



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:47 am BST

PDB ID : 4S0F
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 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

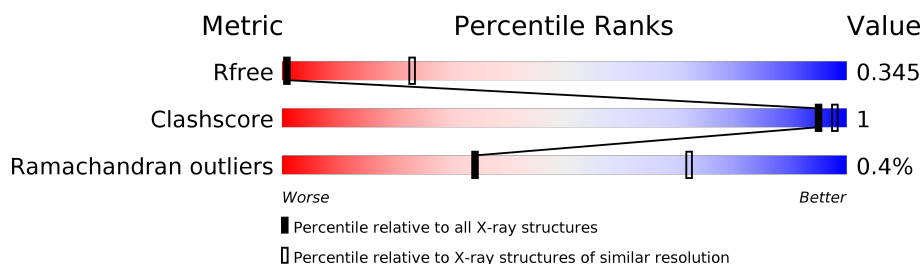
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1000 (7.20-3.84)
Clashscore	141614	1011 (7.12-3.90)
Ramachandran outliers	138981	1015 (7.20-3.82)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	730	
1	B	730	

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.

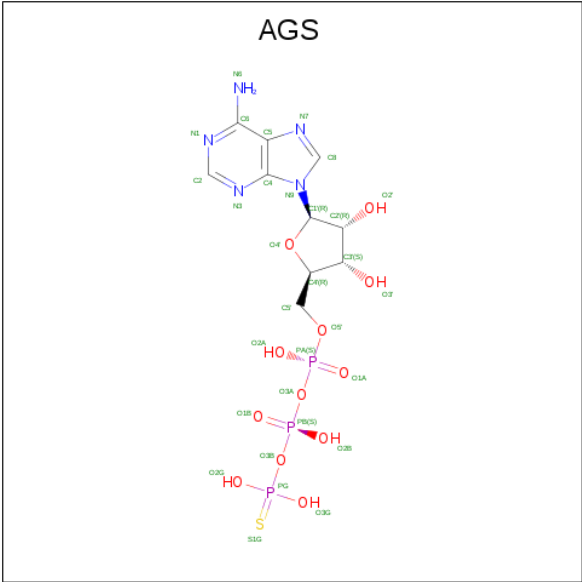
- Molecule 1 is a protein called ABC-type bacteriocin transporter.

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 (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



- Molecule 1: ABC-type bacteriocin transporter

- Molecule 1: ABC-type bacteriocin transporter

Chain B:

76% 23%

Position	Most Conserved Residue	Approx. Information Content (bits)
1	SER	0.14
2	ASN	0.13
3	ALA	0.12
4	ALA	0.11
5	MET	0.10
6	LEU	0.09
7	ARG	0.08
8	ARG	0.07
9	LEU	0.06
10	LEU	0.05
11	GLY	0.04
12	PHE	0.03
13	LYS	0.02
14	LYS	0.01
15	LYS	0.01
16	VAL	0.01
17	VAL	0.01
18	CYS	0.01
19	VAL	0.01
20	LYS	0.01
21	ALA	0.01
22	ARG	0.01
23	GLN	0.01
24	TYR	0.01
25	ASP	0.01
26	ASP	0.01
27	LEU	0.01
28	THR	0.01
29	ASP	0.01
30	CYS	0.01
31	GLY	0.01
32	ALA	0.01
33	ALA	0.01
34	ALA	0.01
35	CYS	0.01
36	LEU	0.01
37	LEU	0.01
38	SER	0.01
39	ILE	0.01
40	ASN	0.01
41	VAL	0.01
42	GLN	0.01
43	TYR	0.01
44	VAL	0.01
45	ASP	0.01
46	ASN	0.01
47	ASN	0.01
48	ARG	0.01
49	LEU	0.01
50	LEU	0.01
51	SER	0.01
52	LEU	0.01
53	ALA	0.01
54	HIS	0.01
55	PHE	0.01
56	VAL	0.01
57	VAL	0.01
58	ILE	0.01
59	TYR	0.01
60	SER	0.01
61	ILE	0.01
62	LYS	0.01
63	ASN	0.01
64	ARG	0.01
65	ILE	0.01
66	THR	0.01
67	VAL	0.01
68	ASP	0.01
69	ALA	0.01
70	ASP	0.01
71	PRO	0.01
72	GLY	0.01
73	ASN	0.01
74	TYR	0.01
75	GLN	0.01
76	ASN	0.01
77	MET	0.01
78	MET	0.01
79	VAL	0.01
80	VAL	0.01
81	LYS	0.01
82	PHE	0.01
83	ALA	0.01
84	ALA	0.01
85	GLU	0.01
86	GLY	0.01
87	GLY	0.01
88	LYS	0.01
89	GLN	0.01
90	THR	0.01
91	THR	0.01
92	ASN	0.01
93	ASN	0.01
94	ASN	0.01
95	ASN	0.01
96	ASN	0.01
97	ASN	0.01
98	ASN	0.01
99	ASN	0.01
100	ASN	0.01

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	230.00 Å 230.00 Å 89.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 5.51 41.66 – 5.51	Depositor EDS
% Data completeness (in resolution range)	80.9 (19.98-5.51) 81.4 (41.66-5.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 5.38 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.300 , 0.314 0.331 , 0.345	Depositor DCC
R_{free} test set	313 reflections (4.72%)	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)	0.56 , 999.0	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	0.75	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	0.23	0/2786	0.42	0/3876
1	B	0.23	0/2786	0.43	0/3876
All	All	0.23	0/5572	0.42	0/7752

There are no bond length outliers.

There are no bond angle outliers.

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:H8	2:B:801:AGS:H5'2	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 [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	563/730 (77%)	535 (95%)	26 (5%)	2 (0%)	34	72
1	B	563/730 (77%)	535 (95%)	26 (5%)	2 (0%)	34	72
All	All	1126/1460 (77%)	1070 (95%)	52 (5%)	4 (0%)	34	72

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 ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	26,33,33	0.70	1 (3%)	26,52,52	1.14	3 (11%)
2	AGS	A	801	-	26,33,33	0.70	0	26,52,52	1.19	3 (11%)

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	-	-	6/17/38/38	0/3/3/3
2	AGS	A	801	-	-	5/17/38/38	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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	801	AGS	PA-O3A-PB	-3.64	120.35	132.83
2	B	801	AGS	PA-O3A-PB	-3.42	121.10	132.83
2	B	801	AGS	C5-C6-N6	2.28	123.81	120.35
2	A	801	AGS	C5-C6-N6	2.23	123.74	120.35
2	A	801	AGS	O3G-PG-O3B	2.01	111.36	104.64
2	B	801	AGS	C3'-C2'-C1'	2.00	103.99	100.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

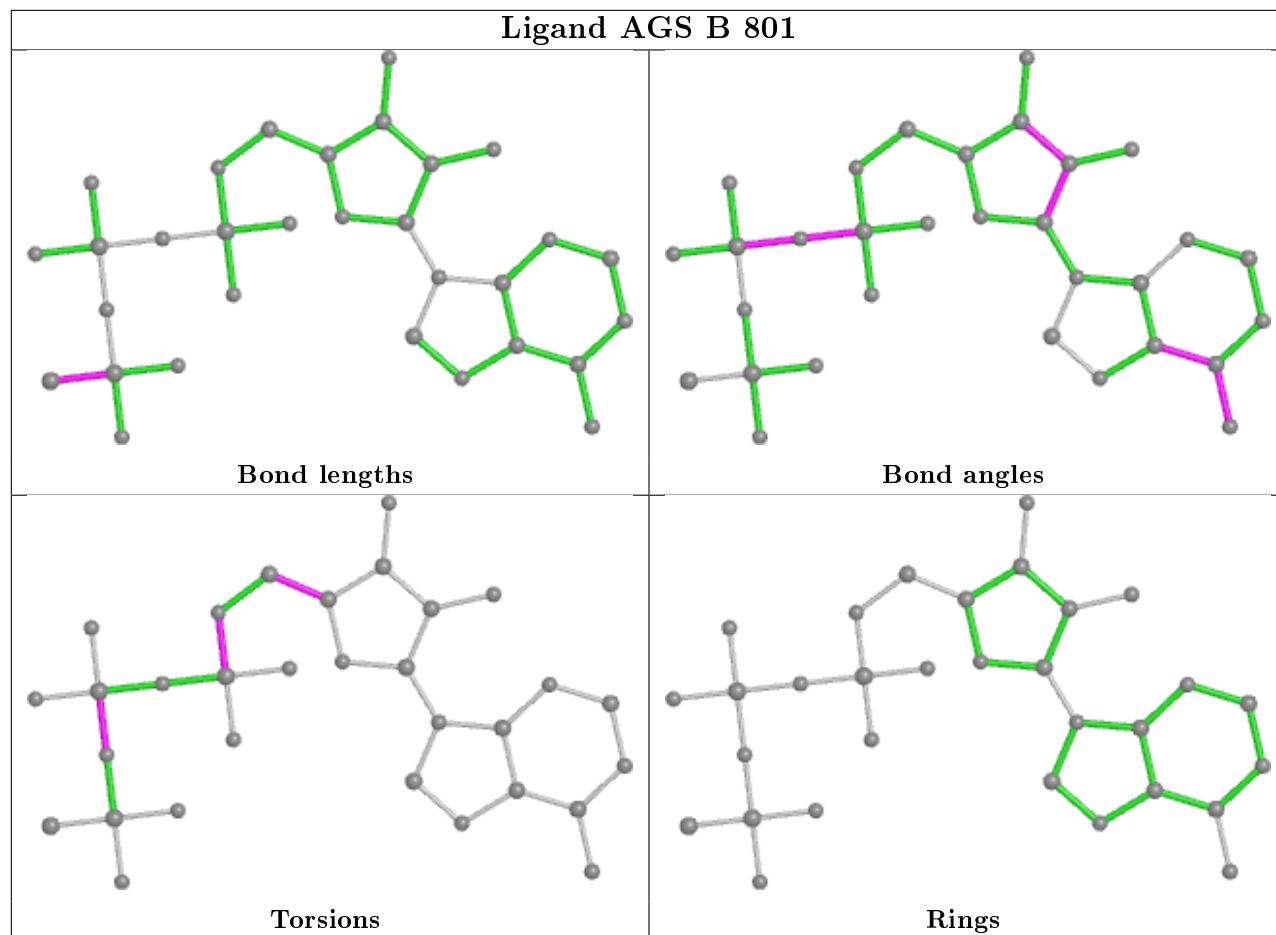
There are no ring outliers.

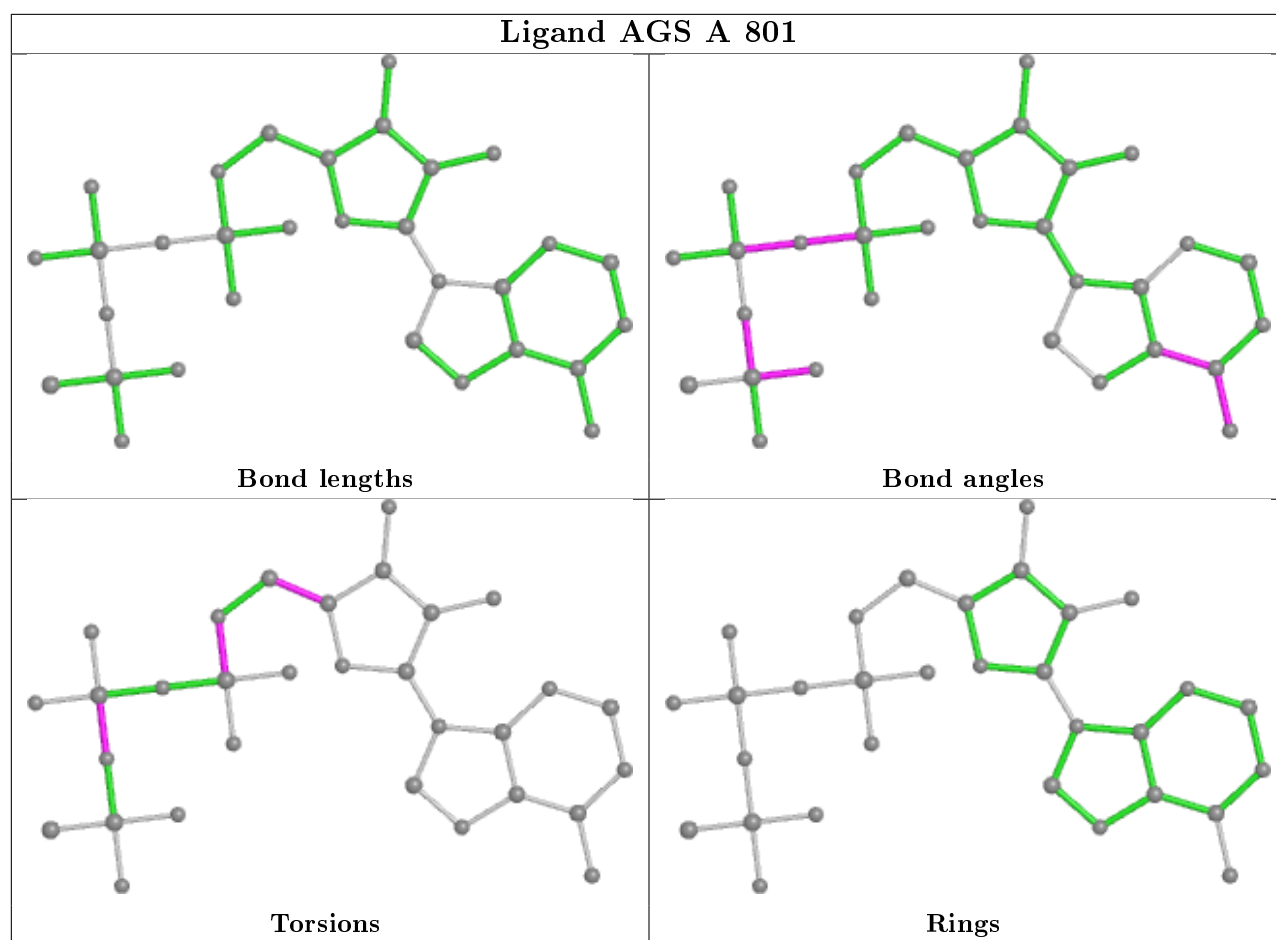
2 monomers are involved in 5 short contacts:

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

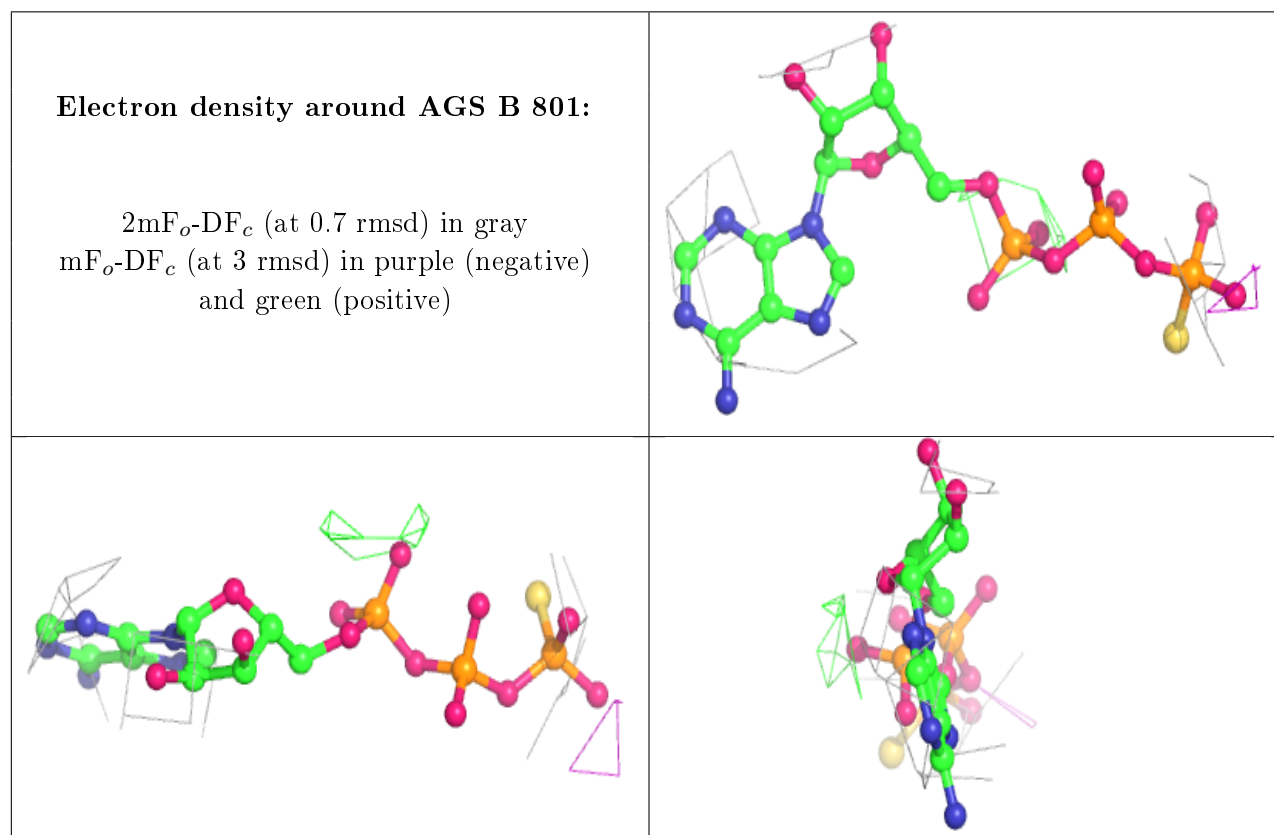
6.3 Carbohydrates [i](#)

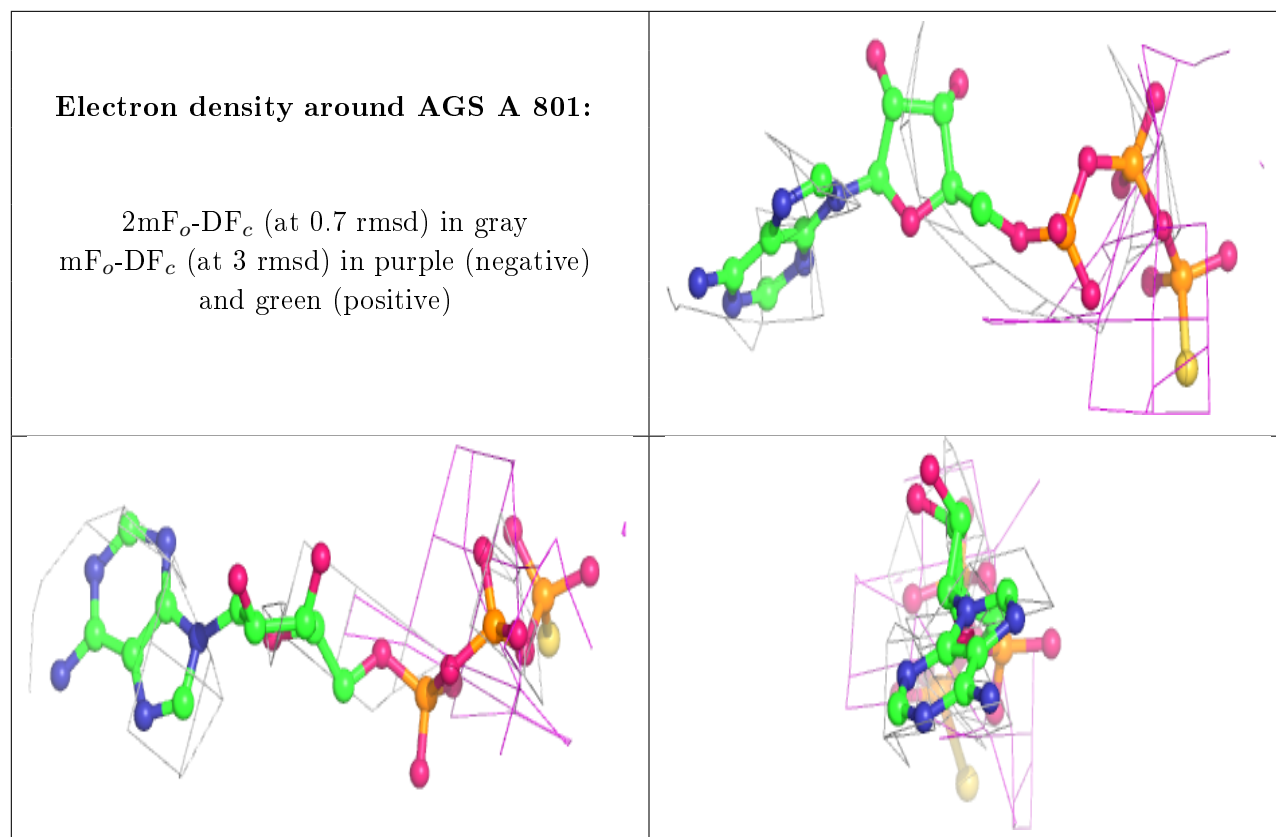
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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 [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.