



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2022 – 12:42 AM EST

PDB ID : 3SUC
Title : Crystal structure of the pre-mature bacteriophage phi29 gene product 12
Authors : Xiang, Y.; Rossmann, M.G.
Deposited on : 2011-07-11
Resolution : 2.15 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

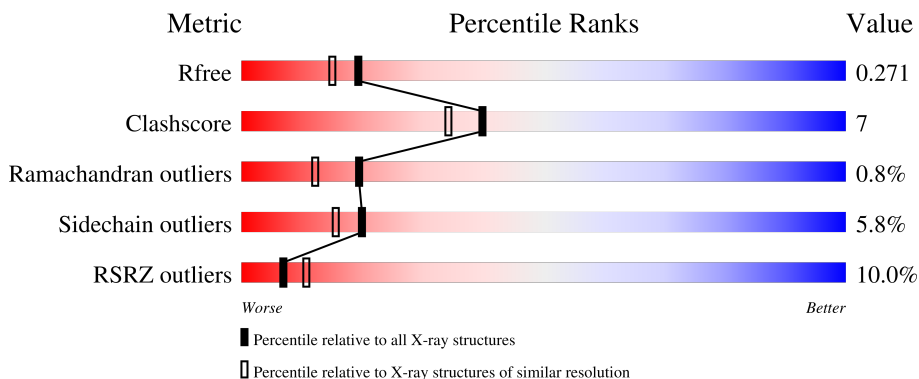
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	772	<div> <div>10%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5875 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 Preneck appendage protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	767	Total	C	N	O	S	0	5	0
			5767	3587	1006	1159	15			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	HIS	-	expression tag	UNP B3VMP8
A	84	HIS	-	expression tag	UNP B3VMP8
A	85	HIS	-	expression tag	UNP B3VMP8
A	86	HIS	-	expression tag	UNP B3VMP8
A	87	HIS	-	expression tag	UNP B3VMP8
A	88	HIS	-	expression tag	UNP B3VMP8
A	166	ARG	LYS	variant	UNP B3VMP8
A	627	GLN	LYS	variant	UNP B3VMP8
A	695	GLN	GLU	engineered mutation	UNP B3VMP8
A	701	GLY	ASP	variant	UNP B3VMP8
A	817	SER	GLY	variant	UNP B3VMP8

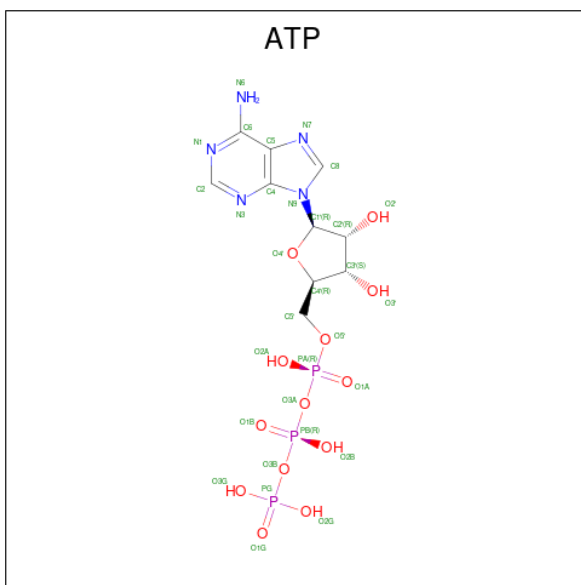
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	73	Total O 74 74	0	1

- Molecule 1: Preneck appendage protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	95.89Å 95.89Å 795.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.27 – 2.15 49.26 – 2.15	Depositor EDS
% Data completeness (in resolution range)	65.5 (49.27-2.15) 65.5 (49.26-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.88 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.261 , 0.291 0.246 , 0.271	Depositor DCC
R_{free} test set	2533 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: MG, CA, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/5882	0.54	1/7972 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	549	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5767	0	5628	84	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	31	0	12	0	0
5	A	74	0	0	3	0
All	All	5875	0	5640	84	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 7.

All (84) 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:A:644:ASN:HD21	1:A:654:THR:CG2	1.55	1.18
1:A:644:ASN:ND2	1:A:654:THR:HG22	1.66	1.11
1:A:644:ASN:HD21	1:A:654:THR:HG22	0.85	1.00
1:A:517:THR:HG22	1:A:519:ASN:O	1.78	0.82
1:A:558:THR:HG21	1:A:570:ILE:HG22	1.59	0.82
1:A:792:ARG:HG2	1:A:792:ARG:HH11	1.43	0.81
1:A:336:ALA:HB2	1:A:342:ALA:HA	1.65	0.79
1:A:496[B]:VAL:HG23	1:A:522:PRO:HB3	1.67	0.77
1:A:514:LEU:HG	1:A:529:SER:HB3	1.73	0.71
1:A:578:GLU:HB3	1:A:593:LYS:HG2	1.74	0.70
1:A:572:GLY:O	1:A:588:THR:HA	1.93	0.68
1:A:644:ASN:ND2	1:A:654:THR:CG2	2.39	0.65
1:A:517:THR:HG21	1:A:522:PRO:HG2	1.77	0.65
1:A:182:ASN:H	1:A:187:ASN:HD21	1.45	0.63
1:A:696:TYR:CE1	1:A:741:GLU:HG2	2.36	0.60
1:A:451:THR:HB	1:A:480:ASN:HB3	1.84	0.60
1:A:519:ASN:HD21	1:A:521:ASN:CG	2.05	0.60
1:A:641:GLY:H	1:A:644:ASN:HD22	1.49	0.59
1:A:792:ARG:HG2	1:A:792:ARG:NH1	2.15	0.58
1:A:521:ASN:HA	1:A:551:ASN:ND2	2.19	0.58
1:A:494:GLU:HG3	5:A:72:HOH:O	2.03	0.58
1:A:473[B]:ASN:ND2	5:A:12:HOH:O	2.38	0.56
1:A:656:GLY:HA3	1:A:659:LYS:HG3	1.86	0.56
1:A:517:THR:CG2	1:A:522:PRO:HG2	2.36	0.55
1:A:288:GLN:HE21	1:A:316:ARG:HE	1.52	0.55
1:A:696:TYR:HE1	1:A:741:GLU:HG2	1.70	0.55
1:A:512:VAL:HG12	1:A:537:ARG:HH12	1.71	0.54
1:A:502:SER:HA	1:A:528:SER:O	2.07	0.54
1:A:277:PHE:CE2	1:A:300:PRO:HB3	2.43	0.54
1:A:646:ILE:HD11	1:A:654:THR:HB	1.89	0.53
1:A:496[B]:VAL:CG2	1:A:522:PRO:HB3	2.36	0.53
1:A:564:ILE:HG12	1:A:570:ILE:CD1	2.39	0.53
1:A:521:ASN:N	1:A:522:PRO:CD	2.73	0.52
1:A:636:GLN:O	1:A:651:GLY:HA2	2.10	0.52
1:A:577:CYS:HB2	5:A:3:HOH:O	2.10	0.51
1:A:514:LEU:HD13	1:A:515:VAL:HG23	1.92	0.51
1:A:159:GLY:HA2	1:A:194:SER:HB3	1.92	0.51
1:A:517:THR:CG2	1:A:519:ASN:O	2.56	0.51
1:A:446:ASN:HD21	1:A:476:ASN:HD22	1.58	0.50
1:A:710:LEU:HD23	1:A:730:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASP:CG	1:A:313:ASP:H	2.15	0.49
1:A:803:GLN:HG2	1:A:834:GLN:HE22	1.77	0.49
1:A:521:ASN:HA	1:A:551:ASN:HD21	1.77	0.49
1:A:472:VAL:HG13	1:A:496[B]:VAL:HG12	1.95	0.48
1:A:475:SER:HA	1:A:499:THR:O	2.13	0.48
1:A:403:PRO:HG2	1:A:428:LEU:O	2.14	0.47
1:A:564:ILE:HG12	1:A:570:ILE:HD13	1.95	0.47
1:A:558:THR:HB	1:A:573:SER:O	2.15	0.46
1:A:315:SER:O	1:A:343:ALA:HA	2.15	0.46
1:A:704:VAL:HG22	1:A:793:ARG:HG2	1.97	0.46
1:A:336:ALA:CB	1:A:342:ALA:HA	2.41	0.46
1:A:239:LEU:HB3	1:A:240:HIS:H	1.55	0.46
1:A:288:GLN:NE2	1:A:316:ARG:HE	2.14	0.45
1:A:324:ARG:HG3	1:A:352:MET:HB3	1.98	0.45
1:A:404:ARG:HD3	1:A:432:THR:O	2.16	0.45
1:A:326:LYS:HA	1:A:354:VAL:O	2.16	0.45
1:A:808:ILE:HG22	1:A:825:ALA:HB3	1.99	0.45
1:A:662:GLY:HA3	1:A:669:TRP:CE2	2.52	0.45
1:A:763:VAL:HB	1:A:771:PHE:CE2	2.52	0.44
1:A:281:GLY:HA3	1:A:297[A]:SER:OG	2.16	0.44
1:A:326:LYS:HG3	1:A:354:VAL:HB	1.99	0.44
1:A:309:PHE:CZ	1:A:323:ASN:HB3	2.53	0.44
1:A:443[B]:CYS:HB3	1:A:472:VAL:HB	1.99	0.44
1:A:672:ASP:OD1	1:A:675:ASN:HB2	2.18	0.44
1:A:480:ASN:C	1:A:480:ASN:HD22	2.22	0.42
1:A:311:ILE:HD11	1:A:320:LEU:HD21	2.01	0.42
1:A:240:HIS:CE1	1:A:279:ASP:HB3	2.54	0.42
1:A:437:GLN:HB3	1:A:463:ILE:HD12	2.01	0.42
1:A:211:ILE:H	1:A:211:ILE:HG13	1.70	0.42
1:A:710:LEU:HD22	1:A:727:ILE:HG21	2.02	0.42
1:A:775:LEU:HA	1:A:776:PRO:HD3	1.92	0.42
1:A:642:ASN:HB3	1:A:657:SER:HB3	2.02	0.41
1:A:446:ASN:ND2	1:A:475:SER:OG	2.50	0.41
1:A:700:LEU:O	1:A:703:GLN:HG3	2.20	0.41
1:A:772:LYS:HB3	1:A:772:LYS:HE2	1.88	0.41
1:A:165:ILE:HB	1:A:197:LEU:HD23	2.02	0.41
1:A:409:SER:HB3	1:A:438:PHE:HB2	2.02	0.41
1:A:649:SER:OG	1:A:662:GLY:HA2	2.21	0.41
1:A:430:THR:O	1:A:456:SER:HA	2.21	0.41
1:A:303:THR:HG22	1:A:303:THR:O	2.20	0.40
1:A:173:ARG:HH12	1:A:208:ILE:HG21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:ILE:HA	1:A:788:PRO:HD3	1.90	0.40
1:A:746:TRP:HA	1:A:786:TYR:CE2	2.57	0.40

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	A	770/772 (100%)	717 (93%)	47 (6%)	6 (1%)	19 12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	606	THR
1	A	689	THR
1	A	304	ALA
1	A	380	ASN
1	A	216	GLU
1	A	521	ASN

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	629/630 (100%)	592 (94%)	37 (6%)	19 15

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	PHE
1	A	143	VAL
1	A	156	THR
1	A	167	PHE
1	A	177	LEU
1	A	180	ASN
1	A	239	LEU
1	A	259	THR
1	A	316	ARG
1	A	379	LYS
1	A	451	THR
1	A	466	SER
1	A	467	ARG
1	A	472	VAL
1	A	478	THR
1	A	480	ASN
1	A	514	LEU
1	A	518	ILE
1	A	519	ASN
1	A	547	LEU
1	A	549	LEU
1	A	558	THR
1	A	567[A]	GLU
1	A	567[B]	GLU
1	A	570	ILE
1	A	606	THR
1	A	610	LYS
1	A	636	GLN
1	A	654	THR
1	A	655	THR
1	A	674	LEU
1	A	703	GLN
1	A	707	THR
1	A	738	VAL
1	A	747	GLN
1	A	792	ARG
1	A	793	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	187	ASN
1	A	200	ASN
1	A	288	GLN
1	A	361	ASN
1	A	374	GLN
1	A	417	ASN
1	A	437	GLN
1	A	446	ASN
1	A	480	ASN
1	A	519	ASN
1	A	551	ASN
1	A	614	ASN
1	A	636	GLN
1	A	644	ASN
1	A	661	ASN
1	A	668	ASN
1	A	703	GLN
1	A	747	GLN
1	A	816	HIS
1	A	834	GLN

5.3.3 RNA [i](#)

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	ATP	A	856	3	26,33,33	1.00	2 (7%)	31,52,52	1.49	5 (16%)

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	ATP	A	856	3	-	3/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	856	ATP	C5-C4	2.71	1.48	1.40
4	A	856	ATP	C2-N3	2.01	1.35	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	856	ATP	C3'-C2'-C1'	3.50	106.25	100.98
4	A	856	ATP	N3-C2-N1	-3.19	123.69	128.68
4	A	856	ATP	C4-C5-N7	-2.74	106.55	109.40
4	A	856	ATP	PA-O3A-PB	-2.69	123.60	132.83
4	A	856	ATP	PB-O3B-PG	-2.64	123.75	132.83

There are no chirality outliers.

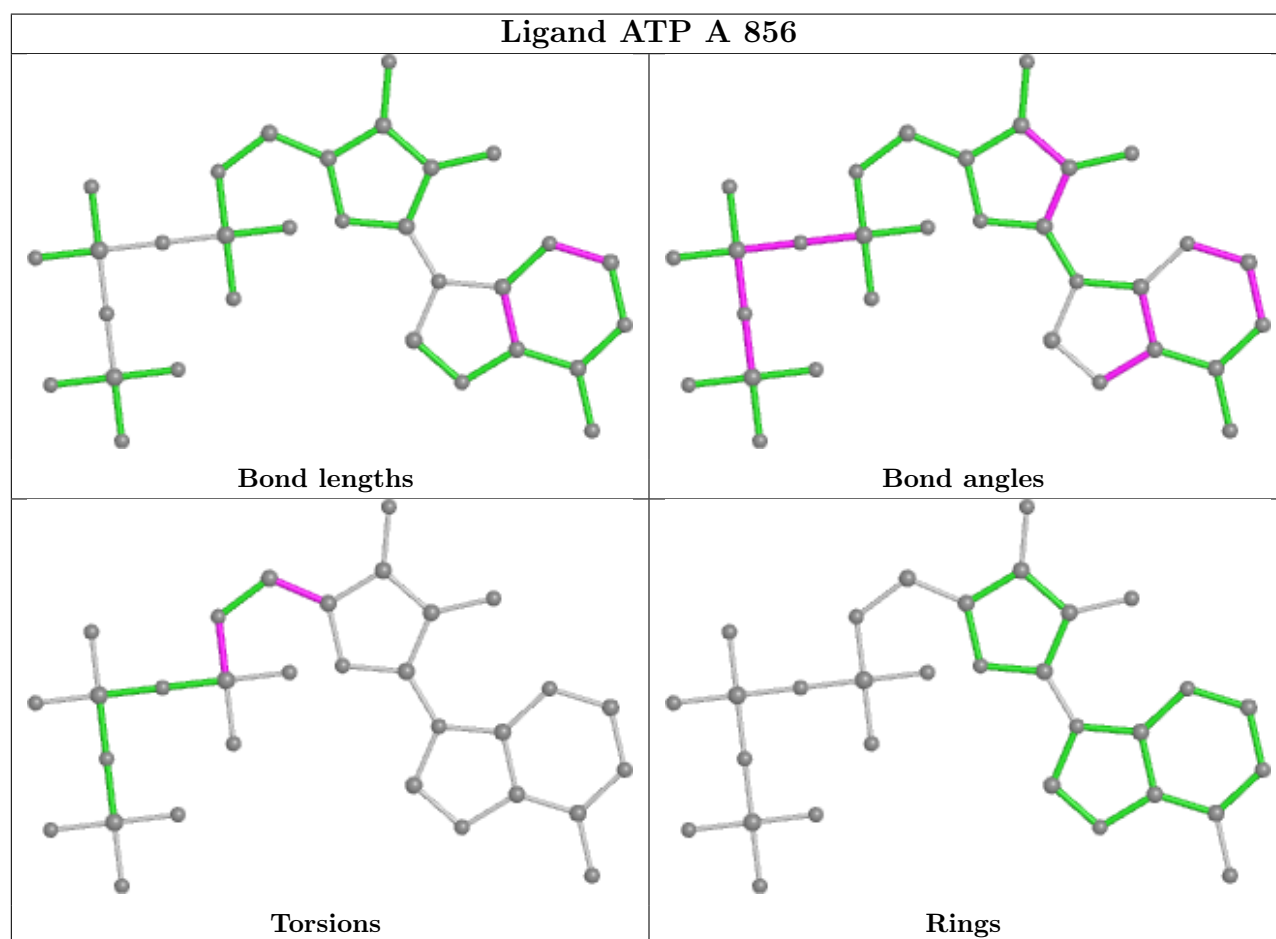
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	856	ATP	C5'-O5'-PA-O1A
4	A	856	ATP	O4'-C4'-C5'-O5'
4	A	856	ATP	C3'-C4'-C5'-O5'

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.



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

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	767/772 (99%)	0.58	77 (10%) 7 11	12, 42, 96, 155	3 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ASN	8.6
1	A	293	LEU	4.6
1	A	319	VAL	4.6
1	A	690	TRP	4.4
1	A	269	ILE	4.4
1	A	302	LEU	4.2
1	A	292	ILE	4.2
1	A	249	LEU	4.1
1	A	320	LEU	4.0
1	A	348	ILE	4.0
1	A	272	CYS	3.7
1	A	268	TRP	3.6
1	A	386	LEU	3.5
1	A	107	VAL	3.4
1	A	349	ASN	3.3
1	A	321	SER	3.3
1	A	92	LEU	3.3
1	A	322	ASN	3.3
1	A	204	LEU	3.2
1	A	384	SER	3.2
1	A	786	TYR	3.2
1	A	271	ASN	3.1
1	A	229	ILE	3.1
1	A	173	ARG	3.1
1	A	199	GLY	3.0
1	A	232	ILE	3.0
1	A	294	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	415	VAL	2.9
1	A	416	ILE	2.9
1	A	387	VAL	2.8
1	A	254	LEU	2.8
1	A	145	ARG	2.7
1	A	382	VAL	2.7
1	A	783	ASN	2.7
1	A	124	PHE	2.7
1	A	290	ILE	2.6
1	A	103	PHE	2.6
1	A	323	ASN	2.6
1	A	230	ARG	2.6
1	A	746	TRP	2.6
1	A	192	LEU	2.5
1	A	267	ILE	2.5
1	A	126	LYS	2.4
1	A	350	GLY	2.4
1	A	347	SER	2.4
1	A	723	LYS	2.4
1	A	181	GLU	2.4
1	A	448	VAL	2.4
1	A	99	GLU	2.4
1	A	206	GLN	2.4
1	A	291	ASN	2.4
1	A	227	VAL	2.3
1	A	168	MET	2.3
1	A	383	ALA	2.3
1	A	89	PHE	2.3
1	A	211	ILE	2.3
1	A	261	PRO	2.3
1	A	782	PRO	2.3
1	A	445	LEU	2.3
1	A	303	THR	2.3
1	A	687	GLY	2.3
1	A	296	TYR	2.2
1	A	691	SER	2.2
1	A	419	LEU	2.2
1	A	129	GLU	2.2
1	A	365	ILE	2.2
1	A	477	VAL	2.1
1	A	228	TYR	2.1
1	A	762	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	295	CYS	2.1
1	A	332	ILE	2.0
1	A	785	ASN	2.0
1	A	270	GLU	2.0
1	A	94	ILE	2.0
1	A	689	THR	2.0
1	A	780	PHE	2.0
1	A	128	ILE	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](#)

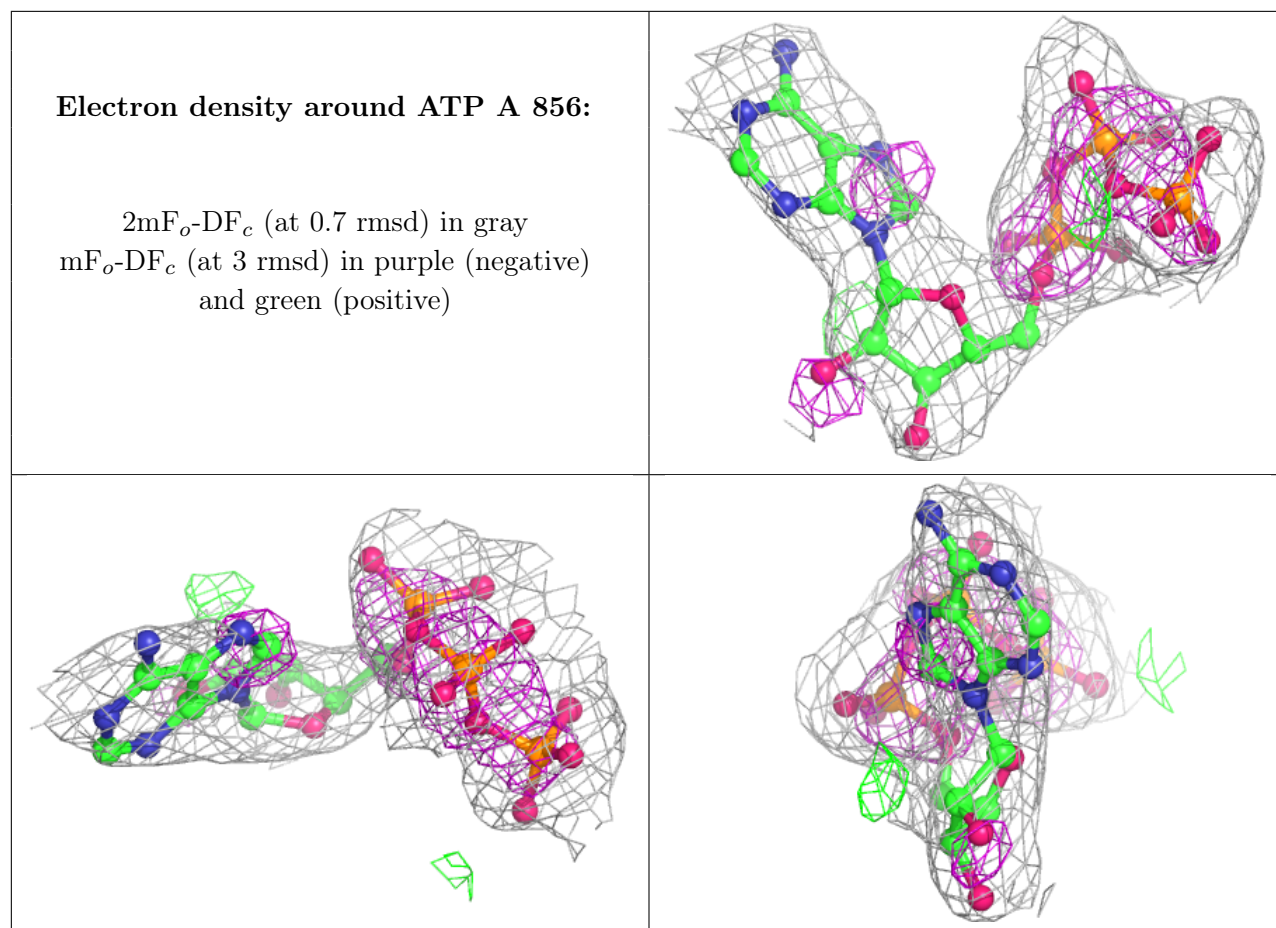
There are no monosaccharides in this entry.

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
4	ATP	A	856	31/31	0.85	0.27	49,59,60,62	0
3	MG	A	857	1/1	0.87	0.07	47,47,47,47	0
2	CA	A	1	1/1	0.90	0.04	49,49,49,49	0
3	MG	A	855	1/1	0.96	0.09	47,47,47,47	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.