



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:43 AM UTC

PDB ID : 2IUT / pdb_00002iut
Title : P. aeruginosa FtsK motor domain, dimeric
Authors : Massey, T.H.; Mercoglian, C.P.; Yates, J.; Sherratt, D.J.; Lowe, J.
Deposited on : 2006-06-07
Resolution : 2.25 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

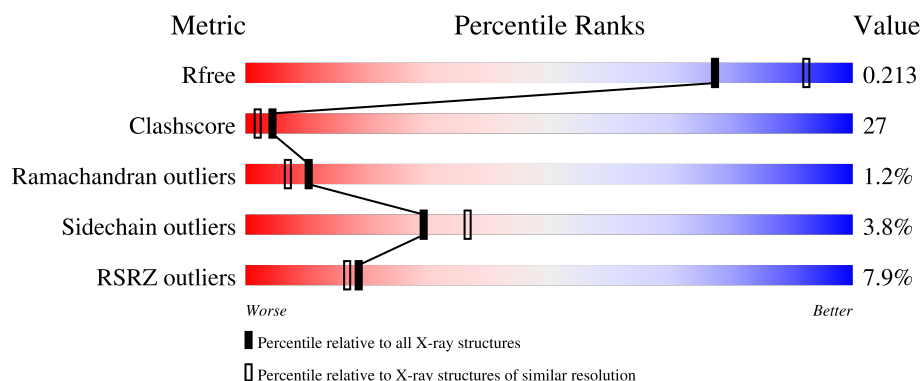
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	574	5% 41% 27% • 29%
1	B	574	6% 42% 26% • 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6673 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.

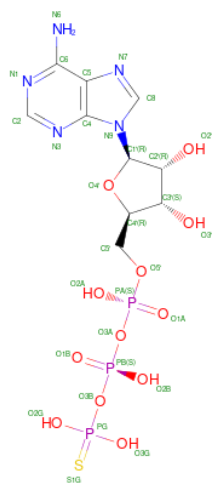
- Molecule 1 is a protein called DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	1
			3122	1983	541	583	15			
1	B	409	Total	C	N	O	S	0	0	1
			3122	1983	541	583	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	MET	-	expression tag	UNP Q9I0M3
A	812	LYS	-	expression tag	UNP Q9I0M3
A	813	LEU	-	expression tag	UNP Q9I0M3
A	814	HIS	-	expression tag	UNP Q9I0M3
A	815	HIS	-	expression tag	UNP Q9I0M3
A	816	HIS	-	expression tag	UNP Q9I0M3
A	817	HIS	-	expression tag	UNP Q9I0M3
A	818	HIS	-	expression tag	UNP Q9I0M3
A	819	HIS	-	expression tag	UNP Q9I0M3
B	246	MET	-	expression tag	UNP Q9I0M3
B	812	LYS	-	expression tag	UNP Q9I0M3
B	813	LEU	-	expression tag	UNP Q9I0M3
B	814	HIS	-	expression tag	UNP Q9I0M3
B	815	HIS	-	expression tag	UNP Q9I0M3
B	816	HIS	-	expression tag	UNP Q9I0M3
B	817	HIS	-	expression tag	UNP Q9I0M3
B	818	HIS	-	expression tag	UNP Q9I0M3
B	819	HIS	-	expression tag	UNP Q9I0M3

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



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

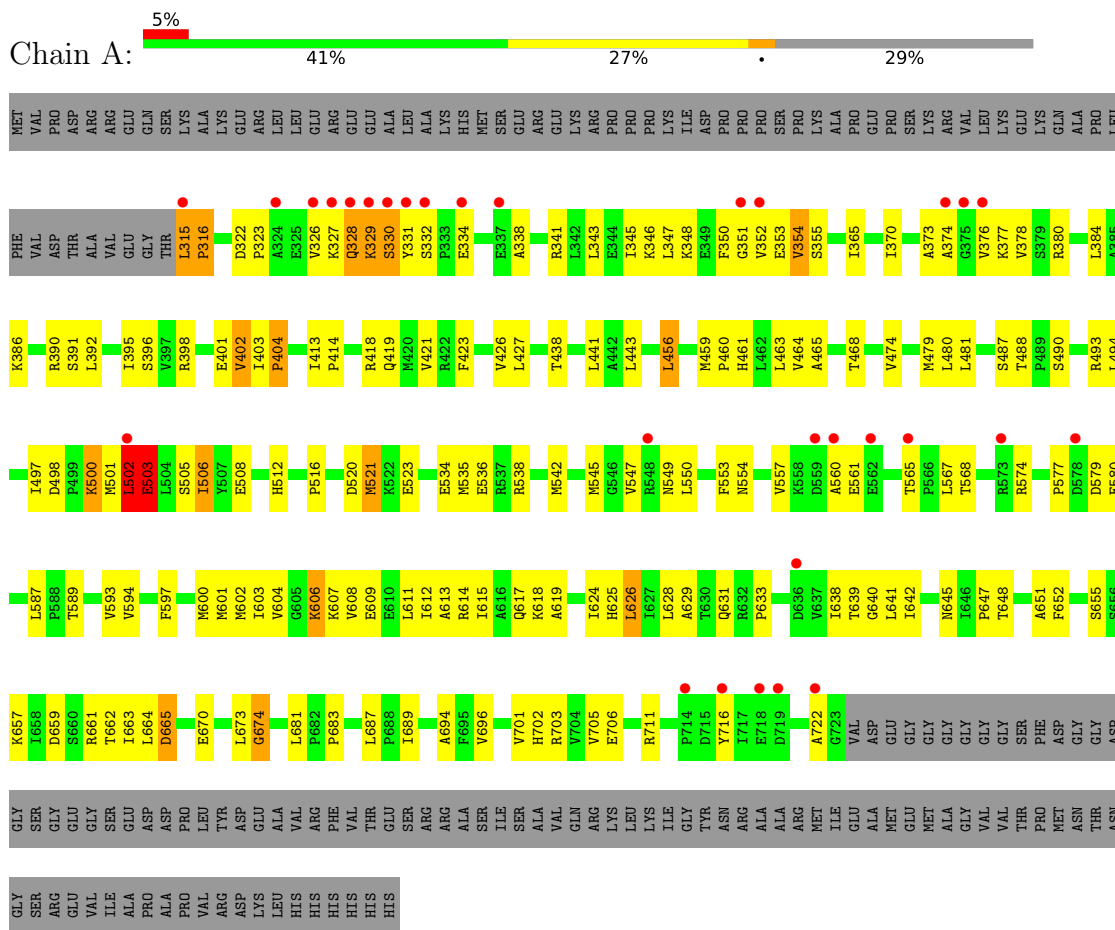
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	172	Total O 172 172	0	0
4	B	193	Total O 193 193	0	0

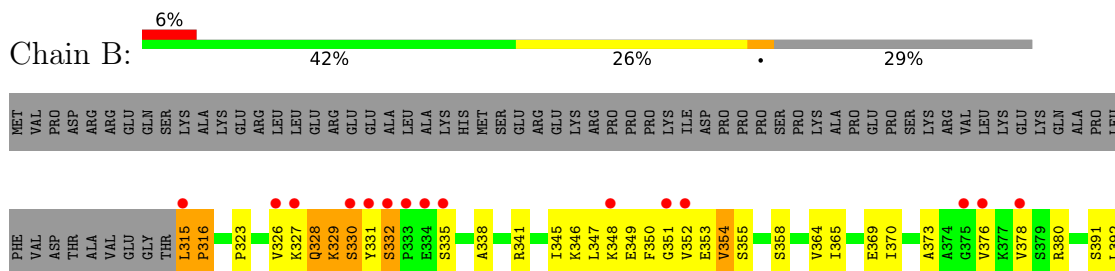
3 Residue-property plots

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: DNA TRANSLOCASE FTSK



• Molecule 1: DNA TRANSLOCASE FTSK



ALA	ASP	I663	V593	L594	I395
PRO	PRO	L664	V594	SS05	S396
VAL	LEU	D665	D595	IS06	V397
ARG	TYR	E666	E596	Y507	R398
ASP	ASP	E670	F597	E508	E401
LYS	GLU	L673	M600	H512	V402
LEU	ALA	G674	M601	P516	I403
HIS	VAL	L681	L603	T519	P404
HIS	PHE	P682	K606	D520	I413
HIS	THR	P683	E609	M521	P414
HIS	GLU	L687	E610	K522	D417
	SER	P698	L611	E523	R418
	ARG	I689	I612	A524	Q419
	ALA	R690	A613	E534	F423
	SER	V691	R614	M535	V426
	ILE	H692	I615	R538	E431
	SER	G693	A616	Y539	L441
	ALA	A694	Q617	M542	L456
	VAL	F695	K618	H545	M459
	GLN	V696	A619	V547	P460
	ARG	V701	R620	L550	H461
	LYS	H702	A621	F553	V464
	LEU	L705	I624	N554	A465
	LYS	G705	H625	R555	G466
	ILE	R711	L626	K556	T467
	TYR	Y716	A629	V557	T468
	ASN	I717	I630	A560	V474
	ARG	E718	Q631	E561	L480
	ALA	A722	R632	A562	L481
	ARG	G723	P633	G564	L484
	MET	V723	S634	T565	S487
	ILE	VAL	V635	P566	T488
	GLU	ASP	D636	L567	P489
	ALA	GLU	V637	T568	S490
	MET	GLU	I638	R573	S490
	GLU	GLY	L641	R574	R493
	ALA	GLY	K642	P577	M496
	GLY	VAL	A644	D578	I497
	VAL	THR	N645	D579	D498
	THR	SER	R649	L587	P499
	PRO	PHE	T650	P588	K500
	MET	ASP	A651	T589	M501
	ASN	GLY	F652	V592	L502
	THR	GLY	G655		E503
	ASN	GLY	S655		
	GLY	SER	S656		
	SER	ARG	K657		
	ARG	GLY	I658		
	GLU	GLU	R661		
	VAL	GLY	T662		
	ILE	SER			
	ALA	GLU			
	PRO	ASP			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.17Å 57.43Å 98.06Å 94.57° 93.80° 107.66°	Depositor
Resolution (Å)	100.00 – 2.25 97.30 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.8 (100.00-2.25) 93.8 (97.30-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.25Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.267 0.213 , 0.213	Depositor DCC
R_{free} test set	2278 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.21% 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, 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	0.44	1/3178 (0.0%)	1.01	17/4314 (0.4%)
1	B	0.45	1/3178 (0.0%)	1.01	17/4314 (0.4%)
All	All	0.44	2/6356 (0.0%)	1.01	34/8628 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	722	ALA	C-N	-5.57	1.25	1.33
1	B	722	ALA	C-N	-5.57	1.25	1.33

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	LEU	N-CA-C	6.88	125.45	110.80
1	B	643	LYS	N-CA-C	6.42	118.27	111.28
1	B	655	SER	N-CA-C	6.17	120.07	112.54
1	A	665	ASP	N-CA-C	-6.12	105.40	112.86
1	A	502	LEU	N-CA-C	6.02	123.63	110.80

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	3122	0	3237	174	0
1	B	3122	0	3237	169	0
2	A	31	0	12	4	0
2	B	31	0	12	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	172	0	0	29	0
4	B	193	0	0	30	0
All	All	6673	0	6498	340	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 27.

The worst 5 of 340 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:329:LYS:H	1:A:329:LYS:HD3	1.20	1.06
1:A:329:LYS:HG2	1:A:330:SER:H	1.23	1.04
1:B:329:LYS:H	1:B:329:LYS:HD3	1.21	1.03
1:B:329:LYS:HG2	1:B:330:SER:H	1.21	1.03
1:A:554:ASN:HD21	1:A:587:LEU:H	1.04	1.01

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	407/574 (71%)	389 (96%)	13 (3%)	5 (1%)	10	7
1	B	407/574 (71%)	387 (95%)	15 (4%)	5 (1%)	10	7
All	All	814/1148 (71%)	776 (95%)	28 (3%)	10 (1%)	10	7

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	LEU
1	B	502	LEU
1	A	328	GLN
1	B	328	GLN
1	A	503	GLU

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	346/481 (72%)	332 (96%)	14 (4%)	28	34
1	B	346/481 (72%)	334 (96%)	12 (4%)	32	39
All	All	692/962 (72%)	666 (96%)	26 (4%)	29	36

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	315	LEU
1	B	402	VAL
1	B	626	LEU
1	B	354	VAL
1	B	404	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	554	ASN
1	B	583	GLN
1	B	625	HIS
1	A	617	GLN
1	A	645	ASN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 2 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$
2	AGS	B	1724	3	32,33,33	2.61	10 (31%)	45,52,52	1.50	8 (17%)
2	AGS	A	1723	3	32,33,33	2.56	10 (31%)	45,52,52	1.44	7 (15%)

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	1724	3	-	5/21/38/38	0/3/3/3
2	AGS	A	1723	3	-	5/21/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1724	AGS	PB-O3A	-8.55	1.50	1.59
2	A	1723	AGS	PB-O3A	-6.79	1.52	1.59
2	A	1723	AGS	PA-O3A	6.40	1.66	1.59
2	B	1724	AGS	PG-S1G	-6.23	1.77	1.90
2	A	1723	AGS	C6-N6	5.12	1.47	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1723	AGS	N9-C8-N7	4.20	119.89	113.94
2	B	1724	AGS	N9-C8-N7	4.10	119.75	113.94
2	B	1724	AGS	C4-N9-C8	-3.73	101.82	105.74
2	A	1723	AGS	C4-N9-C8	-3.63	101.93	105.74
2	B	1724	AGS	O3A-PB-O1B	-3.07	101.47	110.70

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

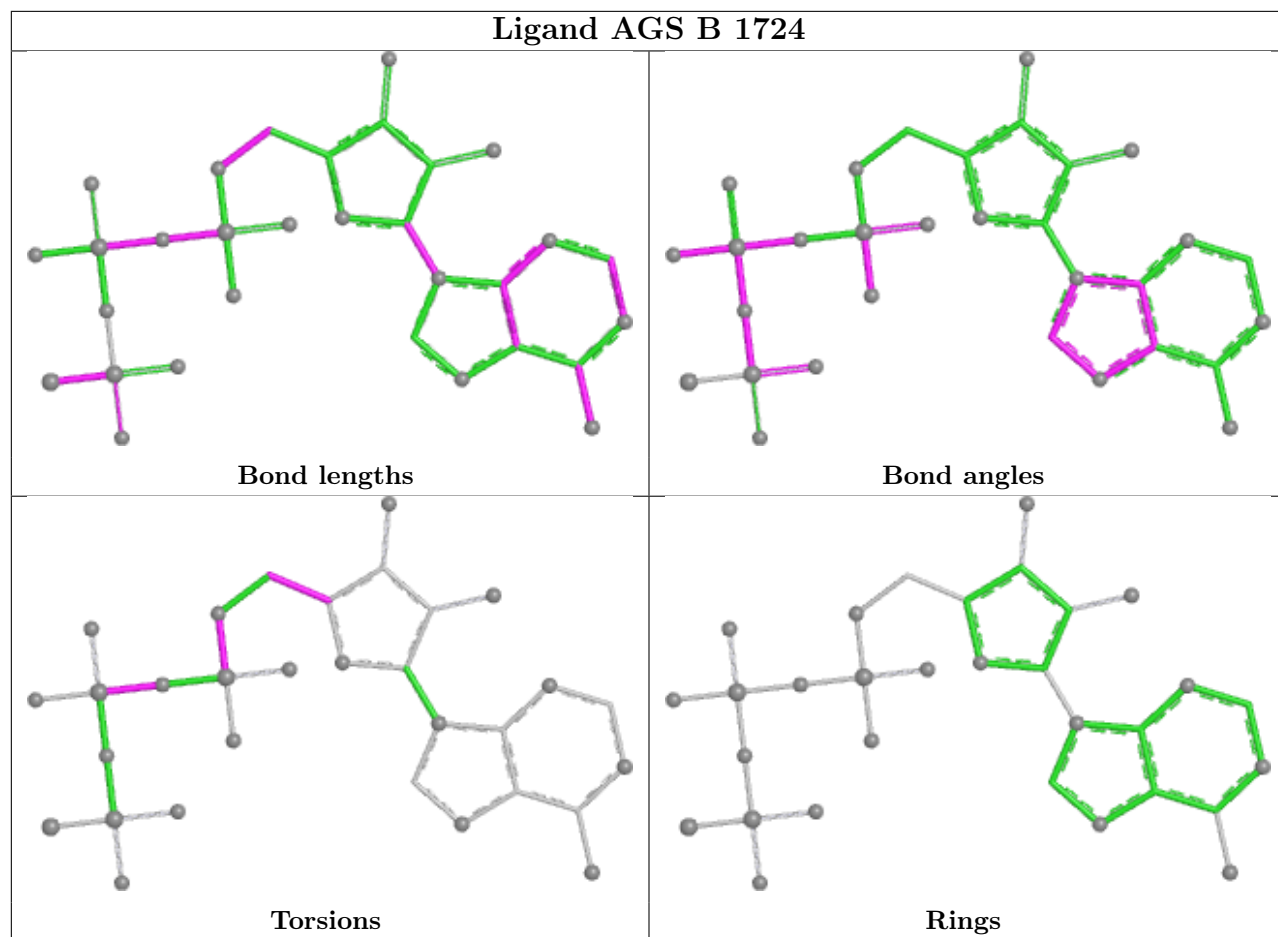
Mol	Chain	Res	Type	Atoms
2	A	1723	AGS	C5'-O5'-PA-O1A
2	B	1724	AGS	C5'-O5'-PA-O1A
2	B	1724	AGS	PA-O3A-PB-O2B
2	A	1723	AGS	O4'-C4'-C5'-O5'
2	A	1723	AGS	C3'-C4'-C5'-O5'

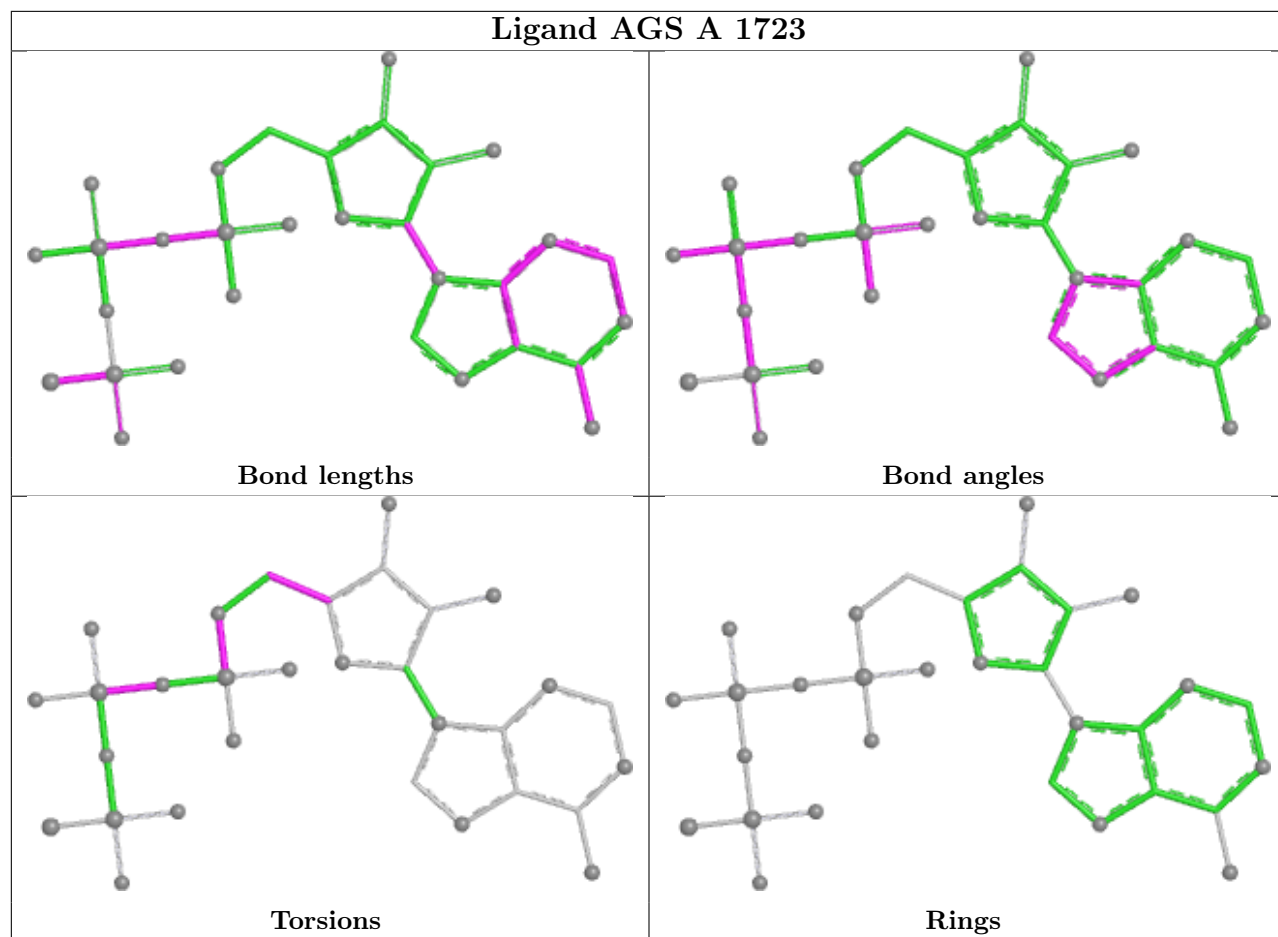
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1724	AGS	4	0
2	A	1723	AGS	4	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	409/574 (71%)	0.43	30 (7%)	21 19	10, 30, 57, 97	0
1	B	409/574 (71%)	0.38	35 (8%)	16 15	11, 30, 57, 97	0
All	All	818/1148 (71%)	0.40	65 (7%)	18 17	10, 30, 57, 97	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	TYR	7.5
1	A	375	GLY	5.2
1	A	718	GLU	4.3
1	A	327	LYS	4.3
1	A	331	TYR	4.3

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](#)

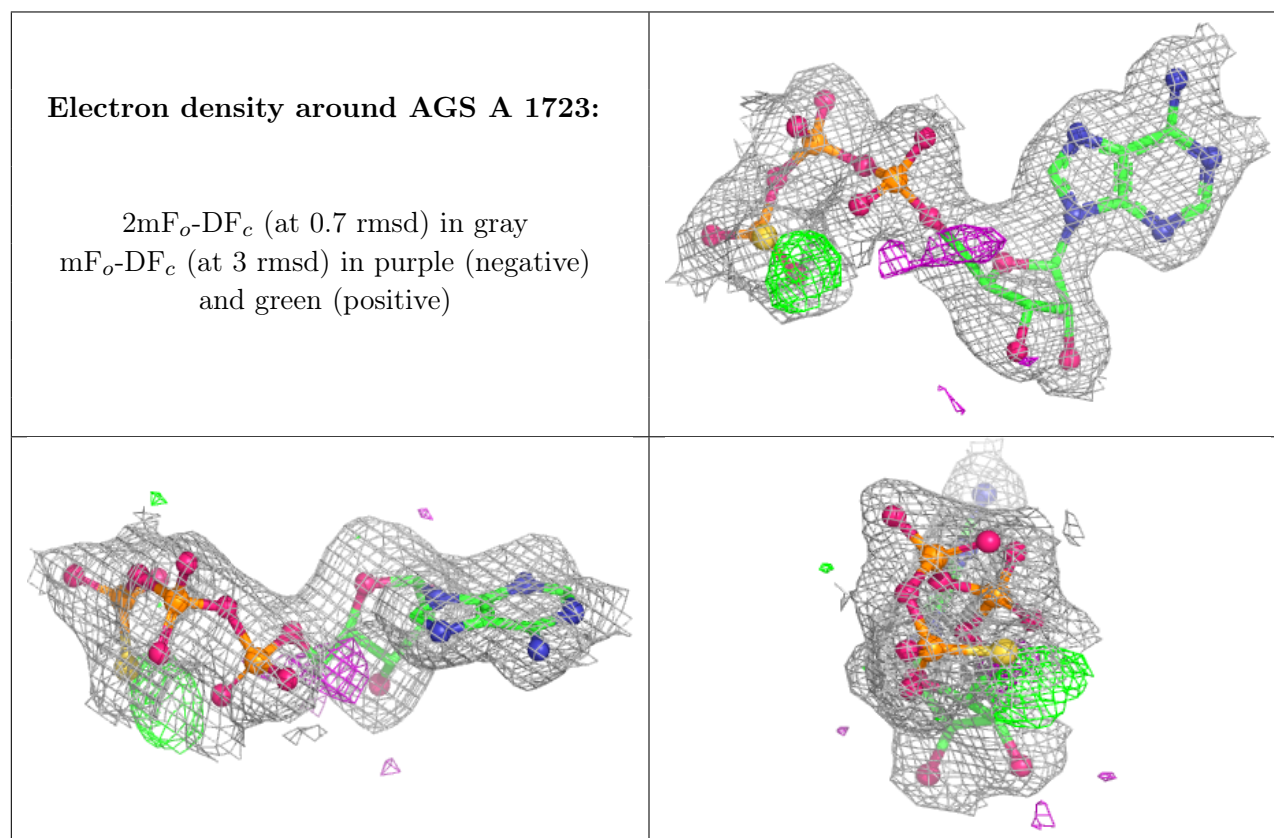
There are no oligosaccharides in this entry.

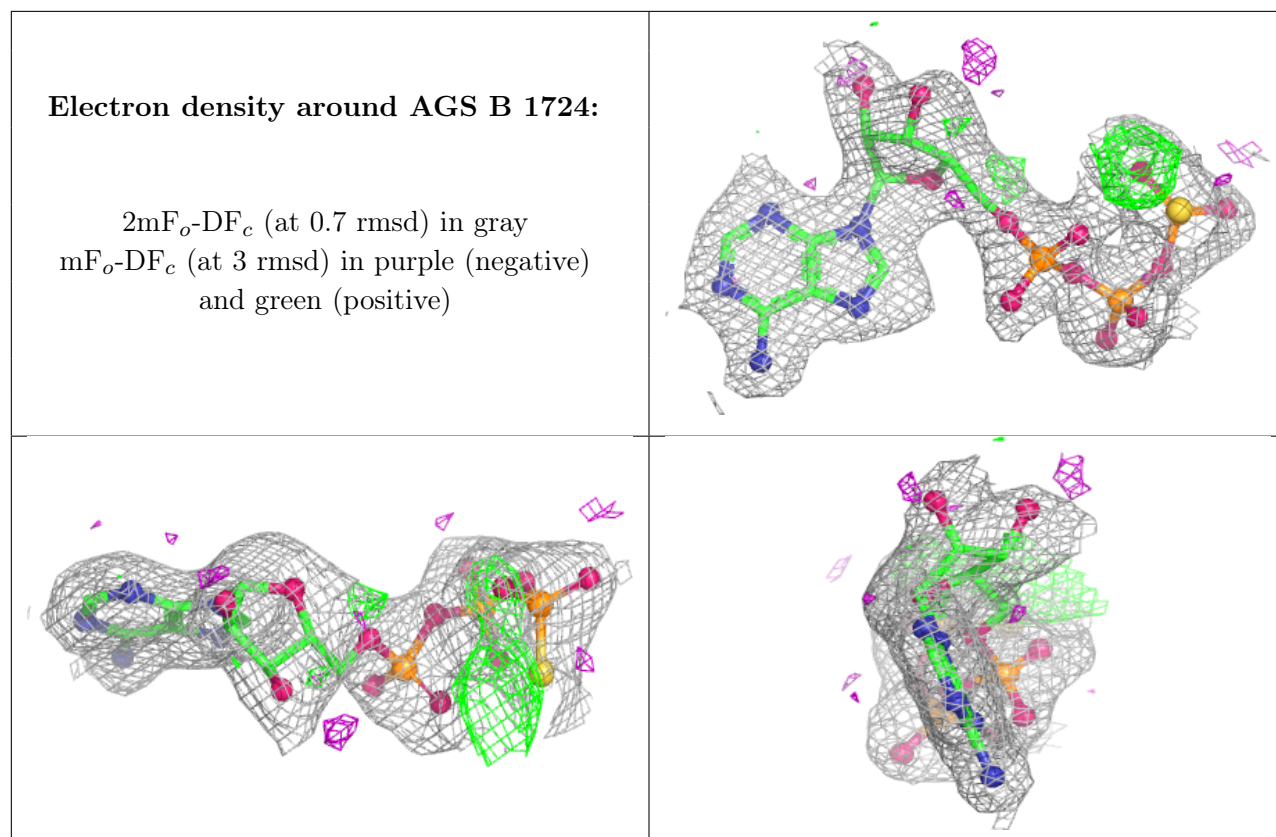
6.4 Ligands [i](#)

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
2	AGS	A	1723	31/31	0.95	0.08	8,21,28,33	0
2	AGS	B	1724	31/31	0.97	0.07	4,19,26,32	0
3	MG	A	1724	1/1	0.99	0.02	1,1,1,1	0
3	MG	B	1723	1/1	0.99	0.03	2,2,2,2	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 [i](#)

There are no such residues in this entry.