



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:12 PM UTC

PDB ID : 6Z4X / pdb_00006z4x
Title : Structure of the CAK complex form Chaetomium thermophilum bound to ATP-gamma-S
Authors : Peissert, S.; Kuper, J.; Kisker, C.
Deposited on : 2020-05-26
Resolution : 2.98 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

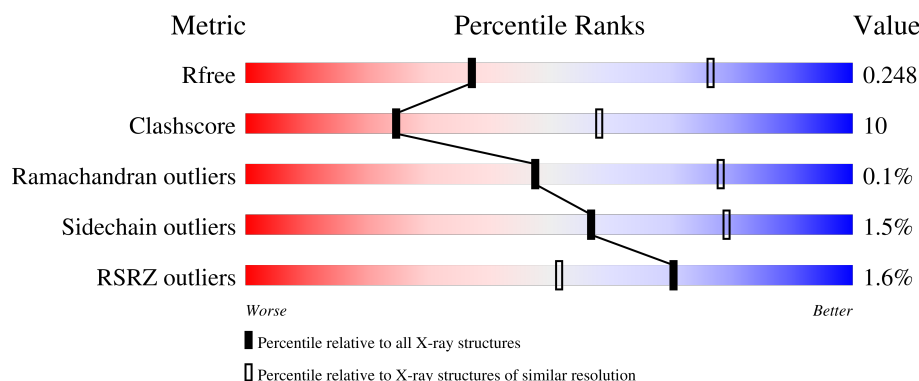
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	425	2% 54%19%27%
1	D	425	% 54%20%26%
2	B	437	% 54%19%26%
2	E	437	% 58%15%26%
3	C	69	3% 74%20%. .

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Mol	Chain	Length	Quality of chain
3	F	69	% 74% 22% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11470 atoms, of which 28 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 CYCLIN domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2522	1599	449	463	11			
1	D	314	Total	C	N	O	S	0	0	0
			2533	1605	451	466	11			

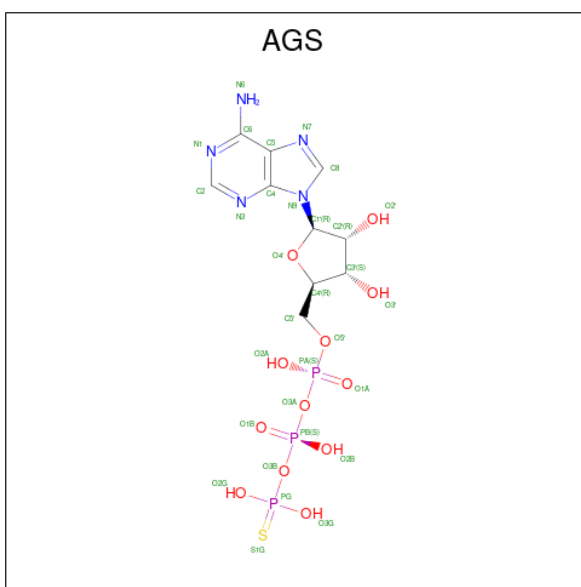
- Molecule 2 is a protein called Protein kinase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2613	1678	462	460	13			
2	E	323	Total	C	N	O	S	0	0	0
			2620	1682	463	462	13			

- Molecule 3 is a protein called RING-type domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	66	Total	C	N	O	S	0	0	0
			538	344	90	102	2			
3	F	67	Total	C	N	O	S	0	0	0
			550	353	91	104	2			

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	S	0	0
			45	10	14	5	12	3	1		
4	E	1	Total	C	H	N	O	P	S	0	0
			45	10	14	5	12	3	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		

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.

[illegible][illegible]

Chain B:

Amino Acid	Score
MET	E181
GLY	R232
MET	I184
VAL	L296
GLU	P297
ASP	G298
GLU	K198
ASN	A199
GLY	W200
PRO	L307
PRO	I312
ARG	L326
GLY	D331
SER	P332
VAL	E213
ALA	F349
ARG	H218
LYS	R219
LEU	D220
ASP	I221
PHE	K222
GLY	P223
GLN	N224
LEU	W225
GLN	L226
LYS	K228
GLY	A229
GLN	D238
GLN	L241
PRO	A242
GLN	R243
PRO	A246
GLY	R251
ASN	M252
LYS	T253
LYS	A254
LYS	N255
LYS	V256
LYS	L257
LYS	T258
LYS	R259
LYS	W260
GLY	R271
GLU	G274
ASP	V277
LYS	D278
ALA	I279
ASP	W280
LEU	P176
LYS	M284
ARG	L180

Chain E:

Residue	Category
THR	Green
ILE	Green
ALA	Green
ASN	Green
VAL	Green
THR	Green
SER	Green
ALA	Green
ALA	Green
PRO	Green
PHE	Green
SER	Green
SER	Green
ARG	Green
PRO	Green
ALA	Green
GLN	Green
ILE	Green
T77	Yellow
F78	Yellow
D79	Yellow
P80	Yellow
V81	Yellow
E82	Yellow
Q83	Yellow
R90	Yellow
R112	Yellow
V119	Yellow
K122	Yellow
K123	Yellow
I124	Yellow
K125	Yellow
V126	Yellow
D132	Yellow
D137	Yellow
A138	Yellow
V139	Yellow
L142	Yellow
N153	Yellow
L157	Yellow
V160	Yellow
D165	Yellow
Q166	Yellow
N167	Yellow
L168	Yellow
V171	Yellow
L172	Yellow
L175	Yellow
E181	Yellow
I184	Yellow
Y192	Yellow
G193	Yellow
I197	Yellow
L204	Yellow
A207	Yellow
R219	Yellow
K222	Yellow
P223	Yellow
N224	Yellow
N225	Yellow
L226	Yellow
L227	Yellow
R243	Yellow
A246	Yellow
R251	Yellow
M252	Yellow
T253	Yellow
A254	Yellow
N255	Yellow
V256	Yellow
I257	Yellow
P263	Yellow
P264	Yellow
E265	Yellow
G269	Yellow
A270	Yellow
R271	Yellow
G274	Yellow
V277	Yellow
D278	Yellow
I279	Yellow
M284	Yellow
T290	Yellow
L291	Yellow
R292	Yellow
F295	Yellow
L296	Yellow
E318	Yellow
L296	Yellow

Chain C:

Residue	State	Count
GLY	Grey	1
PRO	Grey	1
TYR	Grey	1
D273	Red	3
R286	Green	1
V287	Green	1
R288	Green	1
L296	Green	1
D297	Green	1
K298	Green	1
Y299	Green	1
R300	Green	1
I306	Green	1
L313	Yellow	1
I316	Yellow	1
F324	Yellow	1
A323	Green	1
A325	Green	1
G326	Green	1
L327	Green	1
A328	Green	1
V329	Green	1
F330	Green	1
I331	Green	1
G338	Green	1

Chain F:

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.97Å 84.90Å 154.48Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	46.65 – 2.98 46.65 – 2.98	Depositor EDS
% Data completeness (in resolution range)	61.1 (46.65-2.98) 61.1 (46.65-2.98)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.96Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.18rc4_3812	Depositor
R, R_{free}	0.203 , 0.246 0.208 , 0.248	Depositor DCC
R_{free} test set	1469 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11470	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 5.66% 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, CL, 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	0.12	0/2574	0.30	0/3471
1	D	0.13	0/2585	0.32	0/3486
2	B	0.11	0/2684	0.30	0/3635
2	E	0.12	0/2691	0.32	0/3646
3	C	0.09	0/552	0.26	0/742
3	F	0.10	0/565	0.27	0/760
All	All	0.12	0/11651	0.31	0/15740

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 [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	2522	0	2517	59	0
1	D	2533	0	2527	61	0
2	B	2613	0	2624	56	0
2	E	2620	0	2630	47	0
3	C	538	0	502	12	0
3	F	550	0	511	14	0
4	B	31	14	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	31	14	12	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
All	All	11442	28	11335	224	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 10.

The worst 5 of 224 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)
2:E:253:THR:HG22	2:E:255:ASN:H	1.28	0.96
2:B:253:THR:HG22	2:B:255:ASN:H	1.34	0.92
2:E:246:ALA:HB2	2:E:252:MET:HE3	1.55	0.88
1:A:381:ARG:HD3	1:A:385:ASP:HA	1.56	0.86
3:C:313:LEU:HD22	3:C:313:LEU:H	1.48	0.77

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	306/425 (72%)	297 (97%)	9 (3%)	0	100	100
1	D	308/425 (72%)	298 (97%)	10 (3%)	0	100	100
2	B	320/437 (73%)	311 (97%)	8 (2%)	1 (0%)	36	67
2	E	321/437 (74%)	312 (97%)	8 (2%)	1 (0%)	36	67
3	C	64/69 (93%)	64 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	65/69 (94%)	65 (100%)	0	0	100	100
All	All	1384/1862 (74%)	1347 (97%)	35 (2%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	257	ILE
2	E	257	ILE

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	267/354 (75%)	264 (99%)	3 (1%)	65	82
1	D	268/354 (76%)	265 (99%)	3 (1%)	65	82
2	B	275/370 (74%)	272 (99%)	3 (1%)	65	82
2	E	276/370 (75%)	272 (99%)	4 (1%)	59	80
3	C	55/57 (96%)	52 (94%)	3 (6%)	19	51
3	F	56/57 (98%)	54 (96%)	2 (4%)	31	63
All	All	1197/1562 (77%)	1179 (98%)	18 (2%)	57	79

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	326	LEU
3	F	327	LEU
3	F	288	ARG
3	C	327	LEU
2	E	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	215	GLN
2	E	105	ASN
2	E	166	GLN
2	E	116	ASN
2	B	116	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 5 ligands modelled in this entry, 3 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	$\# Z > 2$
4	AGS	E	501	-	32,33,33	2.09	8 (25%)	45,52,52	2.02	12 (26%)
4	AGS	B	501	5	32,33,33	2.08	7 (21%)	45,52,52	1.93	11 (24%)

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	AGS	E	501	-	-	5/21/38/38	0/3/3/3
4	AGS	B	501	5	-	6/21/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	AGS	PG-S1G	8.12	2.08	1.90
4	E	501	AGS	PG-S1G	8.01	2.08	1.90
4	B	501	AGS	C5-C4	4.75	1.47	1.39
4	E	501	AGS	C5-C4	4.70	1.47	1.39
4	E	501	AGS	PA-O3A	2.61	1.62	1.59

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	AGS	C5-C4-N3	-6.11	118.31	126.72
4	B	501	AGS	C5-C4-N3	-6.10	118.32	126.72
4	E	501	AGS	N3-C4-N9	5.09	135.82	127.17
4	B	501	AGS	N3-C4-N9	5.02	135.71	127.17
4	E	501	AGS	C2-N3-C4	4.07	121.76	111.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	AGS	PB-O3B-PG-O2G
4	B	501	AGS	O4'-C1'-N9-C8
4	B	501	AGS	O4'-C1'-N9-C4
4	E	501	AGS	PB-O3B-PG-O2G
4	E	501	AGS	PB-O3B-PG-O3G

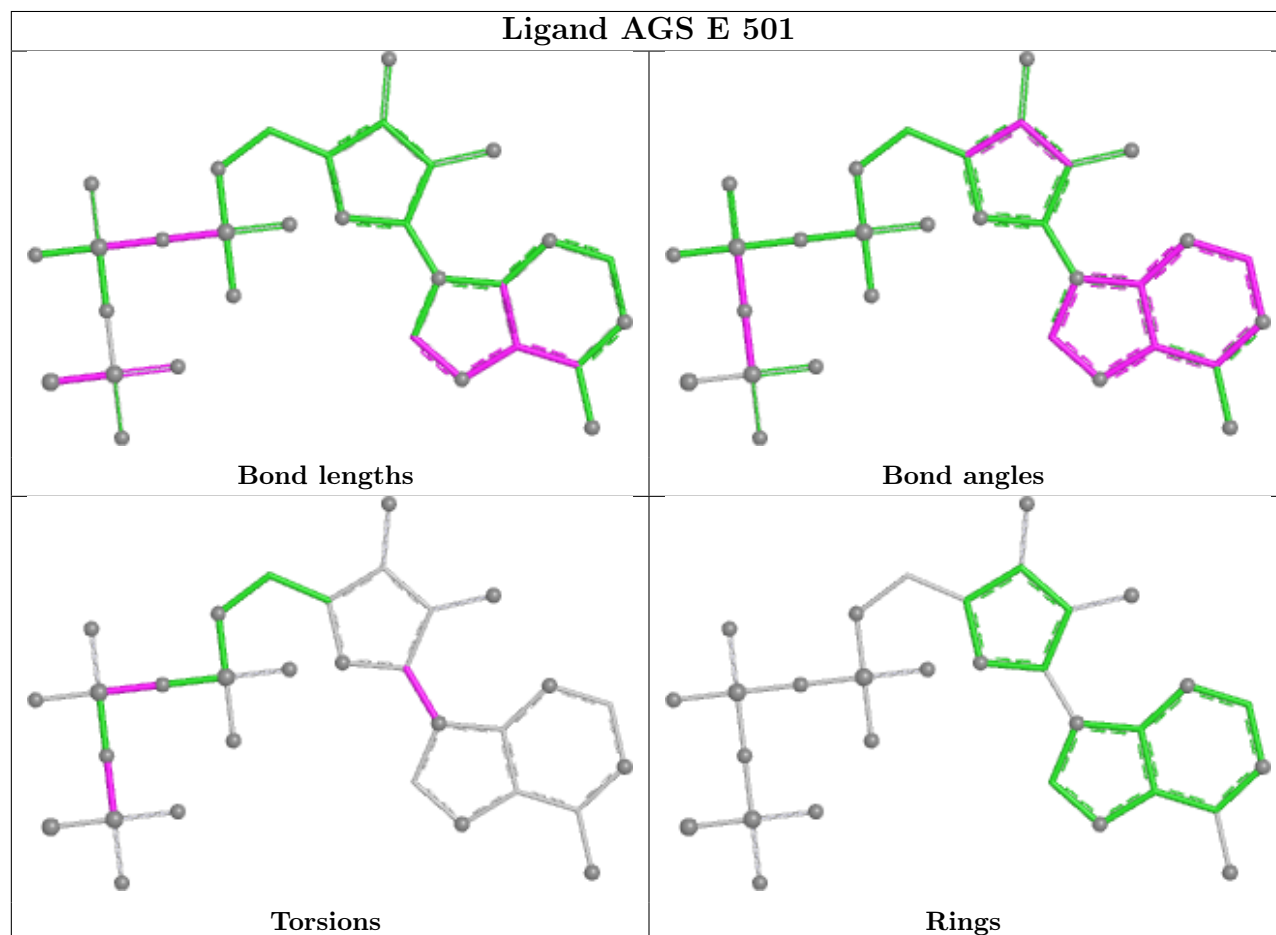
There are no ring outliers.

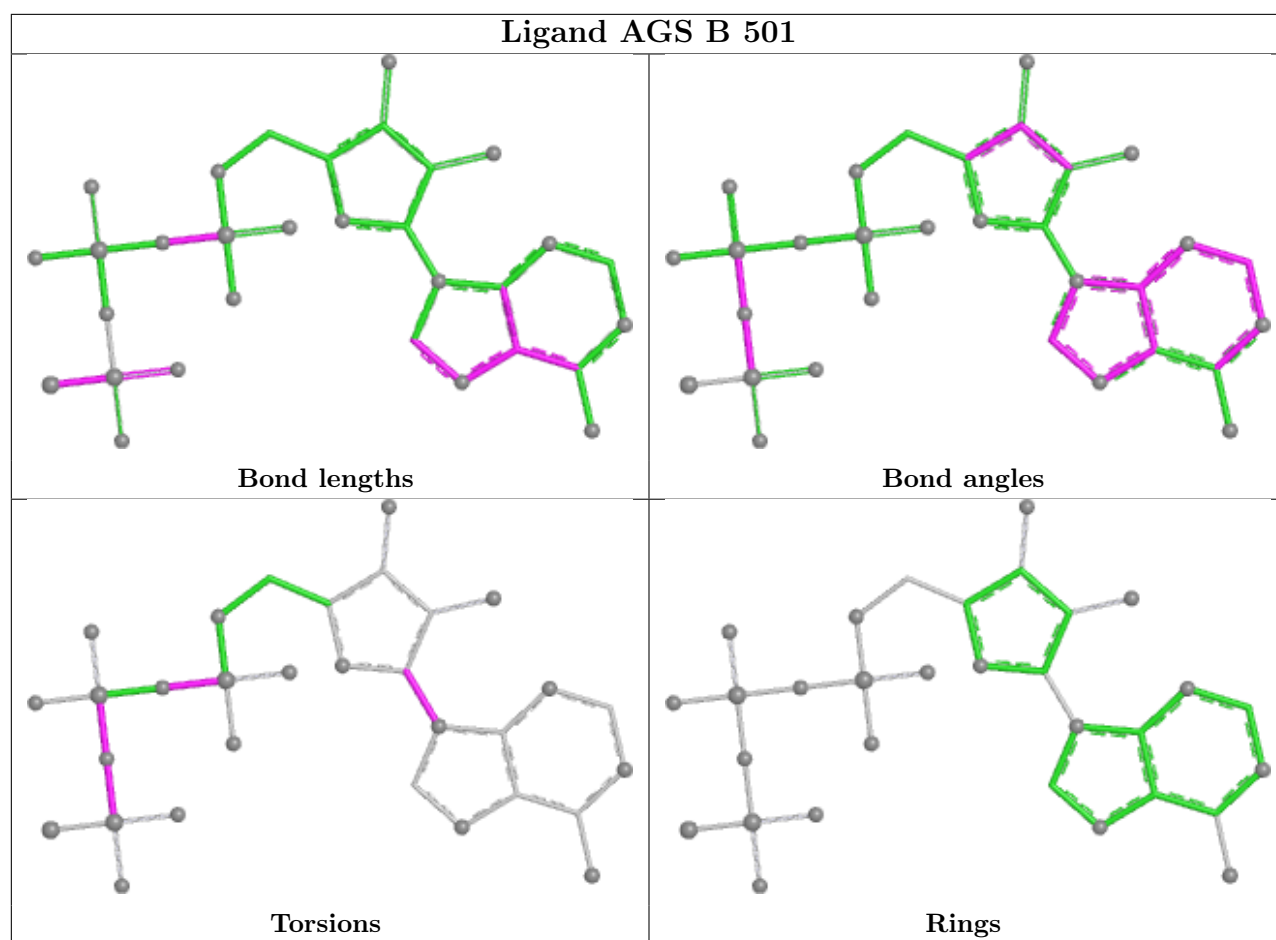
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	AGS	1	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	312/425 (73%)	0.30	8 (2%) 57 38	31, 65, 100, 127	0
1	D	314/425 (73%)	-0.08	6 (1%) 66 47	14, 40, 81, 124	0
2	B	322/437 (73%)	-0.14	3 (0%) 81 65	18, 40, 86, 110	0
2	E	323/437 (73%)	-0.29	3 (0%) 81 65	13, 30, 79, 124	0
3	C	66/69 (95%)	0.09	2 (3%) 52 34	38, 61, 84, 94	0
3	F	67/69 (97%)	-0.30	1 (1%) 72 53	17, 37, 67, 96	0
All	All	1404/1862 (75%)	-0.06	23 (1%) 70 51	13, 44, 88, 127	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	78	PRO	4.4
1	A	5	ILE	4.1
2	E	77	THR	3.8
1	A	384	PHE	3.7
1	D	384	PHE	3.7

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 ⓘ

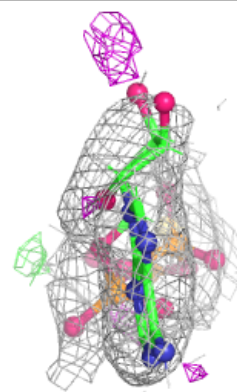
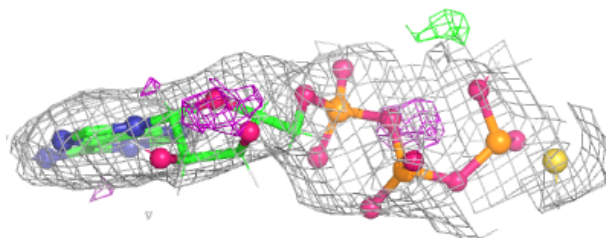
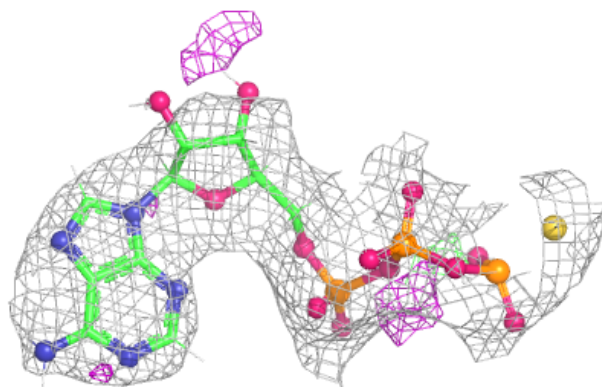
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

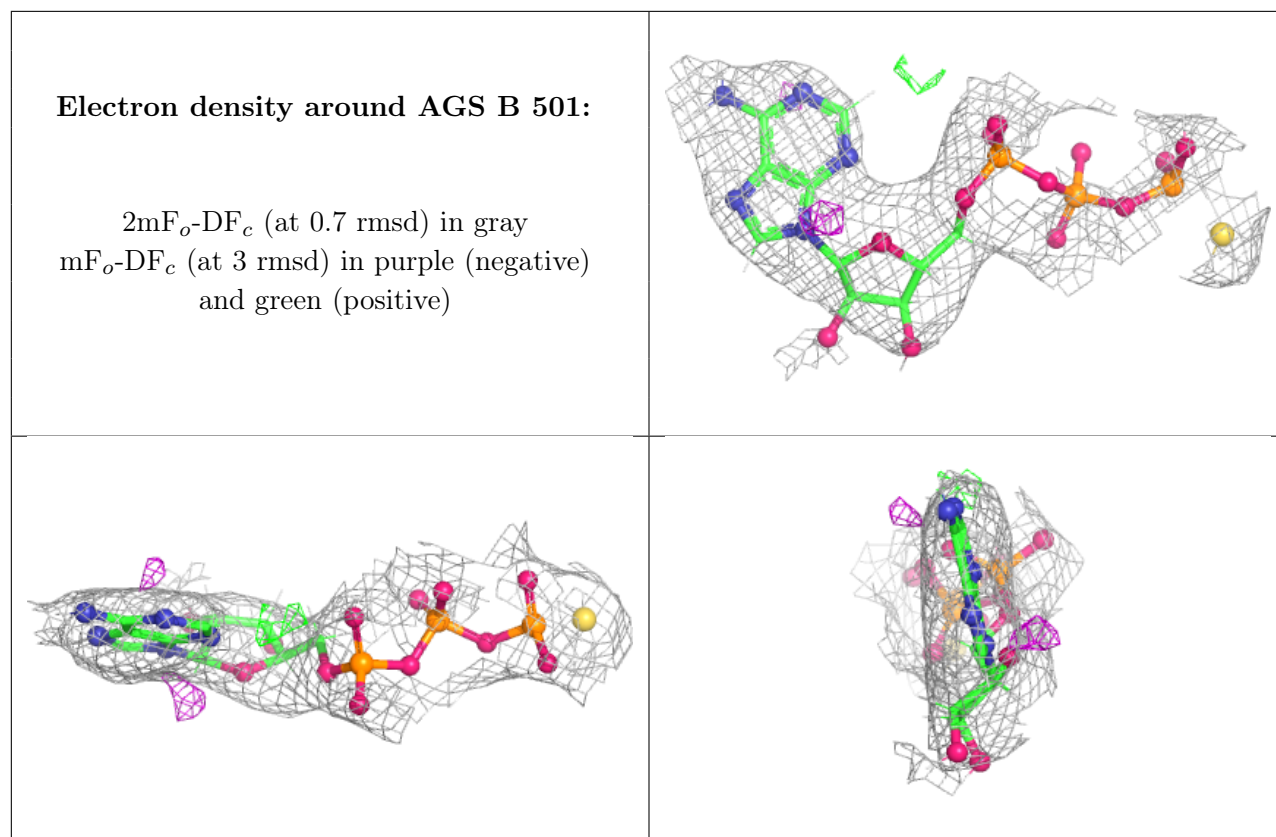
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AGS	E	501	31/31	0.85	0.12	35,77,136,146	0
5	MG	E	502	1/1	0.86	0.21	36,36,36,36	0
4	AGS	B	501	31/31	0.90	0.09	29,76,118,144	0
5	MG	B	502	1/1	0.92	0.11	19,19,19,19	0
6	CL	B	503	1/1	0.97	0.05	43,43,43,43	0

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 E 501:

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.