



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 05:16 AM UTC

PDB ID : 8CAV / pdb_00008cav
Title : Discovery of the lanthipeptide Curvocidin and structural insights into its tri-functional synthetase CuvL
Authors : Sigurdsson, A.; Martins, B.M.; Duettmann, S.A.; Jasyk, M.; Dimos-Roehl, B.; Schoepf, F.; Gemanter, M.; Knittel, C.H.; Schnegotyzki, R.; Schmid, B.; Kosol, S.; Gonzalez-Viegas, M.; Seidel, M.; Huegelland, M.; Leimkuehler, S.; Dobbek, H.; Mainz, A.; Suessmuth, R.
Deposited on : 2023-01-24
Resolution : 2.87 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	: FAILED
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)

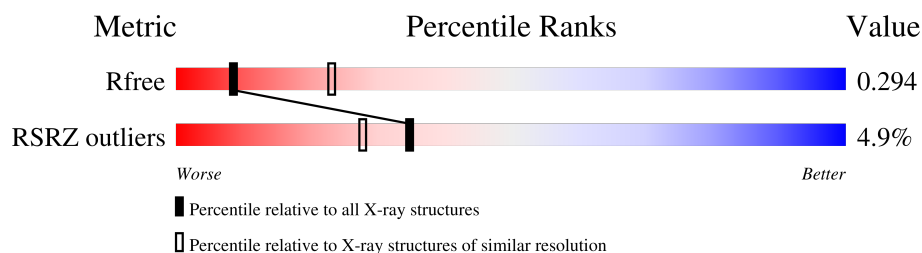
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26231 atoms, of which 12973 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 Serine/threonine protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	860	Total	C	H	N	O	S	0	4	0
			12962	4075	6434	1223	1209	21			
1	B	858	Total	C	H	N	O	S	0	0	0
			12800	4029	6336	1213	1201	21			

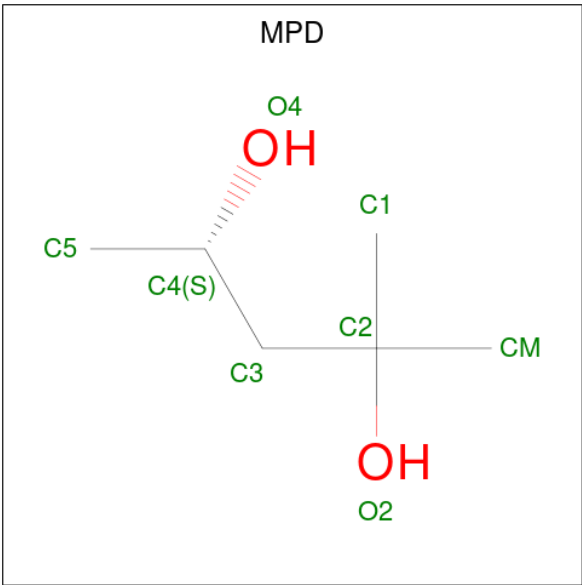
- Molecule 2 is a protein called CuvA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	20	Total	C	H	N	O	0	0	0
			182	59	83	20	20			
2	G	11	Total	C	H	N	O	0	0	0
			94	33	39	11	11			

There are 6 discrepancies between the modelled and reference sequences:

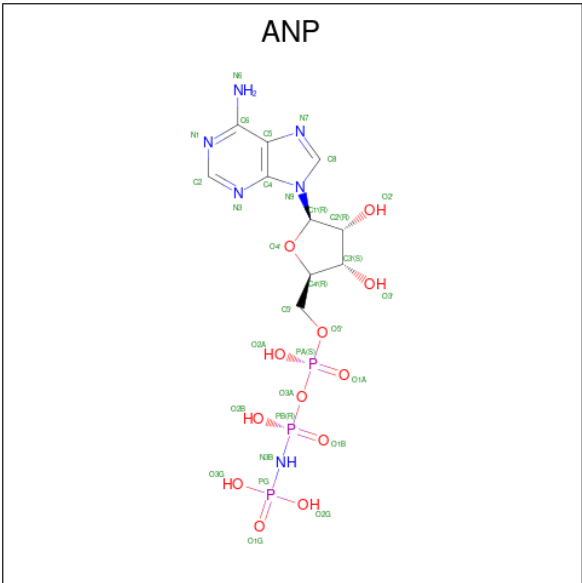
Chain	Residue	Modelled	Actual	Comment	Reference
D	12	ILE	VAL	conflict	UNP D1A2F9
D	13	LYS	PRO	conflict	UNP D1A2F9
D	14	TRP	SER	conflict	UNP D1A2F9
G	116	ILE	VAL	conflict	UNP D1A2F9
G	117	LYS	PRO	conflict	UNP D1A2F9
G	118	TRP	SER	conflict	UNP D1A2F9

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	B	1	Total	C	H	O	0	0
			22	6	14	2		
3	B	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	
			44	10	13	6	12	3	
4	B	1	Total	C	H	N	O	P	
			43	10	12	6	12	3	

- 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	1	Total	Mg		
			1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O		
			13	13	0	0
6	B	3	Total	O		
			3	3	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.37Å 116.13Å 97.41Å 90.00° 106.25° 90.00°	Depositor
Resolution (Å)	46.76 – 2.87 46.76 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.2 (46.76-2.87) 98.4 (46.76-2.87)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.237 , 0.293 0.237 , 0.294	Depositor DCC
R_{free} test set	2039 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 71.9	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	0.91	EDS
Total number of atoms	26231	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 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	$\# Z > 2$
4	ANP	B	1102	5	33,33,33	0.95	4 (12%)	45,52,52	0.72	1 (2%)
3	MPD	A	1001	-	7,7,7	0.31	0	9,10,10	0.42	0
3	MPD	B	1103	-	7,7,7	0.29	0	9,10,10	0.33	0
3	MPD	A	1002	-	7,7,7	0.35	0	9,10,10	0.33	0
4	ANP	A	1003	5	33,33,33	1.02	4 (12%)	45,52,52	0.71	1 (2%)
3	MPD	B	1101	-	7,7,7	0.43	0	9,10,10	0.79	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
4	ANP	B	1102	5	-	5/18/38/38	0/3/3/3
3	MPD	A	1001	-	-	0/5/5/5	-
3	MPD	B	1103	-	-	0/5/5/5	-
3	MPD	A	1002	-	-	1/5/5/5	-
4	ANP	A	1003	5	-	7/18/38/38	0/3/3/3
3	MPD	B	1101	-	-	5/5/5/5	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	ANP	PB-O3A	-2.88	1.55	1.59
4	A	1003	ANP	PG-O1G	2.78	1.50	1.46
4	B	1102	ANP	PG-O1G	2.61	1.50	1.46
4	B	1102	ANP	PG-N3B	2.54	1.70	1.63
4	A	1003	ANP	PG-N3B	2.36	1.69	1.63
4	B	1102	ANP	PB-O1B	2.36	1.49	1.46
4	A	1003	ANP	PB-O1B	2.31	1.49	1.46
4	B	1102	ANP	PB-O3A	-2.12	1.56	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	ANP	O1G-PG-N3B	-2.21	108.52	111.77
4	B	1102	ANP	O1G-PG-N3B	-2.13	108.63	111.77

There are no chirality outliers.

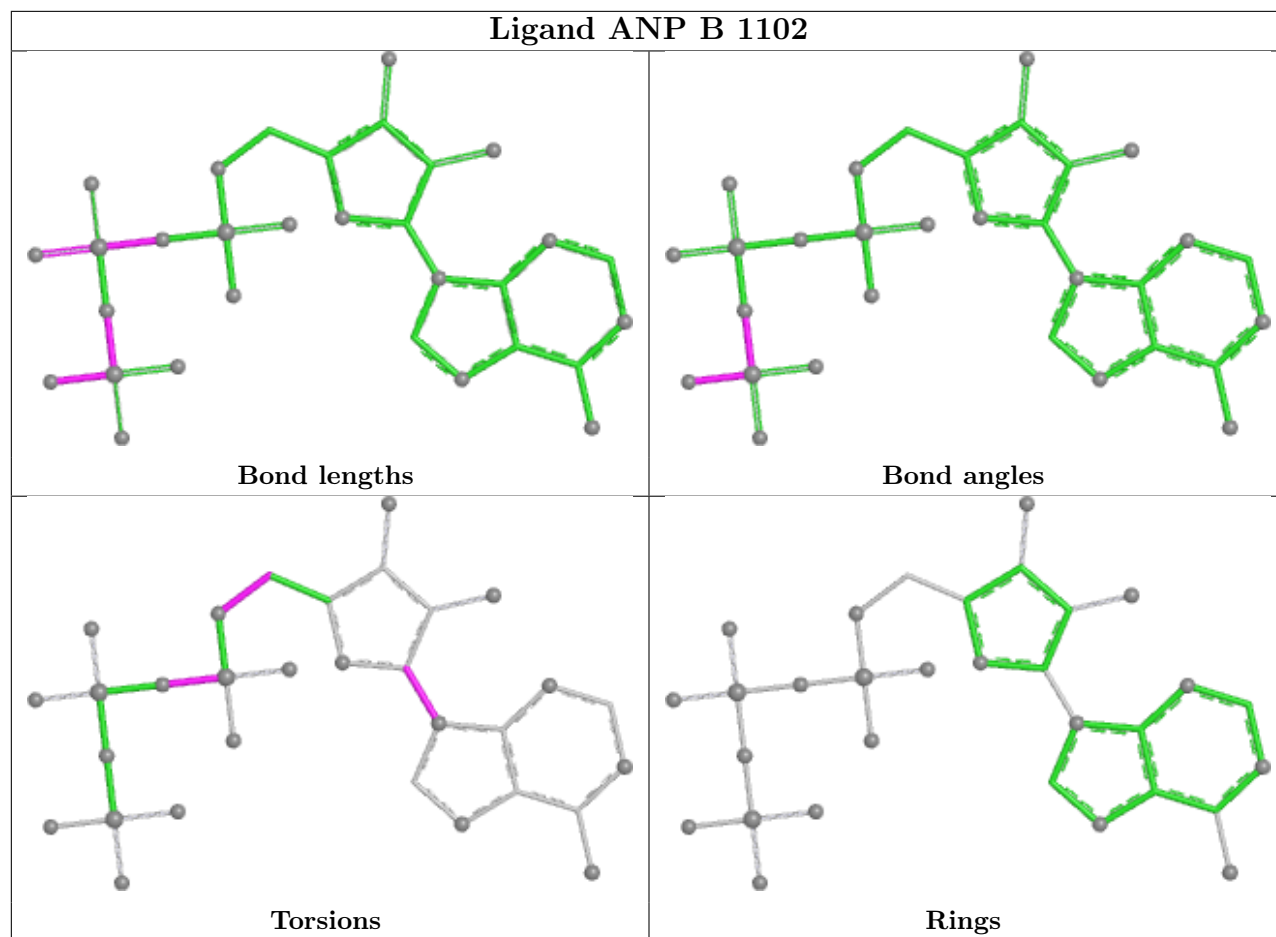
All (18) torsion outliers are listed below:

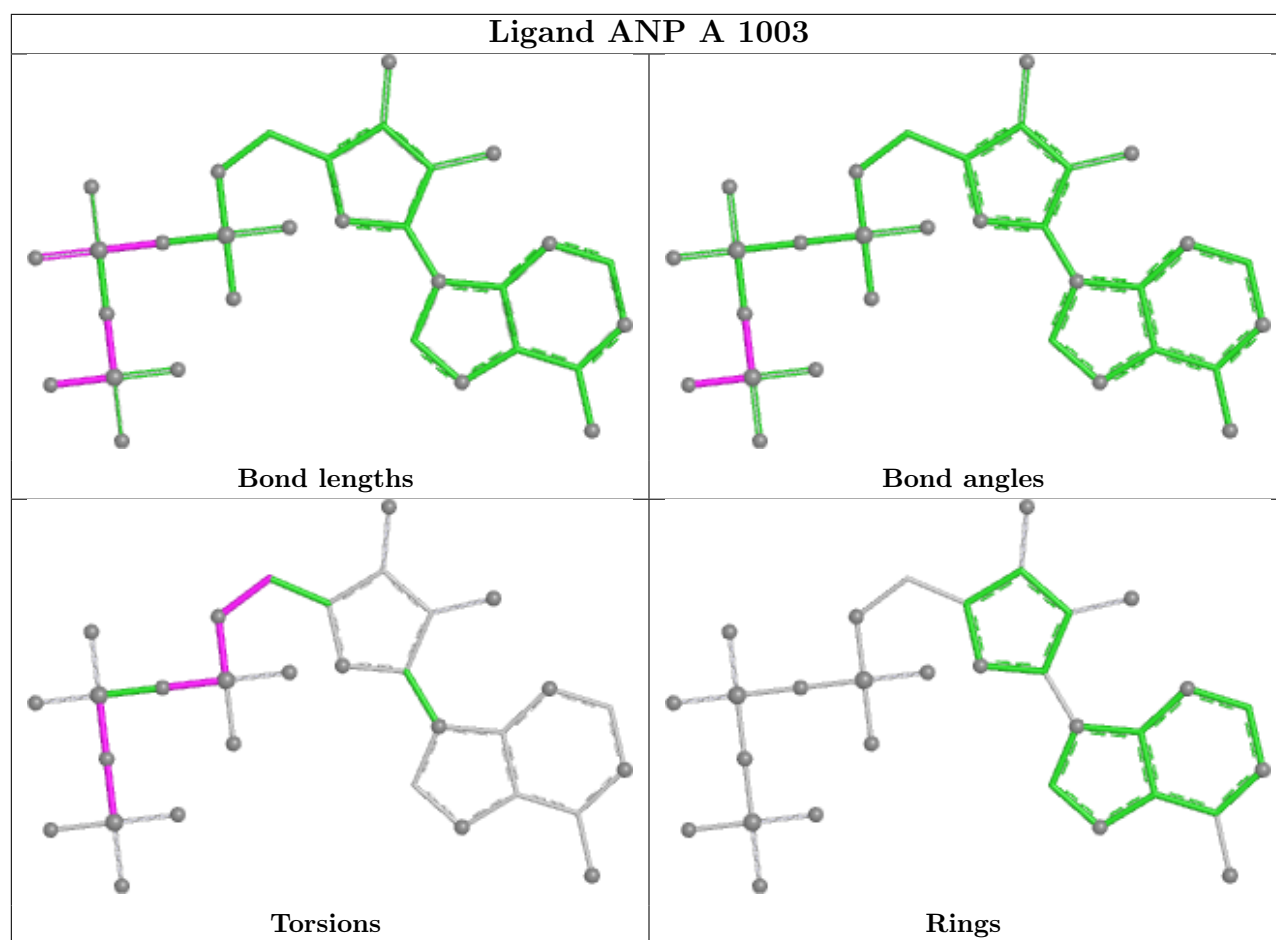
Mol	Chain	Res	Type	Atoms
3	B	1101	MPD	C2-C3-C4-C5
4	A	1003	ANP	PB-N3B-PG-O1G
4	A	1003	ANP	PG-N3B-PB-O1B
4	A	1003	ANP	PB-O3A-PA-O5'
4	A	1003	ANP	C5'-O5'-PA-O2A
4	A	1003	ANP	C5'-O5'-PA-O3A
4	B	1102	ANP	PB-O3A-PA-O5'
4	B	1102	ANP	C4'-C5'-O5'-PA
3	A	1002	MPD	O2-C2-C3-C4
4	B	1102	ANP	C2'-C1'-N9-C4
4	B	1102	ANP	C2'-C1'-N9-C8
4	A	1003	ANP	C4'-C5'-O5'-PA
4	B	1102	ANP	PB-O3A-PA-O1A
3	B	1101	MPD	O2-C2-C3-C4
3	B	1101	MPD	C2-C3-C4-O4
3	B	1101	MPD	C1-C2-C3-C4
3	B	1101	MPD	CM-C2-C3-C4
4	A	1003	ANP	PG-N3B-PB-O3A

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 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.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	860/865 (99%)	0.25	32 (3%) 45 37	29, 62, 123, 196	4 (0%)
1	B	858/865 (99%)	0.32	40 (4%) 36 29	32, 70, 126, 191	0
2	D	20/51 (39%)	1.94	7 (35%) 1 1	78, 95, 124, 158	0
2	G	11/51 (21%)	1.68	6 (54%) 0 0	73, 102, 137, 138	0
All	All	1749/1832 (95%)	0.32	85 (4%) 35 28	29, 67, 126, 196	4 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	662	CYS	4.4
1	A	225	ASN	4.2
2	D	18	ALA	3.9
1	A	514	THR	3.7
1	B	361	THR	3.7
1	B	227	LYS	3.4
1	A	221	GLY	3.3
2	D	7	ASP	3.2
2	D	2	GLY	3.2
1	A	650	ALA	3.1
1	B	203	SER	3.1
1	B	481	SER	3.1
1	B	214	GLY	3.0
1	B	480	PRO	3.0
1	A	43[A]	HIS	3.0
1	A	72	LEU	2.9
2	D	4	THR	2.9
1	B	200	PRO	2.9
1	A	648	LEU	2.8
1	A	226	GLY	2.8
1	A	59	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	362	GLY	2.7
1	B	374	ALA	2.7
1	B	94	ASN	2.7
1	A	71	VAL	2.7
1	B	444	MET	2.7
1	B	719	VAL	2.7
1	A	286	HIS	2.6
2	G	121	PRO	2.6
1	B	301	GLY	2.6
1	B	721	ALA	2.6
1	B	720	SER	2.6
1	B	360	ALA	2.6
1	A	6	ALA	2.5
1	B	655	ASN	2.5
1	B	666	SER	2.5
1	A	665	VAL	2.5
1	A	812	ALA	2.5
1	B	649	THR	2.5
1	B	863	THR	2.5
1	A	642[A]	ARG	2.4
2	G	123	HIS	2.4
1	A	20	PRO	2.4
1	B	479	PRO	2.4
1	B	201	ALA	2.3
1	A	655	ASN	2.3
1	B	177	GLY	2.3
1	A	22	THR	2.3
1	B	447	THR	2.3
1	B	386	TYR	2.3
1	A	198	PRO	2.3
1	A	657	PRO	2.3
1	B	209	PRO	2.3
1	B	466	ILE	2.3
2	D	14	TRP	2.3
1	A	862	GLY	2.3
1	B	344	GLY	2.3
1	A	861	ALA	2.2
1	B	293	GLU	2.2
1	B	202	PRO	2.2
2	D	6	LEU	2.2
1	A	121	ALA	2.2
1	A	485	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	117	LYS	2.2
1	A	652	LEU	2.2
2	G	122	ALA	2.2
2	D	19	HIS	2.1
1	A	214	GLY	2.1
1	B	223	THR	2.1
1	B	471	PHE	2.1
1	B	648	LEU	2.1
1	B	439	ALA	2.1
2	G	120	ALA	2.1
2	G	116	ILE	2.1
1	A	649	THR	2.1
1	B	482	ALA	2.1
1	B	650	ALA	2.1
1	A	177	GLY	2.0
1	A	664	ALA	2.0
1	B	55	ALA	2.0
1	A	34	TRP	2.0
1	A	196	ALA	2.0
1	B	184	TRP	2.0
1	A	37	VAL	2.0
1	B	316	VAL	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MPD	B	1103	8/8	0.51	0.19	84,102,110,112	0

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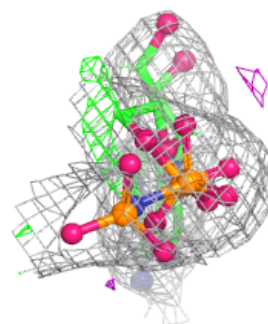
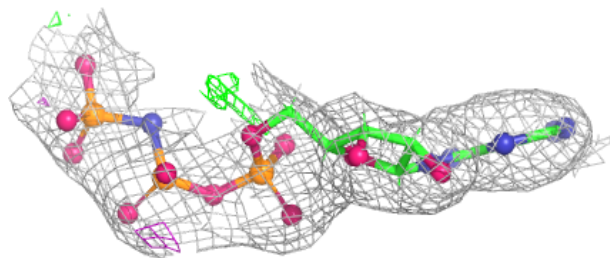
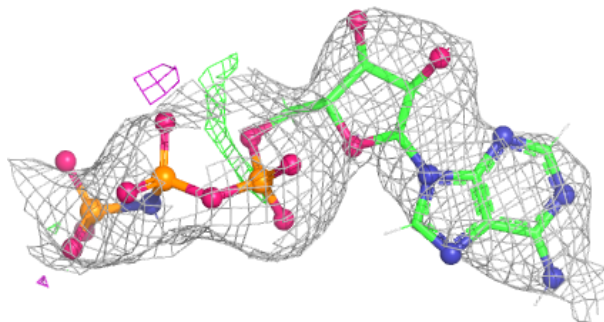
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MPD	A	1002	8/8	0.60	0.14	15,15,81,81	0
3	MPD	B	1101	8/8	0.67	0.14	15,15,88,88	0
5	MG	B	1104	1/1	0.76	0.23	86,86,86,86	0
4	ANP	B	1102	31/31	0.86	0.12	63,88,106,123	0
4	ANP	A	1003	31/31	0.86	0.11	54,74,99,120	0
5	MG	A	1004	1/1	0.94	0.07	56,56,56,56	0
3	MPD	A	1001	8/8	0.94	0.13	15,15,69,69	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.

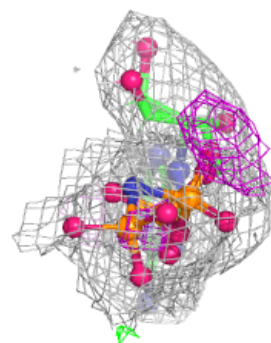
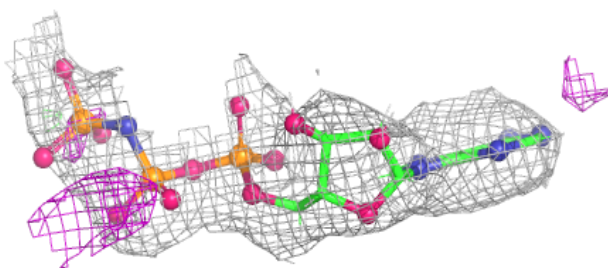
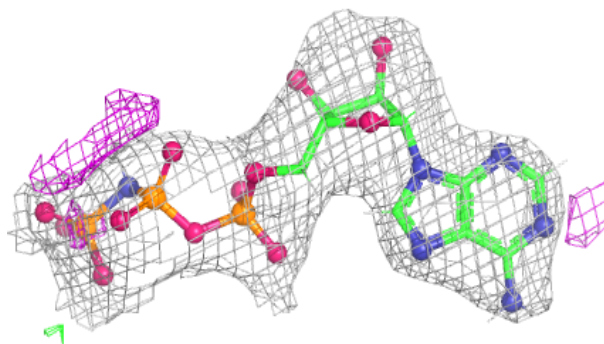
Electron density around ANP B 1102:

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 ANP A 1003:

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



5.5 Other polymers [i](#)

There are no such residues in this entry.