



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:42 AM UTC

PDB ID : 4S0F / pdb_00004s0f
Title : Crystal structure of the peptidase-containing ABC transporter PCAT1 E648Q mutant complexed with ATPgS in an occluded conformation
Authors : Lin, D.L.; Huang, S.; Chen, J.
Deposited on : 2014-12-30
Resolution : 5.51 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

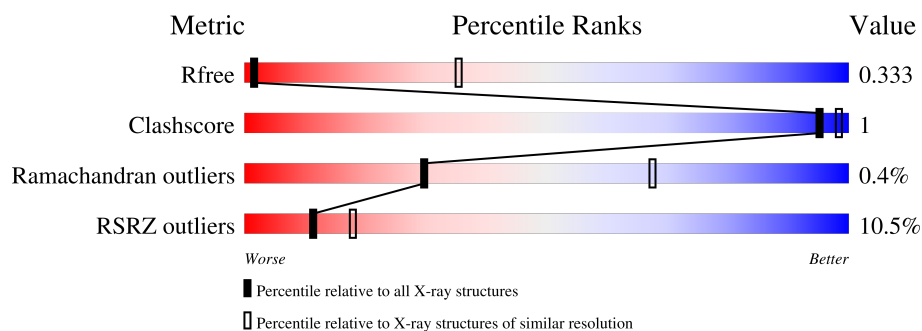
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.51 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	1093 (7.04-4.00)
Clashscore	190562	1152 (7.04-4.00)
Ramachandran outliers	187476	1014 (7.04-3.98)
RSRZ outliers	180081	1086 (7.04-4.00)

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	730	8% 76% 23%
1	B	730	9% 76% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5636 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 ABC-type bacteriocin transporter.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	0	0	0
			2787	1657	565	565			
1	B	565	Total	C	N	O	0	0	0
			2787	1657	565	565			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A3DCU1
A	-1	ASN	-	expression tag	UNP A3DCU1
A	0	ALA	-	expression tag	UNP A3DCU1
A	648	GLN	GLU	engineered mutation	UNP A3DCU1
B	-2	SER	-	expression tag	UNP A3DCU1
B	-1	ASN	-	expression tag	UNP A3DCU1
B	0	ALA	-	expression tag	UNP A3DCU1
B	648	GLN	GLU	engineered mutation	UNP A3DCU1

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

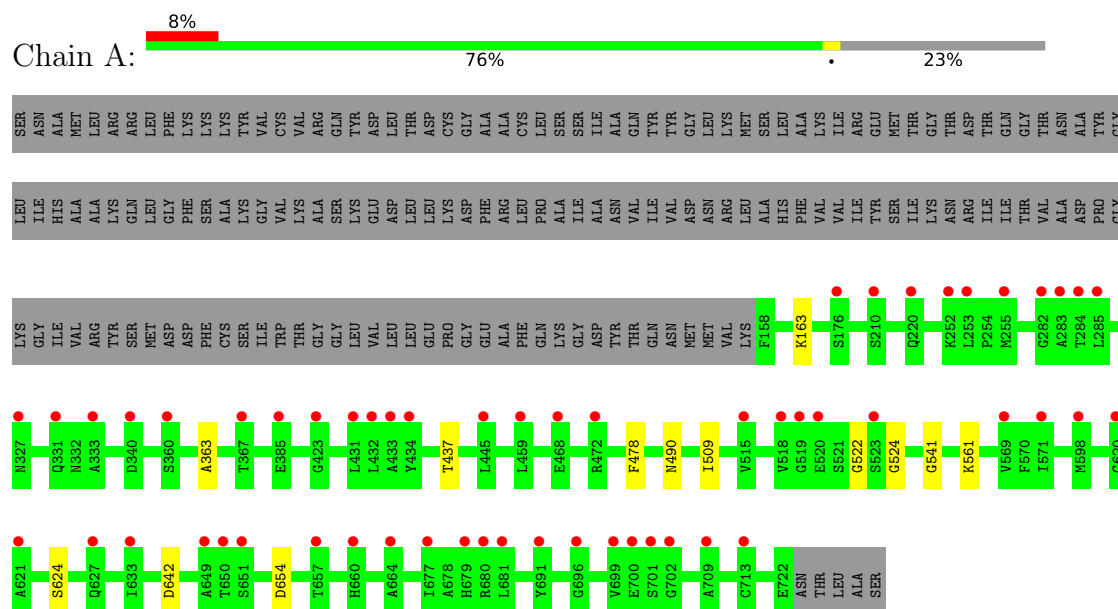


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

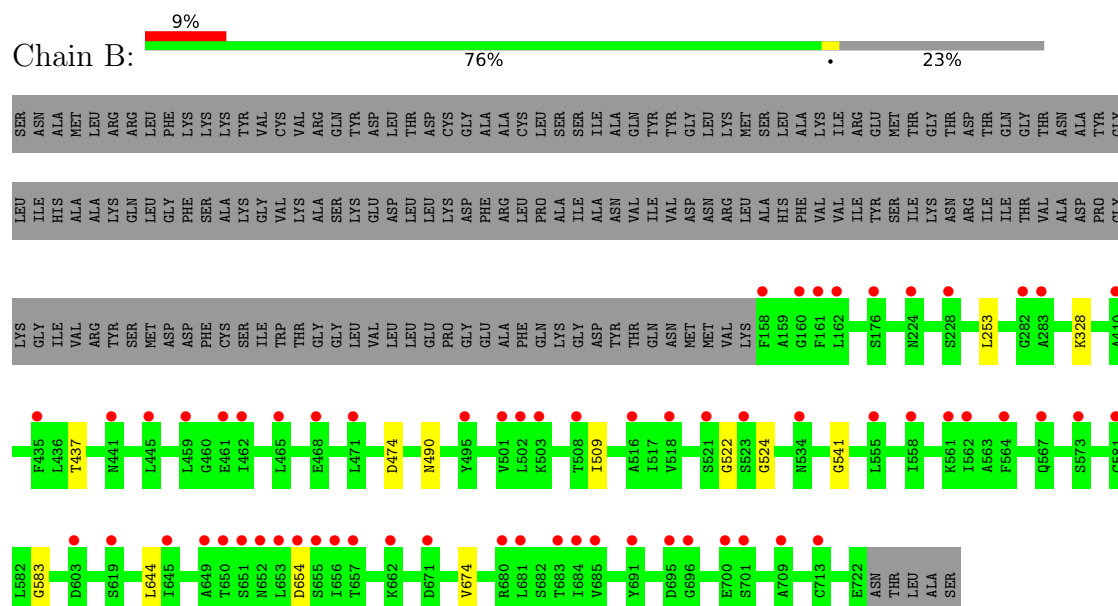
3 Residue-property plots [i](#)

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: ABC-type bacteriocin transporter



• Molecule 1: ABC-type bacteriocin transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	230.00Å 230.00Å 89.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 5.51 19.98 – 5.51	Depositor EDS
% Data completeness (in resolution range)	80.9 (19.98-5.51) 78.9 (19.98-5.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 5.38Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.300 , 0.314 0.332 , 0.333	Depositor DCC
R_{free} test set	313 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å ²)	277.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.08 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5636	wwPDB-VP
Average B, all atoms (Å ²)	223.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.98% 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: AGS

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	0.33	0/2786	0.99	7/3876 (0.2%)
1	B	0.34	0/2786	1.01	9/3876 (0.2%)
All	All	0.34	0/5572	1.00	16/7752 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	509	ILE	CA-C-N	12.01	132.96	119.99
1	B	509	ILE	C-N-CA	12.01	132.96	119.99
1	A	509	ILE	CA-C-N	9.93	130.72	119.99
1	A	509	ILE	C-N-CA	9.93	130.72	119.99
1	B	437	THR	CA-C-N	9.29	128.98	118.85
1	B	437	THR	C-N-CA	9.29	128.98	118.85
1	A	437	THR	CA-C-N	7.18	126.67	118.85
1	A	437	THR	C-N-CA	7.18	126.67	118.85
1	B	654	ASP	N-CA-C	6.92	119.41	111.11
1	B	253	LEU	CA-C-N	5.72	126.52	120.11
1	B	253	LEU	C-N-CA	5.72	126.52	120.11
1	A	163	LYS	CA-C-N	5.18	126.12	120.83
1	A	163	LYS	C-N-CA	5.18	126.12	120.83
1	A	654	ASP	N-CA-C	5.09	117.22	111.11
1	B	328	LYS	CA-C-N	5.07	124.56	119.19
1	B	328	LYS	C-N-CA	5.07	124.56	119.19

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	2787	0	1271	5	0
1	B	2787	0	1271	4	0
2	A	31	0	12	2	0
2	B	31	0	12	3	0
All	All	5636	0	2566	10	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 1.

All (10) 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:522:GLY:HA2	2:B:801:AGS:H4'	1.47	0.95
2:B:801:AGS:H5'2	2:B:801:AGS:H8	1.57	0.85
2:A:801:AGS:O2G	2:A:801:AGS:O2B	2.13	0.67
1:A:522:GLY:HA2	2:A:801:AGS:H5'1	1.90	0.53
1:A:561:LYS:O	1:A:642:ASP:N	2.43	0.51
1:A:363:ALA:HB2	1:B:583:GLY:HA2	1.96	0.47
1:A:490:ASN:O	1:A:541:GLY:HA3	2.16	0.45
1:B:490:ASN:O	1:B:541:GLY:HA3	2.17	0.45
1:B:644:LEU:O	1:B:674:VAL:HA	2.17	0.43
1:A:624:SER:HA	2:B:801:AGS:H5'1	2.01	0.42

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	563/730 (77%)	535 (95%)	26 (5%)	2 (0%)	30	67
1	B	563/730 (77%)	535 (95%)	26 (5%)	2 (0%)	30	67
All	All	1126/1460 (77%)	1070 (95%)	52 (5%)	4 (0%)	30	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	474	ASP
1	A	478	PHE
1	A	524	GLY
1	B	524	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	AGS	B	801	-	32,33,33	0.46	1 (3%)	45,52,52	0.74	1 (2%)
2	AGS	A	801	-	32,33,33	0.58	0	45,52,52	0.87	2 (4%)

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	AGS	B	801	-	-	6/21/38/38	0/3/3/3
2	AGS	A	801	-	-	5/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	AGS	PG-S1G	2.06	1.95	1.90

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	AGS	PB-O3B-PG	-3.79	119.31	133.17
2	B	801	AGS	PB-O3B-PG	-3.38	120.80	133.17
2	A	801	AGS	O3G-PG-O3B	2.01	111.36	104.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

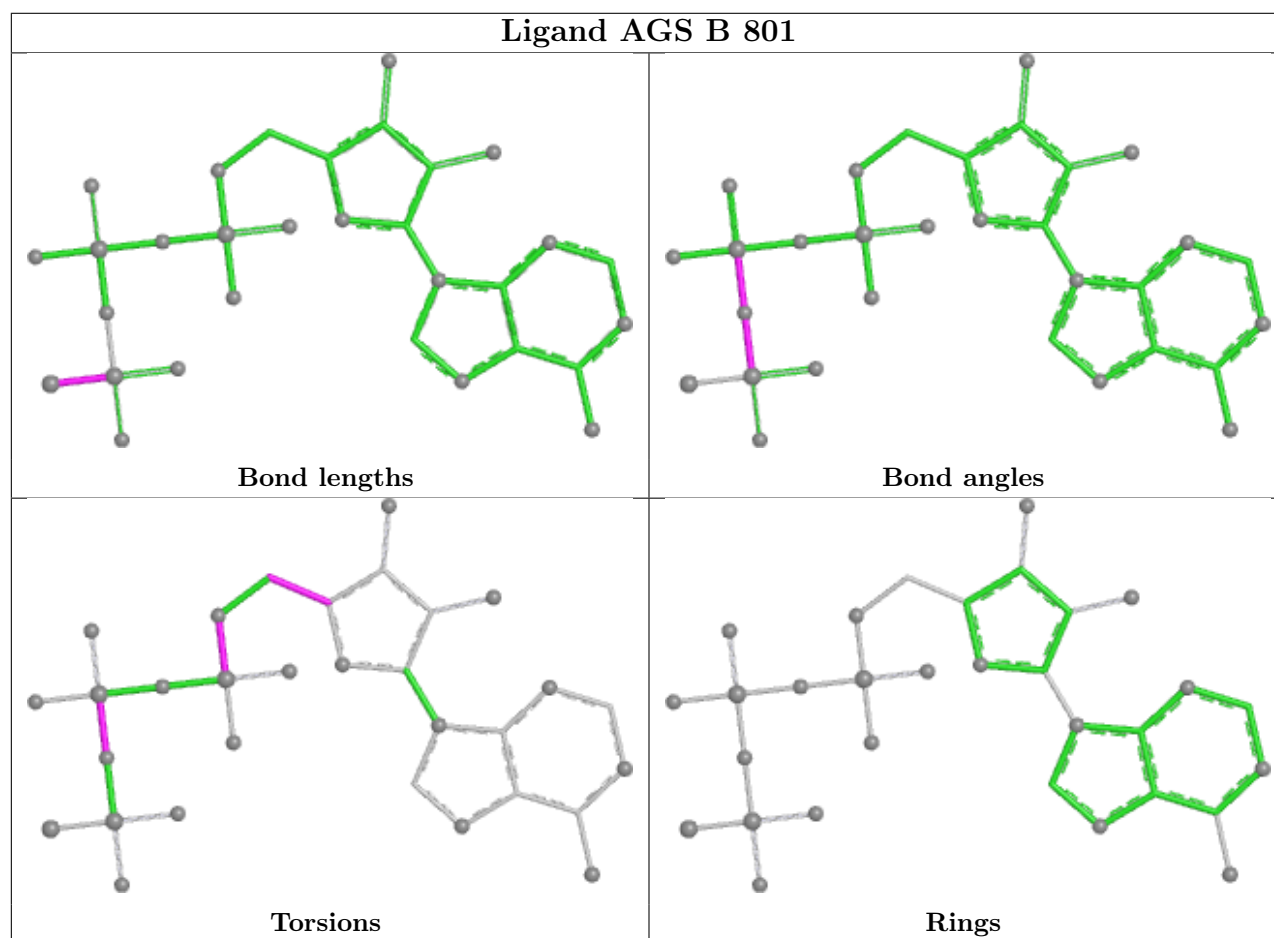
Mol	Chain	Res	Type	Atoms
2	A	801	AGS	O4'-C4'-C5'-O5'
2	B	801	AGS	C5'-O5'-PA-O1A
2	B	801	AGS	C5'-O5'-PA-O2A
2	B	801	AGS	C5'-O5'-PA-O3A
2	B	801	AGS	C3'-C4'-C5'-O5'
2	A	801	AGS	C3'-C4'-C5'-O5'
2	B	801	AGS	O4'-C4'-C5'-O5'
2	A	801	AGS	C5'-O5'-PA-O1A
2	B	801	AGS	PG-O3B-PB-O2B
2	A	801	AGS	PG-O3B-PB-O1B
2	A	801	AGS	PB-O3A-PA-O2A

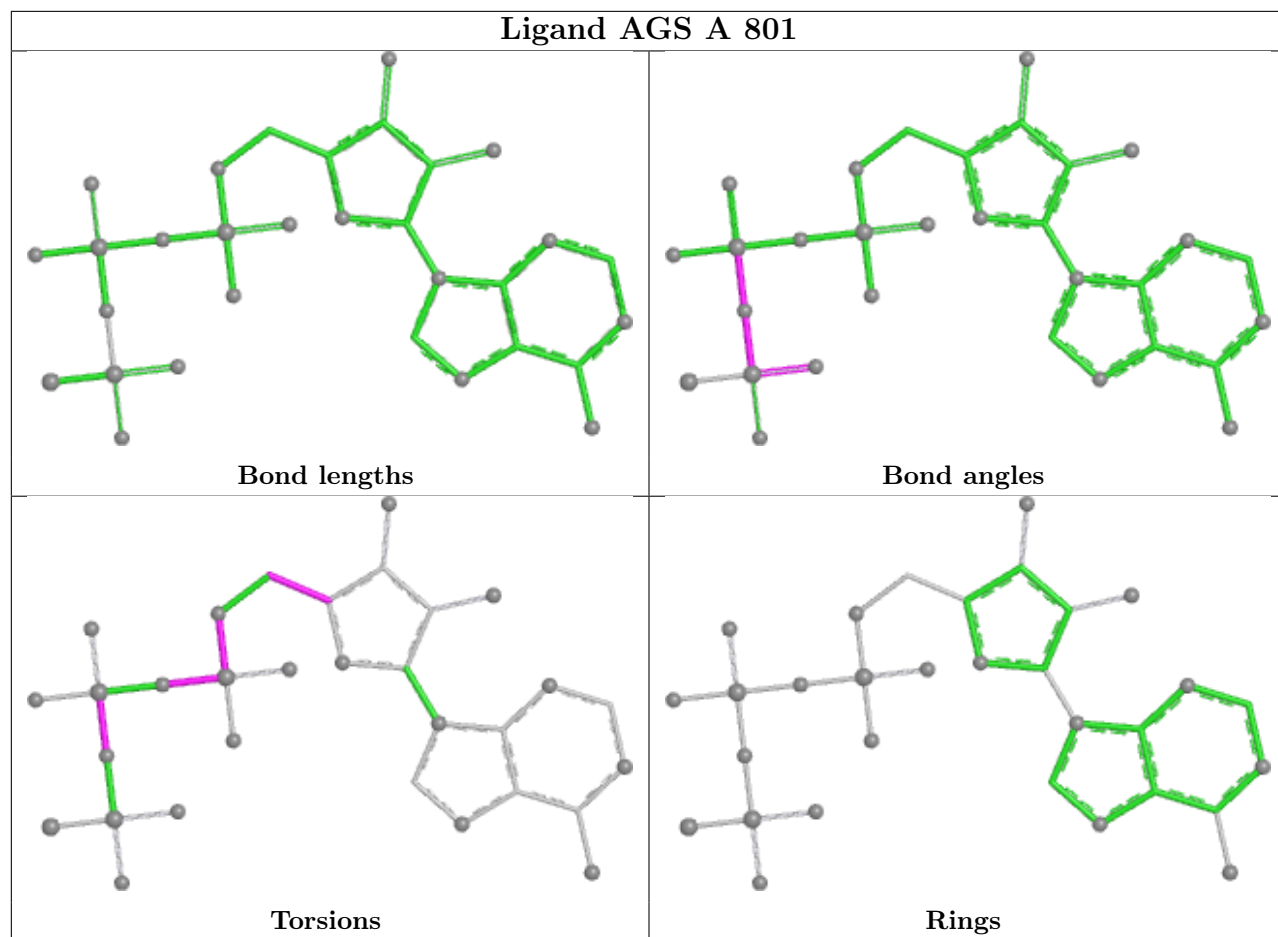
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	AGS	3	0
2	A	801	AGS	2	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

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	565/730 (77%)	0.56	56 (9%)	13 19	79, 201, 310, 383	0
1	B	565/730 (77%)	0.62	63 (11%)	10 17	89, 235, 394, 486	0
All	All	1130/1460 (77%)	0.59	119 (10%)	11 18	79, 214, 375, 486	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	696	GLY	16.2
1	B	695	ASP	9.5
1	B	709	ALA	7.2
1	B	684	ILE	7.0
1	A	680	ARG	6.4
1	A	701	SER	6.1
1	A	699	VAL	6.0
1	B	680	ARG	5.9
1	B	501	VAL	5.8
1	A	432	LEU	5.1
1	B	441	ASN	5.0
1	B	534	ASN	5.0
1	B	523	SER	5.0
1	A	657	THR	4.8
1	A	433	ALA	4.7
1	A	650	THR	4.6
1	B	683	THR	4.4
1	A	519	GLY	4.4
1	B	518	VAL	4.2
1	B	652	ASN	4.1
1	A	649	ALA	4.0
1	A	660	HIS	4.0
1	B	465	LEU	3.8
1	A	679	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	331	GLN	3.6
1	A	360	SER	3.6
1	A	255	MET	3.5
1	A	621	ALA	3.5
1	B	603	ASP	3.4
1	A	283	ALA	3.4
1	B	564	PHE	3.3
1	A	520	GLU	3.3
1	B	567	GLN	3.3
1	B	445	LEU	3.3
1	A	700	GLU	3.3
1	B	650	THR	3.2
1	A	702	GLY	3.2
1	B	228	SER	3.2
1	A	472	ARG	3.2
1	B	435	PHE	3.1
1	B	561	LYS	3.1
1	A	627	GLN	3.1
1	B	691	TYR	3.1
1	B	516	ALA	3.1
1	B	468	GLU	3.1
1	A	664	ALA	3.1
1	B	681	LEU	3.1
1	B	410	ALA	3.0
1	B	558	ILE	3.0
1	A	459	LEU	3.0
1	B	581	CYS	3.0
1	B	700	GLU	3.0
1	A	651	SER	2.9
1	B	645	ILE	2.9
1	A	385	GLU	2.9
1	B	283	ALA	2.9
1	B	158	PHE	2.9
1	B	521	SER	2.9
1	B	555	LEU	2.9
1	A	327	ASN	2.9
1	B	502	LEU	2.9
1	B	160	GLY	2.8
1	A	633	ILE	2.8
1	B	224	ASN	2.8
1	A	677	ILE	2.8
1	B	461	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	681	LEU	2.8
1	B	619	SER	2.8
1	B	657	THR	2.7
1	A	620	GLY	2.7
1	A	523	SER	2.7
1	B	459	LEU	2.7
1	B	161	PHE	2.6
1	A	253	LEU	2.6
1	A	431	LEU	2.6
1	B	503	LYS	2.5
1	B	562	ILE	2.5
1	A	691	TYR	2.5
1	B	282	GLY	2.5
1	B	701	SER	2.5
1	A	468	GLU	2.5
1	B	653	LEU	2.5
1	A	445	LEU	2.5
1	B	685	VAL	2.4
1	A	598	MET	2.4
1	A	518	VAL	2.4
1	A	340	ASP	2.3
1	B	654	ASP	2.3
1	B	671	ASP	2.3
1	A	515	VAL	2.3
1	B	471	LEU	2.3
1	B	495	TYR	2.3
1	B	162	LEU	2.3
1	B	462	ILE	2.3
1	B	508	THR	2.2
1	A	333	ALA	2.2
1	A	709	ALA	2.2
1	A	423	GLY	2.2
1	A	176	SER	2.2
1	B	651	SER	2.2
1	B	662	LYS	2.1
1	B	655	SER	2.1
1	A	571	ILE	2.1
1	A	434	TYR	2.1
1	A	713	CYS	2.1
1	A	252	LYS	2.1
1	B	649	ALA	2.1
1	B	713	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	696	GLY	2.1
1	B	656	ILE	2.1
1	A	210	SER	2.1
1	A	282	GLY	2.1
1	A	367	THR	2.0
1	A	285	LEU	2.0
1	A	220	GLN	2.0
1	A	284	THR	2.0
1	B	176	SER	2.0
1	A	569	VAL	2.0
1	B	573	SER	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](#)

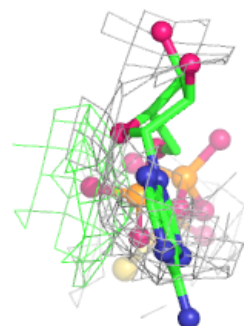
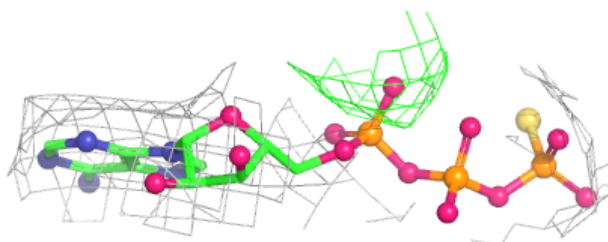
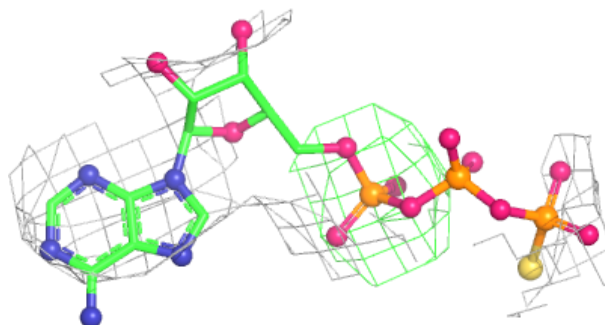
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AGS	B	801	31/31	0.82	0.17	257,257,257,257	0
2	AGS	A	801	31/31	0.86	0.18	248,248,248,248	0

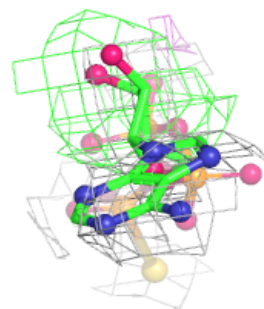
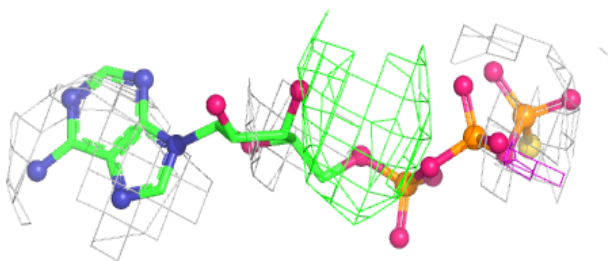
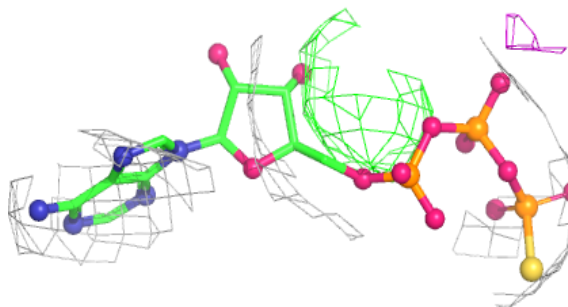
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS B 801:

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

**Electron density around AGS A 801:**

$2mF_o-DF_c$ (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.