



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 08:59 pm BST

PDB ID : 3A6P
Title : Crystal structure of Exportin-5:RanGTP:pre-miRNA complex
Authors : Okada, C.; Yamashita, E.; Lee, S.J.; Shibata, S.; Katahira, J.; Nakagawa, A.; Yoneda, Y.; Tsukihara, T.
Deposited on : 2009-09-07
Resolution : 2.92 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 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 : 2.11
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) : 2.11

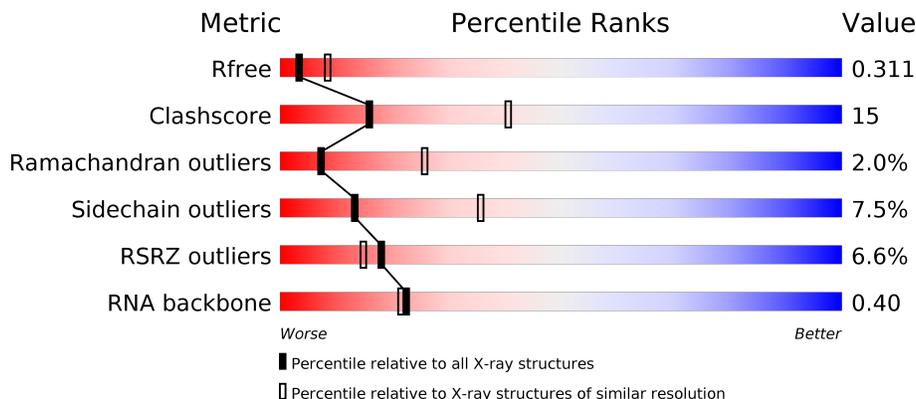
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)
RNA backbone	3102	1001 (3.18-2.66)

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 on 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	1204	 3% 58% 26% 11%
1	F	1204	 8% 60% 24% 5% 11%
2	B	13	 100%
2	G	13	 92% 8%

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Mol	Chain	Length	Quality of chain
3	C	216	
3	H	216	
4	D	24	
4	I	24	
5	E	24	
5	J	24	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GTP	C	1177	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22052 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 Exportin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1072	8570	5480	1442	1574	74	0	0	0
1	F	1072	8570	5480	1442	1574	74	0	0	0

- Molecule 2 is a protein called 13-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	13	66	39	13	14	0	0	0
2	G	13	66	39	13	14	0	0	0

- Molecule 3 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	170	1386	900	244	238	4	0	0	0
3	H	170	1386	900	244	238	4	0	0	0

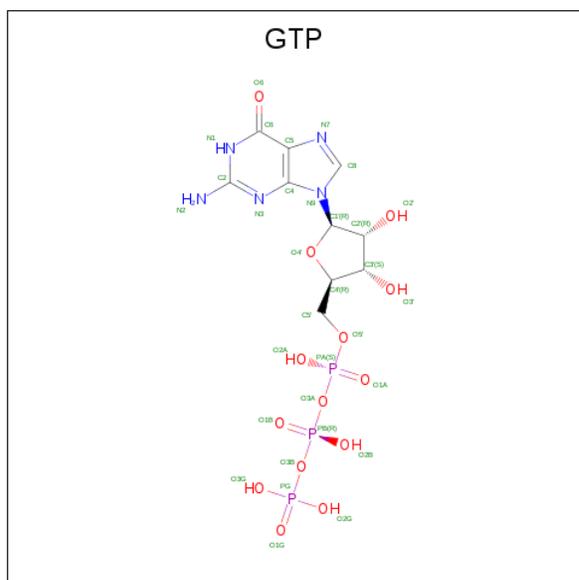
- Molecule 4 is a RNA chain called pre-microRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	22	466	211	88	147	20	0	0	0
4	I	22	466	211	88	147	20	0	0	0

- Molecule 5 is a RNA chain called pre-microRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	E	24	Total 505	C 226	N 84	O 172	P 23	0	0	0
5	J	24	Total 505	C 226	N 84	O 172	P 23	0	0	0

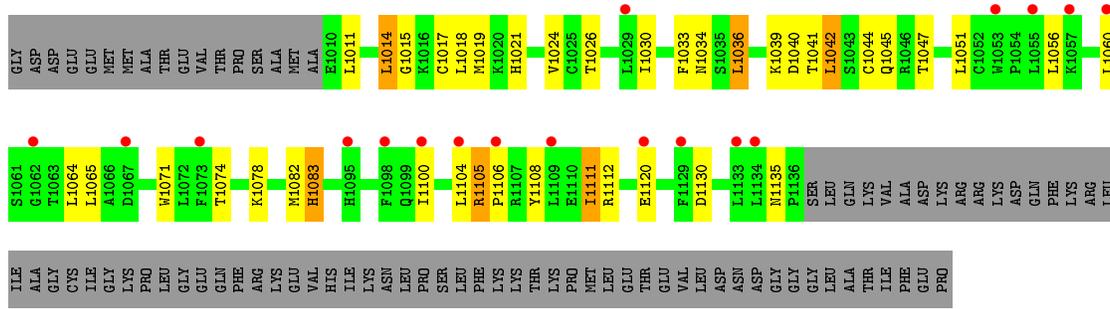
- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



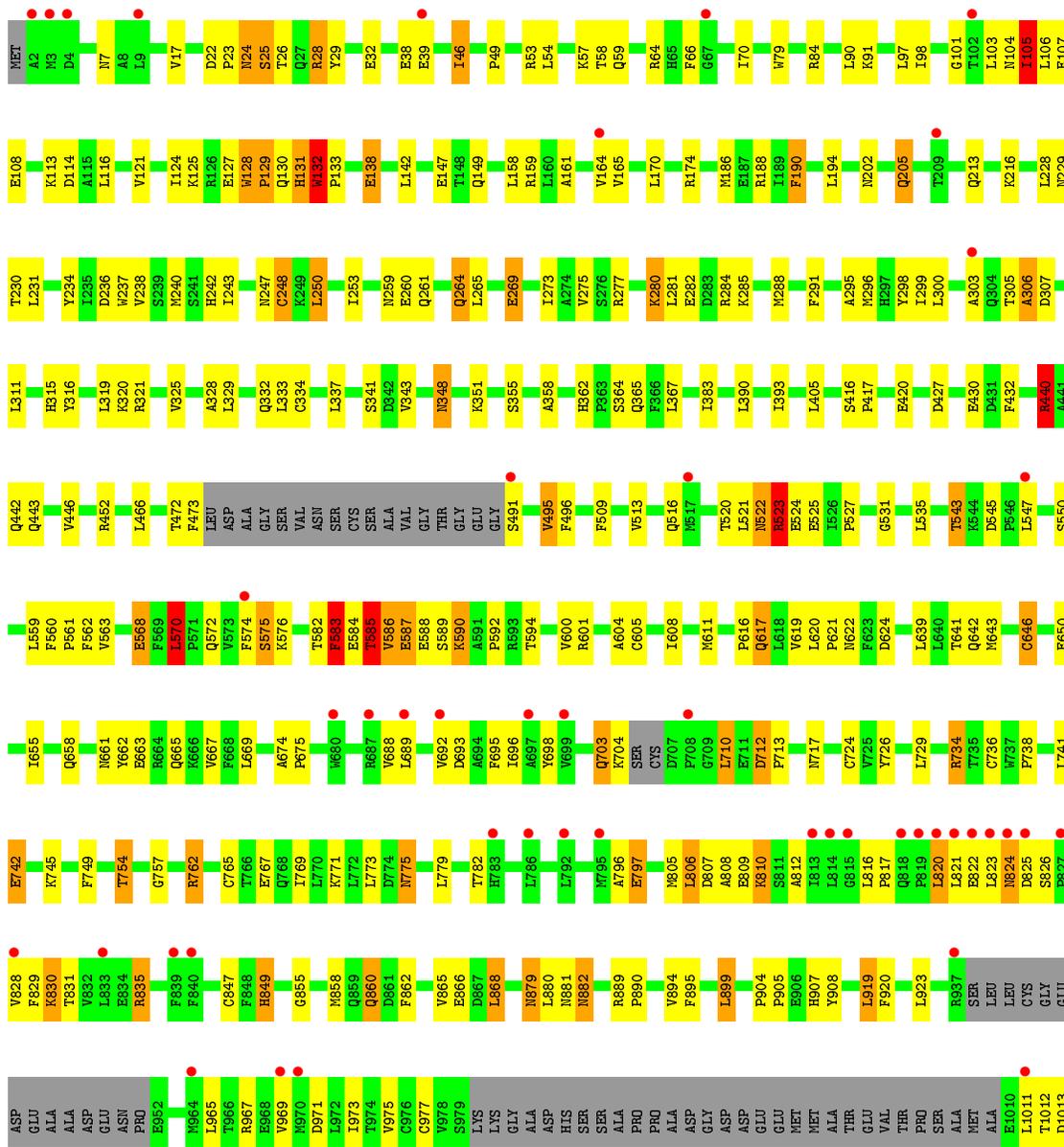
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
6	H	1	Total 32	C 10	N 5	O 14	P 3	0	0

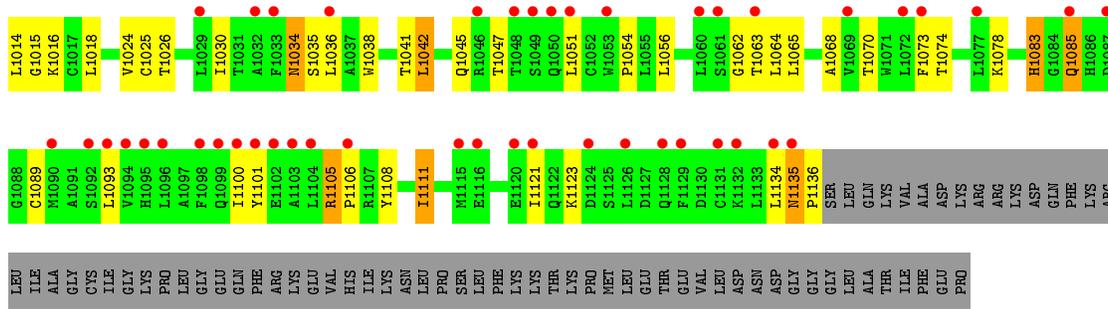
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
7	H	1	Total 1	Mg 1	0	0
7	C	1	Total 1	Mg 1	0	0



• Molecule 1: Exportin-5





- Molecule 2: 13-mer peptide

Chain B: 100%

There are no outlier residues recorded for this chain.

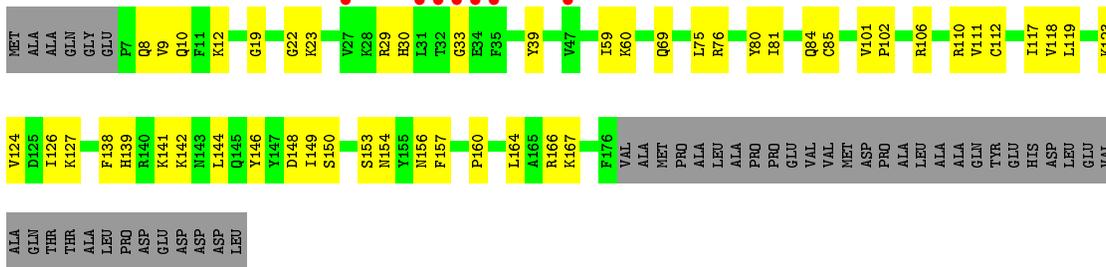
- Molecule 2: 13-mer peptide

Chain G: 92% 8%



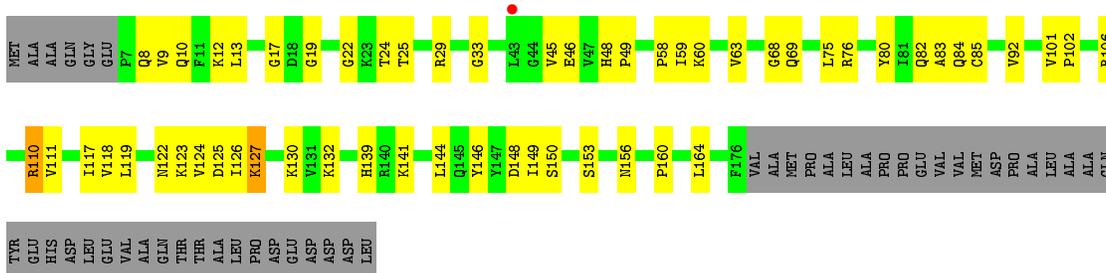
- Molecule 3: GTP-binding nuclear protein Ran

Chain C: 3% 56% 23% 21%



- Molecule 3: GTP-binding nuclear protein Ran

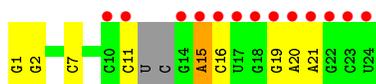
Chain H: 52% 25% 21%



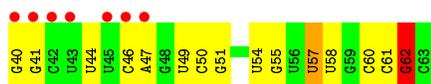
- Molecule 4: pre-microRNA



- Molecule 4: pre-microRNA



- Molecule 5: pre-microRNA



- Molecule 5: pre-microRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.16Å 304.67Å 89.23Å 90.00° 110.79° 90.00°	Depositor
Resolution (Å)	39.84 – 2.92 62.93 – 2.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.84-2.92) 98.2 (62.93-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.312 0.246 , 0.311	Depositor DCC
R_{free} test set	3827 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtrriage
Anisotropy	0.745	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22052	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	1.06	12/8738 (0.1%)	1.00	23/11831 (0.2%)
1	F	0.88	8/8738 (0.1%)	0.86	7/11831 (0.1%)
3	C	0.87	0/1421	0.82	0/1918
3	H	0.84	0/1421	0.83	0/1918
4	D	1.25	3/521 (0.6%)	1.76	12/809 (1.5%)
4	I	1.11	0/521	1.68	9/809 (1.1%)
5	E	1.23	2/562 (0.4%)	1.75	17/874 (1.9%)
5	J	1.06	0/562	1.51	6/874 (0.7%)
All	All	0.98	25/22484 (0.1%)	1.03	74/30864 (0.2%)

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	F	0	1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	TRP	CG-CD2	14.20	1.67	1.43
1	A	237	TRP	CZ3-CH2	13.24	1.61	1.40
1	A	165	VAL	CA-CB	9.13	1.74	1.54
1	A	237	TRP	CG-CD1	-8.79	1.24	1.36
4	D	1	G	N9-C8	-8.53	1.31	1.37

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	G	O4'-C1'-N9	11.60	117.48	108.20
1	A	237	TRP	CD1-NE1-CE2	10.62	118.56	109.00
4	I	2	G	C5-C6-O6	-10.20	122.48	128.60
1	A	237	TRP	CG-CD1-NE1	-10.03	100.07	110.10
4	D	1	G	C4-C5-N7	-9.08	107.17	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	583	PHE	Peptide

5.2 Too-close contacts [i](#)

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	8570	0	8664	292	0
1	F	8570	0	8664	267	0
2	B	66	0	15	0	0
2	G	66	0	15	1	0
3	C	1386	0	1408	34	0
3	H	1386	0	1408	40	0
4	D	466	0	242	1	0
4	I	466	0	242	0	0
5	E	505	0	258	5	0
5	J	505	0	258	6	0
6	C	32	0	12	9	0
6	H	32	0	12	7	0
7	C	1	0	0	0	0
7	H	1	0	0	0	0
All	All	22052	0	21198	630	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 15.

The worst 5 of 630 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:105:ILE:CG1	1:A:105:ILE:CD1	1.78	1.57
1:A:543:THR:HG22	1:A:545:ASP:H	1.17	1.09
1:F:495:VAL:O	1:F:496:PHE:CD1	2.15	0.99
1:A:168:GLN:HB2	1:A:175:ARG:HD2	1.41	0.99
1:A:545:ASP:OD2	1:A:548:ILE:HG12	1.63	0.99

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	1062/1204 (88%)	965 (91%)	73 (7%)	24 (2%)	6	22
1	F	1062/1204 (88%)	948 (89%)	92 (9%)	22 (2%)	7	24
3	C	168/216 (78%)	154 (92%)	11 (6%)	3 (2%)	8	28
3	H	168/216 (78%)	152 (90%)	15 (9%)	1 (1%)	25	57
All	All	2460/2840 (87%)	2219 (90%)	191 (8%)	50 (2%)	7	26

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLU
1	A	211	THR
1	A	245	ALA
1	A	340	ASP
1	A	712	ASP

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	967/1073 (90%)	895 (93%)	72 (7%)	13	36
1	F	967/1073 (90%)	885 (92%)	82 (8%)	10	30
3	C	150/185 (81%)	143 (95%)	7 (5%)	26	58
3	H	150/185 (81%)	144 (96%)	6 (4%)	31	63
All	All	2234/2516 (89%)	2067 (92%)	167 (8%)	13	36

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	84	GLN
1	F	188	ARG
1	F	1041	THR
3	C	141	LYS
1	F	39	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1058	GLN
1	F	149	GLN
1	F	935	ASN
3	C	30	HIS
3	C	173	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	20/24 (83%)	7 (35%)	0
4	I	20/24 (83%)	6 (30%)	0
5	E	23/24 (95%)	4 (17%)	0
5	J	23/24 (95%)	3 (13%)	0
All	All	86/96 (89%)	20 (23%)	0

5 of 20 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	6	A

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Mol	Chain	Res	Type
4	D	11	C
4	D	15	A
4	D	16	C
4	D	19	G

There are no RNA pucker outliers to report.

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 carbohydrates 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
6	GTP	C	1177	7	26,34,34	1.18	2 (7%)	33,54,54	2.11	8 (24%)
6	GTP	H	1177	7	26,34,34	0.97	1 (3%)	33,54,54	2.14	11 (33%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GTP	C	1177	7	-	1/18/38/38	0/3/3/3
6	GTP	H	1177	7	-	2/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1177	GTP	C6-N1	4.05	1.40	1.33
6	C	1177	GTP	C2-N1	2.65	1.40	1.35
6	H	1177	GTP	C6-N1	2.26	1.37	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1177	GTP	N3-C2-N1	-5.32	120.13	127.22
6	C	1177	GTP	PB-O3B-PG	-5.05	115.51	132.83
6	H	1177	GTP	N3-C2-N1	-4.96	120.61	127.22
6	H	1177	GTP	O2G-PG-O3B	4.46	119.59	104.64
6	C	1177	GTP	C2-N3-C4	3.93	119.85	115.36

There are no chirality outliers.

All (3) torsion outliers are listed below:

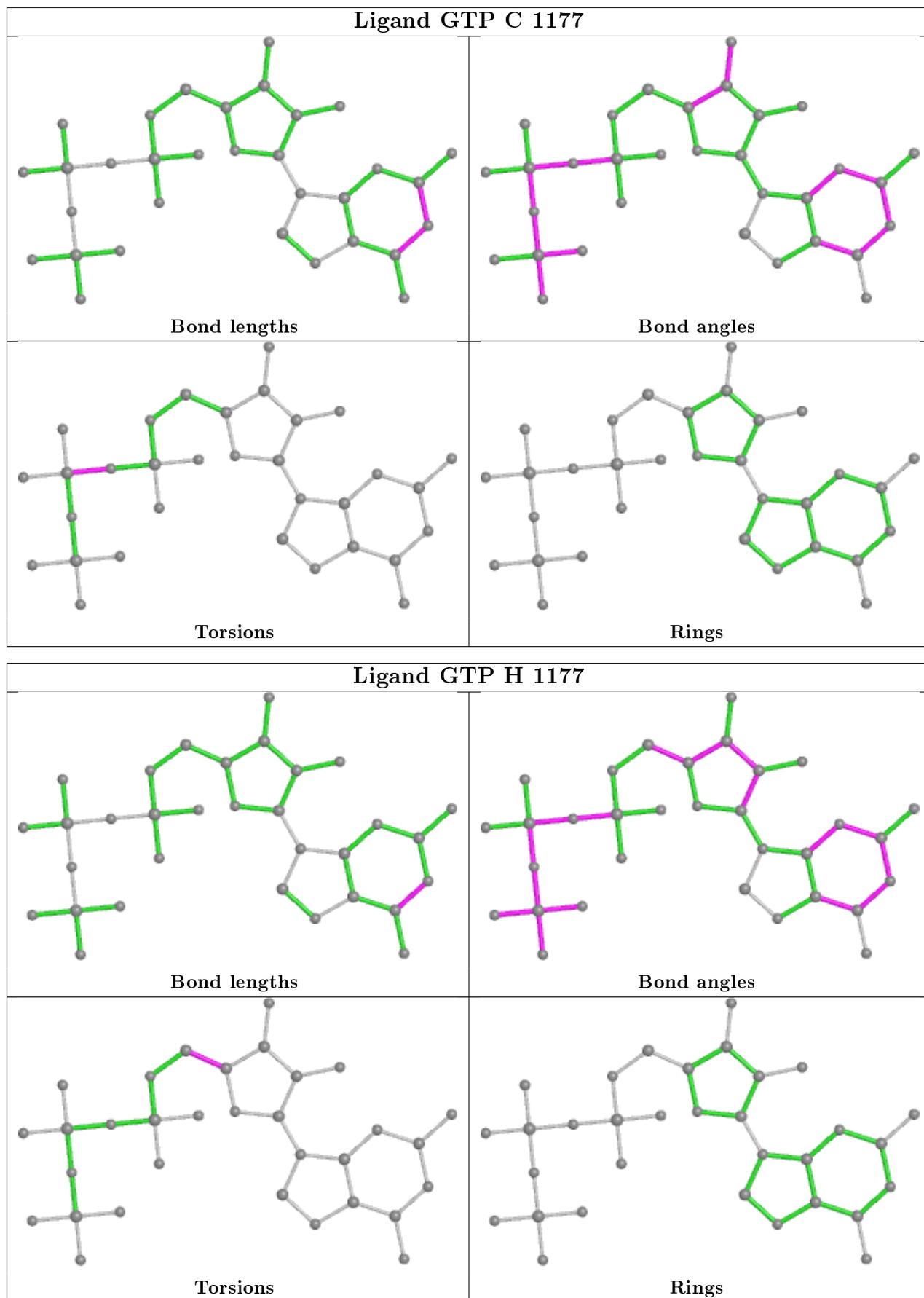
Mol	Chain	Res	Type	Atoms
6	H	1177	GTP	C3'-C4'-C5'-O5'
6	H	1177	GTP	O4'-C4'-C5'-O5'
6	C	1177	GTP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1177	GTP	9	0
6	H	1177	GTP	7	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1072/1204 (89%)	0.19	36 (3%) 45 41	32, 76, 127, 156	0
1	F	1072/1204 (89%)	0.46	91 (8%) 10 8	59, 94, 143, 162	0
2	B	0/13	-	-	-	-
2	G	0/13	-	-	-	-
3	C	170/216 (78%)	0.36	7 (4%) 37 34	59, 90, 115, 127	0
3	H	170/216 (78%)	0.24	1 (0%) 89 89	64, 88, 111, 122	0
4	D	22/24 (91%)	1.08	7 (31%) 0 0	62, 126, 220, 227	0
4	I	22/24 (91%)	2.19	13 (59%) 0 0	71, 191, 259, 263	0
5	E	24/24 (100%)	1.14	7 (29%) 0 0	78, 118, 205, 210	0
5	J	24/24 (100%)	2.14	7 (29%) 0 0	121, 170, 256, 271	0
All	All	2576/2962 (86%)	0.37	169 (6%) 18 15	32, 86, 141, 271	0

The worst 5 of 169 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	40	G	13.2
1	F	819	PRO	8.6
1	F	4	ASP	8.5
1	F	823	LEU	7.5
1	F	820	LEU	6.8

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](#)

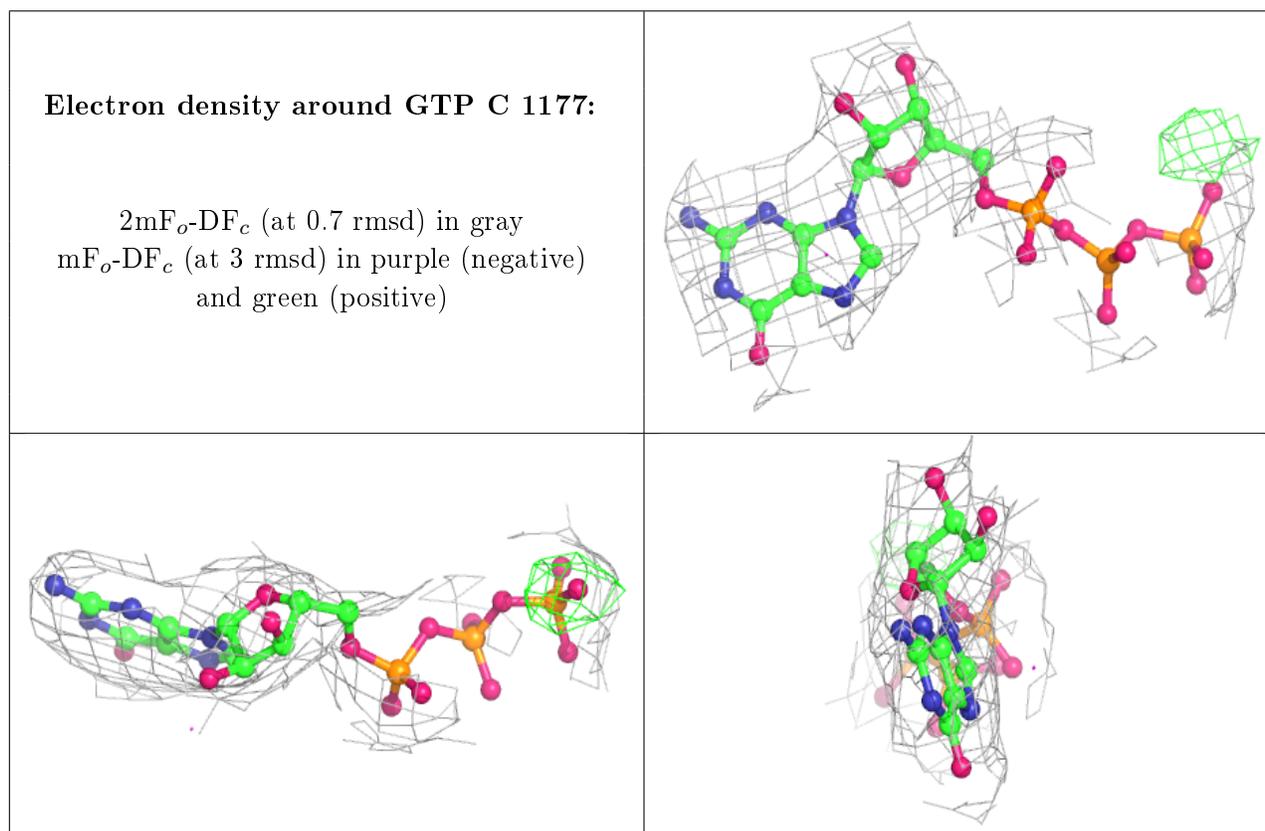
There are no carbohydrates in this entry.

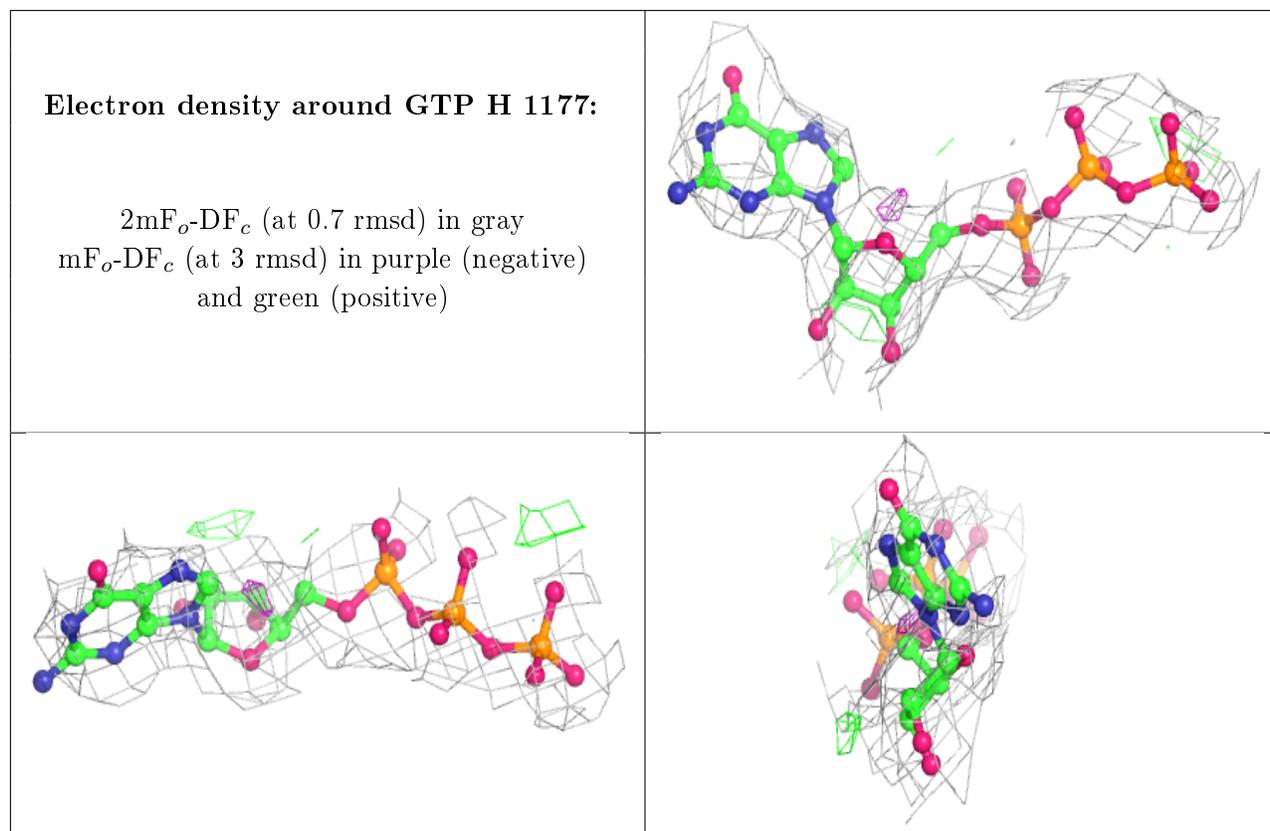
6.4 Ligands [i](#)

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
6	GTP	C	1177	32/32	0.93	0.17	96,101,105,106	0
6	GTP	H	1177	32/32	0.94	0.18	92,100,112,115	0
7	MG	H	1178	1/1	0.96	0.23	74,74,74,74	0
7	MG	C	1178	1/1	0.99	0.16	85,85,85,85	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.