Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 05:12 PM JST

PDB ID	:	5GNS
Title	:	Structures of human Mitofusin 1 provide insight into mitochondrial tethering
Authors	:	Qi, Y.; Yan, L.; Yu, C.; Guo, X.; Zhou, X.; Hu, X.; Huang, X.; Rao, Z.; Lou, Z.; Hu, J.
Deposited on	:	2016-07-24
Resolution	:	2.70 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:

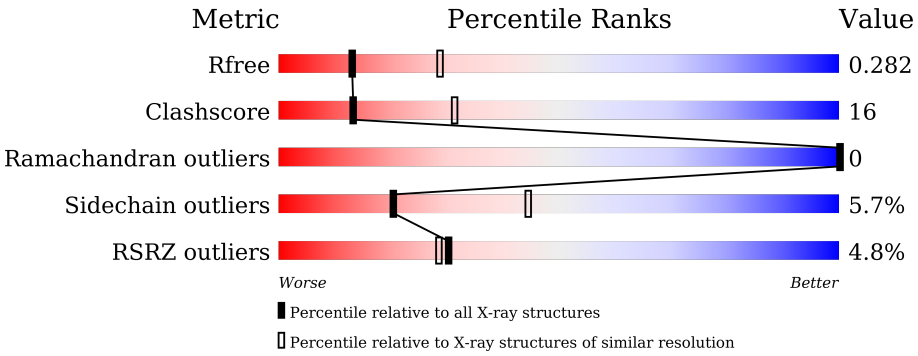
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	421	4% 66% 20% · 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3051 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 Mitofusin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	377	3011	1909	518	570	14	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

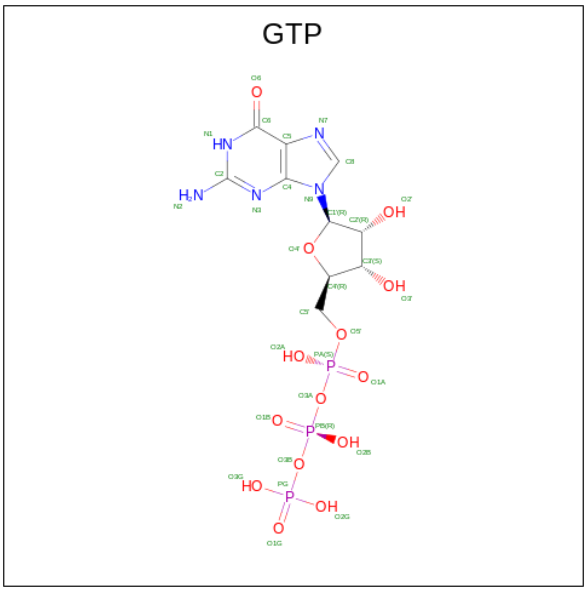
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	ALA	LYS	engineered mutation	UNP Q8IWA4
A	365	GLY	-	expression tag	UNP Q8IWA4
A	366	SER	-	expression tag	UNP Q8IWA4
A	367	GLY	-	expression tag	UNP Q8IWA4
A	368	SER	-	expression tag	UNP Q8IWA4
A	369	GLY	-	expression tag	UNP Q8IWA4
A	370	SER	-	expression tag	UNP Q8IWA4
A	371	GLY	-	expression tag	UNP Q8IWA4
A	372	GLY	-	expression tag	UNP Q8IWA4
A	373	SER	-	expression tag	UNP Q8IWA4
A	374	GLU	-	expression tag	UNP Q8IWA4
A	375	ILE	-	expression tag	UNP Q8IWA4
A	376	ALA	-	expression tag	UNP Q8IWA4
A	377	ARG	-	expression tag	UNP Q8IWA4
A	378	LEU	-	expression tag	UNP Q8IWA4
A	379	PRO	-	expression tag	UNP Q8IWA4
A	380	LYS	-	expression tag	UNP Q8IWA4
A	381	GLU	-	expression tag	UNP Q8IWA4
A	382	ILE	-	expression tag	UNP Q8IWA4
A	383	ASP	-	expression tag	UNP Q8IWA4
A	384	GLN	-	expression tag	UNP Q8IWA4
A	385	LEU	-	expression tag	UNP Q8IWA4
A	386	GLU	-	expression tag	UNP Q8IWA4
A	387	LYS	-	expression tag	UNP Q8IWA4
A	388	ILE	-	expression tag	UNP Q8IWA4
A	389	GLN	-	expression tag	UNP Q8IWA4
A	390	ASN	-	expression tag	UNP Q8IWA4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	ASN	-	expression tag	UNP Q8IWA4
A	392	SER	-	expression tag	UNP Q8IWA4
A	393	LYS	-	expression tag	UNP Q8IWA4
A	394	LEU	-	expression tag	UNP Q8IWA4
A	395	LEU	-	expression tag	UNP Q8IWA4
A	396	ARG	-	expression tag	UNP Q8IWA4
A	397	ASN	-	expression tag	UNP Q8IWA4
A	398	LYS	-	expression tag	UNP Q8IWA4
A	399	ALA	-	expression tag	UNP Q8IWA4
A	400	VAL	-	expression tag	UNP Q8IWA4
A	401	GLN	-	expression tag	UNP Q8IWA4
A	402	LEU	-	expression tag	UNP Q8IWA4
A	403	GLU	-	expression tag	UNP Q8IWA4
A	404	ASN	-	expression tag	UNP Q8IWA4
A	405	GLU	-	expression tag	UNP Q8IWA4
A	406	LEU	-	expression tag	UNP Q8IWA4
A	407	GLU	-	expression tag	UNP Q8IWA4
A	408	ASN	-	expression tag	UNP Q8IWA4
A	409	PHE	-	expression tag	UNP Q8IWA4
A	410	THR	-	expression tag	UNP Q8IWA4
A	411	LYS	-	expression tag	UNP Q8IWA4
A	412	GLN	-	expression tag	UNP Q8IWA4
A	413	PHE	-	expression tag	UNP Q8IWA4
A	414	LEU	-	expression tag	UNP Q8IWA4
A	415	PRO	-	expression tag	UNP Q8IWA4
A	416	SER	-	expression tag	UNP Q8IWA4
A	417	SER	-	expression tag	UNP Q8IWA4
A	418	ASN	-	expression tag	UNP Q8IWA4
A	419	GLU	-	expression tag	UNP Q8IWA4
A	420	GLU	-	expression tag	UNP Q8IWA4
A	421	SER	-	expression tag	UNP Q8IWA4

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is water.

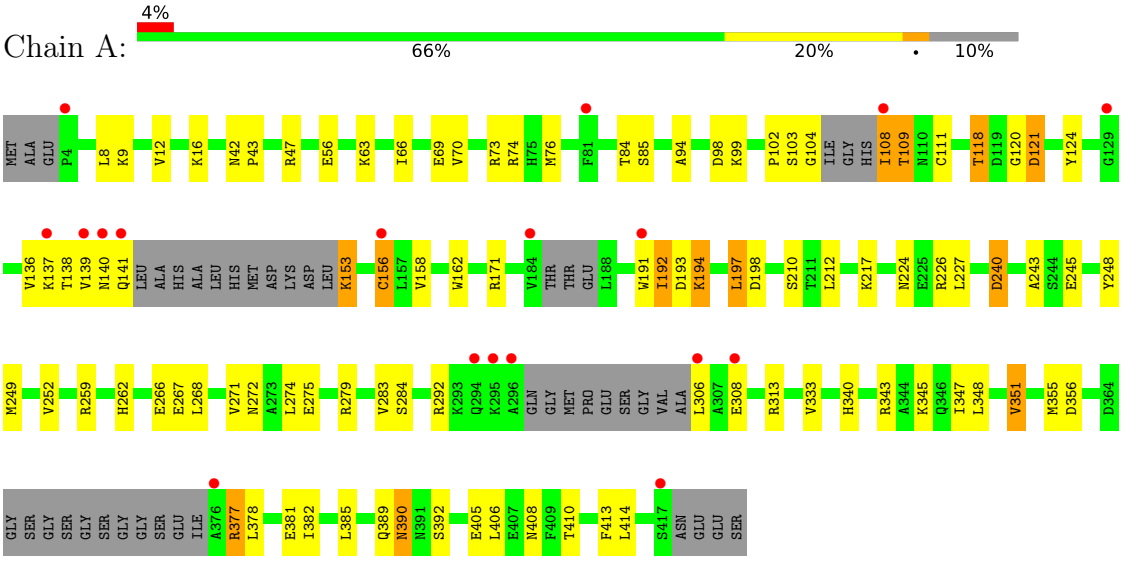
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		

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: Mitofusin-1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.66Å 74.67Å 94.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.01 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.01-2.70) 99.8 (40.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.16 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.212 , 0.283 0.221 , 0.282	Depositor DCC
R_{free} test set	1436 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3051	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GTP

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	0.54	0/3059	0.76	4/4115 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	ASP	N-CA-CB	-19.52	75.45	110.60
1	A	121	ASP	N-CA-C	6.86	129.51	111.00
1	A	192	ILE	N-CA-CB	-6.50	95.84	110.80
1	A	191	TRP	CB-CA-C	-5.46	99.48	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	LYS	Peptide

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	3011	0	3014	98	1
2	A	32	0	12	3	0
3	A	8	0	0	4	0
All	All	3051	0	3026	98	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 16.

All (98) 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:104:GLY:CA	1:A:108:ILE:HB	1.66	1.25
1:A:104:GLY:C	1:A:108:ILE:HG13	1.56	1.25
1:A:104:GLY:C	1:A:108:ILE:CG1	2.04	1.25
1:A:153:LYS:O	1:A:153:LYS:HD2	1.39	1.17
1:A:104:GLY:HA3	1:A:108:ILE:HB	1.25	1.09
1:A:104:GLY:CA	1:A:108:ILE:CB	2.31	1.07
1:A:104:GLY:C	1:A:108:ILE:CB	2.22	1.07
1:A:139:VAL:O	1:A:139:VAL:CG2	1.99	1.07
1:A:139:VAL:O	1:A:139:VAL:HG23	1.23	1.04
1:A:104:GLY:HA2	1:A:108:ILE:HG21	1.38	1.03
1:A:104:GLY:HA2	1:A:108:ILE:CG2	1.89	1.02
1:A:111:CYS:CB	1:A:156:CYS:HB3	1.90	1.00
1:A:85:SER:HB2	2:A:501:GTP:H5'	1.43	1.00
1:A:111:CYS:HB3	1:A:156:CYS:HB3	1.04	0.99
1:A:111:CYS:HB2	1:A:156:CYS:O	1.61	0.98
1:A:104:GLY:C	1:A:108:ILE:HB	1.81	0.97
1:A:197:LEU:HD22	1:A:197:LEU:O	1.62	0.97
1:A:108:ILE:HD13	1:A:109:THR:H	1.26	0.97
1:A:104:GLY:CA	1:A:108:ILE:CG2	2.44	0.95
1:A:111:CYS:HB3	1:A:156:CYS:CB	1.99	0.85
1:A:104:GLY:HA3	1:A:108:ILE:CB	2.08	0.77
1:A:102:PRO:O	1:A:102:PRO:HD2	1.84	0.76
1:A:104:GLY:CA	1:A:108:ILE:HG21	2.12	0.76
1:A:153:LYS:O	1:A:153:LYS:CD	2.30	0.75
1:A:102:PRO:O	1:A:102:PRO:CD	2.33	0.73
1:A:240:ASP:OD2	2:A:501:GTP:N1	2.22	0.72
1:A:85:SER:CB	2:A:501:GTP:H5'	2.19	0.71
1:A:111:CYS:SG	1:A:158:VAL:HG23	2.31	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:O	1:A:259:ARG:NH1	2.24	0.69
1:A:356:ASP:OD2	3:A:601:HOH:O	2.11	0.67
1:A:111:CYS:CB	1:A:156:CYS:O	2.40	0.67
1:A:108:ILE:HD13	1:A:109:THR:N	2.06	0.67
1:A:137:LYS:O	1:A:140:ASN:HB2	1.96	0.66
1:A:140:ASN:C	1:A:140:ASN:OD1	2.34	0.65
1:A:308:GLU:N	1:A:308:GLU:OE1	2.30	0.64
1:A:377:ARG:HG3	1:A:377:ARG:HH11	1.63	0.63
1:A:66:ILE:O	1:A:70:VAL:HG13	1.98	0.63
1:A:377:ARG:HH11	1:A:377:ARG:CG	2.10	0.63
1:A:111:CYS:HB2	1:A:156:CYS:C	2.20	0.62
1:A:108:ILE:CD1	1:A:109:THR:H	2.08	0.61
1:A:197:LEU:HD23	1:A:227:LEU:HD21	1.83	0.61
1:A:377:ARG:HB2	1:A:381:GLU:OE1	2.00	0.60
1:A:9:LYS:HA	1:A:12:VAL:HG12	1.83	0.60
1:A:378:LEU:O	1:A:382:ILE:HG13	2.02	0.59
1:A:377:ARG:HB3	1:A:377:ARG:CZ	2.31	0.59
1:A:118:THR:HG21	1:A:124:TYR:CE2	2.38	0.58
1:A:245:GLU:O	1:A:249:MET:HB2	2.05	0.57
1:A:272:ASN:ND2	1:A:275:GLU:OE2	2.39	0.56
1:A:308:GLU:O	1:A:313:ARG:NH2	2.41	0.54
1:A:217:LYS:NZ	1:A:267:GLU:OE2	2.39	0.53
1:A:279:ARG:NE	3:A:603:HOH:O	2.37	0.53
1:A:153:LYS:HD2	1:A:153:LYS:C	2.21	0.53
1:A:243:ALA:O	1:A:245:GLU:HG2	2.09	0.52
1:A:279:ARG:NH2	3:A:603:HOH:O	2.36	0.52
1:A:377:ARG:CB	1:A:377:ARG:NH1	2.73	0.51
1:A:197:LEU:O	1:A:197:LEU:CD2	2.48	0.51
1:A:69:GLU:HG3	1:A:73:ARG:HH12	1.77	0.50
1:A:108:ILE:O	1:A:141:GLN:NE2	2.43	0.50
1:A:140:ASN:OD1	1:A:140:ASN:O	2.30	0.50
1:A:248:TYR:O	1:A:252:VAL:HG23	2.13	0.49
1:A:377:ARG:CG	1:A:377:ARG:NH1	2.72	0.48
1:A:224:ASN:O	3:A:602:HOH:O	2.19	0.48
1:A:271:VAL:HG22	1:A:275:GLU:HB2	1.95	0.48
1:A:240:ASP:HA	1:A:313:ARG:NH1	2.29	0.48
1:A:405:GLU:O	1:A:408:ASN:HB3	2.13	0.48
1:A:84:THR:O	1:A:84:THR:OG1	2.30	0.47
1:A:390:ASN:N	1:A:390:ASN:OD1	2.46	0.47
1:A:385:LEU:O	1:A:389:GLN:HG3	2.14	0.47
1:A:192:ILE:HG13	1:A:193:ASP:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HB	1:A:120:GLY:H	1.79	0.46
1:A:355:MET:CE	1:A:392:SER:HA	2.47	0.45
1:A:345:LYS:NZ	1:A:410:THR:HG21	2.31	0.45
1:A:406:LEU:O	1:A:410:THR:HG23	2.17	0.45
1:A:94:ALA:O	1:A:292:ARG:NH1	2.46	0.45
1:A:138:THR:OG1	1:A:139:VAL:N	2.48	0.44
1:A:8:LEU:HD22	1:A:76:MET:SD	2.57	0.44
1:A:70:VAL:O	1:A:74:ARG:HG2	2.17	0.44
1:A:333:VAL:HG12	1:A:414:LEU:HD21	1.98	0.44
1:A:377:ARG:CZ	1:A:377:ARG:CB	2.95	0.44
1:A:262:HIS:CD2	1:A:266:GLU:OE2	2.71	0.43
1:A:16:LYS:HE3	1:A:16:LYS:HB2	1.84	0.43
1:A:137:LYS:O	1:A:138:THR:C	2.54	0.43
1:A:347:ILE:O	1:A:351:VAL:HG12	2.18	0.43
1:A:348:LEU:HA	1:A:351:VAL:CG1	2.48	0.43
1:A:63:LYS:HE3	1:A:63:LYS:HB2	1.87	0.43
1:A:224:ASN:ND2	1:A:268:LEU:O	2.51	0.43
1:A:413:PHE:O	1:A:414:LEU:HD23	2.19	0.42
1:A:240:ASP:OD1	1:A:284:SER:OG	2.23	0.42
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.83	0.42
1:A:226:ARG:O	1:A:227:LEU:HD23	2.20	0.42
1:A:98:ASP:OD1	1:A:99:LYS:N	2.49	0.42
1:A:118:THR:HG21	1:A:124:TYR:HE2	1.82	0.42
1:A:42:ASN:HA	1:A:43:PRO:HD3	1.88	0.41
1:A:137:LYS:NZ	1:A:162:TRP:HZ3	2.18	0.41
1:A:137:LYS:O	1:A:140:ASN:CB	2.67	0.41
1:A:340:HIS:CE1	1:A:343:ARG:HH21	2.38	0.41
1:A:8:LEU:HA	1:A:8:LEU:HD23	1.78	0.40
1:A:355:MET:HE2	1:A:392:SER:HA	2.03	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)
1:A:56:GLU:OE2	1:A:210:SER:OG[2_574]	2.19	0.01

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	365/421 (87%)	337 (92%)	28 (8%)	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	334/367 (91%)	315 (94%)	19 (6%)	20 44

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	103	SER
1	A	108	ILE
1	A	109	THR
1	A	118	THR
1	A	121	ASP
1	A	136	VAL
1	A	153	LYS
1	A	156	CYS
1	A	171	ARG
1	A	194	LYS
1	A	197	LEU
1	A	198	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	240	ASP
1	A	283	VAL
1	A	306	LEU
1	A	351	VAL
1	A	377	ARG
1	A	390	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	GTP	A	501	-	26,34,34	1.07	1 (3%)	32,54,54	1.29	4 (12%)

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	GTP	A	501	-	-	5/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GTP	C5-C6	-3.68	1.39	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	GTP	C8-N7-C5	3.06	108.82	102.99
2	A	501	GTP	PB-O3B-PG	-2.95	122.72	132.83
2	A	501	GTP	C5-C6-N1	2.76	118.82	113.95
2	A	501	GTP	C2-N1-C6	-2.41	120.67	125.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GTP	C5'-O5'-PA-O3A
2	A	501	GTP	C5'-O5'-PA-O1A
2	A	501	GTP	PG-O3B-PB-O1B
2	A	501	GTP	PG-O3B-PB-O2B
2	A	501	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

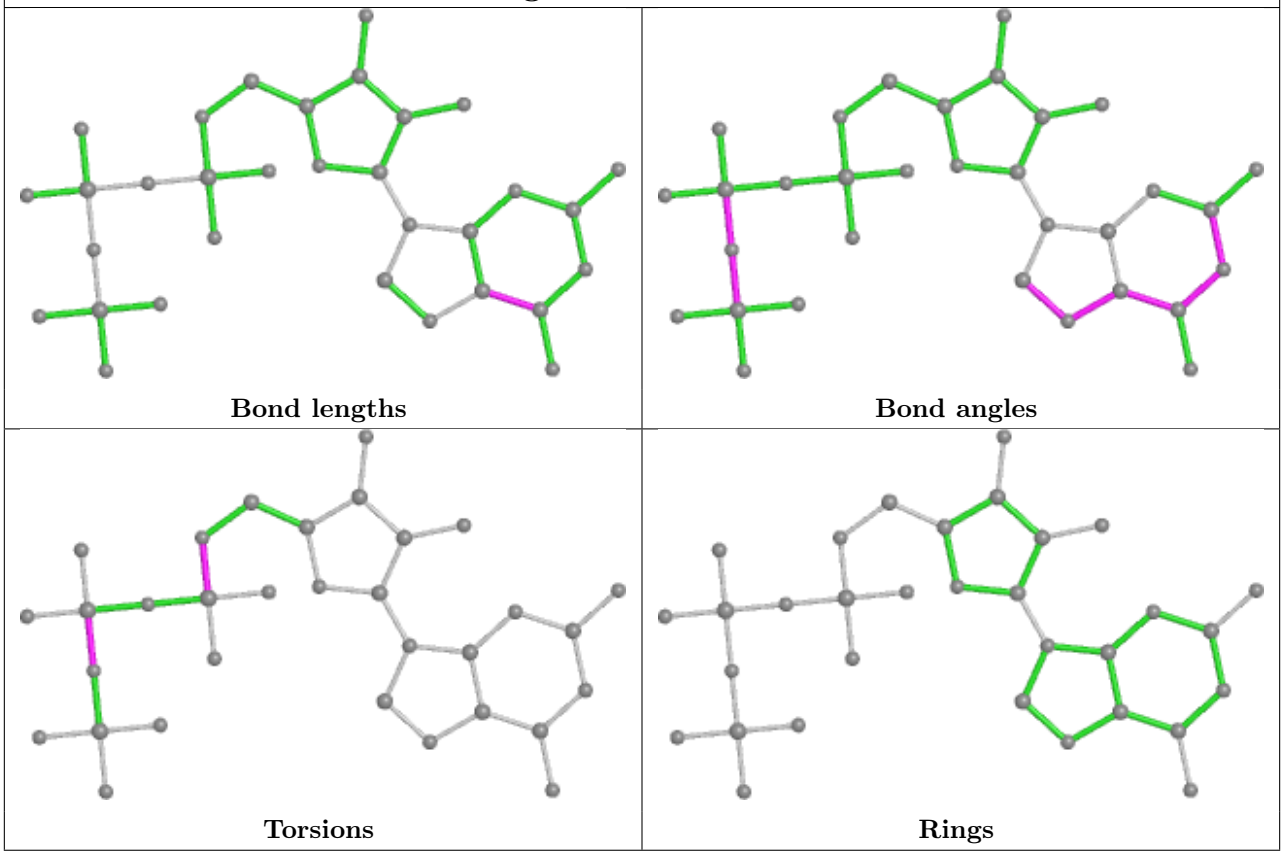
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GTP	3	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 then 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.

Ligand GTP A 501



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, 95^{th} 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	377/421 (89%)	0.23	18 (4%) 30 28	30, 60, 104, 124	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	SER	6.3
1	A	191	TRP	6.2
1	A	306	LEU	4.8
1	A	184	VAL	4.6
1	A	140	ASN	4.0
1	A	4	PRO	4.0
1	A	108	ILE	3.4
1	A	137	LYS	3.3
1	A	296	ALA	3.2
1	A	141	GLN	3.1
1	A	129	GLY	2.9
1	A	308	GLU	2.7
1	A	376	ALA	2.5
1	A	81	PHE	2.4
1	A	139	VAL	2.2
1	A	156	CYS	2.1
1	A	294	GLN	2.0
1	A	295	LYS	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

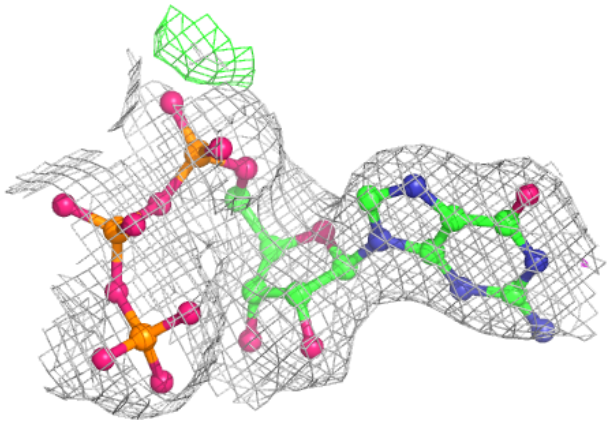
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

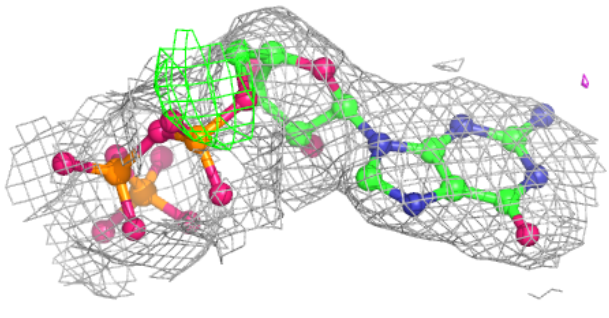
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GTP	A	501	32/32	0.94	0.13	59,74,95,102	0

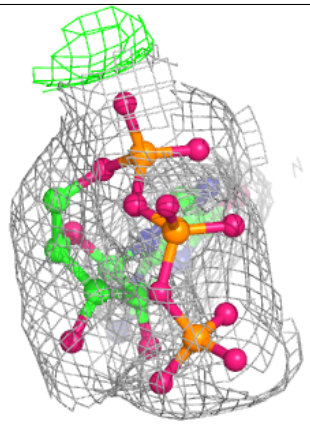
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP A 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.