



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 08:40 pm BST

PDB ID : 1GL9
Title : Archaeoglobus fulgidus reverse gyrase complexed with ADPNP
Authors : Rodriguez, A.C.; Stock, D.
Deposited on : 2001-08-30
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

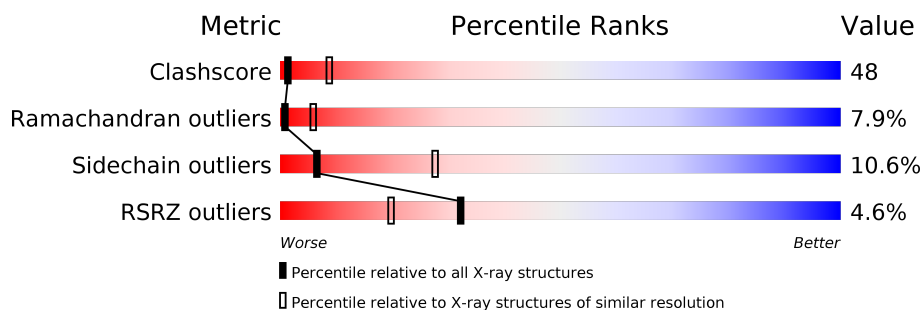
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	B	1054	<div> <div>7%</div> <div>35%</div> <div>50%</div> <div>11%</div> <div>• •</div> </div>
1	C	1054	<div> <div>7%</div> <div>35%</div> <div>50%</div> <div>9%</div> <div>• 5%</div> </div>

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
2	ANP	B	2055	X	-	-	-
3	MG	C	2056	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16398 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.

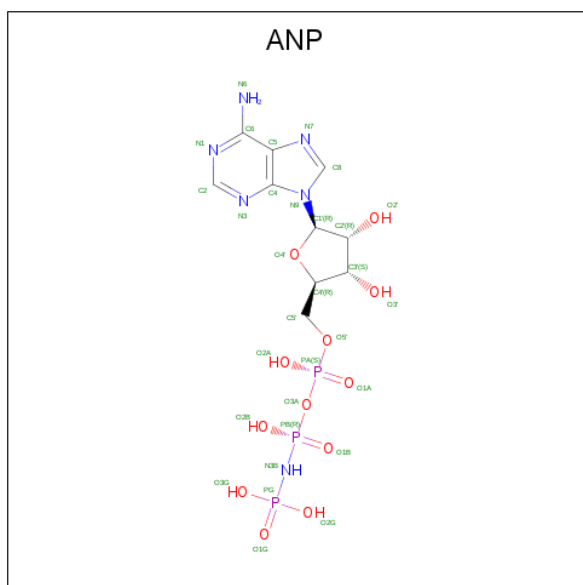
- Molecule 1 is a protein called REVERSE GYRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1020	Total	C	N	O	S	0	0	0
			8226	5246	1450	1505	25			
1	C	1005	Total	C	N	O	S	0	0	0
			8108	5169	1430	1483	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	719	LEU	PRO	engineered mutation	UNP O29238
B	1046	MET	LEU	engineered mutation	UNP O29238
C	719	LEU	PRO	engineered mutation	UNP O29238
C	1046	MET	LEU	engineered mutation	UNP O29238

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: 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	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

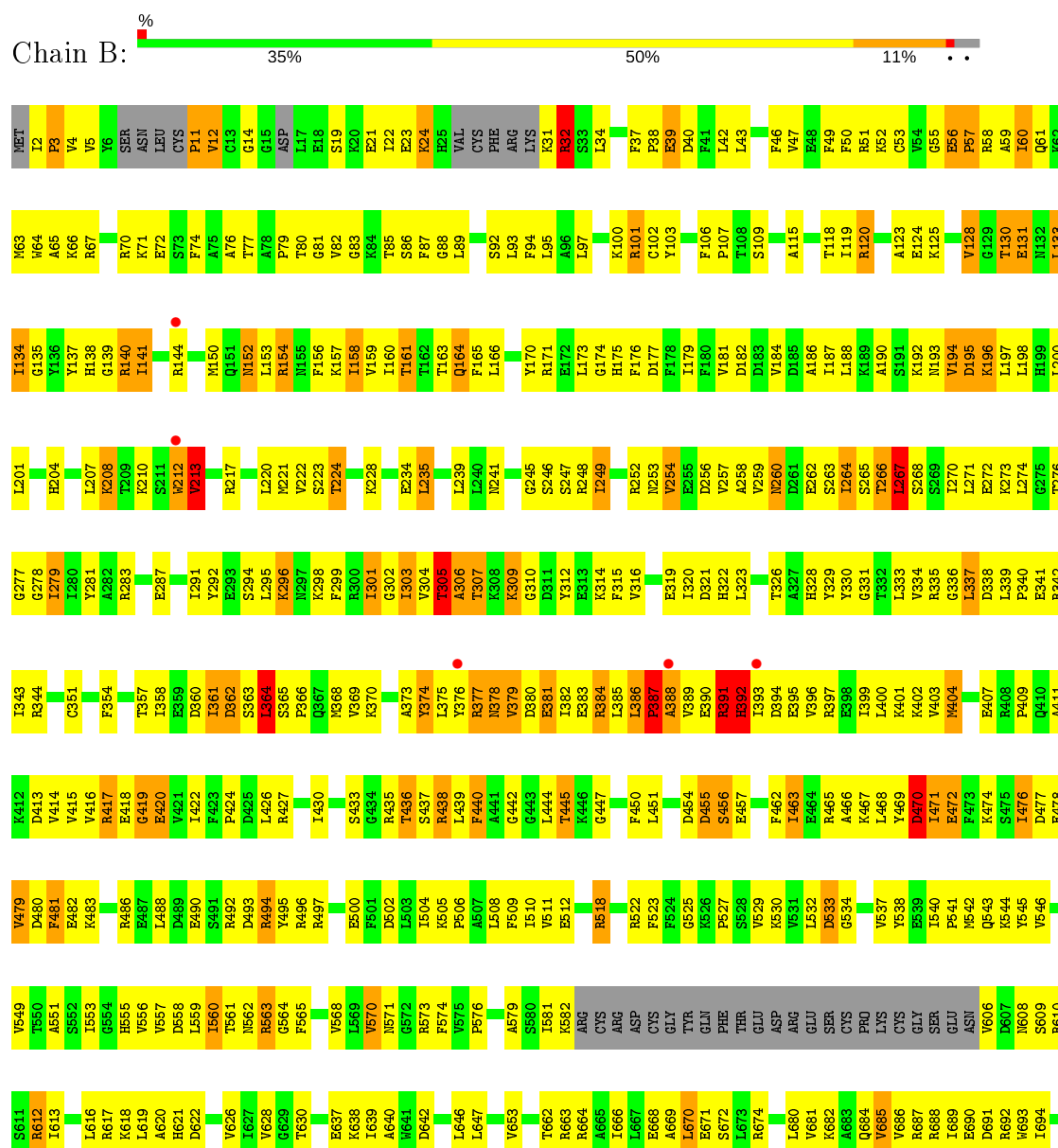
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

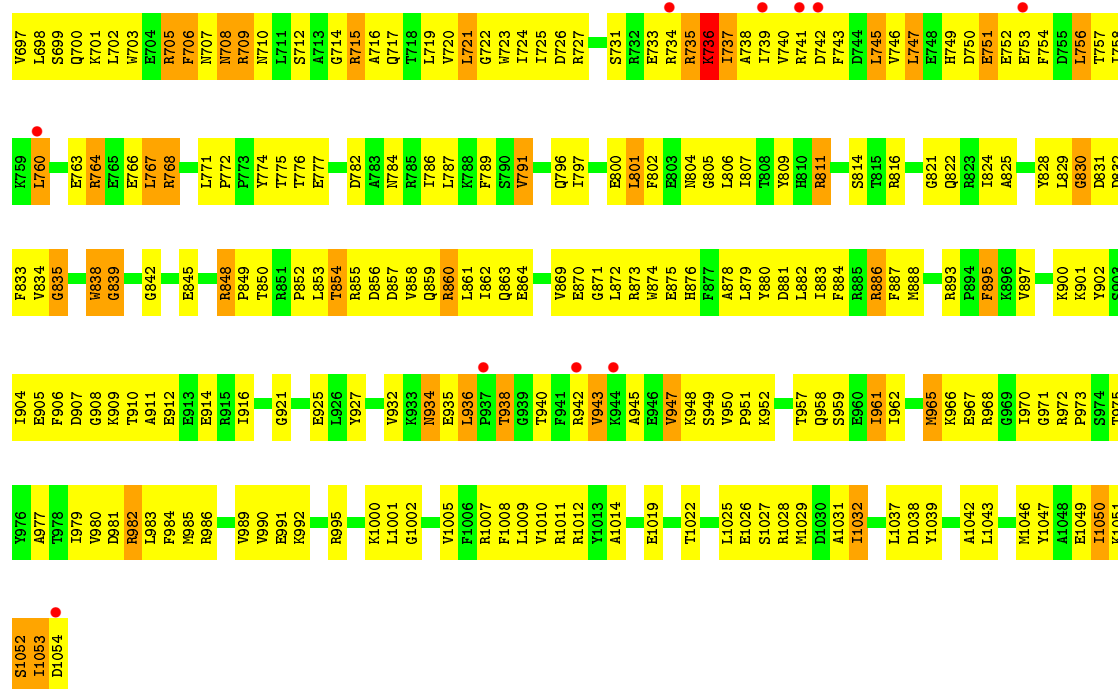
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

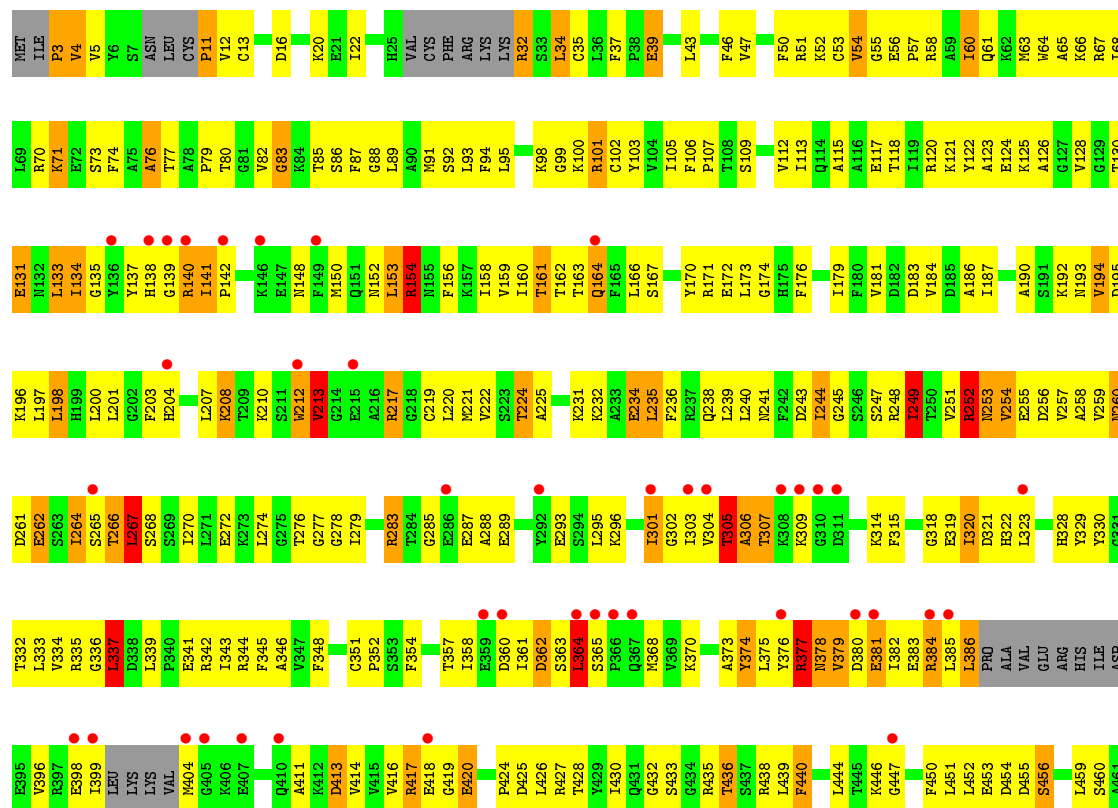
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: REVERSE GYRASE





• Molecule 1: REVERSE GYRASE



L1007	F462	P527	SER	I666	A738	Y809	A878	F941	L1007
F1008	I463	S528	CYS	L667	I739	H810	L879	R942	F1008
L1009	E464	W529	PRO	E668	V740	R811	Y880	Y943	L1009
Y1010	R465	K530	LYS	A669	R741	T812	D881	K944	Y1010
R1011	A466	V531	CYS	L673	D742	D813	L882	A945	R1011
R1012	K467	L532	GLY	F743	F743	S814	L883	E946	R1012
Y1013	L468	D583	SER	D744	D744	T815	F884	V947	Y1013
A1014	Y469	G534	ASN	V681	L745	R816	R885	K948	A1014
Y1017	I471	V537	D606	K682	V746	V817	R886	S949	Y1017
S1018	E472	Y538	P607	A683	L747	S818	F887	V950	S1018
E1019	F473	E539	I608	Q684	GLU	D819	M888	P951	E1019
D1020	K474	T540	S609	V685	HIS	V820	A889	K952	D1020
R1021	S475	P541	R610	V686	D750	G821	S890	V853	R1021
T1022	L476	M542	S611	R687	E751	Q822	Q891	T957	T1022
L1025	D477	Q543	R612	R688	E752	R823	C892	Q958	L1025
E1026	E478	K544	E613	E753	E753	R824	R893	Q959	E1026
S1027	V479	Y545	E614	F754	D755	L829	F894	E960	S1027
R1028	D480	V546	A615	D691	L756	G830	F895	I961	R1028
M1029	F481	V549	L616	I694	T757	D831	K896	I962	M1029
D1030	E482	W549	R617	G695	I758	D832	V897	I963	D1030
A1031	K483	I553	R618	F696	K759	F833	V898	M964	A1031
I1032	L484	I553	R619	V697	L760	V834	K900	M965	I1032
L1037	L488	V556	A620	Q700	V761	G835	K901	K966	L1037
D1038	D489	V557	R621	R701	E762	R836	Y902	E967	D1038
Y1039	E490	D558	D622	L702	E763	E837	S983	R968	Y1039
I1050	S491	L559	A623	L703	R764	W838	I904	G969	I1050
K1051	D502	I571	E624	W703	E765	G839	E905	I970	K1051
S1052	L503	R572	I627	E704	E766	G842	F906	G971	S1052
I1053	L504	R573	W628	R705	L767	Y845	GLY	R972	I1053
R985	K505	R574	R629	F706	R768	C846	LYS	T975	R985
R986	P506	V575	T630	N707	T769	R847	THR	Y976	R986
V989	A507	S580	T634	N708	F770	R848	ALA	A977	V989
V990	L508	I581	E635	N709	L771	P849	E912	T978	V990
E991	P509	R582	E636	N710	Y774	T850	E913	I979	E991
K992	I510	C584	E637	N711	T775	R851	E914	V980	K992
R995	V511	R585	E638	N712	T776	P852	E915	D981	R995
P998	E512	ASP	E639	N713	E777	L853	E920	R982	P998
T999	S513	CYS	C650	N714	D782	T854	G921	L983	T999
K1000	P514	TYR	R654	N715	A783	R855	R922	M984	K1000
L1001	A517	GLY	F658	N716	Q717	D856	A923	R985	L1001
G1002	R518	THR	V661	N717	Q718	D857	Y924	R986	G1002
I1003	R522	GLU	T662	N718	D784	V858	E925	I987	I1003
D1004	F523	ASP	R663	N719	N784	Q859	L926	V989	D1004
F1006	F524	ARG	A665	N720	L787	R860	Y927	E991	F1006
				N721	K788	L861	R928	K992	
				L722	F789	I862	A929	R995	
				W723	S790	Q863	V930		
				I724	V791	V869	W931		
				I725	K792	E870	K933		
				D726	Q793	G871	N934		
				R727	Y796	L872	E935		
				S731	I797	R873	L936		
				R732	Y797	W874	F937		
				E733	L801	E875	T988		
				R734	L806	R876	G939		
				R735	I807	F877	T940		
				K736	T808				
				I737					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.41Å 68.69Å 134.00Å 90.00° 99.70° 90.00°	Depositor
Resolution (Å)	34.00 – 3.20 34.40 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (34.00-3.20) 96.7 (34.40-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.256 , 0.332 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16398	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: MG, ANP

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	B	0.47	0/8371	0.72	5/11265 (0.0%)
1	C	0.35	0/8246	0.61	3/11090 (0.0%)
All	All	0.41	0/16617	0.67	8/22355 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	ARG	N-CA-C	-7.20	91.57	111.00
1	C	305	THR	N-CA-C	6.94	129.73	111.00
1	B	388	ALA	N-CA-C	-6.79	92.68	111.00
1	B	3	PRO	N-CA-CB	5.77	110.23	103.30
1	C	11	PRO	N-CA-CB	5.54	109.95	103.30

There are no chirality outliers.

There are no planarity outliers.

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	B	8226	0	8310	830	0
1	C	8108	0	8178	754	0
2	B	31	0	13	5	0
2	C	31	0	13	5	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
All	All	16398	0	16514	1581	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 48.

The worst 5 of 1581 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:379:VAL:HG12	1:B:380:ASP:H	1.12	1.12
1:B:386:LEU:HD23	1:B:386:LEU:H	1.19	1.06
1:B:638:LYS:HB2	1:B:684:GLN:HG3	1.38	1.06
1:C:192:LYS:HB3	1:C:196:LYS:HE3	1.43	1.00
1:B:540:ILE:HG13	1:B:541:PRO:HD2	1.46	0.97

There are no symmetry-related clashes.

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	B	1010/1054 (96%)	752 (74%)	177 (18%)	81 (8%)	1	6
1	C	987/1054 (94%)	696 (70%)	214 (22%)	77 (8%)	1	6
All	All	1997/2108 (95%)	1448 (72%)	391 (20%)	158 (8%)	1	6

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	PRO
1	B	5	VAL

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Mol	Chain	Res	Type
1	B	12	VAL
1	B	24	LYS
1	B	32	ARG

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	B	876/925 (95%)	782 (89%)	94 (11%)	6	27
1	C	863/925 (93%)	773 (90%)	90 (10%)	7	28
All	All	1739/1850 (94%)	1555 (89%)	184 (11%)	6	27

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	886	ARG
1	C	131	GLU
1	C	873	ARG
1	B	934	ASN
1	B	1050	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	934	ASN
1	C	152	ASN
1	C	876	HIS
1	B	963	GLN
1	C	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	C	2055	-	29,33,33	2.42	9 (31%)	31,52,52	2.25	10 (32%)
2	ANP	B	2055	-	29,33,33	2.01	7 (24%)	31,52,52	2.32	10 (32%)

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	C	2055	-	-	5/14/38/38	0/3/3/3
2	ANP	B	2055	-	1/1/7/8	3/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2055	ANP	PB-O3A	7.85	1.69	1.59
2	B	2055	ANP	C2'-C1'	-4.92	1.46	1.53
2	C	2055	ANP	C2'-C1'	-4.50	1.46	1.53
2	B	2055	ANP	PB-O3A	4.34	1.64	1.59
2	B	2055	ANP	PB-O2B	-3.96	1.46	1.56

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2055	ANP	O1B-PB-N3B	-5.55	103.59	111.77
2	B	2055	ANP	O1B-PB-N3B	-5.46	103.73	111.77
2	B	2055	ANP	O1G-PG-N3B	-5.43	103.78	111.77
2	C	2055	ANP	O1G-PG-N3B	-5.36	103.87	111.77
2	B	2055	ANP	C3'-C2'-C1'	5.12	108.69	100.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2055	ANP	C2'

5 of 8 torsion outliers are listed below:

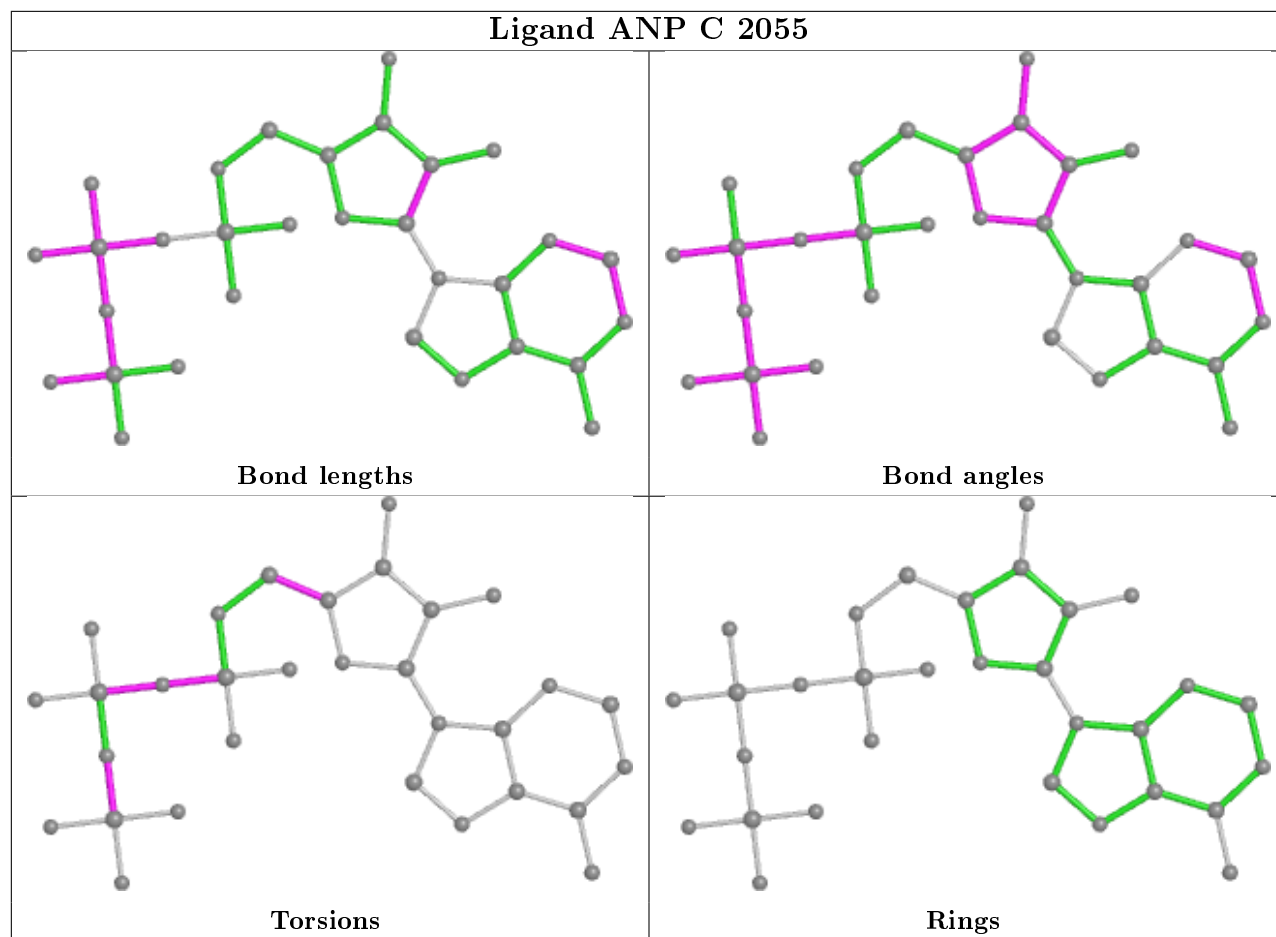
Mol	Chain	Res	Type	Atoms
2	C	2055	ANP	PB-N3B-PG-O1G
2	C	2055	ANP	PA-O3A-PB-O1B
2	C	2055	ANP	PA-O3A-PB-O2B
2	B	2055	ANP	PB-N3B-PG-O1G
2	B	2055	ANP	PA-O3A-PB-O1B

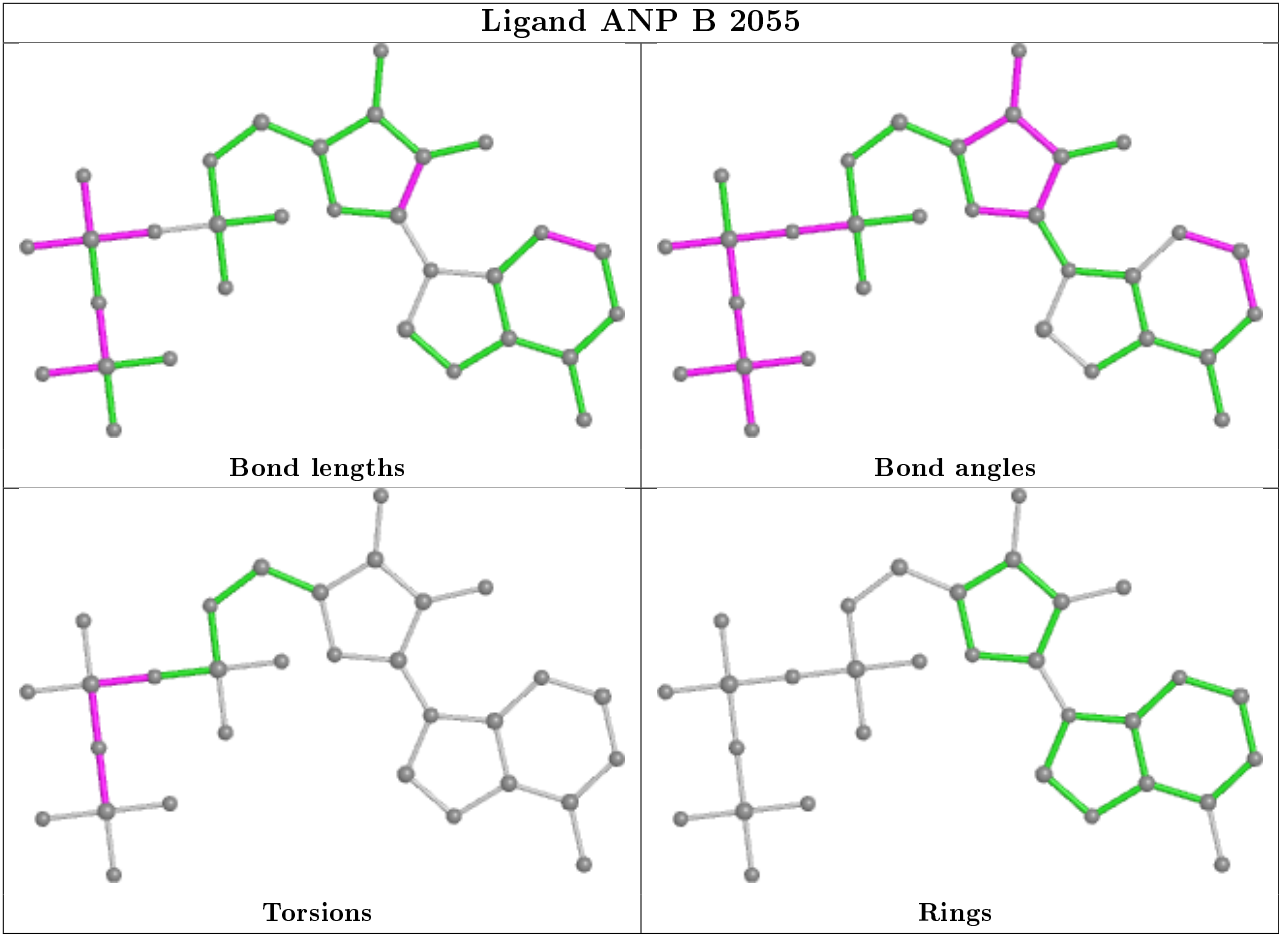
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2055	ANP	5	0
2	B	2055	ANP	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	15:GLY	C	16:ASP	N	13.42

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	B	1020/1054 (96%)	-0.31	15 (1%)	73 61	1, 38, 137, 192	0
1	C	1005/1054 (95%)	0.32	79 (7%)	12 6	24, 92, 160, 195	0
All	All	2025/2108 (96%)	0.00	94 (4%)	32 20	1, 68, 153, 195	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	942	ARG	7.8
1	C	140	ARG	6.4
1	C	139	GLY	6.2
1	C	380	ASP	5.5
1	C	907	ASP	5.5

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](#)

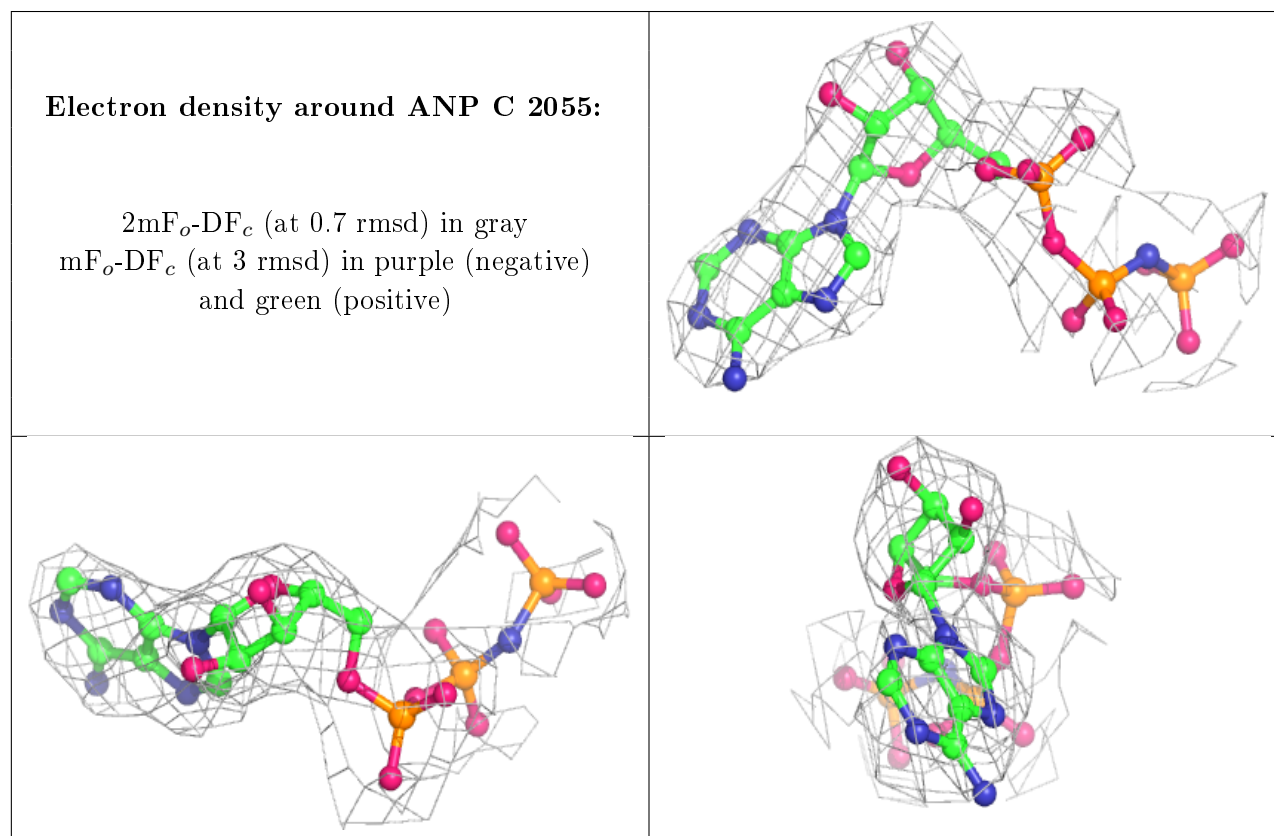
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

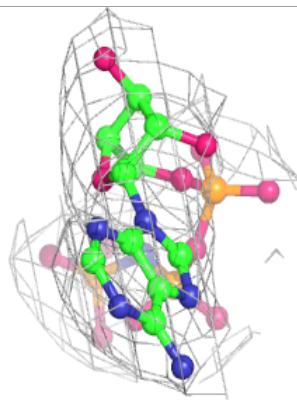
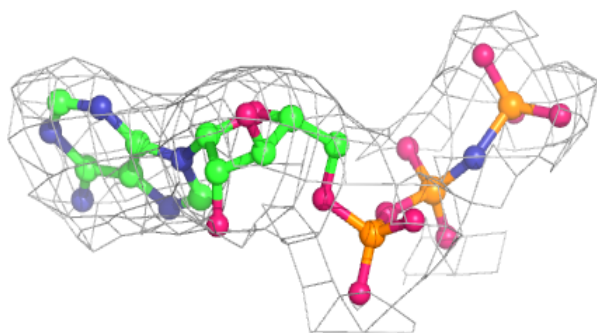
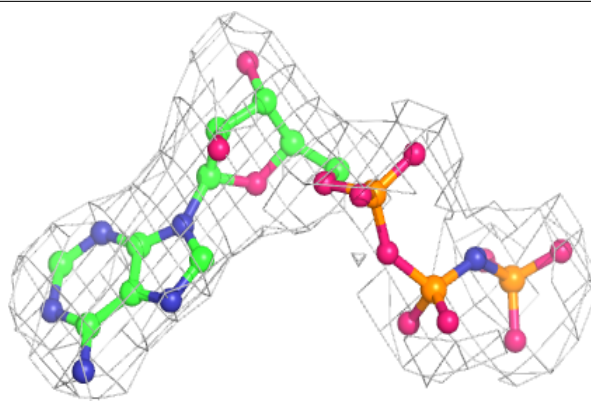
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	C	2056	1/1	0.31	1.04	70,70,70,70	0
3	MG	B	2056	1/1	0.83	0.38	40,40,40,40	0
2	ANP	C	2055	31/31	0.88	0.23	38,57,75,77	0
2	ANP	B	2055	31/31	0.95	0.20	24,34,69,77	0

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 2055:

$2mF_o-DF_c$ (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.