



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:15 PM EDT

PDB ID : 6NZ4 / pdb_00006nz4
Title : YcjX-GDP (type I)
Authors : Lee, S.; Tsai, J.; Tsai, F.T.
Deposited on : 2019-02-12
Resolution : 1.92 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

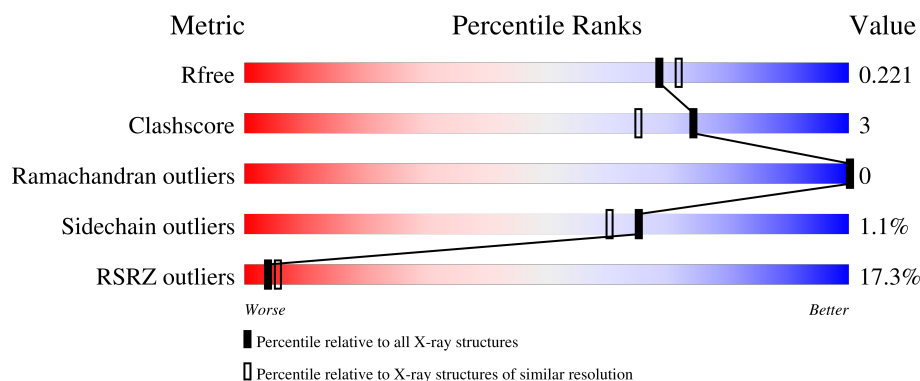
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	485	10% 90% 6%
1	B	485	22% 83% 9% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7976 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.

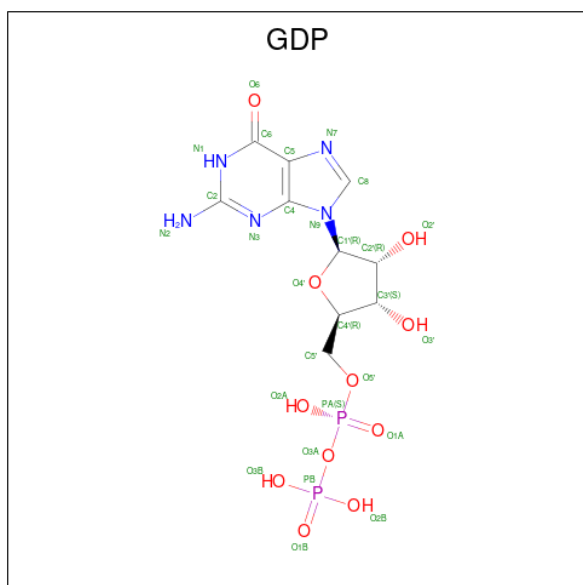
- Molecule 1 is a protein called YcjX Stress Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	9	0
			3714	2371	647	683	13			
1	B	451	Total	C	N	O	S	0	2	0
			3527	2260	609	645	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	LEU	PHE	engineered mutation	UNP Q8EG04
A	218	GLY	ASP	engineered mutation	UNP Q8EG04
B	187	LEU	PHE	engineered mutation	UNP Q8EG04
B	218	GLY	ASP	engineered mutation	UNP Q8EG04

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).

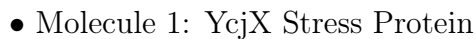


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	425	Total	O	0	0
			425	425		
3	B	254	Total	O	0	0
			254	254		

- Molecule 1: YcjX Stress Protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.31Å 133.94Å 144.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.86 – 1.92 45.86 – 1.92	Depositor EDS
% Data completeness (in resolution range)	75.1 (45.86-1.92) 87.7 (45.86-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 1.91Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.180 , 0.223 0.181 , 0.221	Depositor DCC
R_{free} test set	2010 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.8	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	0.94	EDS
Total number of atoms	7976	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.19	0/3803	0.37	0/5164
1	B	0.15	0/3612	0.35	0/4906
All	All	0.17	0/7415	0.36	0/10070

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	3714	0	3646	18	0
1	B	3527	0	3455	26	0
2	A	28	0	12	0	0
2	B	28	0	12	1	0
3	A	425	0	0	4	0
3	B	254	0	0	2	1
All	All	7976	0	7125	44	1

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 (44) 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:331:GLN:NE2	1:A:380:HIS:O	2.10	0.84
1:A:298:ARG:HD3	1:A:348:ARG:HB2	1.72	0.71
1:B:404:MET:HE1	1:B:413:GLU:HG2	1.72	0.71
1:B:298:ARG:HD3	1:B:348:ARG:HB2	1.74	0.69
1:A:228:ALA:HB3	1:A:234[A]:LEU:HD22	1.76	0.67
1:B:237:GLY:O	3:B:601:HOH:O	2.14	0.65
1:A:159:MET:HE1	1:A:230:PRO:HB3	1.78	0.64
1:B:371:LEU:HA	1:B:374:MET:HE3	1.78	0.64
1:B:110:TRP:CD1	2:B:500:GDP:HO2'	2.16	0.62
1:B:396:ALA:HA	1:B:472:LEU:HD11	1.83	0.61
1:B:26[A]:HIS:NE2	1:B:145:ASP:OD2	2.32	0.60
1:A:206[B]:LYS:NZ	3:A:610:HOH:O	2.36	0.59
1:B:159:MET:HE1	1:B:230:PRO:HB3	1.85	0.59
1:B:127:ARG:NH1	1:B:138:ASP:O	2.37	0.56
1:B:412:VAL:HG13	1:B:429:PRO:HG3	1.89	0.55
1:A:415[B]:VAL:HG12	1:A:427:LEU:HB3	1.88	0.55
1:A:115:ARG:NH1	3:A:612:HOH:O	2.39	0.53
1:B:139:ALA:N	3:B:612:HOH:O	2.42	0.52
1:B:370:LEU:HG	1:B:374:MET:HE2	1.90	0.51
1:A:152:GLU:HG2	1:A:234[A]:LEU:HD21	1.92	0.50
1:B:200:ALA:HB2	1:B:269:ALA:HA	1.92	0.50
1:A:42:PHE:HA	1:A:396:ALA:CB	2.45	0.47
1:B:313:LYS:HB2	1:B:442:TRP:CG	2.51	0.46
1:A:435:ARG:NH2	3:A:619:HOH:O	2.49	0.46
1:B:356:VAL:HG11	1:B:393:ALA:HB1	1.98	0.46
1:A:63:ARG:HH12	1:A:76:GLN:HG2	1.81	0.46
1:B:27:LEU:HD23	1:B:480:VAL:HG23	1.97	0.46
1:B:297:ASP:O	1:B:346:ILE:HA	2.16	0.45
1:A:117:ILE:HA	1:A:148:ASP:O	2.17	0.44
1:A:476:LEU:O	1:A:480[B]:VAL:HG22	2.20	0.42
1:A:231:GLY:O	1:A:234[A]:LEU:HD23	2.20	0.42
1:B:42:PHE:HA	1:B:396:ALA:CB	2.50	0.41
1:B:388:LYS:NZ	1:B:390:GLU:HG3	2.35	0.41
1:A:400:THR:HB	1:A:415[B]:VAL:HG22	2.02	0.41
1:A:473:ASP:N	1:A:473:ASP:OD1	2.53	0.41
1:B:398:LYS:HB3	1:B:468:ASP:HB2	2.03	0.41
1:B:427:LEU:HG	1:B:428:PHE:HD1	1.85	0.41
1:B:419:GLY:C	1:B:421:ASN:H	2.29	0.41
1:B:476:LEU:O	1:B:480:VAL:HG12	2.20	0.41
1:A:72:VAL:HG11	1:A:484:LEU:HD13	2.02	0.41
1:B:117:ILE:HA	1:B:148:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:HB2	3:A:754:HOH:O	2.22	0.40
1:B:366:HIS:HB2	1:B:432:VAL:HG13	2.04	0.40
1:B:106:ASN:HA	1:B:107:PRO:HA	1.97	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:612:HOH:O	3:B:785:HOH:O[4_466]	2.14	0.06

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	474/485 (98%)	462 (98%)	12 (2%)	0	100	100
1	B	449/485 (93%)	434 (97%)	15 (3%)	0	100	100
All	All	923/970 (95%)	896 (97%)	27 (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	389/412 (94%)	387 (100%)	2 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	368/412 (89%)	362 (98%)	6 (2%)	55 44
All	All	757/824 (92%)	749 (99%)	8 (1%)	65 60

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

Mol	Chain	Res	Type
1	A	233	MET
1	A	412	VAL
1	B	415	VAL
1	B	421	ASN
1	B	423	GLN
1	B	425	LEU
1	B	428	PHE
1	B	480	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	217	HIS
1	A	223	GLN
1	A	448	ASN
1	B	211	GLN
1	B	366	HIS

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

2 ligands are 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$
2	GDP	B	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	6 (13%)
2	GDP	A	500	-	29,30,30	1.19	3 (10%)	45,47,47	1.68	6 (13%)

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	GDP	B	500	-	-	0/16/32/32	0/3/3/3
2	GDP	A	500	-	-	2/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	GDP	C5-C4	3.20	1.47	1.38
2	A	500	GDP	C5-C4	3.09	1.47	1.38
2	B	500	GDP	C6-N1	-2.47	1.34	1.38
2	A	500	GDP	C6-N1	-2.46	1.34	1.38
2	B	500	GDP	C5-N7	-2.16	1.34	1.39
2	A	500	GDP	PA-O3A	2.11	1.61	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	GDP	C5-C4-N3	-6.36	118.27	128.39
2	A	500	GDP	C5-C4-N3	-5.72	119.29	128.39
2	B	500	GDP	C2-N3-C4	5.10	121.08	112.30
2	B	500	GDP	N9-C4-N3	4.63	135.21	125.95
2	A	500	GDP	C2-N3-C4	4.58	120.18	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	GDP	N9-C4-N3	4.28	134.50	125.95
2	B	500	GDP	C6-C5-N7	3.20	136.12	130.29
2	A	500	GDP	C6-C5-N7	3.15	136.03	130.29
2	B	500	GDP	C4-C5-N7	-2.76	106.29	110.67
2	A	500	GDP	C4-C5-N7	-2.57	106.60	110.67
2	A	500	GDP	O2B-PB-O3A	2.17	111.92	104.64
2	B	500	GDP	C3'-C2'-C1'	2.07	105.38	101.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

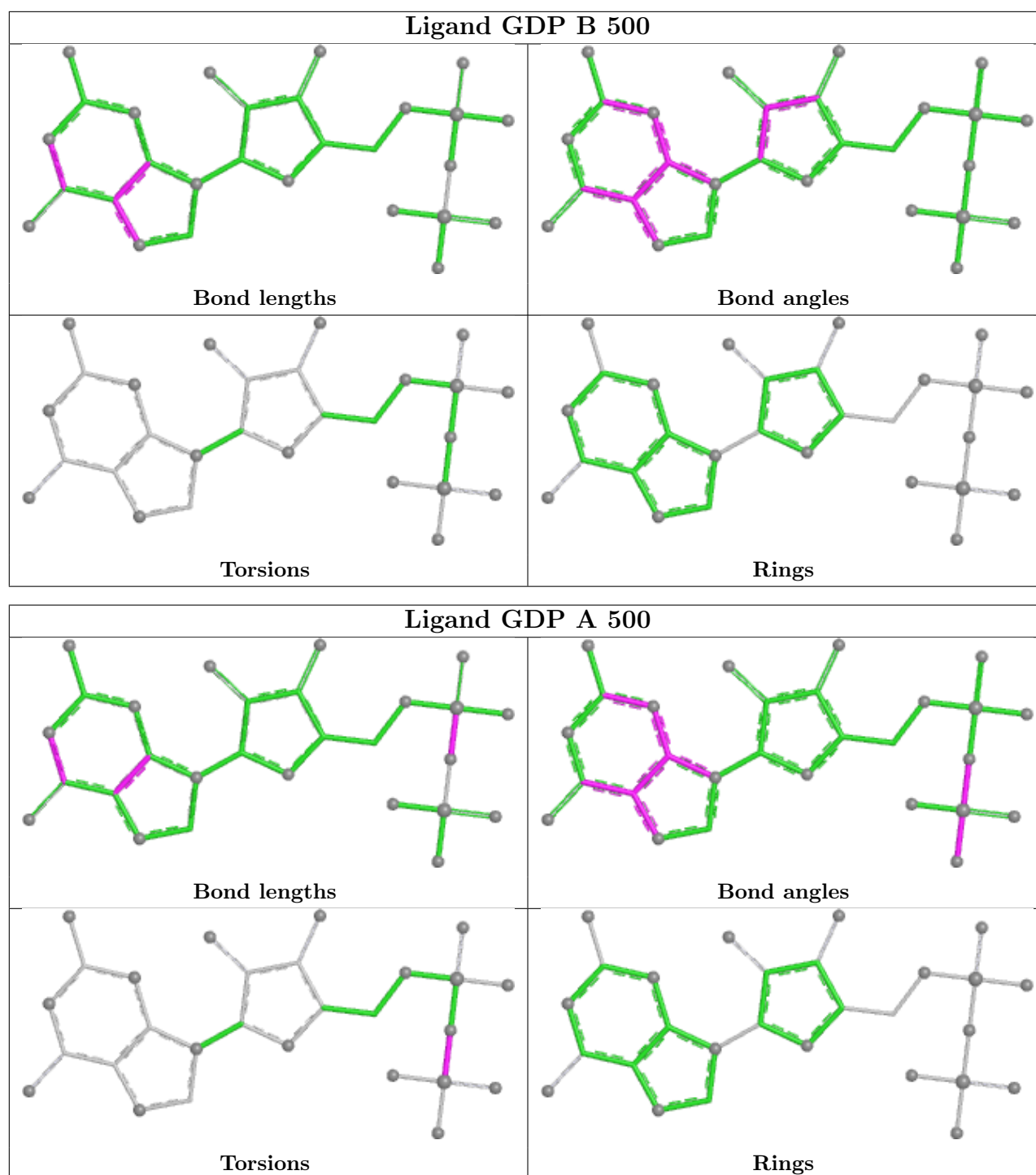
Mol	Chain	Res	Type	Atoms
2	A	500	GDP	PA-O3A-PB-O2B
2	A	500	GDP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	GDP	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

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	467/485 (96%)	0.22	50 (10%)	11 14	5, 20, 66, 119	9 (1%)
1	B	451/485 (92%)	1.19	109 (24%)	2 2	13, 39, 92, 118	2 (0%)
All	All	918/970 (94%)	0.70	159 (17%)	4 5	5, 29, 84, 119	11 (1%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	PHE	8.6
1	B	133	LEU	8.3
1	B	132	LEU	7.7
1	B	415	VAL	7.6
1	A	19	LEU	7.4
1	A	59	VAL	7.3
1	A	447	PHE	6.7
1	B	136	PHE	6.7
1	B	334	GLN	6.7
1	B	429	PRO	6.6
1	B	427	LEU	6.5
1	B	452	PHE	6.2
1	B	137	ALA	6.2
1	B	441	PHE	5.9
1	A	56	VAL	5.7
1	B	134	ALA	5.6
1	B	460	VAL	5.5
1	A	61	HIS	5.2
1	B	131	GLY	5.2
1	B	442	TRP	5.2
1	B	447	PHE	5.1
1	B	440	ASP	5.0
1	A	62	SER	5.0
1	B	387	CYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	386	GLY	4.9
1	A	462	PRO	4.9
1	A	335	SER	4.7
1	A	65	ASN	4.6
1	B	362	ASP	4.6
1	B	446	GLY	4.6
1	B	416	GLN	4.6
1	B	138	ASP	4.6
1	B	432	VAL	4.5
1	B	420	LEU	4.5
1	B	451	GLY	4.5
1	A	20	HIS	4.5
1	A	58	THR	4.5
1	A	382	ALA	4.5
1	B	449	PHE	4.4
1	A	57	SER	4.4
1	B	424	ALA	4.3
1	B	461	ASP	4.3
1	B	421	ASN	4.3
1	A	461	ASP	4.2
1	B	430	GLY	4.2
1	A	459	ASN	4.1
1	B	335	SER	4.1
1	B	135	LYS	4.1
1	A	460	VAL	4.0
1	B	266	LYS	3.9
1	B	444	GLU	3.8
1	B	450	ILE	3.8
1	B	453	ALA	3.7
1	B	423	GLN	3.7
1	A	332	TYR	3.7
1	B	443	ARG	3.7
1	A	384	PHE	3.6
1	A	63	ARG	3.6
1	B	417	GLY	3.6
1	B	437	PRO	3.6
1	B	24	ASP	3.6
1	B	260	ASN	3.6
1	B	332	TYR	3.6
1	A	64	GLN	3.6
1	B	382	ALA	3.5
1	B	459	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	418	THR	3.4
1	B	458	THR	3.4
1	B	439	PRO	3.4
1	B	337	TYR	3.3
1	B	367	VAL	3.3
1	B	448	ASN	3.3
1	B	222	VAL	3.3
1	B	462	PRO	3.3
1	A	333	GLY	3.3
1	A	60	SER	3.3
1	B	422	GLY	3.2
1	A	385	GLU	3.2
1	A	440	ASP	3.2
1	B	106	ASN	3.1
1	A	334	GLN	3.1
1	A	446	GLY	3.1
1	B	425	LEU	3.0
1	B	385	GLU	3.0
1	A	402	HIS	3.0
1	A	409	GLU	3.0
1	B	431	GLU	3.0
1	B	312	GLY	2.9
1	B	360	THR	2.9
1	B	409[A]	GLU	2.9
1	B	310	ASN	2.9
1	B	139	ALA	2.9
1	A	367[A]	VAL	2.9
1	B	225	TYR	2.9
1	A	421	ASN	2.9
1	B	365	SER	2.9
1	B	109	THR	2.8
1	B	435	ARG	2.8
1	A	458	THR	2.8
1	A	336	SER	2.8
1	B	369	SER	2.8
1	B	445	GLN	2.8
1	B	108	PRO	2.8
1	B	314	SER	2.7
1	B	256	ALA	2.7
1	A	379	GLN	2.6
1	B	433	PRO	2.6
1	B	436	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	54	GLY	2.5
1	A	256	ALA	2.5
1	B	221	HIS	2.5
1	A	55	ALA	2.5
1	B	363	GLN	2.5
1	A	441	PHE	2.5
1	A	138	ASP	2.5
1	B	265	ASP	2.5
1	A	337[A]	TYR	2.4
1	B	184	TYR	2.4
1	B	381	PHE	2.4
1	B	364	GLN	2.4
1	B	426	THR	2.4
1	A	386	GLY	2.4
1	A	422	GLY	2.4
1	B	384	PHE	2.4
1	B	414	VAL	2.4
1	A	423	GLN	2.4
1	B	308	ALA	2.3
1	B	199	MET	2.3
1	B	404	MET	2.3
1	B	455	PRO	2.3
1	A	66	GLY	2.3
1	B	403	GLY	2.3
1	B	419	GLY	2.3
1	A	448	ASN	2.3
1	B	103	LEU	2.3
1	B	465	VAL	2.2
1	B	183	LEU	2.2
1	A	408	GLN	2.2
1	B	456	ASP	2.2
1	B	333	GLY	2.2
1	B	185	ALA	2.2
1	B	175	ILE	2.2
1	B	399	ALA	2.2
1	A	127	ARG	2.2
1	A	339	ARG	2.2
1	B	457	ASN	2.1
1	B	413	GLU	2.1
1	B	361	ARG	2.1
1	A	259	SER	2.1
1	B	311	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	359	VAL	2.1
1	A	404	MET	2.1
1	B	234	LEU	2.1
1	B	315	GLN	2.1
1	A	485	GLU	2.1
1	B	402	HIS	2.1
1	A	405	VAL	2.1
1	B	309	LEU	2.0
1	B	66	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](#)

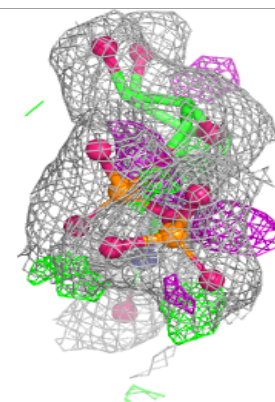
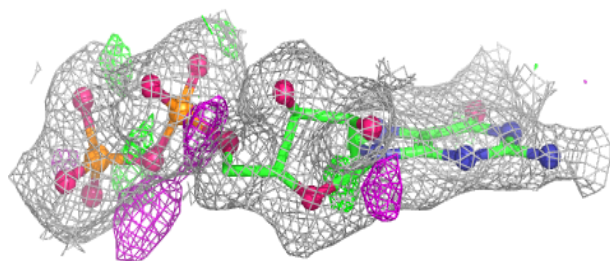
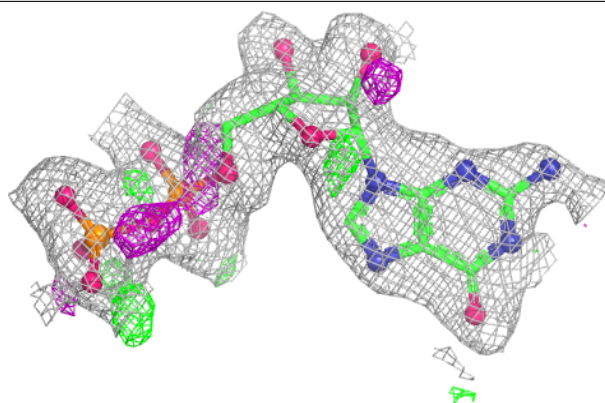
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	GDP	B	500	28/28	0.93	0.11	20,37,53,54	0
2	GDP	A	500	28/28	0.99	0.04	6,12,16,17	0

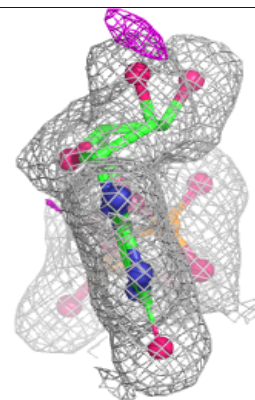
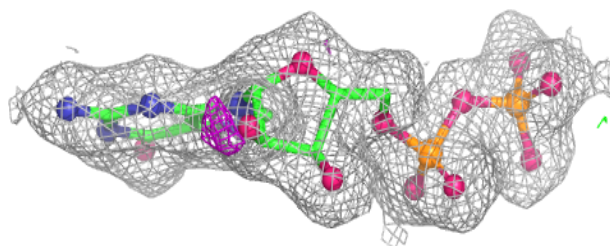
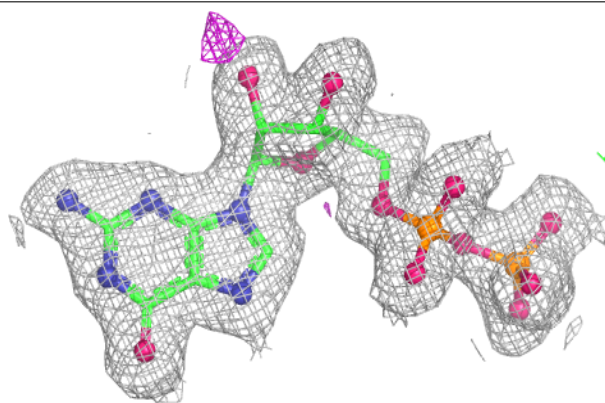
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP B 500:

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

**Electron density around 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.