1	A	350	GLY	3.4
1	A	232	ASP	3.3
1	A	264	ALA	3.3
1	A	262	ALA	3.3
1	A	265	PRO	3.1
1	A	213	ALA	3.0
1	A	214	ALA	2.9
1	A	229	VAL	2.9
1	A	220	GLU	2.8
1	A	254	VAL	2.7
1	A	233	GLY	2.7
1	A	224	ARG	2.6
1	A	289	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	218	VAL	2.5
1	B	320	PHE	2.4
1	A	206	TYR	2.4
1	A	230	ASP	2.4
1	A	227	ARG	2.4
1	A	85[A]	ARG	2.3
1	A	235	PRO	2.3
1	B	321	ALA	2.2
1	A	90	GLU	2.2
1	A	255	LEU	2.2
1	A	209	GLY	2.2
1	B	350	GLY	2.1
1	A	236	VAL	2.1
1	A	237	PHE	2.1
1	A	221	ASN	2.1
1	A	189[A]	VAL	2.1
1	A	269	VAL	2.1
1	A	216	GLY	2.1
1	A	228	SER	2.0
1	A	210	GLY	2.0
1	A	198	ALA	2.0
1	A	253	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	1355	6/6	0.69	0.21	48,54,55,55	0

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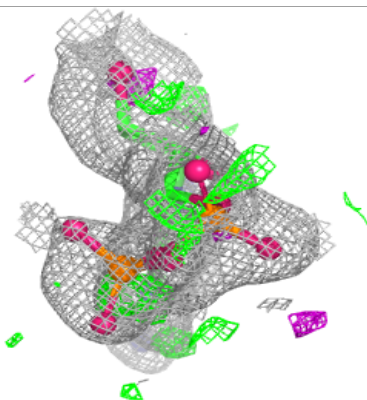
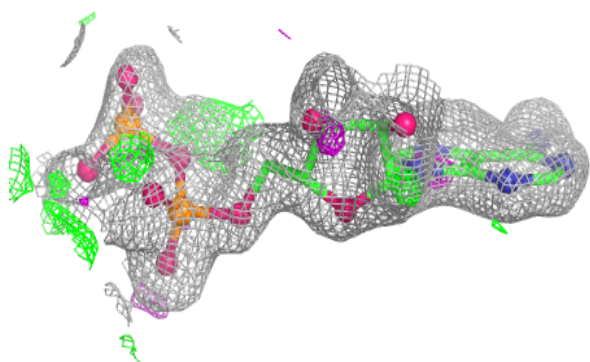
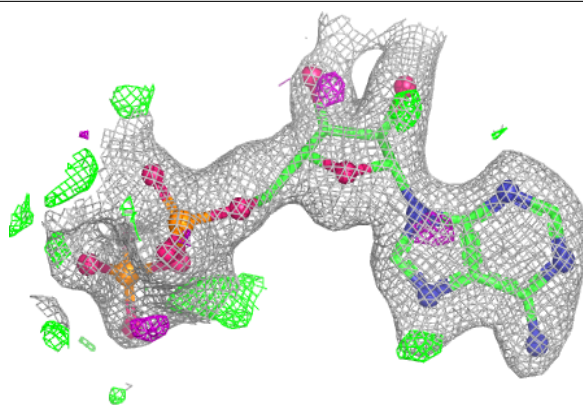
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	1356	6/6	0.83	0.16	17,22,31,34	6
2	ADP	A	1352[A]	27/27	0.87	0.11	29,34,45,48	27
2	ADP	A	1352[B]	27/27	0.87	0.11	17,26,31,34	27
3	GOL	A	1353	6/6	0.90	0.12	21,33,36,38	0
3	GOL	A	1354	6/6	0.91	0.10	28,36,37,41	0
3	GOL	B	1353	6/6	0.91	0.11	16,21,32,35	0
3	GOL	A	1355	6/6	0.95	0.07	24,24,26,27	0
3	GOL	B	1354	6/6	0.95	0.07	21,22,23,24	0
5	MG	B	1359	1/1	0.96	0.08	21,21,21,21	0
4	K	B	1357	1/1	0.97	0.09	26,26,26,26	1
5	MG	B	1361	1/1	0.97	0.06	26,26,26,26	0
6	CA	A	1359	1/1	0.97	0.14	30,30,30,30	0
4	K	B	1358	1/1	0.98	0.05	16,16,16,16	0
4	K	A	1357[A]	1/1	0.98	0.05	32,32,32,32	1
5	MG	B	1360	1/1	0.98	0.06	28,28,28,28	0
4	K	A	1357[B]	1/1	0.98	0.05	15,15,15,15	1
4	K	A	1356	1/1	0.98	0.04	18,18,18,18	0
2	ADP	B	1352	27/27	0.99	0.04	12,14,18,26	0
5	MG	A	1358	1/1	0.99	0.11	18,18,18,18	1

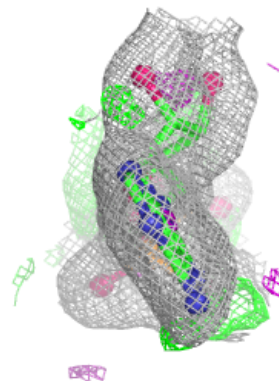
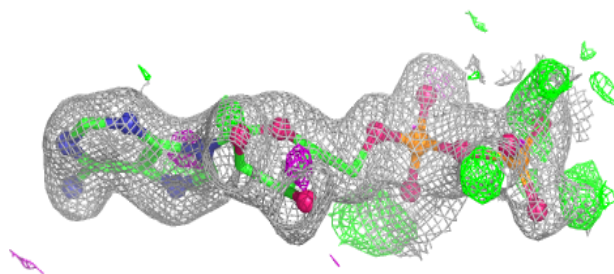
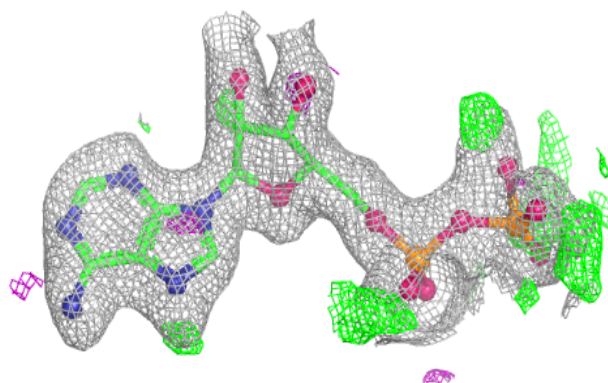
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

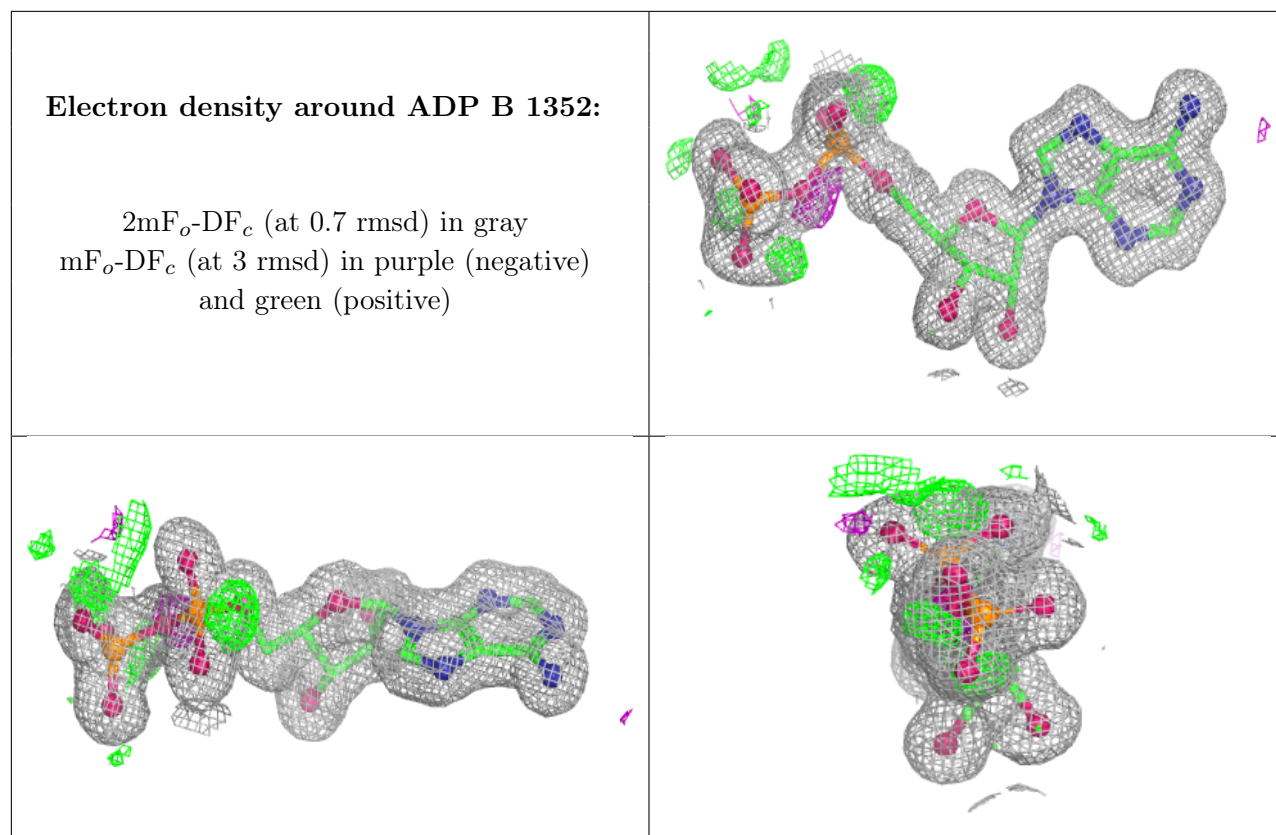
Electron density around ADP A 1352 (A):

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

**Electron density around ADP A 1352 (B):**

$2mF_o-DF_c$ (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.