



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:11 AM UTC

PDB ID : 4YIY / pdb_00004yiy
Title : Structure of MRB1590 bound to AMP-PNP
Authors : Shaw, P.L.R.; Schumacher, M.A.
Deposited on : 2015-03-02
Resolution : 3.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

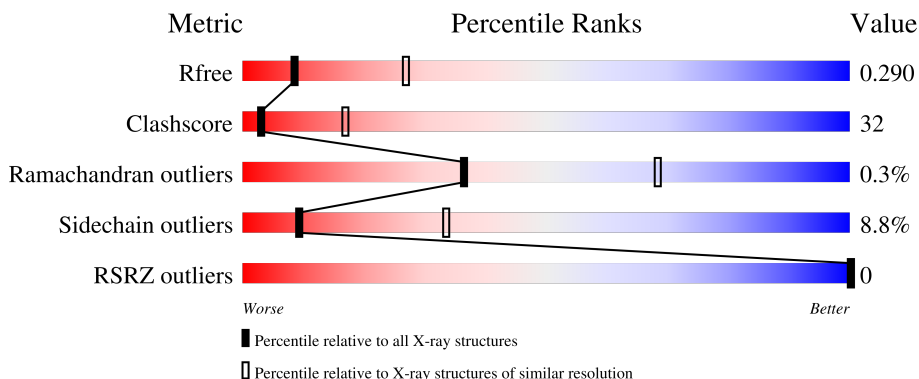
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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 $\leq 5\%$. 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	680	
1	B	680	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8916 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 kRNA Editing A6 Specific Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	577	Total	C	N	O	S	0	0	0
			4416	2763	782	845	26			
1	A	577	Total	C	N	O	S	0	0	0
			4418	2763	783	846	26			

There are 46 discrepancies between the modelled and reference sequences:

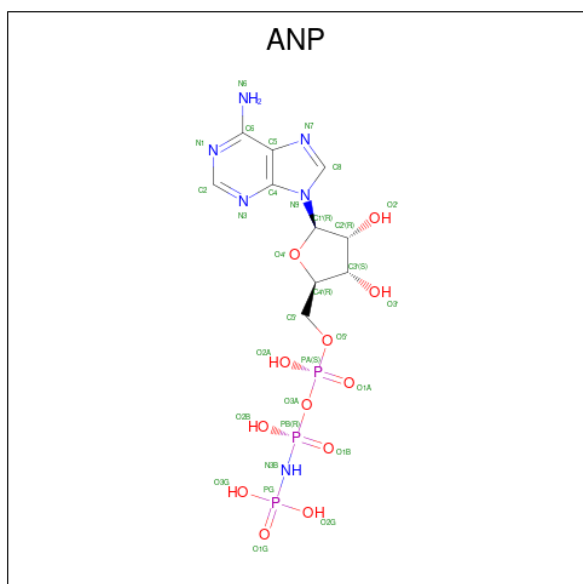
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP Q57ZF2
B	-10	HIS	-	expression tag	UNP Q57ZF2
B	-9	HIS	-	expression tag	UNP Q57ZF2
B	-8	HIS	-	expression tag	UNP Q57ZF2
B	-7	HIS	-	expression tag	UNP Q57ZF2
B	-6	HIS	-	expression tag	UNP Q57ZF2
B	-5	HIS	-	expression tag	UNP Q57ZF2
B	-4	SER	-	expression tag	UNP Q57ZF2
B	-3	SER	-	expression tag	UNP Q57ZF2
B	-2	GLY	-	expression tag	UNP Q57ZF2
B	-1	VAL	-	expression tag	UNP Q57ZF2
B	0	ASP	-	expression tag	UNP Q57ZF2
B	1	LEU	-	expression tag	UNP Q57ZF2
B	2	GLY	-	expression tag	UNP Q57ZF2
B	3	THR	-	expression tag	UNP Q57ZF2
B	4	GLU	-	expression tag	UNP Q57ZF2
B	5	ASN	-	expression tag	UNP Q57ZF2
B	6	LEU	-	expression tag	UNP Q57ZF2
B	7	TYR	-	expression tag	UNP Q57ZF2
B	8	PHE	-	expression tag	UNP Q57ZF2
B	9	GLN	-	expression tag	UNP Q57ZF2
B	10	SER	-	expression tag	UNP Q57ZF2
B	242	GLU	VAL	conflict	UNP Q57ZF2
A	-11	MET	-	initiating methionine	UNP Q57ZF2
A	-10	HIS	-	expression tag	UNP Q57ZF2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP Q57ZF2
A	-8	HIS	-	expression tag	UNP Q57ZF2
A	-7	HIS	-	expression tag	UNP Q57ZF2
A	-6	HIS	-	expression tag	UNP Q57ZF2
A	-5	HIS	-	expression tag	UNP Q57ZF2
A	-4	SER	-	expression tag	UNP Q57ZF2
A	-3	SER	-	expression tag	UNP Q57ZF2
A	-2	GLY	-	expression tag	UNP Q57ZF2
A	-1	VAL	-	expression tag	UNP Q57ZF2
A	0	ASP	-	expression tag	UNP Q57ZF2
A	1	LEU	-	expression tag	UNP Q57ZF2
A	2	GLY	-	expression tag	UNP Q57ZF2
A	3	THR	-	expression tag	UNP Q57ZF2
A	4	GLU	-	expression tag	UNP Q57ZF2
A	5	ASN	-	expression tag	UNP Q57ZF2
A	6	LEU	-	expression tag	UNP Q57ZF2
A	7	TYR	-	expression tag	UNP Q57ZF2
A	8	PHE	-	expression tag	UNP Q57ZF2
A	9	GLN	-	expression tag	UNP Q57ZF2
A	10	SER	-	expression tag	UNP Q57ZF2
A	242	GLU	VAL	conflict	UNP Q57ZF2

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

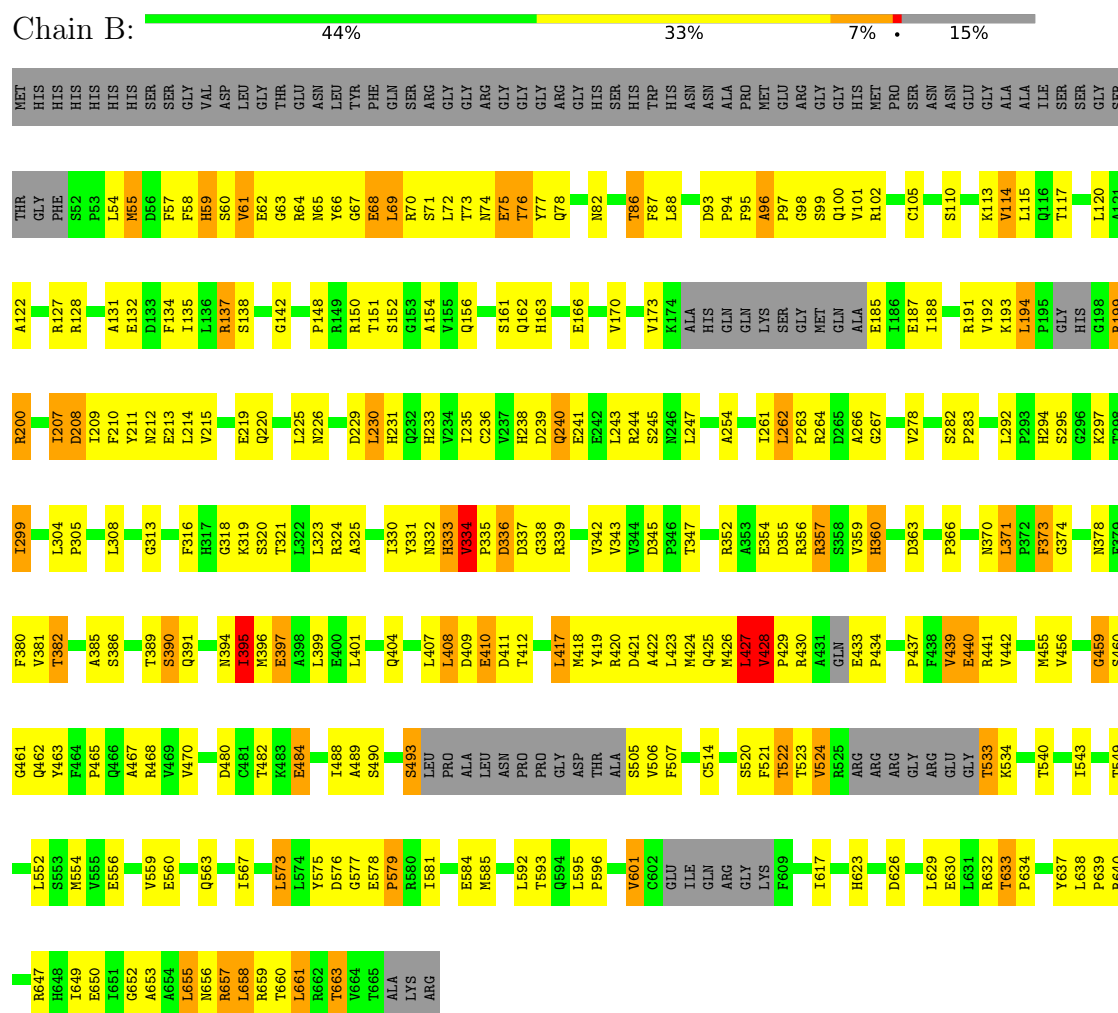
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	12	Total	O	0	0
			12	12		
4	A	4	Total	O	0	0
			4	4		

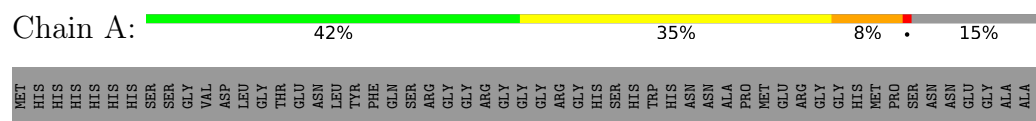
3 Residue-property plots

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: kRNA Editing A6 Specific Protein



• Molecule 1: kRNA Editing A6 Specific Protein



L631	ARG	L445	T368	H294	E200	V114	THR
G632	GLY	L445	T368	H294	E200	V114	GLY
T633	ARG	L445	T368	H294	E200	V114	PHE
P634	GLU	N448	T378	K297	G203	G126	S52
G635	GLY	H449	T378	K297	H204	R127	P53
G636	T633	L445	T378	G301	G205	L54	L54
G637	K534	S452	T379	G301	A206	A130	M55
L638	L445	S452	T379	G301	A206	A130	S55
P639	E556	S453	T381	P305	T207	A131	S56
G640	L454	T382	T382	P305	D208	E132	F57
G641	M455	M455	A383	L308	D209	D133	F58
G642	V456	V456	A383	L308	F210	F134	H59
T643	V559	V559	A383	L310	Y211	I135	S60
G644	V560	V560	A385	L310	M212	L136	V61
G645	E561	G458	S386	G313	E213	R137	G62
G646	G562	G459	S387	G313	L214	G62	G63
G647	G563	G461	T389	G315	Y215	I147	R64
G648	L567	Q462	S390	F316	P216	P148	N65
I649	A568	Y463	Q391	H317	L217	R149	Y66
G650	Q569	Q466	T395	G318	Q220	R150	G87
G651	L573	Q466	T395	K319	Q221	A154	E88
A653	L574	A467	S392	G320	V222	V155	R69
A654	L574	A467	E397	S320	Q221	V155	L70
L655	Y575	V469	A398	L322	L225	Q156	S71
M656	D576	V470	L399	L323	R226	R159	L72
G657	G577	Y470	E400	R324	E227	P160	T73
L658	E578	Y476	L401	Q324	Q227	S161	N74
R659	PRO	Y476	L401	Q324	Q227	S161	E75
T660	D480	D480	L405	G329	L230	Q162	T76
L661	L581	C481	L406	L330	H231	H163	Y77
R662	V582	T482	L407	T331	Q232	H163	Y77
T663	P583	L408	L408	S332	H233	V164	Q78
V664	A584	A485	D409	H333	V234	L165	I79
T665	M585	E584	E410	P335	T235	V170	S80
ALA	T586	L488	D411	P335	C236	G171	N82
LYS	T587	L488	T412	D337	V237	L172	V83
ARG	K588	S493	T412	D337	H238	V173	R84
L690	L592	L590	L417	G338	D239	K174	C85
L691	L592	L590	N418	R339	Q240	ALA	T86
L692	L592	L590	N418	R339	Q240	ALA	F87
L693	L592	L590	N418	R339	Q240	ALA	F87
L694	L592	L590	N418	R339	Q240	ALA	F87
L695	L592	L590	N418	R339	Q240	ALA	F87
L696	L592	L590	N418	R339	Q240	ALA	F87
L697	L592	L590	N418	R339	Q240	ALA	F87
L698	L592	L590	N418	R339	Q240	ALA	F87
L699	L592	L590	N418	R339	Q240	ALA	F87
L700	L592	L590	N418	R339	Q240	ALA	F87
L701	L592	L590	N418	R339	Q240	ALA	F87
L702	L592	L590	N418	R339	Q240	ALA	F87
L703	L592	L590	N418	R339	Q240	ALA	F87
L704	L592	L590	N418	R339	Q240	ALA	F87
L705	L592	L590	N418	R339	Q240	ALA	F87
L706	L592	L590	N418	R339	Q240	ALA	F87
L707	L592	L590	N418	R339	Q240	ALA	F87
L708	L592	L590	N418	R339	Q240	ALA	F87
L709	L592	L590	N418	R339	Q240	ALA	F87
L710	L592	L590	N418	R339	Q240	ALA	F87
L711	L592	L590	N418	R339	Q240	ALA	F87
L712	L592	L590	N418	R339	Q240	ALA	F87
L713	L592	L590	N418	R339	Q240	ALA	F87
L714	L592	L590	N418	R339	Q240	ALA	F87
L715	L592	L590	N418	R339	Q240	ALA	F87
L716	L592	L590	N418	R339	Q240	ALA	F87
L717	L592	L590	N418	R339	Q240	ALA	F87
L718	L592	L590	N418	R339	Q240	ALA	F87
L719	L592	L590	N418	R339	Q240	ALA	F87
L720	L592	L590	N418	R339	Q240	ALA	F87
L721	L592	L590	N418	R339	Q240	ALA	F87
L722	L592	L590	N418	R339	Q240	ALA	F87
L723	L592	L590	N418	R339	Q240	ALA	F87
L724	L592	L590	N418	R339	Q240	ALA	F87
L725	L592	L590	N418	R339	Q240	ALA	F87
L726	L592	L590	N418	R339	Q240	ALA	F87
L727	L592	L590	N418	R339	Q240	ALA	F87
L728	L592	L590	N418	R339	Q240	ALA	F87
L729	L592	L590	N418	R339	Q240	ALA	F87
L730	L592	L590	N418	R339	Q240	ALA	F87
L731	L592	L590	N418	R339	Q240	ALA	F87
L732	L592	L590	N418	R339	Q240	ALA	F87
L733	L592	L590	N418	R339	Q240	ALA	F87
L734	L592	L590	N418	R339	Q240	ALA	F87
L735	L592	L590	N418	R339	Q240	ALA	F87
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L737	L592	L590	N418	R339	Q240	ALA	F87
L738	L592	L590	N418	R339	Q240	ALA	F87
L739	L592	L590	N418	R339	Q240	ALA	F87
L740	L592	L590	N418	R339	Q240	ALA	F87
L741	L592	L590	N418	R339	Q240	ALA	F87
L742	L592	L590	N418	R339	Q240	ALA	F87
L743	L592	L590	N418	R339	Q240	ALA	F87
L744	L592	L590	N418	R339	Q240	ALA	F87
L745	L592	L590	N418	R339	Q240	ALA	F87
L746	L592	L590	N418	R339	Q240	ALA	F87
L747	L592	L590	N418	R339	Q240	ALA	F87
L748	L592	L590	N418	R339	Q240	ALA	F87
L749	L592	L590	N418	R339	Q240	ALA	F87
L750	L592	L590	N418	R339	Q240	ALA	F87
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L752	L592	L590	N418	R339	Q240	ALA	F87
L753	L592	L590	N418	R339	Q240	ALA	F87
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L757	L592	L590	N418	R339	Q240	ALA	F87
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L759	L592	L590	N418	R339	Q240	ALA	F87
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L761	L592	L590	N418	R339	Q240	ALA	F87
L762	L592	L590	N418	R339	Q240	ALA	F87
L763	L592	L590	N418	R339	Q240	ALA	F87
L764	L592	L590	N418	R339	Q240	ALA	F87
L765	L592	L590	N418	R339	Q240	ALA	F87
L766	L592	L590	N418	R339	Q240	ALA	F87
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L769	L592	L590	N418	R339	Q240	ALA	F87
L770	L592	L590	N418	R339	Q240	ALA	F87
L771	L592	L590	N418	R339	Q240	ALA	F87
L772	L592	L590	N418	R339	Q240	ALA	F87
L773	L592	L590	N418	R339	Q240	ALA	F87
L774	L592	L590	N418	R339	Q240	ALA	F87
L775	L592	L590	N418	R339	Q240	ALA	F87
L776	L592	L590	N418	R339	Q240	ALA	F87
L777	L592	L590	N418	R339	Q240	ALA	F87
L778	L592	L590	N418	R339	Q240	ALA	F87
L779	L592	L590	N418	R339	Q240	ALA	F87
L780	L592	L590	N418	R339	Q240	ALA	F87
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L782	L592	L590	N418	R339	Q240	ALA	F87
L783	L592	L590	N418	R339	Q240	ALA	F87
L784	L592	L590	N418	R339	Q240	ALA	F87
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L786	L592	L590	N418	R339	Q240	ALA	F87
L787	L592	L590	N418	R339	Q240	ALA	F87
L788	L592	L590	N418	R339	Q240	ALA	F87
L789	L592	L590	N418	R339	Q240	ALA	F87
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L793	L592	L590	N418	R339	Q240	ALA	F87
L794	L592	L590	N418	R339	Q240	ALA	F87
L795	L592	L590	N418	R339	Q240	ALA	F87
L796	L592	L590	N418	R339	Q240	ALA	F87
L797	L592	L590	N418	R339	Q240	ALA	F87
L798	L592	L590	N418	R339	Q240	ALA	F87
L799	L592	L590	N418	R339	Q240	ALA	F87
L800	L592	L590	N418	R339	Q240	ALA	F87
L801	L592	L590	N418	R339	Q240	ALA	F87
L802	L592	L590	N418	R339	Q240	ALA	F87
L803	L592	L590	N418	R339	Q240	ALA	F87
L804	L592	L590	N418	R339	Q240	ALA	F87
L805	L592	L590	N418	R339	Q240	ALA	F87
L806	L592	L590	N418	R339	Q240	ALA	F87
L807	L592	L590	N418	R339	Q240	ALA	F87
L808	L592	L590	N418	R339	Q240	ALA	F87
L809	L592	L590	N418	R339	Q240	ALA	F87
L810	L592	L590	N418	R339	Q240	ALA	F87
L811	L592	L590	N418	R339	Q240	ALA	F87
L812	L592	L590	N418	R339	Q240	ALA	F87
L813	L592	L590	N418	R339	Q240	ALA	F87
L814	L592	L590	N418	R339	Q240	ALA	F87
L815	L592	L590	N418	R339	Q240	ALA	F87
L816	L592	L590	N418	R339	Q240	ALA	F87
L817	L592	L590	N418	R339	Q240	ALA	F87
L818	L592	L590	N418	R339	Q240	ALA	F87
L819	L592	L590	N418	R339	Q240	ALA	F87
L820	L592	L590	N418	R339	Q240	ALA	F87
L821	L592	L590	N418	R339	Q240	ALA	F87
L822	L592	L590	N418	R339	Q240	ALA	F87
L823	L592	L590	N418	R339	Q240	ALA	F87
L824	L592	L590	N418	R339	Q240	ALA	F87
L825	L592	L590	N418	R339	Q240	ALA	F87
L826	L592	L590	N418	R339	Q240	ALA	F87
L827	L592	L590	N418	R339	Q240	ALA	F87
L828	L592	L590	N418	R339	Q240	ALA	F87
L829	L592	L590	N418	R339	Q240	ALA	F87
L830	L592	L590	N418	R339	Q240	ALA	F87
L831	L592	L590	N418	R339	Q240	ALA	F87
L832	L592	L590	N418	R339	Q240	ALA	F87
L833	L592	L590	N418	R339	Q240	ALA	F87
L834	L592	L590	N418	R339	Q240	ALA	F87
L835	L592	L590	N418	R339	Q240	ALA	F87
L836	L592	L590	N418	R339	Q240	ALA	F87
L837	L592	L590	N418	R339	Q240	ALA	F87
L838	L592	L590	N418	R339	Q240	ALA	F87
L839	L592	L590	N418	R339	Q240	ALA	F87

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.18Å 71.52Å 103.54Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	44.82 – 3.02 44.82 – 3.02	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.82-3.02) 97.6 (44.82-3.02)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.297 0.251 , 0.290	Depositor DCC
R_{free} test set	2004 reflections (7.87%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.781	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for l,k,-h-l 0.036 for -h-l,k,h 0.047 for h,-k,-h-l 0.378 for l,-k,h 0.044 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8916	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MG

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	1.10	7/4495 (0.2%)	1.27	53/6091 (0.9%)
1	B	1.10	9/4494 (0.2%)	1.20	46/6091 (0.8%)
All	All	1.10	16/8989 (0.2%)	1.24	99/12182 (0.8%)

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
1	A	0	1
1	B	0	2
All	All	0	3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	634	PRO	N-CD	-13.46	1.28	1.47
1	B	199	ARG	CA-C	6.90	1.62	1.52
1	A	659	ARG	CA-C	6.59	1.62	1.52
1	B	262	LEU	C-N	6.09	1.40	1.33
1	B	355	ASP	CA-C	-5.88	1.45	1.52

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	631	LEU	N-CA-C	-18.12	83.70	110.52
1	B	408	LEU	N-CA-C	11.08	126.92	109.07
1	B	592	LEU	N-CA-C	10.88	127.52	109.46
1	A	201	ILE	N-CA-C	10.75	121.59	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	657	ARG	CB-CA-C	-10.74	93.84	111.13

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASP	Peptide
1	B	336	ASP	Peptide
1	B	96	ALA	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	4418	0	4382	262	50
1	B	4416	0	4381	317	50
2	A	31	0	13	4	0
2	B	31	0	13	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	0	3	0
4	B	12	0	0	4	0
All	All	8916	0	8789	558	50

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 32.

The worst 5 of 558 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:114:VAL:HG23	1:B:115:LEU:CD1	1.70	1.21
1:B:576:ASP:OD2	1:B:634:PRO:HD2	1.03	1.19
1:A:57:PHE:O	1:A:60:SER:HB2	1.38	1.17
1:A:244:ARG:NH2	1:A:332:ASN:OD1	1.78	1.16
1:B:430:ARG:HA	1:B:433:GLU:HB3	1.25	1.14

The worst 5 of 50 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)
1:B:63:GLY:C	1:A:580:ARG:NH1[2_455]	0.27	1.93
1:B:69:LEU:C	1:A:632:ARG:NH2[2_455]	0.39	1.81
1:B:70:ARG:CA	1:A:632:ARG:NE[2_455]	0.55	1.65
1:B:584:GLU:CD	1:A:64:ARG:NE[2_455]	0.57	1.63
1:B:584:GLU:CG	1:A:64:ARG:NH2[2_455]	0.63	1.57

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	563/680 (83%)	535 (95%)	28 (5%)	0	100	100
1	B	563/680 (83%)	534 (95%)	26 (5%)	3 (0%)	24	59
All	All	1126/1360 (83%)	1069 (95%)	54 (5%)	3 (0%)	36	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	GLU
1	B	410	GLU
1	B	579	PRO

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	491/567 (87%)	449 (91%)	42 (9%)	10	34
1	B	491/567 (87%)	447 (91%)	44 (9%)	9	32
All	All	982/1134 (87%)	896 (91%)	86 (9%)	9	33

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	HIS
1	A	439	VAL
1	A	357	ARG
1	A	397	GLU
1	A	493	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	612	ASN
1	A	656	ASN
1	B	656	ASN
1	A	91	GLN
1	A	162	GLN

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	ANP	B	701	3	33,33,33	2.04	11 (33%)	45,52,52	2.06	13 (28%)
2	ANP	A	701	3	33,33,33	2.20	11 (33%)	45,52,52	2.83	15 (33%)

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	ANP	B	701	3	-	6/18/38/38	0/3/3/3
2	ANP	A	701	3	-	7/18/38/38	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ANP	C5-C4	4.70	1.47	1.39
2	B	701	ANP	PG-N3B	4.66	1.75	1.63
2	A	701	ANP	PB-O2B	-4.62	1.44	1.56
2	B	701	ANP	PB-N3B	4.61	1.75	1.63
2	A	701	ANP	PG-O3G	-4.41	1.45	1.56

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ANP	O1G-PG-N3B	-11.17	95.32	111.77
2	A	701	ANP	O2B-PB-O1B	6.83	124.52	109.87
2	B	701	ANP	C5-C4-N3	-5.81	118.71	126.72
2	A	701	ANP	C5-C4-N3	-5.43	119.24	126.72
2	A	701	ANP	N3-C4-N9	5.30	136.18	127.17

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

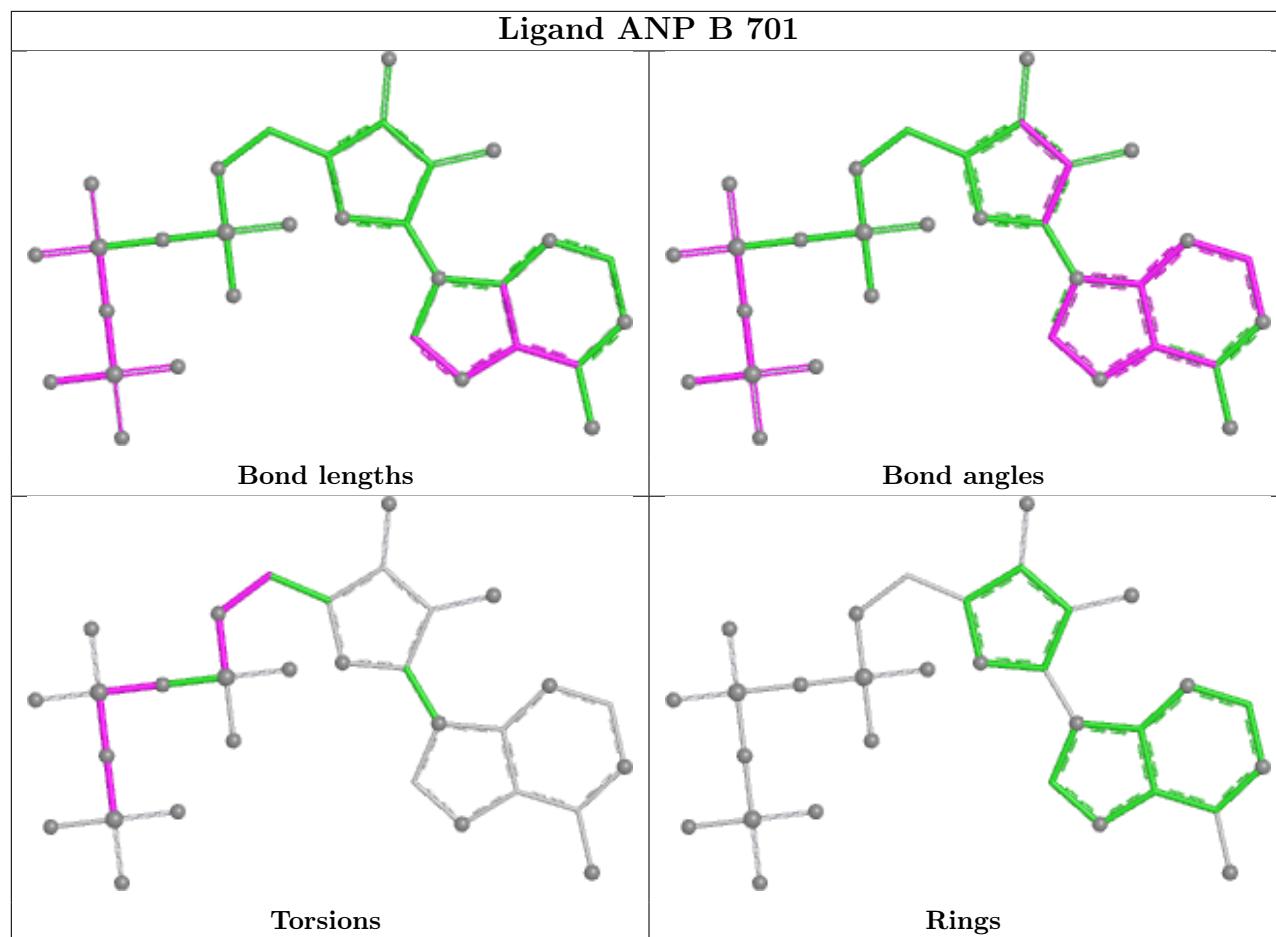
Mol	Chain	Res	Type	Atoms
2	B	701	ANP	PB-N3B-PG-O1G
2	B	701	ANP	PG-N3B-PB-O1B
2	B	701	ANP	C5'-O5'-PA-O2A
2	B	701	ANP	C5'-O5'-PA-O3A
2	A	701	ANP	PB-N3B-PG-O1G

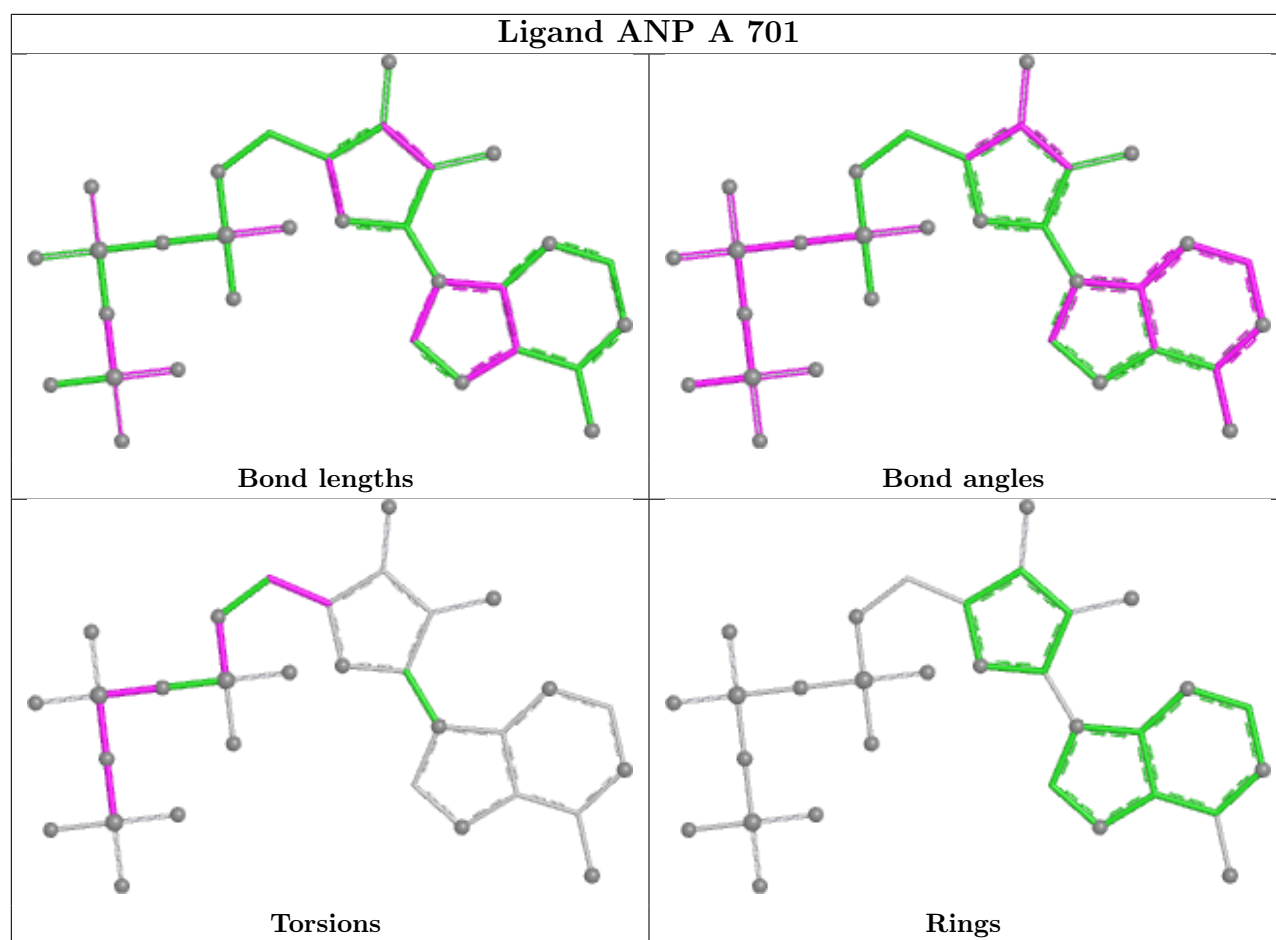
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ANP	7	0
2	A	701	ANP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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(Å ²)	Q<0.9
1	A	577/680 (84%)	-1.36	0 100 100	26, 43, 72, 80	0
1	B	577/680 (84%)	-1.31	0 100 100	26, 42, 74, 81	0
All	All	1154/1360 (84%)	-1.34	0 100 100	26, 42, 73, 81	0

There are no RSRZ outliers to report.

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](#)

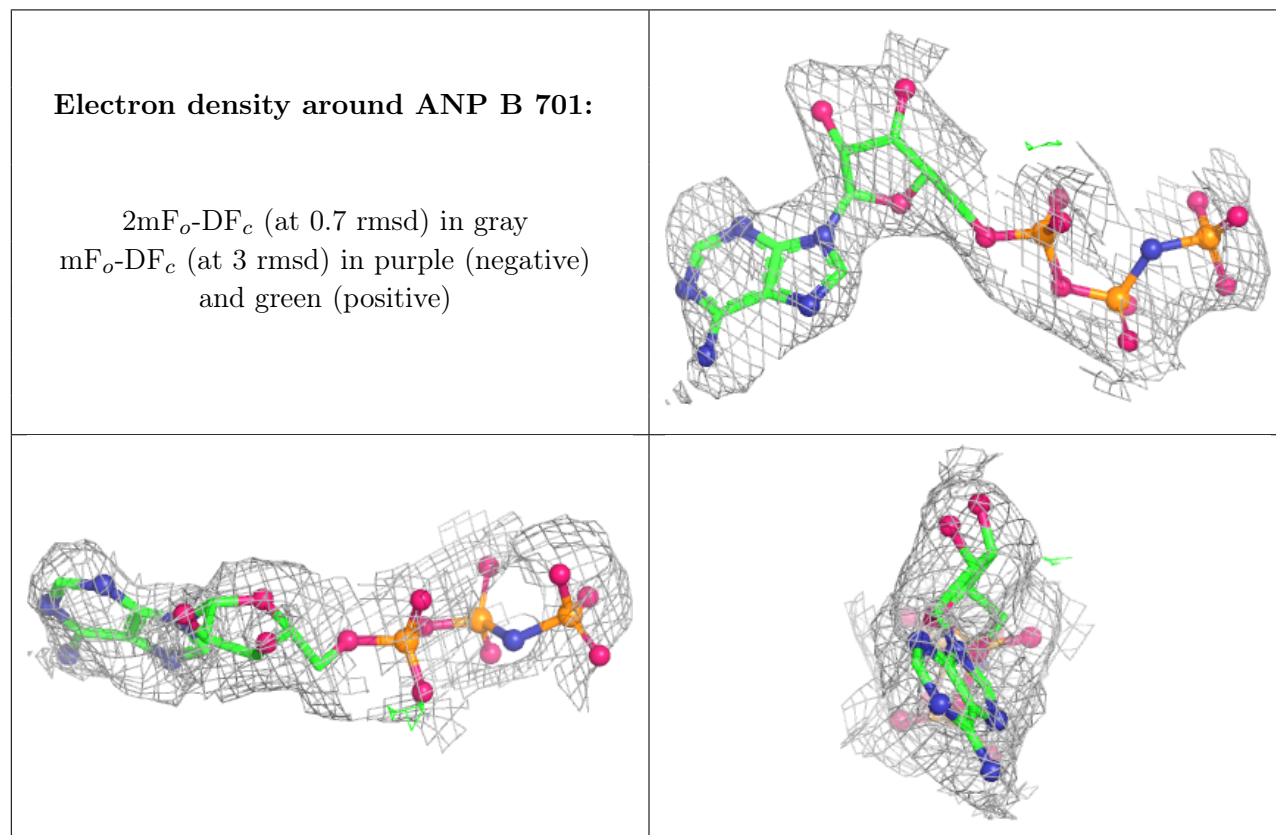
There are no oligosaccharides in this entry.

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.

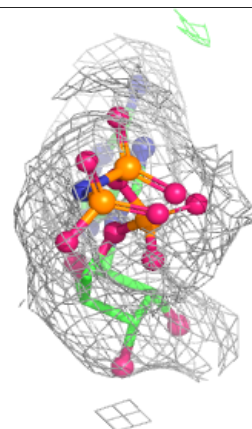
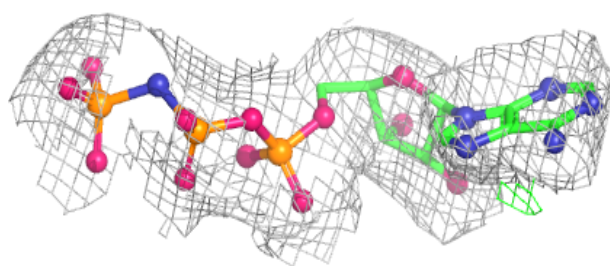
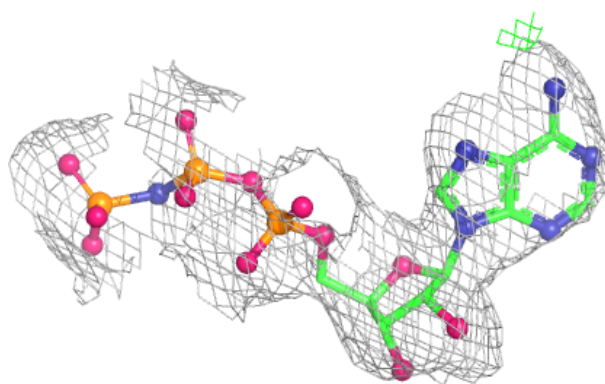
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	703	1/1	0.97	0.05	79,79,79,79	0
3	MG	A	702	1/1	0.98	0.05	45,45,45,45	0
2	ANP	B	701	31/31	0.99	0.04	36,37,40,40	0
3	MG	B	703	1/1	1.00	0.03	37,37,37,37	0
2	ANP	A	701	31/31	1.00	0.03	36,40,44,45	0
3	MG	B	702	1/1	1.00	0.05	43,43,43,43	0

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 A 701:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.