



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5YT0 / pdb_00005yt0
Title : Crystal structure of the complex of archaeal ribosomal stalk protein aP1 and archaeal translation initiation factor aIF5B
Authors : Murakami, R.; Singh, C.R.; Morris, J.; Tang, L.; Harmon, I.; Miyoshi, T.; Ito, K.; Asano, K.; Uchiumi, T.
Deposited on : 2017-11-16
Resolution : 1.89 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

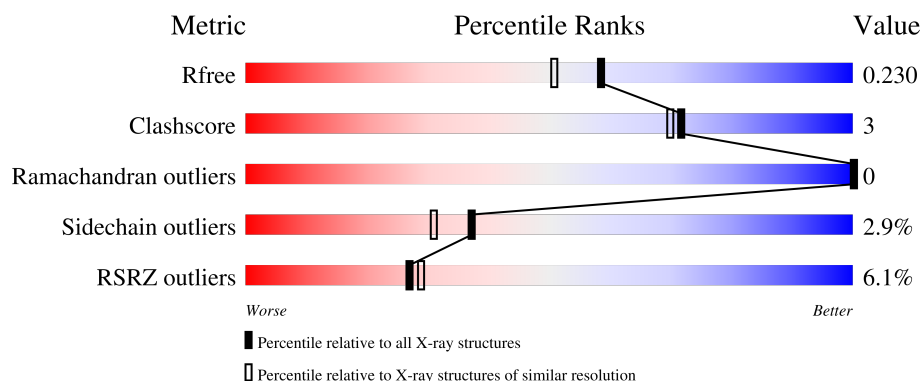
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	364	6% 65% 24% 9%
2	B	21	43% 5% 5% 48%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2839 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 Probable translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	1	0
			2581	1662	454	460	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	HIS	-	expression tag	UNP Q9Y9B3
A	360	HIS	-	expression tag	UNP Q9Y9B3
A	361	HIS	-	expression tag	UNP Q9Y9B3
A	362	HIS	-	expression tag	UNP Q9Y9B3
A	363	HIS	-	expression tag	UNP Q9Y9B3
A	364	HIS	-	expression tag	UNP Q9Y9B3

- Molecule 2 is a protein called Archaeal ribosomal stalk protein aP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	S	0	0	0
			79	51	11	16	1			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	146	Total O 146 146	0	0
4	B	5	Total O 5 5	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.72Å 79.02Å 101.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 1.89 42.70 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.3 (42.70-1.89) 98.4 (42.70-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.171 , 0.217 0.185 , 0.230	Depositor DCC
R_{free} test set	1758 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.9	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	0.96	EDS
Total number of atoms	2839	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: GDP

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	2.00	61/2614 (2.3%)	1.55	25/3536 (0.7%)
2	B	2.24	4/80 (5.0%)	1.64	1/103 (1.0%)
All	All	2.00	65/2694 (2.4%)	1.56	26/3639 (0.7%)

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	PRO	C-O	-10.94	1.11	1.23
1	A	25	VAL	CA-CB	10.26	1.66	1.54
1	A	119	LYS	N-CA	9.92	1.52	1.46
1	A	284	VAL	CA-C	-8.46	1.41	1.52
1	A	167	LYS	CA-C	8.46	1.64	1.52
1	A	87	ASP	CG-OD1	8.32	1.41	1.25
1	A	188	LEU	C-O	-8.32	1.18	1.25
1	A	80	ILE	CA-C	-7.99	1.44	1.52
2	B	109	PHE	CA-C	7.75	1.63	1.52
1	A	157	PHE	C-O	7.55	1.32	1.24
2	B	109	PHE	N-CA	-7.25	1.37	1.46
1	A	57	ILE	C-N	-7.13	1.27	1.33
1	A	149	TRP	CA-CB	7.07	1.65	1.53
1	A	211	ARG	N-CA	6.87	1.54	1.46
1	A	96	ASN	CA-CB	-6.84	1.41	1.53
1	A	348	GLU	N-CA	6.75	1.54	1.46
1	A	157	PHE	N-CA	-6.74	1.38	1.46
1	A	73	VAL	N-CA	-6.64	1.38	1.46
1	A	179	ILE	CA-C	-6.62	1.44	1.52
1	A	241	PRO	CA-C	6.60	1.60	1.52
1	A	239	GLU	C-O	-6.59	1.16	1.23
1	A	353	GLU	CA-C	-6.54	1.44	1.52
1	A	171	ILE	CA-C	6.45	1.60	1.52
1	A	354	ILE	N-CA	-6.41	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	GLN	N-CA	-6.38	1.38	1.45
1	A	121	GLN	C-O	-6.37	1.15	1.24
2	B	109	PHE	C-O	-6.31	1.16	1.23
1	A	182	LYS	CA-C	-6.30	1.44	1.52
1	A	292	MET	C-O	6.26	1.30	1.24
1	A	15	ARG	CA-C	6.26	1.61	1.53
1	A	159	GLU	N-CA	6.13	1.53	1.46
1	A	238	ALA	N-CA	6.05	1.53	1.46
1	A	58	VAL	N-CA	6.01	1.51	1.46
1	A	251	GLU	CA-C	-5.94	1.45	1.52
1	A	322	ALA	C-O	5.92	1.30	1.24
1	A	293	PRO	C-O	-5.87	1.17	1.23
1	A	244	GLY	C-O	5.83	1.29	1.23
1	A	68	GLU	N-CA	5.82	1.52	1.46
1	A	181	GLY	N-CA	5.68	1.52	1.45
1	A	153	PRO	CA-C	-5.61	1.45	1.52
1	A	179	ILE	CA-CB	5.61	1.60	1.54
1	A	21	VAL	N-CA	5.47	1.53	1.46
1	A	50	THR	N-CA	5.46	1.52	1.46
1	A	226	LEU	N-CA	-5.46	1.39	1.46
1	A	291	LEU	N-CA	5.46	1.52	1.46
1	A	209	SER	N-CA	5.46	1.52	1.46
1	A	38	ARG	CD-NE	-5.45	1.38	1.46
1	A	277	GLY	CA-C	-5.44	1.43	1.52
1	A	270	LYS	CA-C	5.44	1.59	1.52
1	A	89	PRO	C-O	5.44	1.30	1.23
1	A	158	ILE	N-CA	5.43	1.53	1.46
1	A	50	THR	CA-C	-5.43	1.46	1.52
1	A	119	LYS	C-O	5.36	1.28	1.24
1	A	123	TYR	CA-C	-5.33	1.45	1.52
1	A	268	LEU	CA-C	-5.31	1.46	1.52
1	A	193	PHE	N-CA	-5.30	1.39	1.46
1	A	295	PRO	N-CA	5.29	1.54	1.47
1	A	138	ILE	CA-C	-5.24	1.46	1.52
1	A	127	GLU	N-CA	5.20	1.52	1.46
1	A	50	THR	C-O	5.18	1.30	1.24
1	A	220	LEU	CA-C	-5.16	1.46	1.52
1	A	60	ALA	N-CA	5.15	1.52	1.46
1	A	332	SER	CA-C	-5.03	1.48	1.53
1	A	35	LYS	N-CA	5.01	1.52	1.46
2	B	108	MET	CA-CB	5.00	1.62	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	MET	CG-SD-CE	7.46	117.32	100.90
1	A	68	GLU	CA-C-N	-7.33	112.64	119.82
1	A	68	GLU	C-N-CA	-7.33	112.64	119.82
1	A	224	ALA	CA-C-N	6.20	126.82	119.94
1	A	224	ALA	C-N-CA	6.20	126.82	119.94
1	A	42	ALA	N-CA-C	6.17	118.97	111.82
1	A	25	VAL	N-CA-C	6.09	117.27	109.30
1	A	37	ARG	CA-CB-CG	5.93	125.95	114.10
1	A	163	ARG	N-CA-C	5.76	119.29	112.72
1	A	37	ARG	CA-C-O	-5.73	114.80	120.82
1	A	40	ALA	CA-C-O	-5.67	114.86	120.70
1	A	234	ARG	CB-CA-C	-5.58	99.96	110.67
1	A	178	GLU	CA-CB-CG	-5.56	102.97	114.10
1	A	160	THR	N-CA-C	5.53	118.23	111.82
1	A	37	ARG	O-C-N	5.44	127.68	122.07
1	A	87	ASP	CB-CG-OD2	-5.41	105.97	118.40
2	B	108	MET	CA-CB-CG	-5.29	103.51	114.10
1	A	281	GLY	CA-C-N	5.22	125.38	119.90
1	A	281	GLY	C-N-CA	5.22	125.38	119.90
1	A	212	THR	N-CA-C	5.18	119.60	113.28
1	A	274	ILE	O-C-N	5.17	128.53	123.00
1	A	322	ALA	CA-C-N	-5.15	114.48	119.78
1	A	322	ALA	C-N-CA	-5.15	114.48	119.78
1	A	347	MET	N-CA-C	-5.13	105.77	111.36
1	A	71	LYS	N-CA-C	5.05	117.51	111.71
1	A	157	PHE	N-CA-CB	5.02	117.42	109.94

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	2581	0	2723	18	0
2	B	79	0	71	0	0
3	A	28	0	12	0	0
4	A	146	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
All	All	2839	0	2806	18	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 3.

All (18) 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:52:HIS:HD2	1:A:317:GLY:H	1.32	0.76
1:A:52:HIS:CD2	1:A:317:GLY:H	2.17	0.60
1:A:93:LEU:C	1:A:93:LEU:HD13	2.30	0.56
1:A:199:PHE:HB3	1:A:226:LEU:HD21	1.89	0.54
1:A:109:ILE:HD11	1:A:223:LEU:HD11	1.91	0.52
1:A:91:HIS:CD2	1:A:128:LEU:HD11	2.46	0.50
1:A:52:HIS:HD2	1:A:317:GLY:N	2.07	0.50
1:A:114:ILE:O	1:A:175:ARG:HD3	2.12	0.49
1:A:258:VAL:HG21	1:A:319:ARG:HD3	1.95	0.47
1:A:115:MET:CE	1:A:115:MET:HA	2.47	0.45
1:A:52:HIS:CE1	1:A:57:ILE:HD12	2.52	0.44
1:A:76:VAL:O	1:A:76:VAL:HG12	2.17	0.44
1:A:341:GLU:HG2	1:A:344:ARG:NH2	2.33	0.44
1:A:344:ARG:NH1	4:A:604:HOH:O	2.50	0.43
1:A:76:VAL:O	1:A:76:VAL:CG1	2.66	0.43
1:A:52:HIS:CD2	1:A:316:ALA:HA	2.54	0.43
1:A:338:GLU:HG2	4:A:654:HOH:O	2.18	0.42
1:A:84:LEU:C	1:A:84:LEU:HD23	2.45	0.41

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	323/364 (89%)	321 (99%)	2 (1%)	0	100	100
2	B	9/21 (43%)	9 (100%)	0	0	100	100
All	All	332/385 (86%)	330 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	272/296 (92%)	265 (97%)	7 (3%)	40	35
2	B	8/18 (44%)	7 (88%)	1 (12%)	4	1
All	All	280/314 (89%)	272 (97%)	8 (3%)	37	31

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	71	LYS
1	A	115	MET
1	A	279	ARG
1	A	288	ARG
1	A	334	ILE
1	A	355	GLU
2	B	108	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	91	HIS
1	A	174	GLN
1	A	308	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
3	GDP	A	500	-	29,30,30	1.64	5 (17%)	45,47,47	1.36	8 (17%)

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
3	GDP	A	500	-	-	1/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	GDP	PA-O3A	-4.07	1.55	1.59
3	A	500	GDP	C5-C4	4.00	1.49	1.38
3	A	500	GDP	C8-N9	3.19	1.44	1.37
3	A	500	GDP	PA-O2A	-2.66	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	GDP	C4-N9	-2.58	1.31	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	GDP	C6-C5-N7	3.16	136.03	130.29
3	A	500	GDP	C6-C5-C4	-2.99	114.33	118.83
3	A	500	GDP	O6-C6-C5	-2.55	119.79	126.53
3	A	500	GDP	O3A-PA-O1A	2.47	118.13	110.70
3	A	500	GDP	C5-C4-N3	-2.40	124.56	128.39
3	A	500	GDP	N9-C4-N3	2.29	130.52	125.95
3	A	500	GDP	O4'-C1'-N9	-2.16	103.46	108.36
3	A	500	GDP	O2'-C2'-C1'	-2.00	103.22	110.10

There are no chirality outliers.

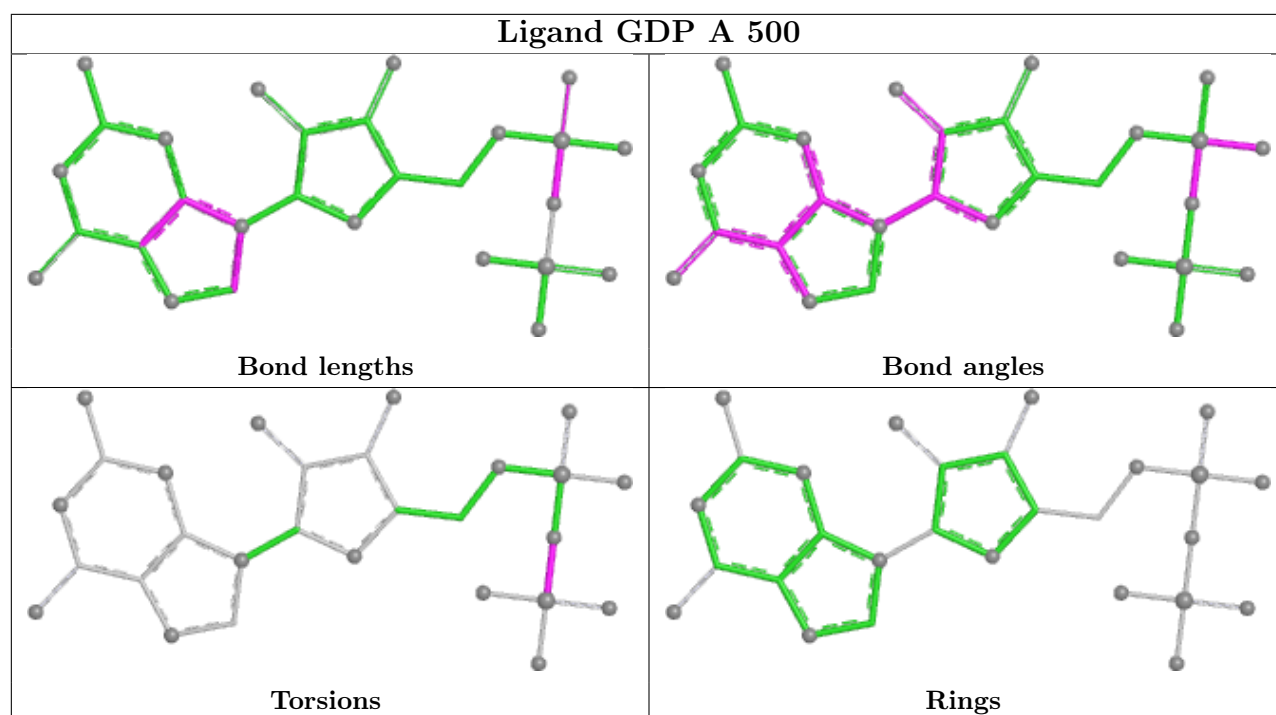
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	GDP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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	331/364 (90%)	0.41	21 (6%) 26 27	24, 35, 63, 83	1 (0%)
2	B	11/21 (52%)	0.63	0 100 100	32, 35, 46, 49	0
All	All	342/385 (88%)	0.41	21 (6%) 27 29	24, 35, 63, 83	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	TYR	3.9
1	A	50	THR	3.7
1	A	295	PRO	3.3
1	A	51	GLN	3.1
1	A	162[B]	ARG	3.0
1	A	294	ALA	2.8
1	A	165	ASP	2.7
1	A	95	SER	2.7
1	A	238	ALA	2.6
1	A	49	ILE	2.6
1	A	177	TYR	2.6
1	A	48	GLY	2.5
1	A	87	ASP	2.5
1	A	42	ALA	2.4
1	A	71	LYS	2.4
1	A	44	LYS	2.3
1	A	306	PHE	2.2
1	A	357	LEU	2.2
1	A	280	GLU	2.1
1	A	355	GLU	2.1
1	A	254	GLY	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](#)

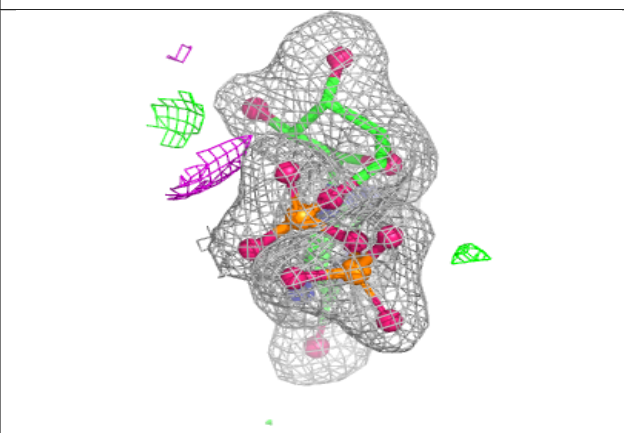
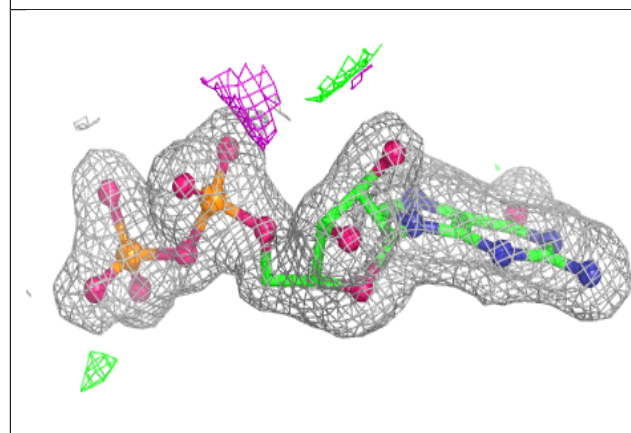
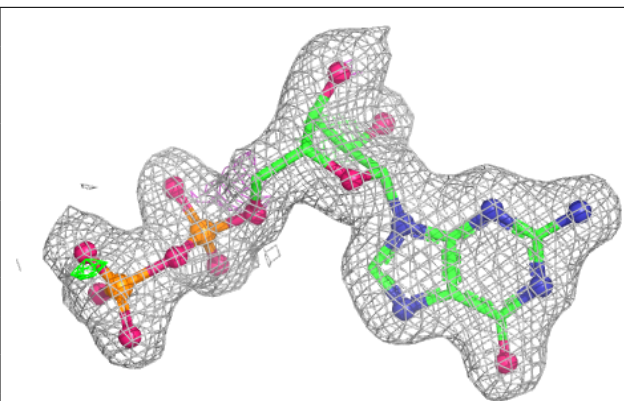
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GDP	A	500	28/28	0.98	0.05	24,28,33,35	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 GDP A 500:

$2mF_o-DF_c$ (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.