



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 01:21 PM EDT

PDB ID : 6HRC / pdb_00006hrc
Title : Outward-facing PglK with ATPgammaS bound
Authors : Perez, C.; Locher, K.P.
Deposited on : 2018-09-26
Resolution : 3.30 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

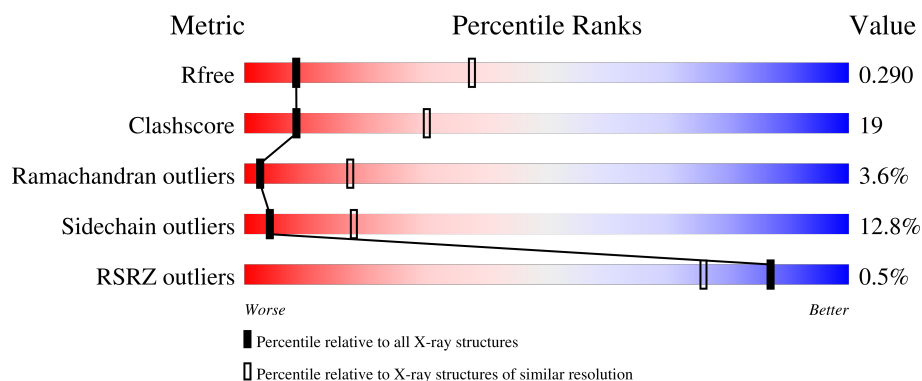
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	564	57% 37% 6%
1	B	564	55% 36% 9%
1	C	564	53% 37% 9%
1	D	564	55% 37% 7%

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	AGS	B	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18482 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.

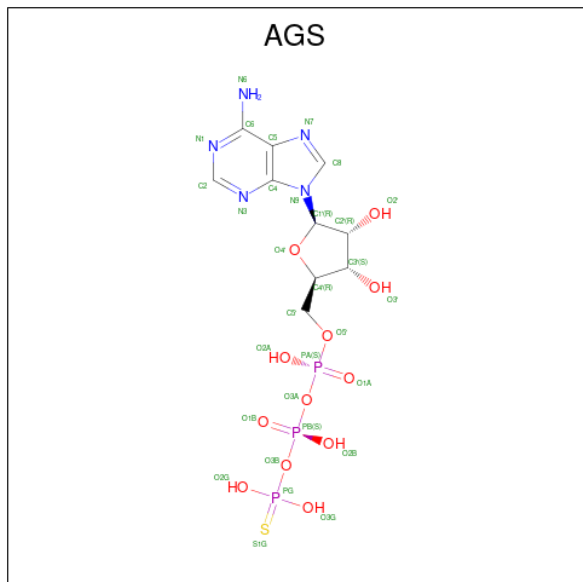
- Molecule 1 is a protein called WlaB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4555	2998	732	811	14			
1	B	564	Total	C	N	O	S	0	0	0
			4555	2998	732	811	14			
1	C	564	Total	C	N	O	S	0	0	0
			4555	2998	732	811	14			
1	D	564	Total	C	N	O	S	0	0	0
			4555	2998	732	811	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	conflict	UNP O86150
A	105	LYS	TYR	conflict	UNP O86150
A	338	ALA	LEU	conflict	UNP O86150
A	339	ALA	GLY	conflict	UNP O86150
A	510	GLN	GLU	engineered mutation	UNP O86150
B	2	VAL	LEU	conflict	UNP O86150
B	105	LYS	TYR	conflict	UNP O86150
B	338	ALA	LEU	conflict	UNP O86150
B	339	ALA	GLY	conflict	UNP O86150
B	510	GLN	GLU	engineered mutation	UNP O86150
C	2	VAL	LEU	conflict	UNP O86150
C	105	LYS	TYR	conflict	UNP O86150
C	338	ALA	LEU	conflict	UNP O86150
C	339	ALA	GLY	conflict	UNP O86150
C	510	GLN	GLU	engineered mutation	UNP O86150
D	2	VAL	LEU	conflict	UNP O86150
D	105	LYS	TYR	conflict	UNP O86150
D	338	ALA	LEU	conflict	UNP O86150
D	339	ALA	GLY	conflict	UNP O86150
D	510	GLN	GLU	engineered mutation	UNP O86150

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: 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		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	36	Total	O	0	0
			36	36		

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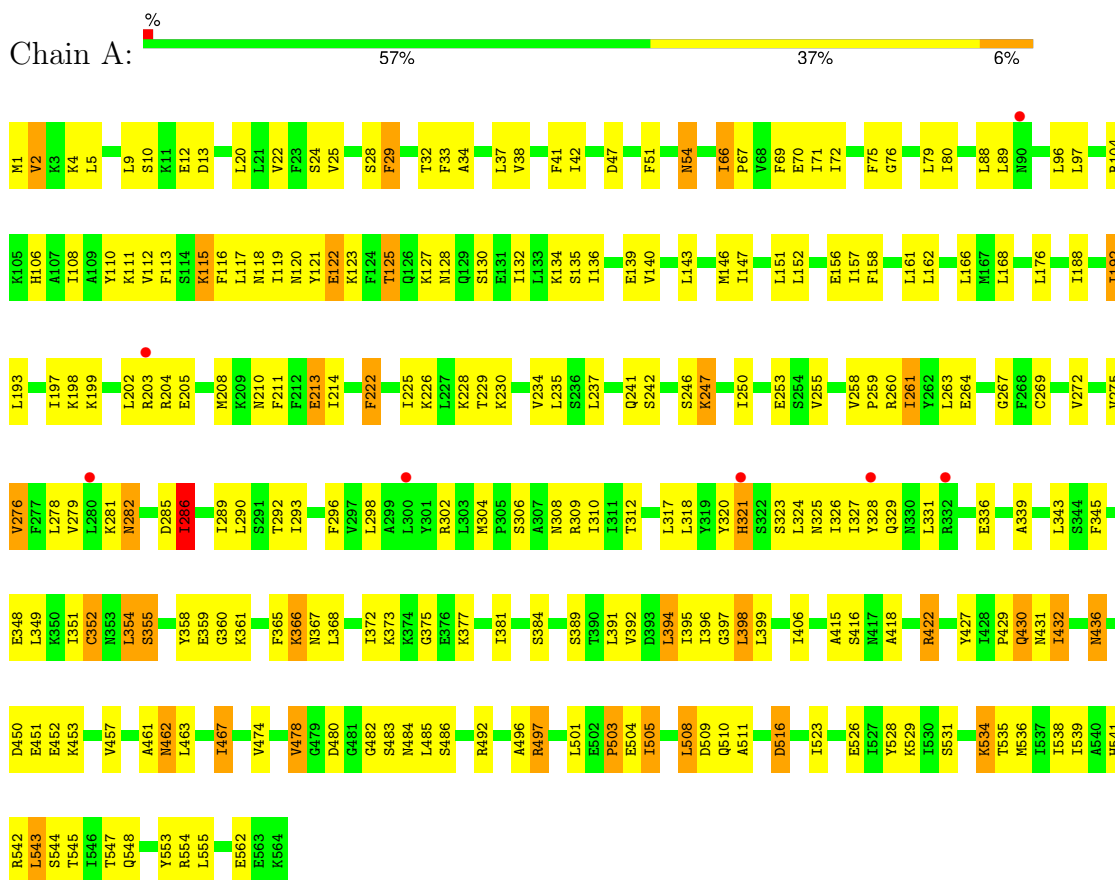
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	37	Total 37	O 37	0	0
4	D	31	Total 31	O 31	0	0

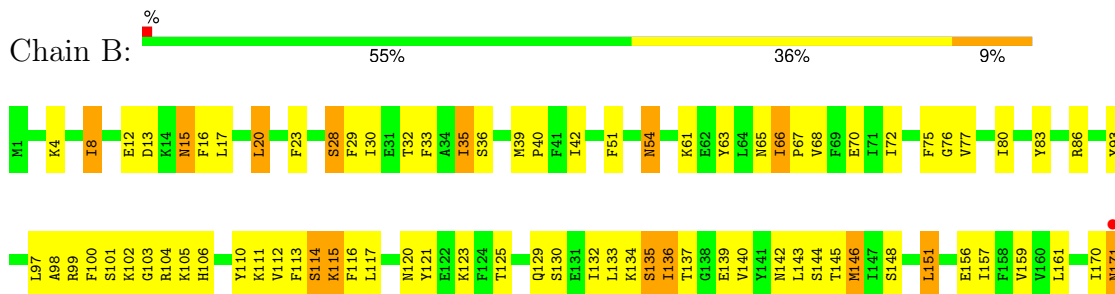
3 Residue-property plots

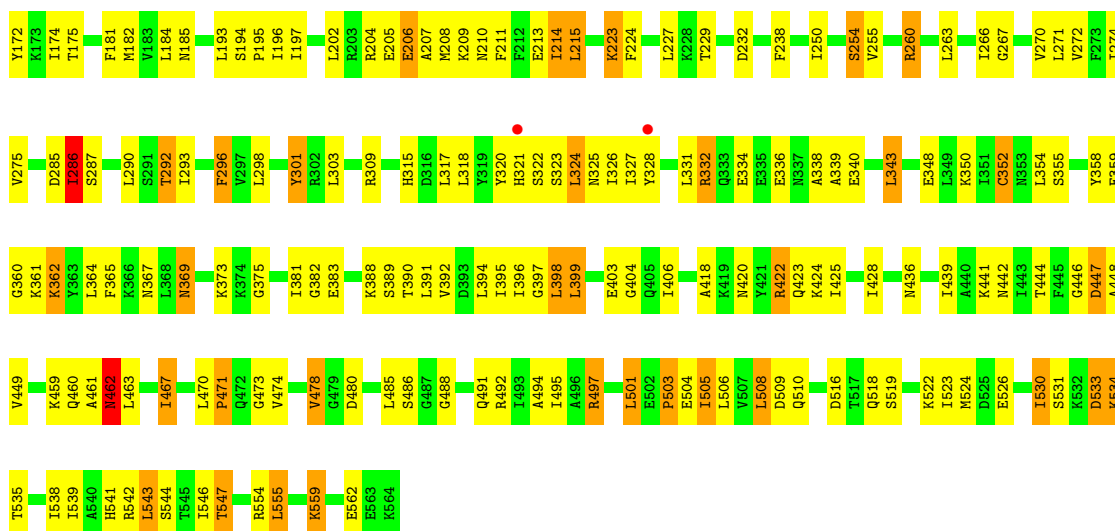
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: WlaB protein



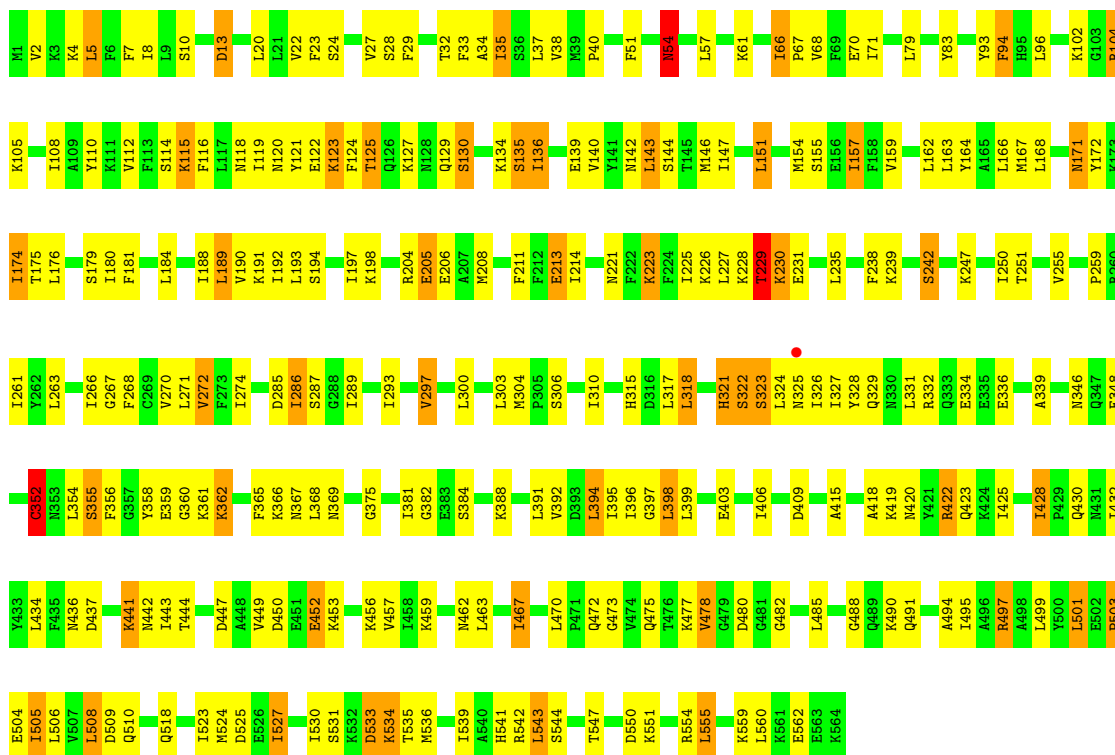
• Molecule 1: WlaB protein





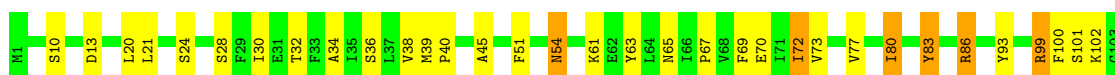
• Molecule 1: WlaB protein

Chain C: 53% 37% 9%



• Molecule 1: WlaB protein

Chain D: 55% 37% 7%



T535		V457		K373		F296		M208		R104	
T539		I458		K374		V297		K209		K105	
A540		K459		G375		L298		A299		H106	
H541		Q460				A299		N210		A107	
A461		A461		A379		L300		F211		I108	
N462		N462		F380		Y301		F212		A109	
L463		L463		I381		R302		E213		Y110	
				G382		L303		L214		K111	
				E383		M304		L215		V112	
				S384		P305					
						S306		N220		K115	
T547		P471		G387		A307				F116	
Q548		Q472		K388		K308		K223			
C549		V474		S389		R309		F224		I119	
Y553				T390		I310		I225		M120	
R554		K477		L391				K226		Y121	
L555		V478		V392		L317		L227		E122	
				D393		L318		K228		K123	
K559		G482		L394				T229		F124	
L560				L395		H321		K230		T125	
K561		L485		I396		S322					
E562		S486		G397		S323		V234		S130	
E563				L398		L324				E131	
K564		Q489		L399				Q241		I132	
						I327		S242		I133	
		R492		I406		Y328		E243		K134	
		I493								S135	
		A494		D409		L331		S246		I136	
		I495		K410		R332		K247			
						Q333				E139	
		A496		N414				L250		V140	
		R497		A415		E340				Y141	
		K498		S416				V255		M142	
		L499		N417		L343					
		Y500		A418		S344		V258		L151	
		L501				F345		P259		L152	
		P502		Y421		N346		R260		L153	
		E503		R422		Q347				M154	
		E504		Q423		E348		L263		S155	
		I505		K424		L349				E156	
		L506		I425		K350		F268		I157	
		Y507				I351				F158	
		L508		N431		C352		L271		V159	
		D509		I432		N353				V160	
						L354		I274		L161	
		L515		D437		S355		V275			
								V276		Y164	
		S519		K441		Y358		F277		L168	
				N442				L278			
		I523		I443		K362		V279		M171	
		M524				Y363					
		B525		D447		L364		D285		F181	
		E526				F365		I286			
		I527		D450		K366		S287		I197	
		Y528				N367				K198	
		K529		E451		I368		L290		K199	
				E452		N369		S291			
		I530		K453		L370		I292		R204	
		S531		L454		N371		I293		E205	
		R532		N455							
		D533		K456							
		K534									

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.68Å 145.98Å 206.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.8 (20.00-3.30) 90.3 (20.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.232 , 0.284 0.244 , 0.290	Depositor DCC
R_{free} test set	2695 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 99.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18482	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: AGS, 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	0.23	0/4639	0.49	0/6244
1	B	0.31	0/4639	0.55	0/6244
1	C	0.27	0/4639	0.54	2/6244 (0.0%)
1	D	0.25	0/4639	0.53	2/6244 (0.0%)
All	All	0.27	0/18556	0.53	4/24976 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ILE	CA-C-N	-5.79	115.55	122.44
1	C	136	ILE	C-N-CA	-5.79	115.55	122.44
1	D	136	ILE	CA-C-N	-5.38	116.03	122.44
1	D	136	ILE	C-N-CA	-5.38	116.03	122.44

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	A	4555	0	4760	176	0
1	B	4555	0	4760	187	0
1	C	4555	0	4760	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4555	0	4760	186	0
2	A	31	0	12	3	0
2	B	31	0	12	10	0
2	C	31	0	12	3	0
2	D	31	0	12	5	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	32	0	0	7	0
4	B	36	0	0	6	0
4	C	37	0	0	9	0
4	D	31	0	0	4	0
All	All	18482	0	19088	707	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 19.

The worst 5 of 707 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:125:THR:HG21	2:B:601:AGS:HN62	1.27	1.00
1:C:509:ASP:HA	1:C:539:ILE:HB	1.54	0.90
1:C:38:VAL:HG22	1:C:83:TYR:OH	1.70	0.89
1:A:397:GLY:HA3	1:A:422:ARG:HD2	1.58	0.86
1:D:142:ASN:HB2	1:D:324:LEU:HD22	1.59	0.84

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	562/564 (100%)	499 (89%)	47 (8%)	16 (3%)	4 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	562/564 (100%)	484 (86%)	57 (10%)	21 (4%)	2	17
1	C	562/564 (100%)	490 (87%)	50 (9%)	22 (4%)	2	16
1	D	562/564 (100%)	486 (86%)	55 (10%)	21 (4%)	2	17
All	All	2248/2256 (100%)	1959 (87%)	209 (9%)	80 (4%)	2	17

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	503	PRO
1	B	68	VAL
1	B	338	ALA
1	B	462	ASN
1	B	503	PRO

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	A	504/504 (100%)	453 (90%)	51 (10%)	7	26
1	B	504/504 (100%)	426 (84%)	78 (16%)	2	12
1	C	504/504 (100%)	433 (86%)	71 (14%)	3	14
1	D	504/504 (100%)	445 (88%)	59 (12%)	5	20
All	All	2016/2016 (100%)	1757 (87%)	259 (13%)	4	18

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	302	ARG
1	D	369	ASN
1	B	309	ARG
1	B	292	THR
1	D	431	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	436	ASN
1	D	185	ASN
1	D	484	ASN
1	D	455	ASN
1	B	171	ASN

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	AGS	A	601	-	32,33,33	2.04	6 (18%)	45,52,52	1.89	10 (22%)
2	AGS	C	601	3	32,33,33	2.03	6 (18%)	45,52,52	1.89	10 (22%)
2	AGS	B	601	3	32,33,33	2.04	6 (18%)	45,52,52	1.89	10 (22%)
2	AGS	D	601	-	32,33,33	2.04	6 (18%)	45,52,52	1.90	10 (22%)

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	A	601	-	-	2/21/38/38	0/3/3/3
2	AGS	C	601	3	-	5/21/38/38	0/3/3/3
2	AGS	B	601	3	-	6/21/38/38	0/3/3/3
2	AGS	D	601	-	-	1/21/38/38	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	AGS	PG-S1G	7.99	2.08	1.90
2	A	601	AGS	PG-S1G	7.96	2.07	1.90
2	B	601	AGS	PG-S1G	7.95	2.07	1.90
2	C	601	AGS	PG-S1G	7.94	2.07	1.90
2	A	601	AGS	C5-C4	4.74	1.47	1.39

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	AGS	C5-C4-N3	-5.87	118.63	126.72
2	C	601	AGS	C5-C4-N3	-5.86	118.65	126.72
2	D	601	AGS	C5-C4-N3	-5.85	118.66	126.72
2	A	601	AGS	C5-C4-N3	-5.85	118.67	126.72
2	B	601	AGS	N3-C4-N9	4.62	135.02	127.17

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	AGS	PB-O3B-PG-O2G
2	C	601	AGS	PB-O3B-PG-O3G
2	B	601	AGS	O4'-C4'-C5'-O5'
2	B	601	AGS	C3'-C4'-C5'-O5'
2	B	601	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 21 short contacts:

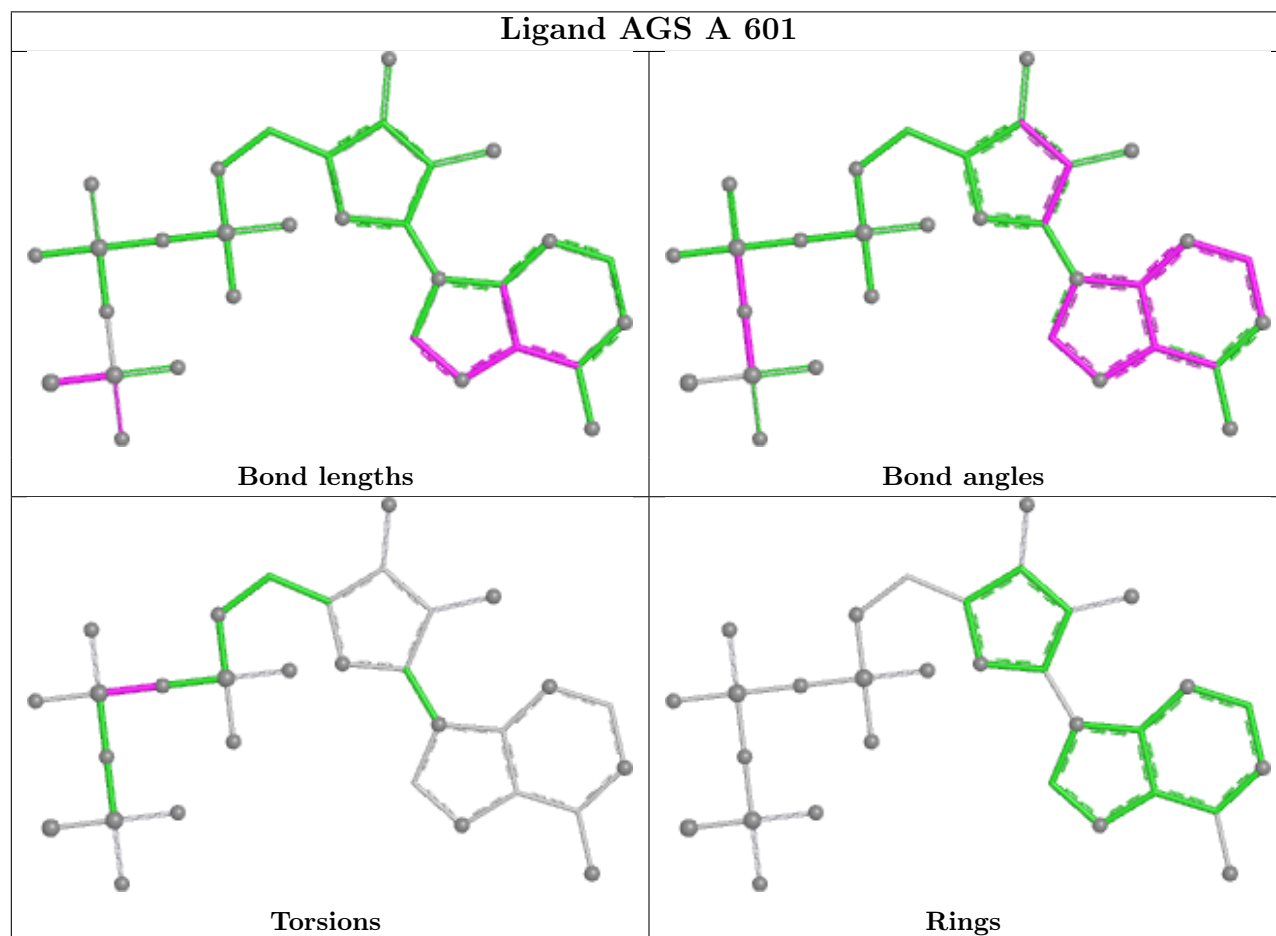
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	AGS	3	0

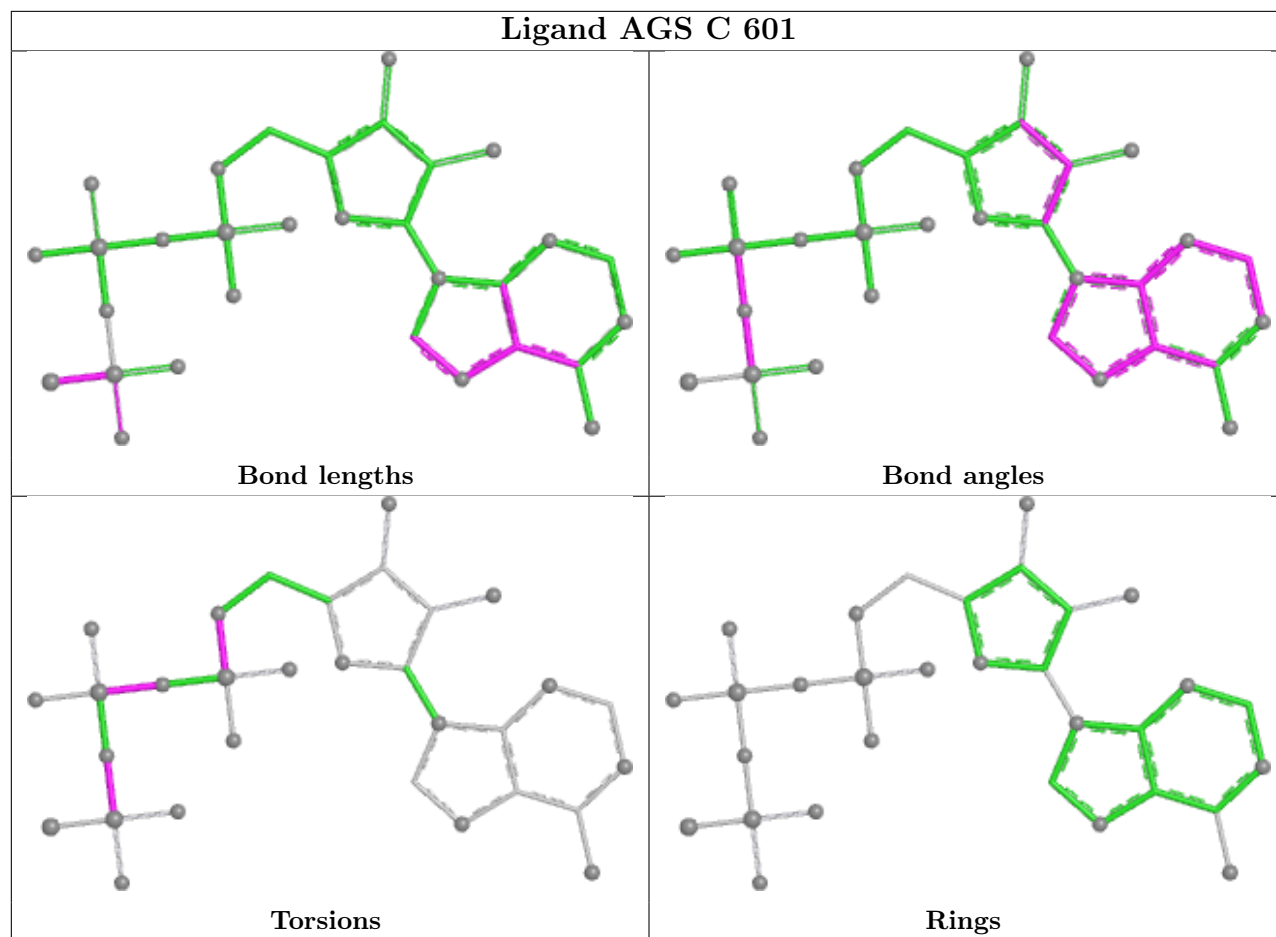
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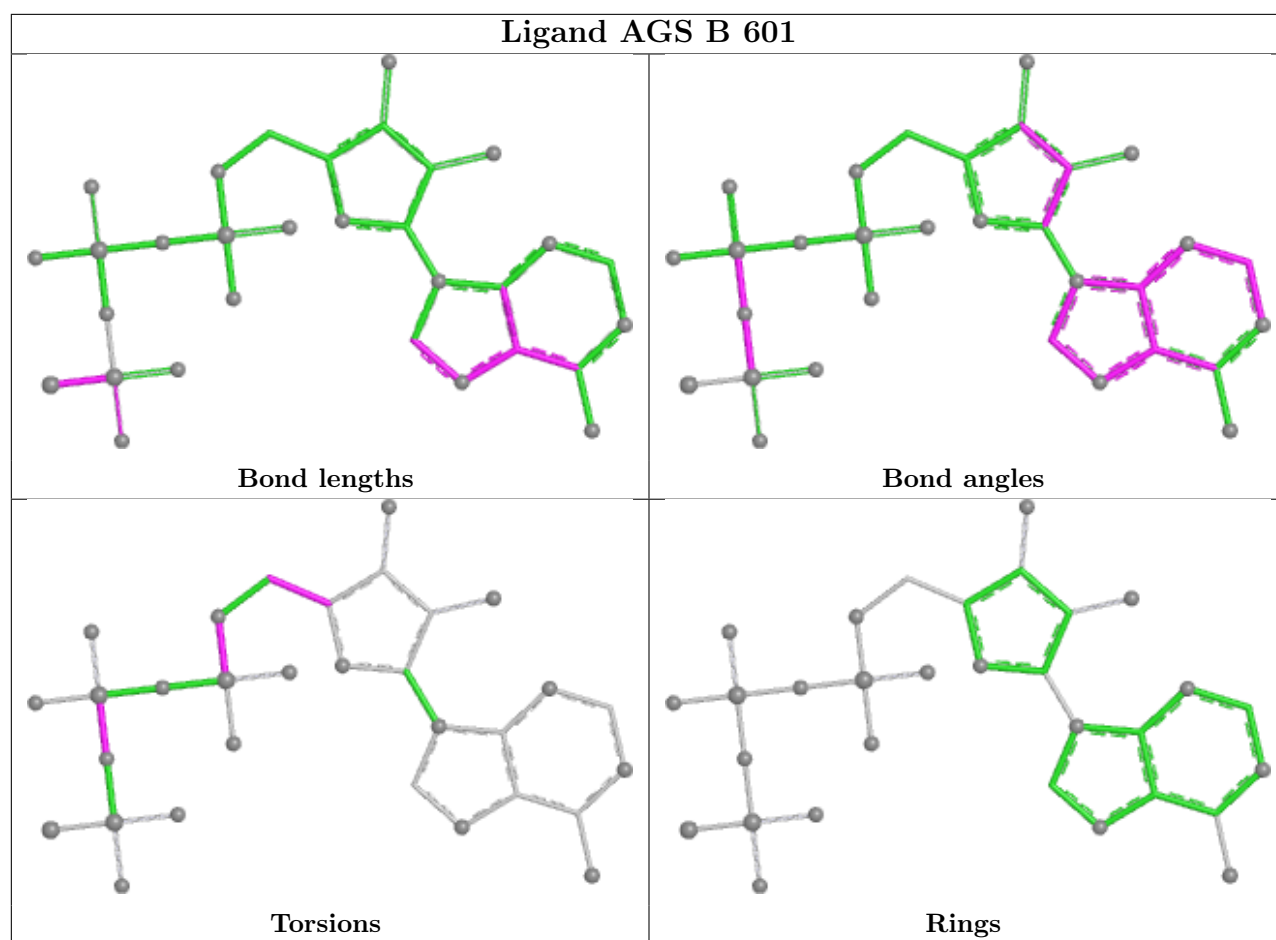
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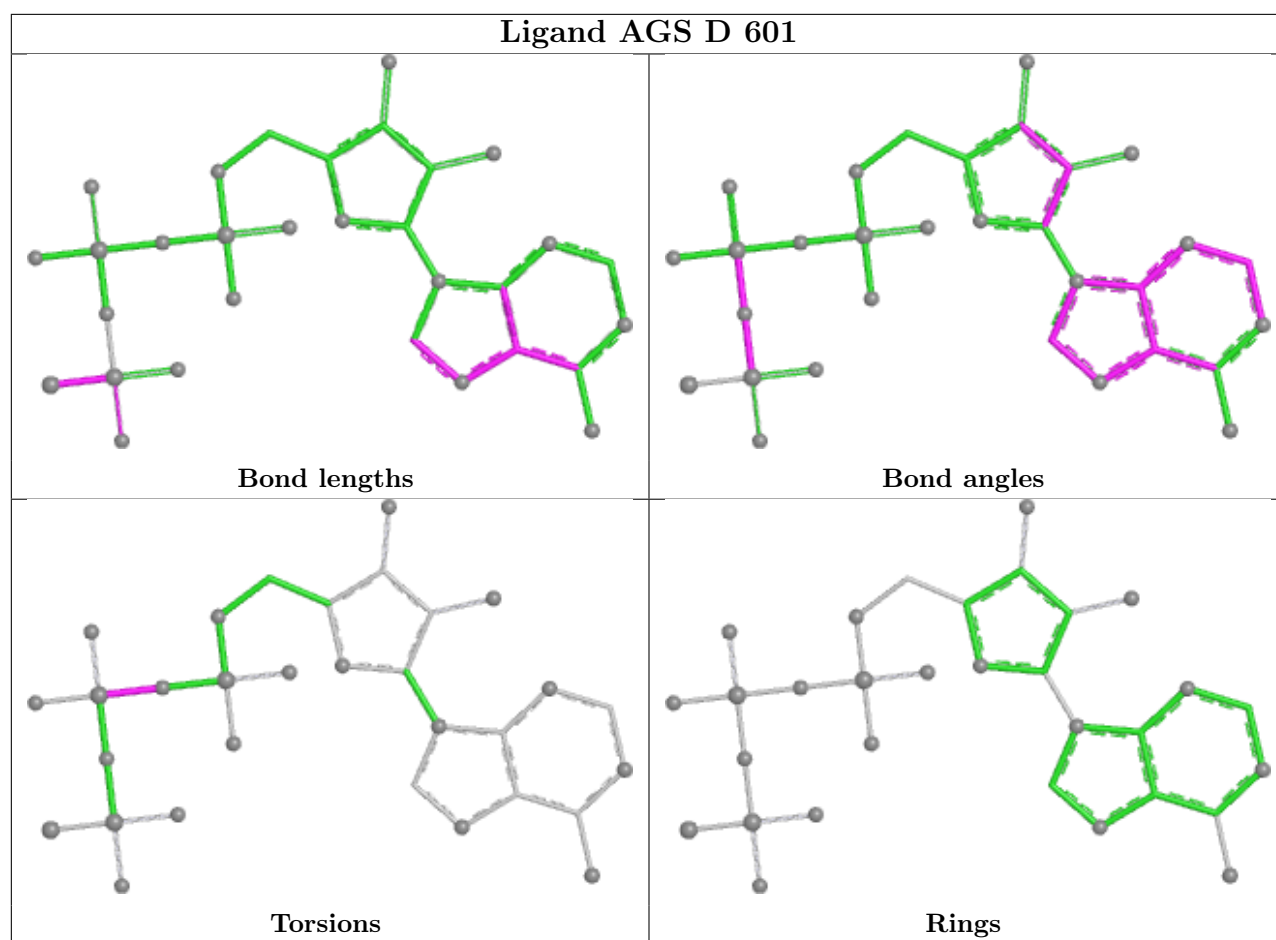
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	AGS	3	0
2	B	601	AGS	10	0
2	D	601	AGS	5	0

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 [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	564/564 (100%)	-0.26	7 (1%) 76 58	64, 143, 291, 584	0
1	B	564/564 (100%)	-0.30	3 (0%) 87 76	44, 115, 261, 366	0
1	C	564/564 (100%)	-0.29	1 (0%) 91 86	58, 119, 275, 346	0
1	D	564/564 (100%)	-0.27	1 (0%) 91 86	60, 131, 288, 450	0
All	All	2256/2256 (100%)	-0.28	12 (0%) 87 76	44, 127, 280, 584	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	HIS	4.7
1	A	321	HIS	4.6
1	A	280	LEU	3.4
1	A	328	TYR	3.0
1	D	321	HIS	2.9

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](#)

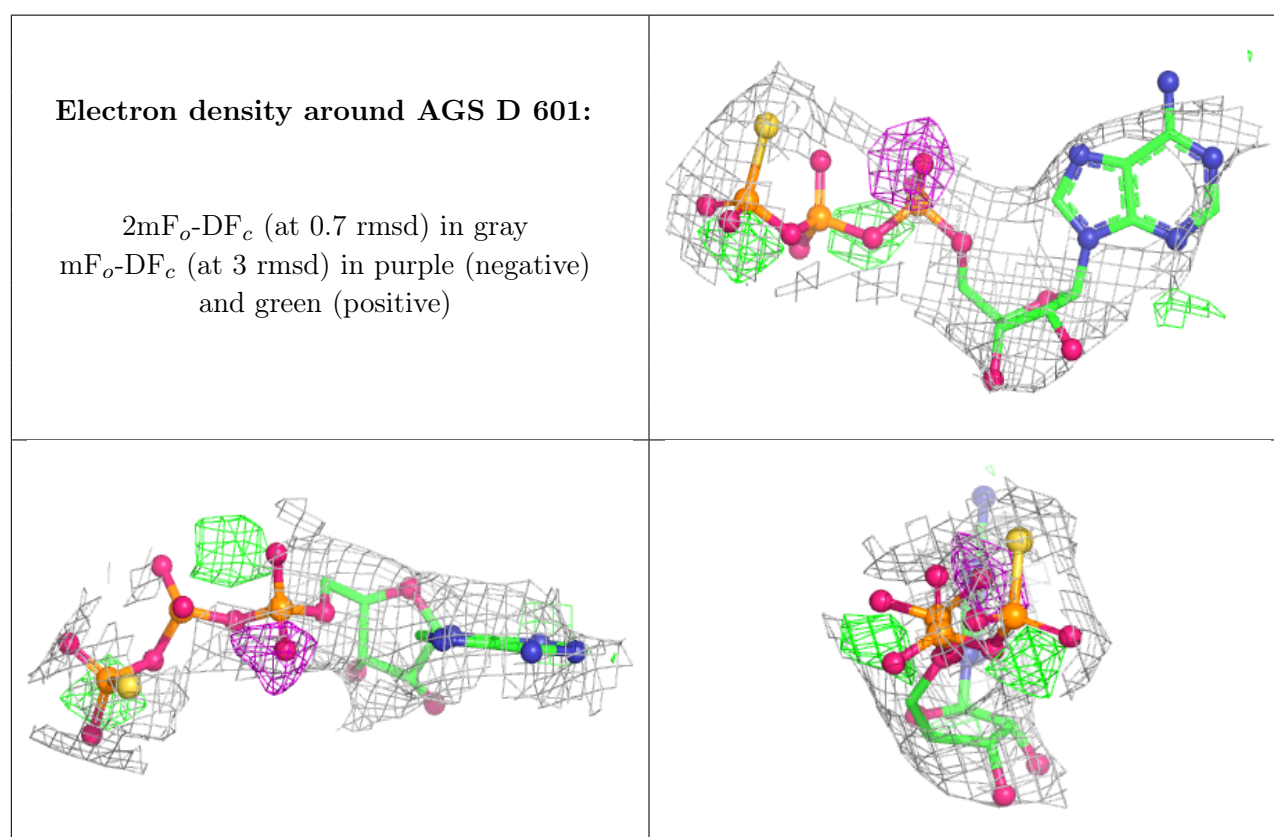
There are no oligosaccharides in this entry.

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.

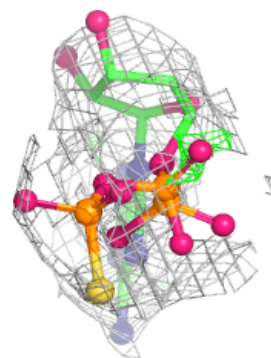
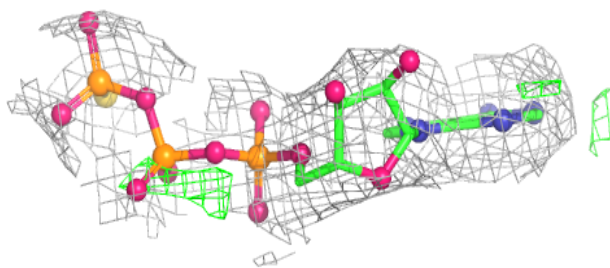
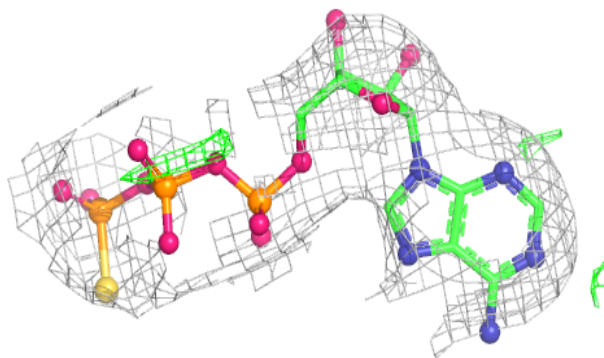
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	602	1/1	0.90	0.09	104,104,104,104	0
2	AGS	D	601	31/31	0.92	0.11	43,121,168,276	0
2	AGS	A	601	31/31	0.92	0.11	59,118,158,208	0
2	AGS	B	601	31/31	0.94	0.08	71,92,130,225	0
2	AGS	C	601	31/31	0.96	0.07	45,81,139,289	0
3	MG	C	602	1/1	0.99	0.05	112,112,112,112	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.

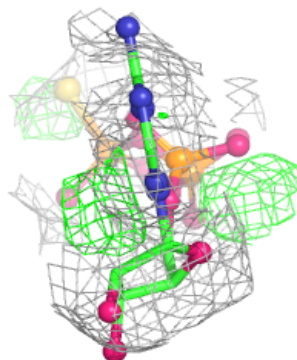
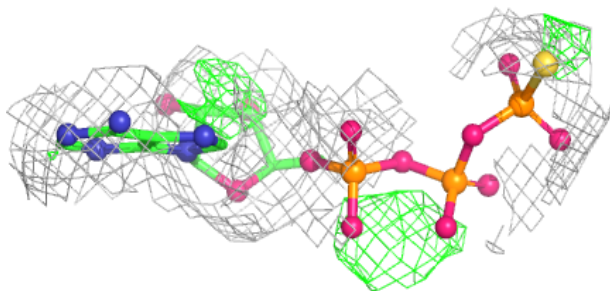
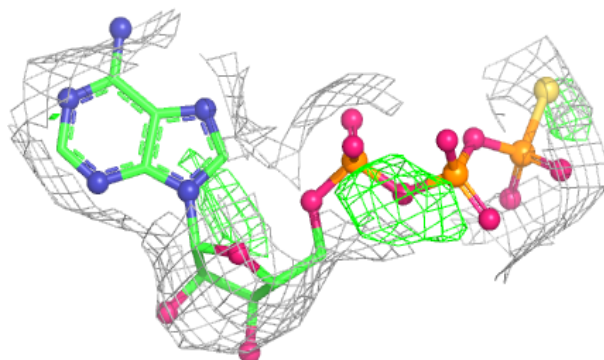


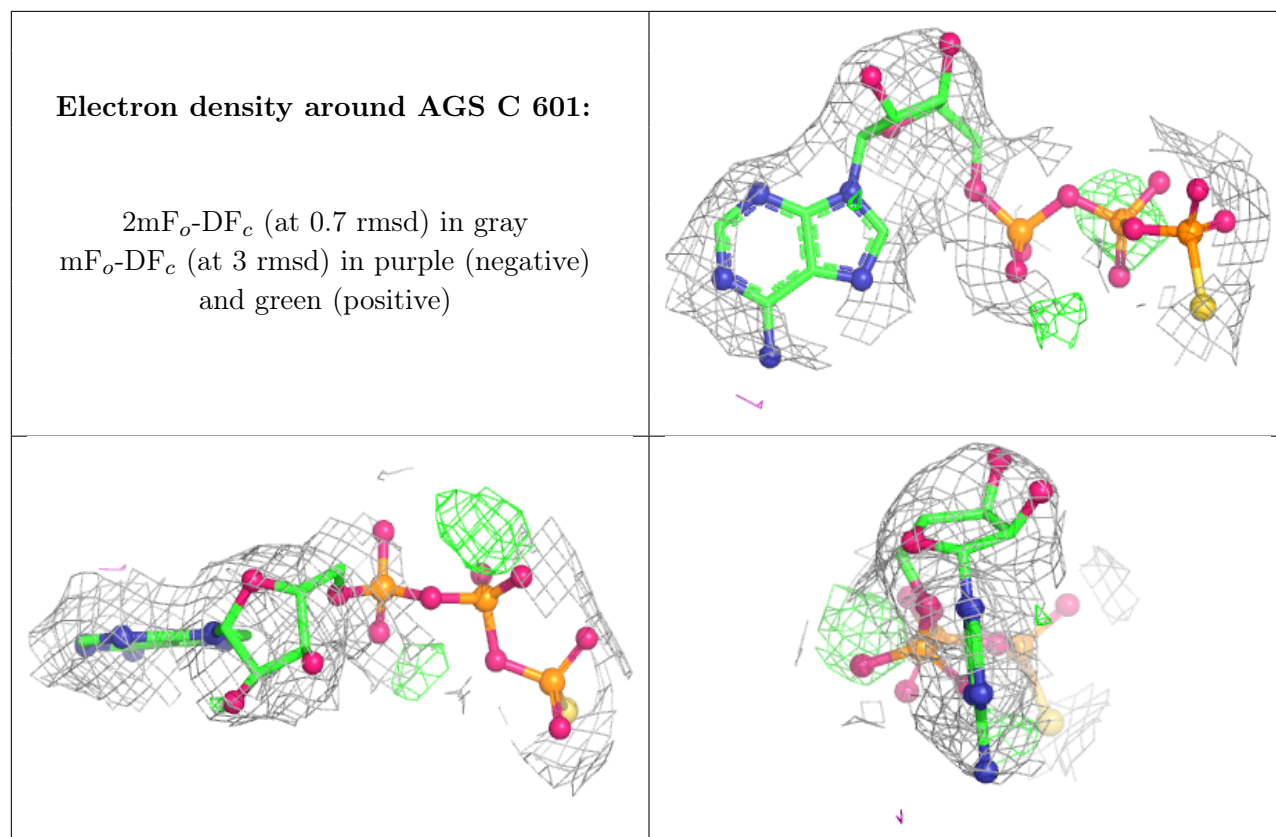
Electron density around AGS A 601:

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

**Electron density around AGS B 601:**

$2mF_o-DF_c$ (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.