



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:13 PM GMT

PDB ID : 3A6P  
Title : Crystal structure of Exportin-5:RanGTP:pre-miRNAcomplex  
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 validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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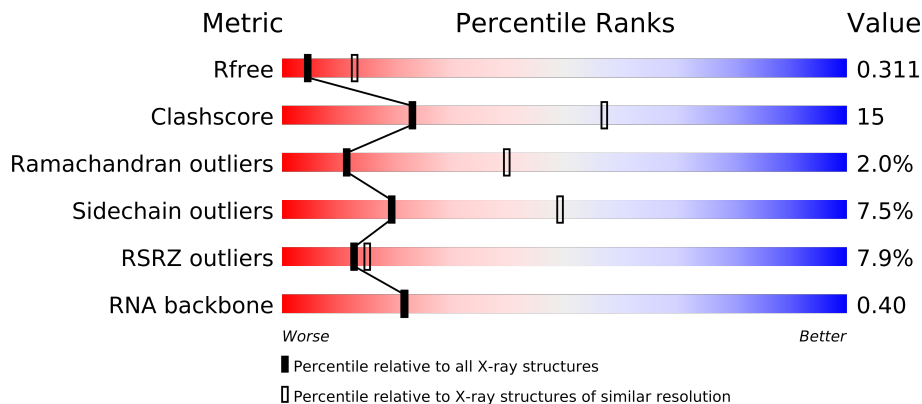
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)
RNA backbone	1838	1003 (3.42-2.42)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1204	
1	F	1204	
2	B	13	
2	G	13	
3	C	216	
3	H	216	
4	D	24	
4	I	24	
5	E	24	
5	J	24	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22052 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	1072	Total	C	N	O	S	0	0	0
			8570	5480	1442	1574	74			
1	F	1072	Total	C	N	O	S	0	0	0
			8570	5480	1442	1574	74			

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

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

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

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

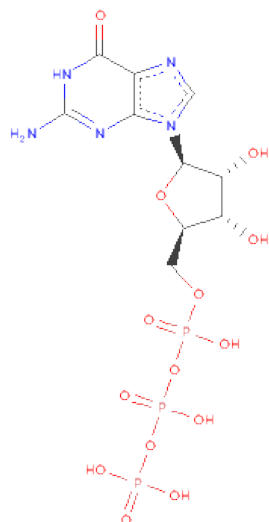
- Molecule 4 is a RNA chain called pre-microRNA.

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

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

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

- 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
6	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
6	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

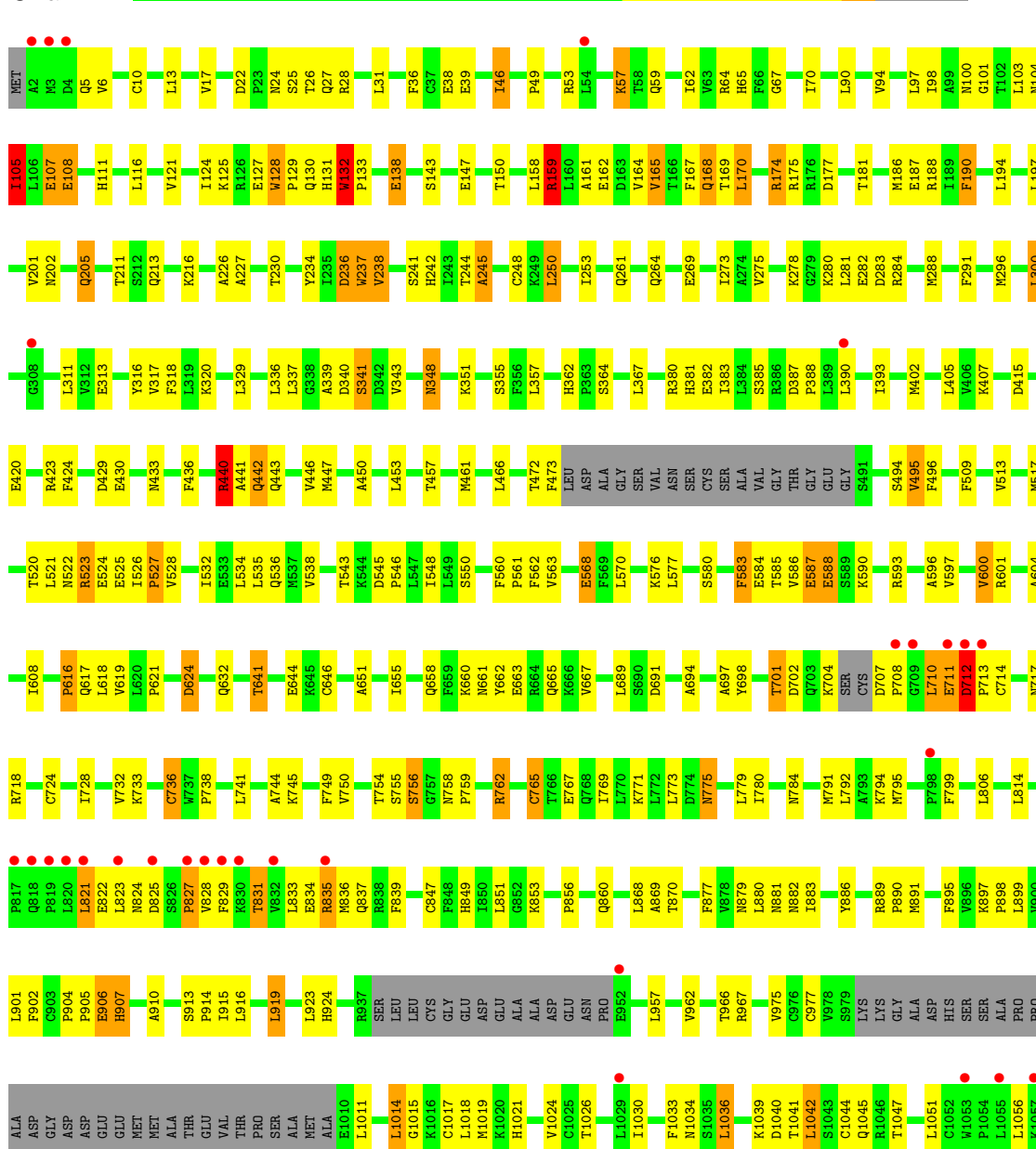
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

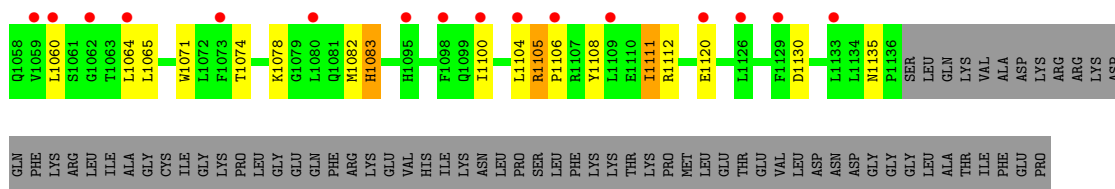
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Exportin-5

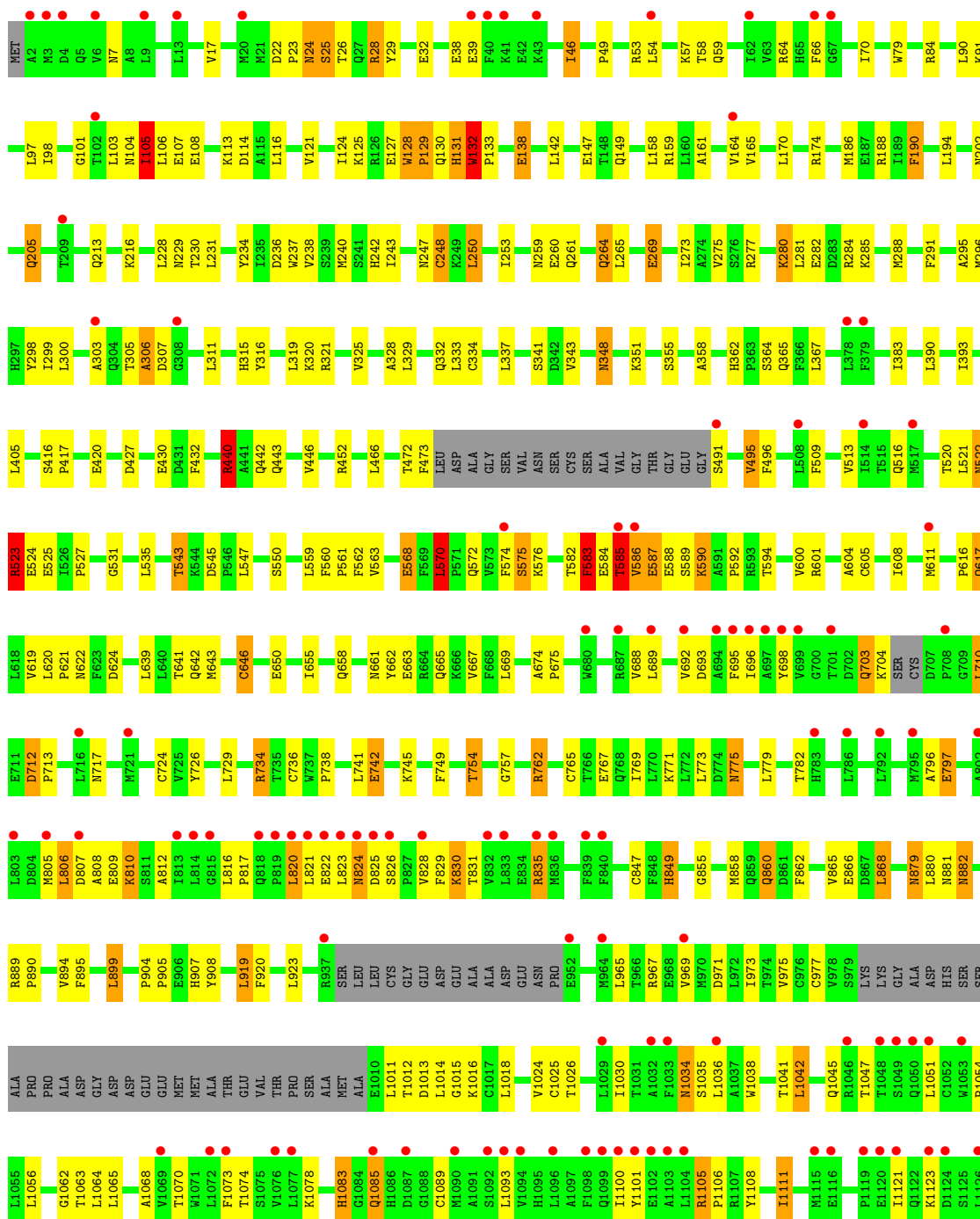
Chain A:

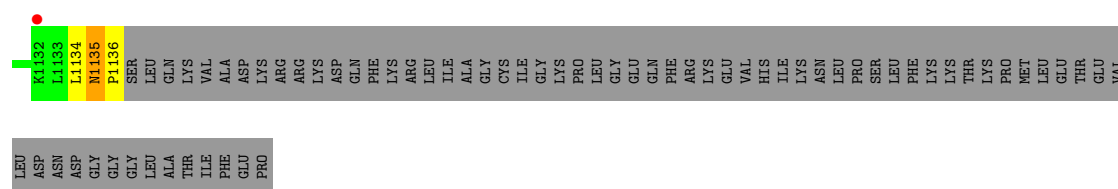




## • Molecule 1: Exportin-5

Chain F:





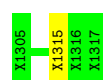
- Molecule 2: 13-mer peptide

Chain B:

There are no outlier residues recorded for this chain.

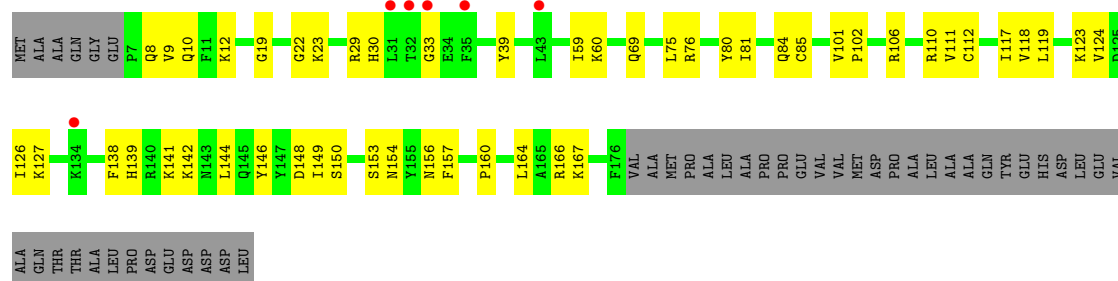
- Molecule 2: 13-mer peptide

Chain G:



- Molecule 3: GTP-binding nuclear protein Ran

Chain C:



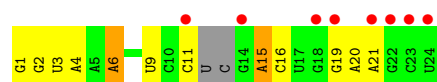
- Molecule 3: GTP-binding nuclear protein Ran

Chain H:



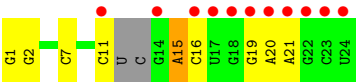
- Molecule 4: pre-microRNA

Chain D:



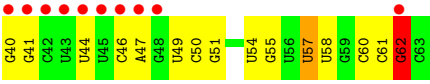
- Molecule 4: pre-microRNA

Chain I: 



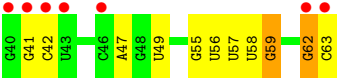
• Molecule 5: pre-microRNA

Chain E: 



• Molecule 5: pre-microRNA

Chain J: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.247 , 0.312 0.249 , 0.311	Depositor DCC
$R_{free}$ test set	3827 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.5	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.0	EDS
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74910 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 630 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

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%)	10	35
1	F	1062/1204 (88%)	948 (89%)	92 (9%)	22 (2%)	11	38
3	C	168/216 (78%)	154 (92%)	11 (6%)	3 (2%)	13	43
3	H	168/216 (78%)	152 (90%)	15 (9%)	1 (1%)	33	75
All	All	2460/2840 (87%)	2219 (90%)	191 (8%)	50 (2%)	11	40

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 ⓘ

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%)	20	50
1	F	967/1073 (90%)	885 (92%)	82 (8%)	15	42
3	C	150/185 (81%)	143 (95%)	7 (5%)	36	75
3	H	150/185 (81%)	144 (96%)	6 (4%)	42	80
All	All	2234/2516 (89%)	2067 (92%)	167 (8%)	19	49

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 ⓘ

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
4	D	11	C
4	D	15	A

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Mol	Chain	Res	Type
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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	34,34,34	1.23	2 (5%)	51,54,54	2.20	12 (23%)
6	GTP	H	1177	7	34,34,34	1.02	1 (2%)	51,54,54	2.99	14 (27%)

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
6	GTP	C	1177	7	-	0/22/38/38	0/1/3/3
6	GTP	H	1177	7	-	0/22/38/38	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1177	GTP	C2-N3	5.46	1.40	1.33
6	H	1177	GTP	C2-N3	3.50	1.37	1.33
6	C	1177	GTP	C2-N1	2.12	1.40	1.36

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1177	GTP	C6-C5-N7	-15.70	132.03	134.14
6	C	1177	GTP	C6-C5-N7	-8.47	133.00	134.14
6	H	1177	GTP	O4'-C1'-N9	7.56	115.47	108.44
6	C	1177	GTP	PB-O3B-PG	-5.51	115.51	131.68
6	C	1177	GTP	O3A-PB-O3B	-4.40	92.72	101.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1072/1204 (89%)	0.22	46 (4%) 34 40	32, 76, 127, 156	0
1	F	1072/1204 (89%)	0.59	113 (10%) 7 8	59, 94, 143, 162	0
2	B	0/13	-	-	-	-
2	G	0/13	-	-	-	-
3	C	170/216 (78%)	0.34	6 (3%) 42 49	59, 90, 115, 127	0
3	H	170/216 (78%)	0.28	3 (1%) 65 75	64, 88, 111, 122	0
4	D	22/24 (91%)	1.67	8 (36%) 1 1	62, 126, 220, 227	0
4	I	22/24 (91%)	2.48	11 (50%) 0 0	71, 191, 259, 263	0
5	E	24/24 (100%)	1.67	10 (41%) 1 0	78, 118, 205, 210	0
5	J	24/24 (100%)	2.65	7 (29%) 1 1	121, 170, 256, 271	0
All	All	2576/2962 (86%)	0.46	204 (7%) 13 15	32, 86, 141, 271	0

The worst 5 of 204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	40	G	14.9
1	F	823	LEU	11.0
1	F	819	PRO	9.9
1	F	820	LEU	9.5
1	F	4	ASP	8.9

### 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 carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	H	1178	1/1	0.23	0.35	74,74,74,74	0
6	GTP	H	1177	32/32	0.19	-0.43	92,100,112,115	0
6	GTP	C	1177	32/32	0.18	-0.57	96,101,105,106	0
7	MG	C	1178	1/1	0.15	-3.03	85,85,85,85	0

## 6.5 Other polymers

There are no such residues in this entry.