



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:27 PM UTC

PDB ID : 4ZKD / pdb_00004zkd
Title : Crystal structure of the *S. cerevisiae* Ski7 GTPase-like domain, bound to GDP and inorganic phosphate.
Authors : Kowalinski, E.; Conti, E.
Deposited on : 2015-04-30
Resolution : 2.18 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

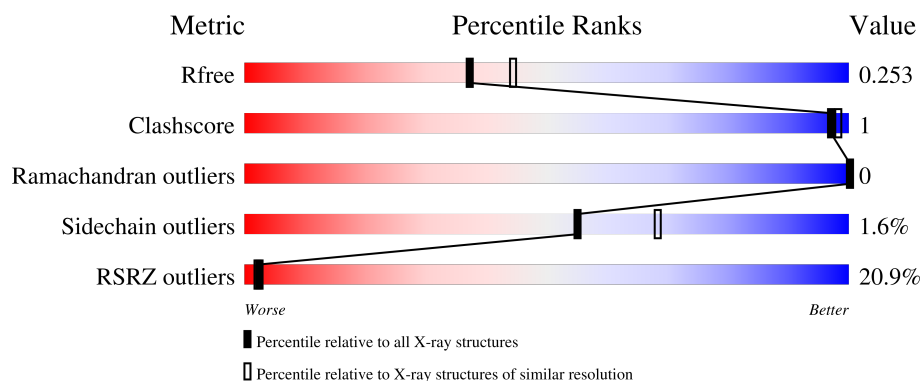
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	499	20% 90% 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7720 atoms, of which 3867 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.

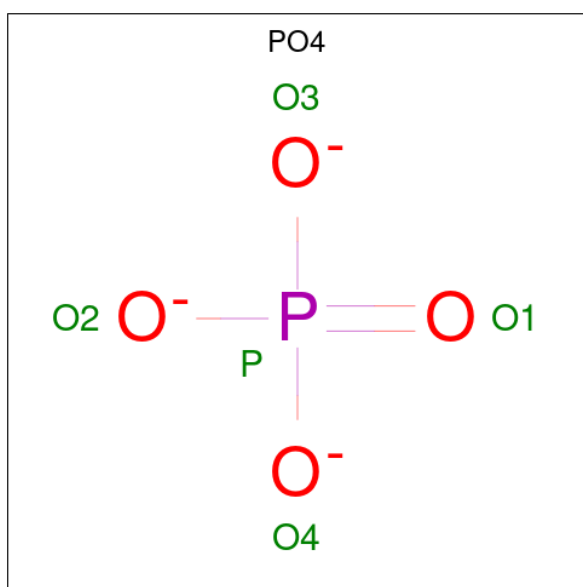
- Molecule 1 is a protein called Superkiller protein 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	470	7666	2442	3857	628	727	12	0	9	0

There are 5 discrepancies between the modelled and reference sequences:

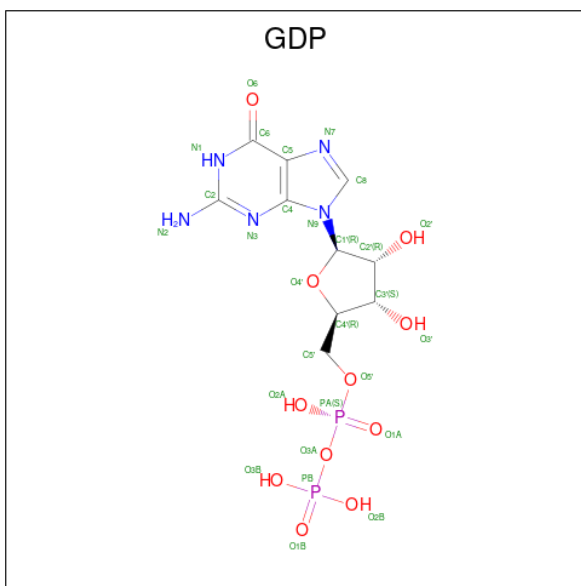
Chain	Residue	Modelled	Actual	Comment	Reference
A	249	GLY	-	expression tag	UNP Q08491
A	250	PRO	-	expression tag	UNP Q08491
A	251	ASP	-	expression tag	UNP Q08491
A	252	SER	-	expression tag	UNP Q08491
A	253	MET	-	expression tag	UNP Q08491

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

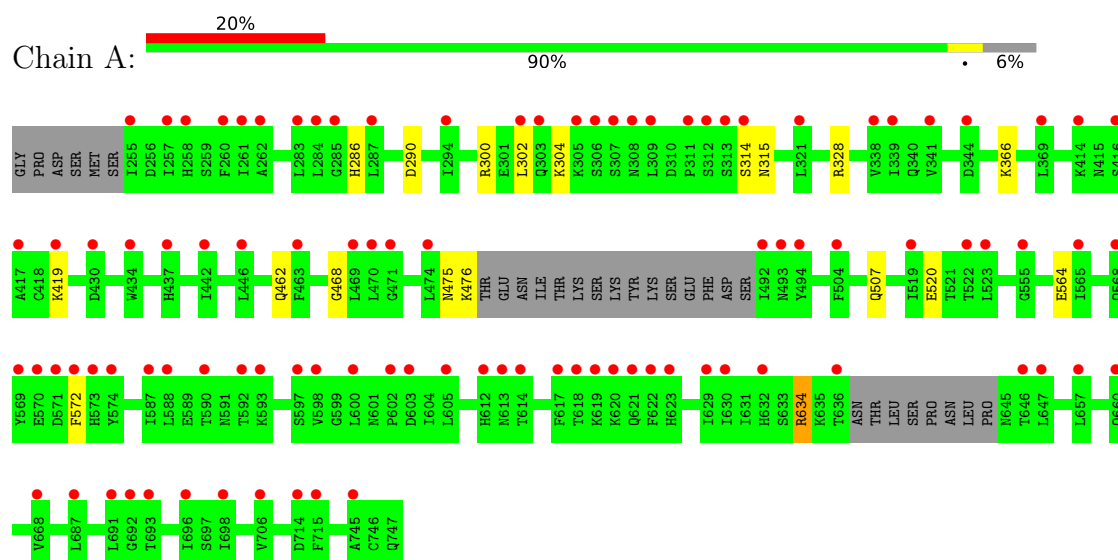
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0

3 Residue-property plots [i](#)

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: Superkiller protein 7



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	93.14Å 120.62Å 105.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.72 – 2.18 73.72 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.1 (73.72-2.18) 99.5 (73.72-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.217 , 0.246 0.226 , 0.253	Depositor DCC
R_{free} test set	1587 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7720	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: PO4, MG, 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	0.27	0/3909	0.60	0/5301

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	3809	3857	3841	7	0
2	A	5	0	0	0	0
3	A	28	10	12	0	0
4	A	1	0	0	0	0
5	A	10	0	0	1	0
All	All	3853	3867	3853	7	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 (7) 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:476:LYS:N	5:A:901:HOH:O	2.19	0.74
1:A:286:HIS:ND1	1:A:468:GLY:O	2.38	0.56
1:A:564:GLU:OE1	1:A:634:ARG:NH1	2.41	0.54
1:A:462:GLN:OE1	1:A:507:GLN:NE2	2.48	0.47
1:A:300:ARG:O	1:A:304:LYS:N	2.45	0.46
1:A:290:ASP:OD2	1:A:475:ASN:ND2	2.47	0.45
1:A:314[A]:SER:OG	1:A:315:ASN:N	2.51	0.43

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	473/499 (95%)	457 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	449/468 (96%)	441 (98%)	8 (2%)	51	65

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

Mol	Chain	Res	Type
1	A	302	LEU
1	A	328	ARG
1	A	366	LYS
1	A	419[A]	LYS
1	A	419[B]	LYS
1	A	520	GLU
1	A	572	PHE
1	A	634	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	A	553	ASN
1	A	586	GLN
1	A	662	HIS
1	A	728	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 3 ligands modelled in this entry, 1 is 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	PO4	A	801	4	4,4,4	1.01	0	6,6,6	0.44	0
3	GDP	A	802	4	29,30,30	1.14	3 (10%)	45,47,47	1.76	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
3	GDP	A	802	4	-	1/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	GDP	C5-C4	3.03	1.47	1.38
3	A	802	GDP	C6-N1	-2.42	1.34	1.38
3	A	802	GDP	C5-N7	-2.03	1.35	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	GDP	C5-C4-N3	-5.84	119.10	128.39
3	A	802	GDP	C2-N3-C4	4.93	120.79	112.30
3	A	802	GDP	N9-C4-N3	4.32	134.59	125.95
3	A	802	GDP	C6-C5-N7	3.46	136.59	130.29
3	A	802	GDP	C4-C5-N7	-2.64	106.49	110.67
3	A	802	GDP	O6-C6-C5	-2.10	120.99	126.53
3	A	802	GDP	C2'-C3'-C4'	2.04	106.55	102.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

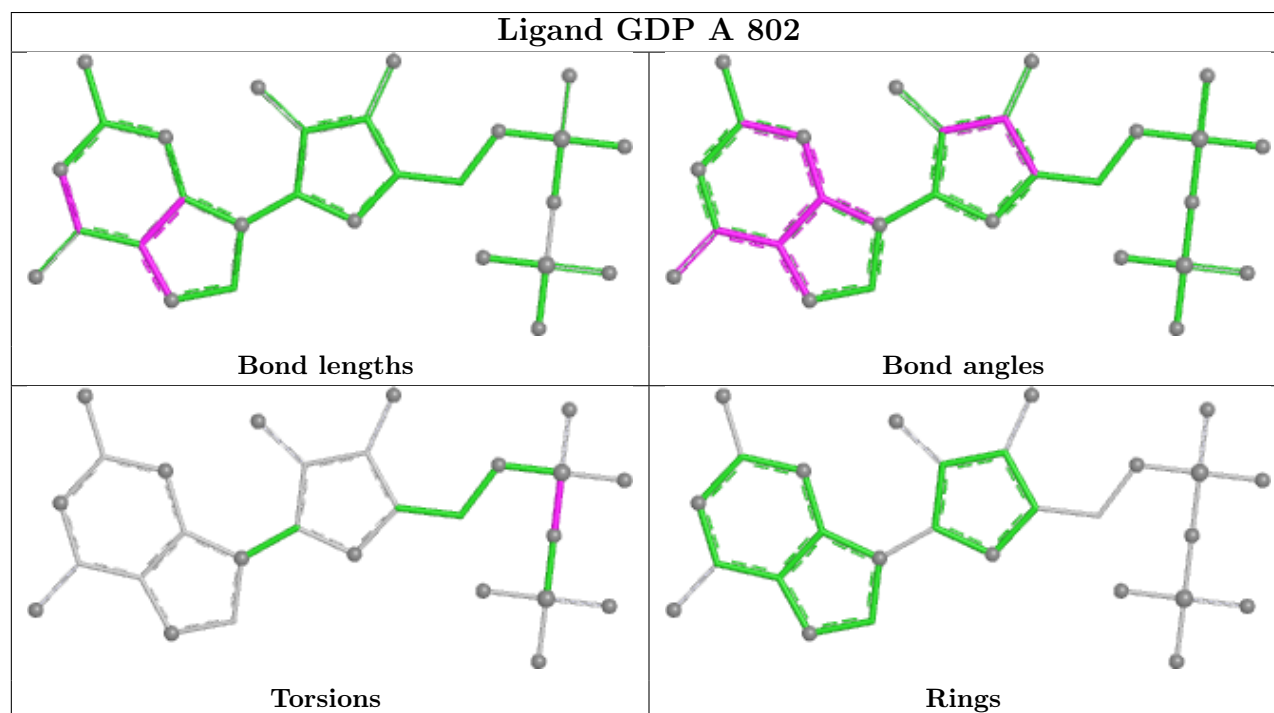
Mol	Chain	Res	Type	Atoms
3	A	802	GDP	PB-O3A-PA-O2A

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	470/499 (94%)	1.32	98 (20%) 2 2	32, 79, 127, 149	7 (1%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	ILE	6.6
1	A	572	PHE	6.4
1	A	492	ILE	6.0
1	A	494	TYR	5.6
1	A	612[A]	HIS	5.3
1	A	309	LEU	5.0
1	A	470	LEU	5.0
1	A	255	ILE	5.0
1	A	523	LEU	4.7
1	A	311	PRO	4.5
1	A	260	PHE	4.4
1	A	569	TYR	4.3
1	A	302	LEU	4.2
1	A	600	LEU	4.2
1	A	419[A]	LYS	4.1
1	A	417	ALA	4.0
1	A	287	LEU	4.0
1	A	636	THR	4.0
1	A	622	PHE	3.9
1	A	714	ASP	3.8
1	A	307	SER	3.8
1	A	605	LEU	3.7
1	A	657	LEU	3.7
1	A	442	ILE	3.7
1	A	588	LEU	3.6
1	A	414	LYS	3.6
1	A	306	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	437[A]	HIS	3.5
1	A	493	ASN	3.5
1	A	706	VAL	3.5
1	A	691	LEU	3.4
1	A	668	VAL	3.4
1	A	471	GLY	3.4
1	A	519	ILE	3.3
1	A	504	PHE	3.3
1	A	258	HIS	3.3
1	A	696	ILE	3.3
1	A	474	LEU	3.3
1	A	261	ILE	3.2
1	A	446	LEU	3.2
1	A	619	LYS	3.2
1	A	715	PHE	3.1
1	A	573	HIS	3.1
1	A	339	ILE	3.1
1	A	621	GLN	3.0
1	A	314[A]	SER	3.0
1	A	692	GLY	3.0
1	A	369	LEU	2.9
1	A	555	GLY	2.9
1	A	522	THR	2.9
1	A	623	HIS	2.9
1	A	646	THR	2.8
1	A	614	THR	2.7
1	A	294	ILE	2.7
1	A	618	THR	2.7
1	A	463	PHE	2.6
1	A	617	PHE	2.6
1	A	284	LEU	2.6
1	A	598	VAL	2.6
1	A	632	HIS	2.6
1	A	698	ILE	2.6
1	A	338	VAL	2.5
1	A	430	ASP	2.5
1	A	693	THR	2.5
1	A	587	ILE	2.5
1	A	568	GLN	2.4
1	A	629	ILE	2.4
1	A	597	SER	2.4
1	A	602	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	305	LYS	2.4
1	A	308	ASN	2.4
1	A	262	ALA	2.3
1	A	745	ALA	2.3
1	A	647	LEU	2.3
1	A	313	SER	2.3
1	A	341	VAL	2.3
1	A	570	GLU	2.2
1	A	613[A]	ASN	2.2
1	A	283	LEU	2.2
1	A	687	LEU	2.2
1	A	603	ASP	2.2
1	A	593	LYS	2.2
1	A	344	ASP	2.2
1	A	285	GLY	2.2
1	A	416	SER	2.1
1	A	303	GLN	2.1
1	A	321	LEU	2.1
1	A	565	ILE	2.1
1	A	434	TRP	2.1
1	A	312	SER	2.1
1	A	469	LEU	2.1
1	A	574	TYR	2.1
1	A	590	THR	2.1
1	A	630	ILE	2.1
1	A	620	LYS	2.0
1	A	660	GLN	2.0
1	A	571	ASP	2.0
1	A	592	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

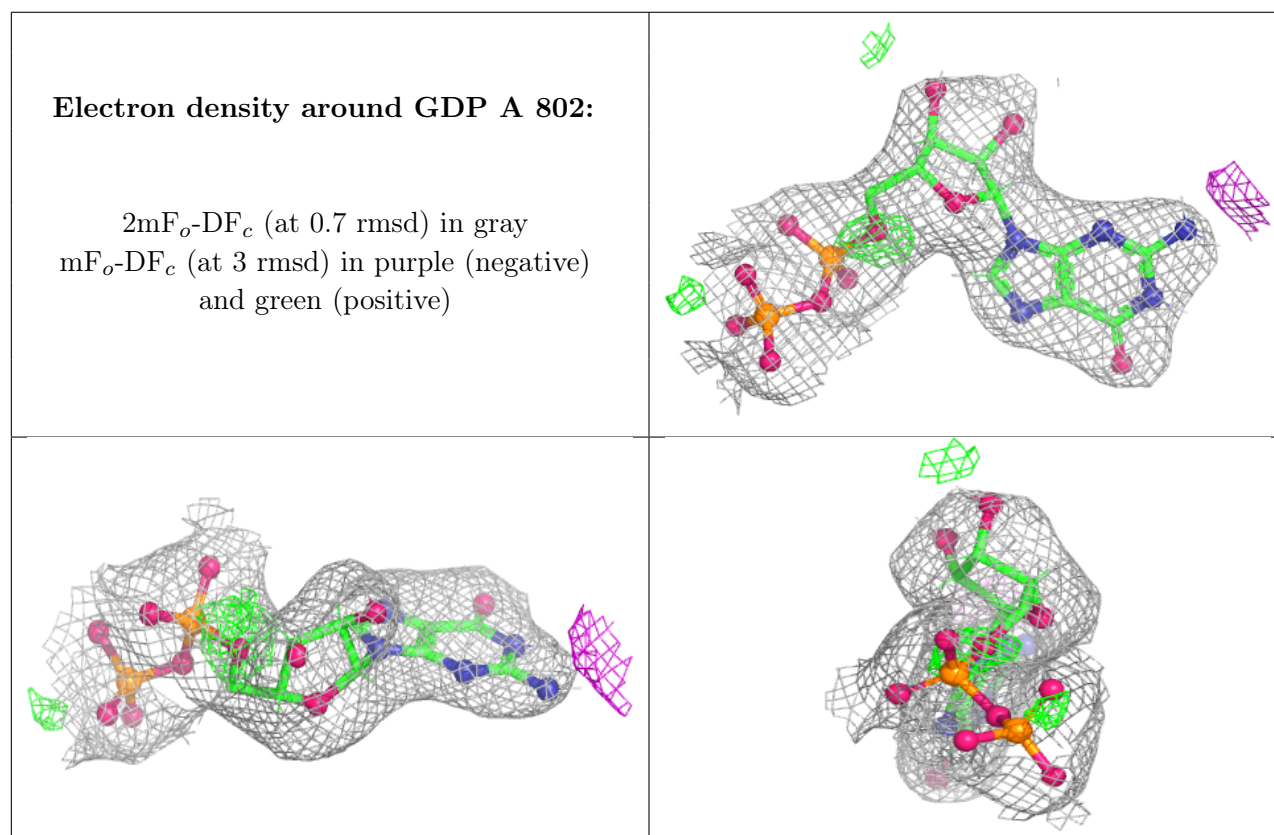
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	GDP	A	802	28/28	0.95	0.11	51,63,90,108	0
2	PO4	A	801	5/5	0.96	0.09	52,55,61,61	0
4	MG	A	803	1/1	0.99	0.07	59,59,59,59	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.