wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2021 – 01:01 AM EDT

PDB ID	:	3GJX
Title	:	Crystal Structure of the Nuclear Export Complex CRM1-Snurportin1-RanGTP
Authors	:	Monecke, T.; Guettler, T.; Neumann, P.; Dickmanns, A.; Goerlich, D.; Ficner, R.
Deposited on	:	2009-03-09
Resolution	:	2.50 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 (i) symbol.

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

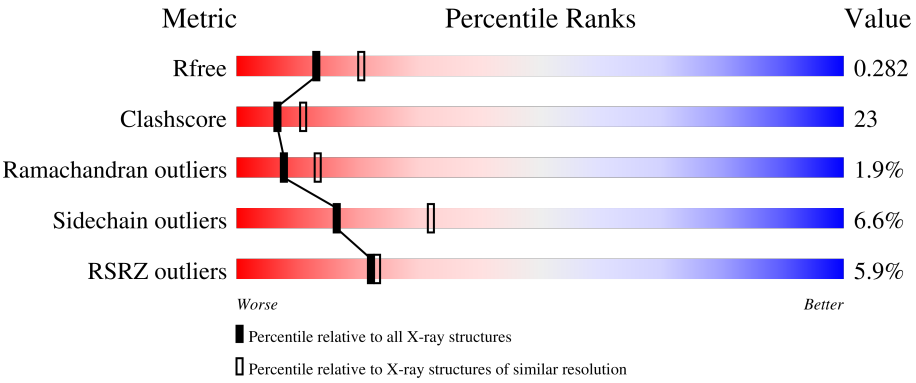
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	B	365	2% 44% 26% 5% 25%
1	E	365	2% 43% 30% 24%
2	C	216	% 47% 28% 21%
2	F	216	53% 23% 21%
3	A	1073	6% 56% 36% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1073	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 25280 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 Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	274	Total	C	N	O	S	0	2	0
			2222	1413	379	415	15			
1	E	279	Total	C	N	O	S	0	8	0
			2303	1466	394	427	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP O95149
B	-3	PRO	-	expression tag	UNP O95149
B	-2	LEU	-	expression tag	UNP O95149
B	-1	GLY	-	expression tag	UNP O95149
B	0	SER	-	expression tag	UNP O95149
E	-4	GLY	-	expression tag	UNP O95149
E	-3	PRO	-	expression tag	UNP O95149
E	-2	LEU	-	expression tag	UNP O95149
E	-1	GLY	-	expression tag	UNP O95149
E	0	SER	-	expression tag	UNP O95149

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	1	0
			1399	910	246	238	5			
2	F	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	engineered mutation	UNP P62826
F	69	LEU	GLN	engineered mutation	UNP P62826

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1041	Total	C	N	O	S	0	5	0
			8456	5424	1421	1557	54			
3	D	1041	Total	C	N	O	S	0	8	0
			8483	5438	1427	1564	54			

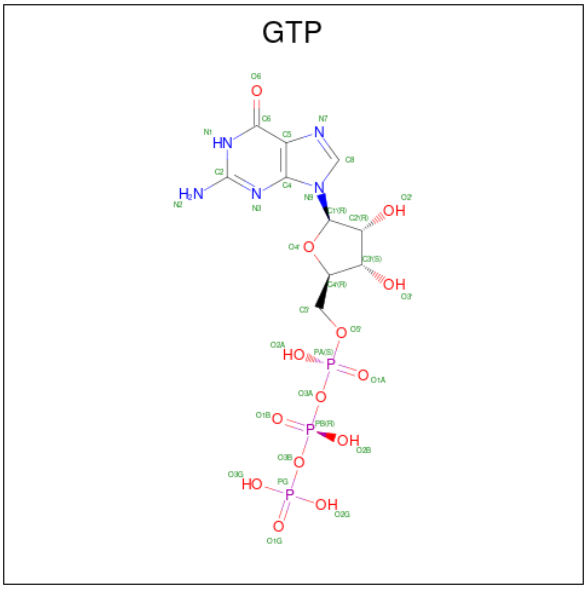
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6P5F9
A	0	SER	-	expression tag	UNP Q6P5F9
D	-1	GLY	-	expression tag	UNP Q6P5F9
D	0	SER	-	expression tag	UNP Q6P5F9

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	E	1	Total	Na	0	0
			1	1		

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

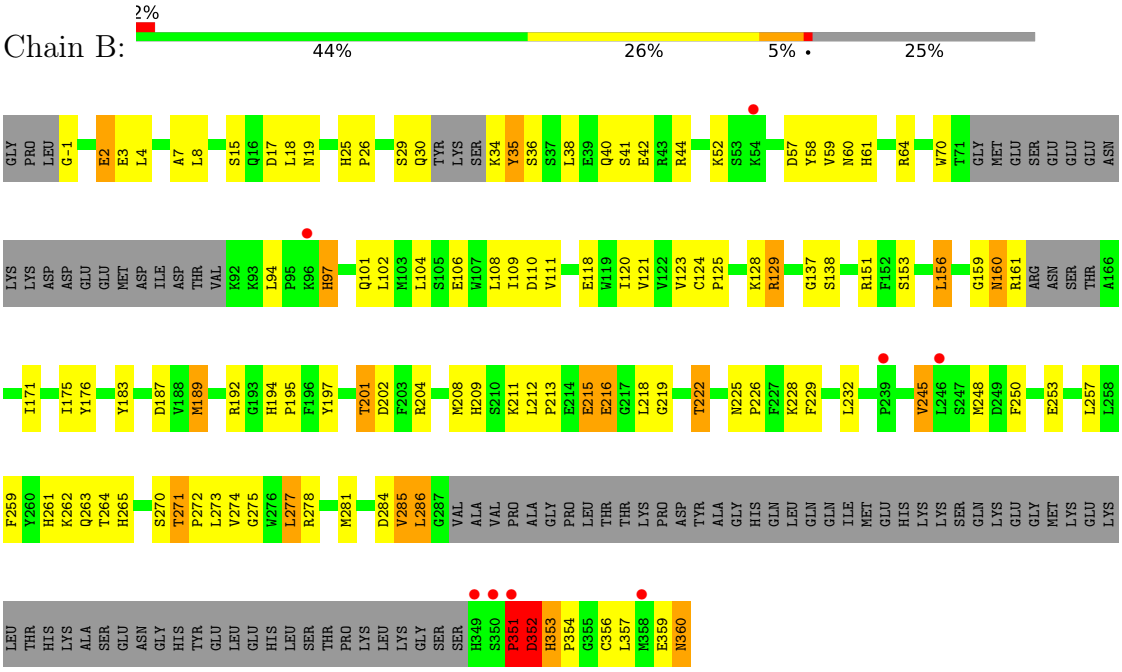
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	134	Total	O	0	0
			134	134		
8	C	58	Total	O	0	0
			58	58		
8	A	258	Total	O	0	0
			258	258		
8	E	130	Total	O	0	0
			130	130		
8	F	46	Total	O	0	0
			46	46		
8	D	333	Total	O	0	0
			333	333		

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.

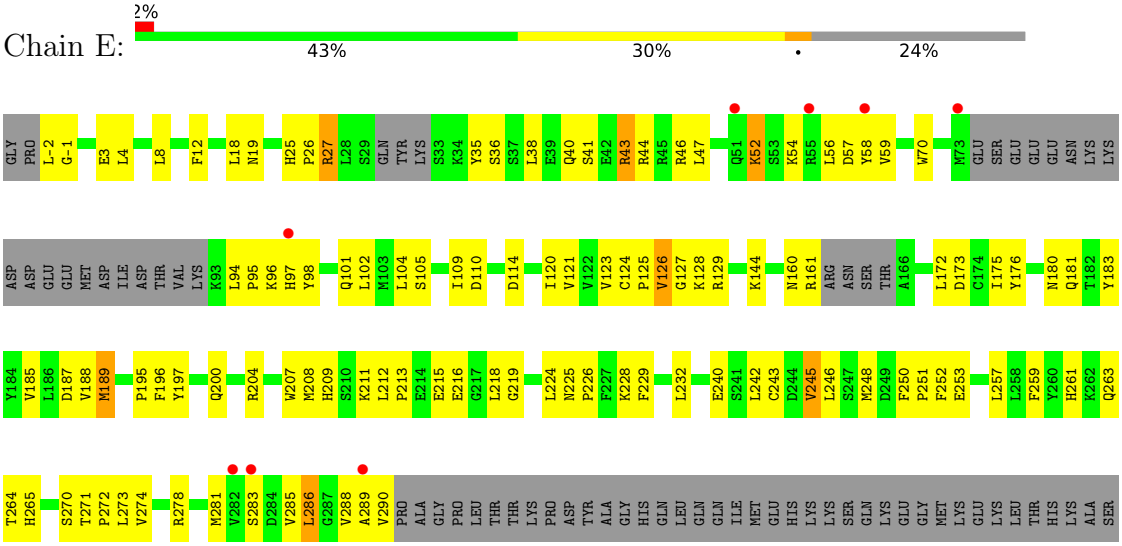
• Molecule 1: Snurportin-1

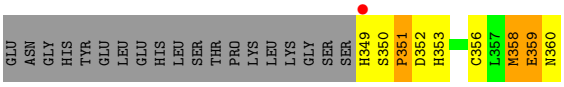
Chain B:



• Molecule 1: Snurportin-1

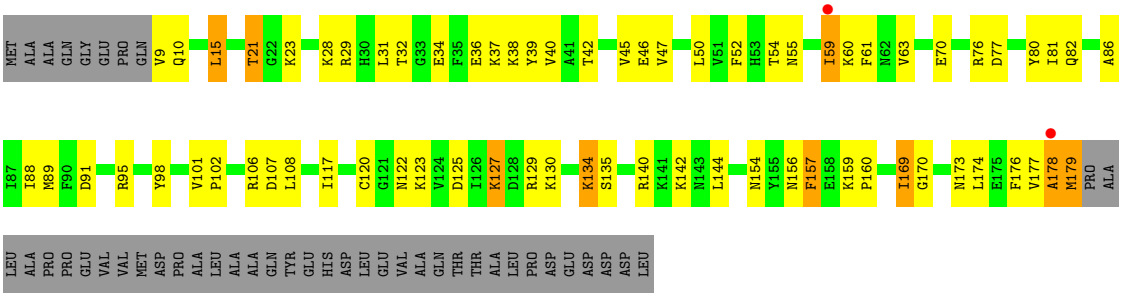
Chain E:





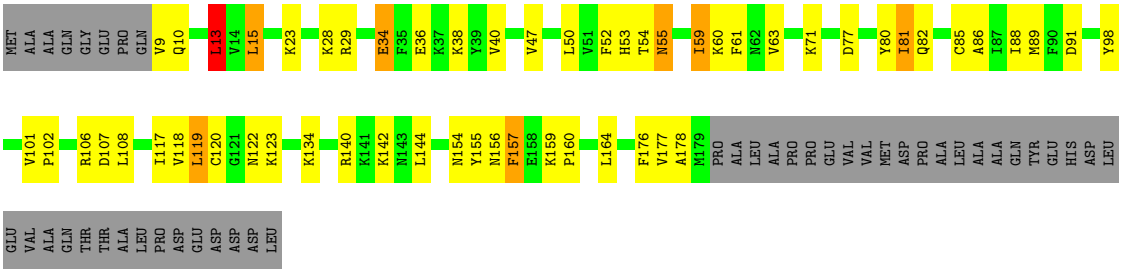
• Molecule 2: GTP-binding nuclear protein Ran

Chain C:



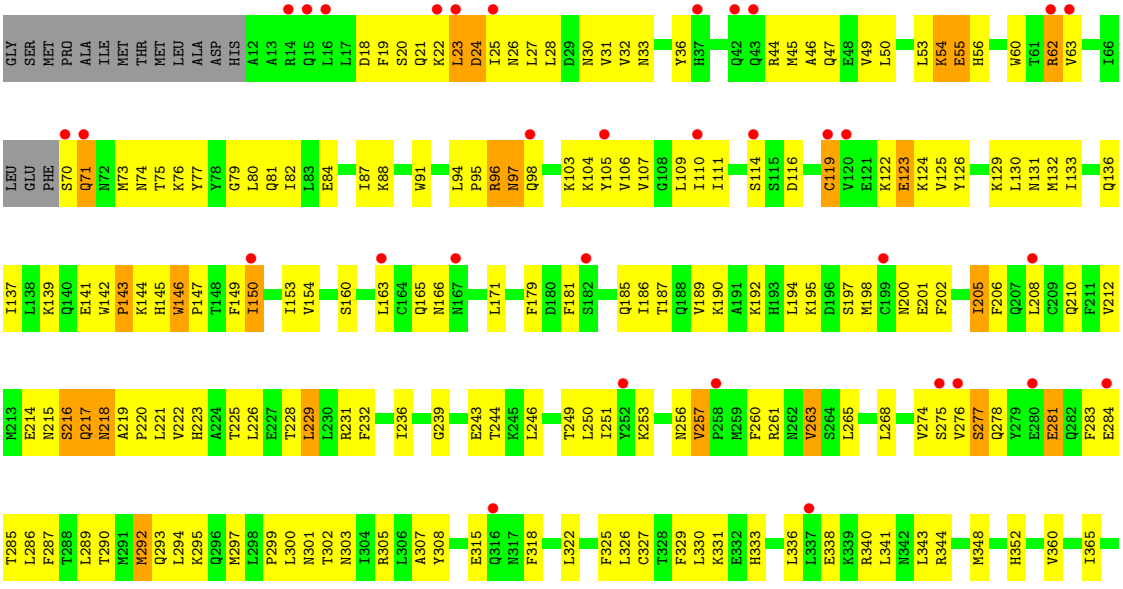
• Molecule 2: GTP-binding nuclear protein Ran

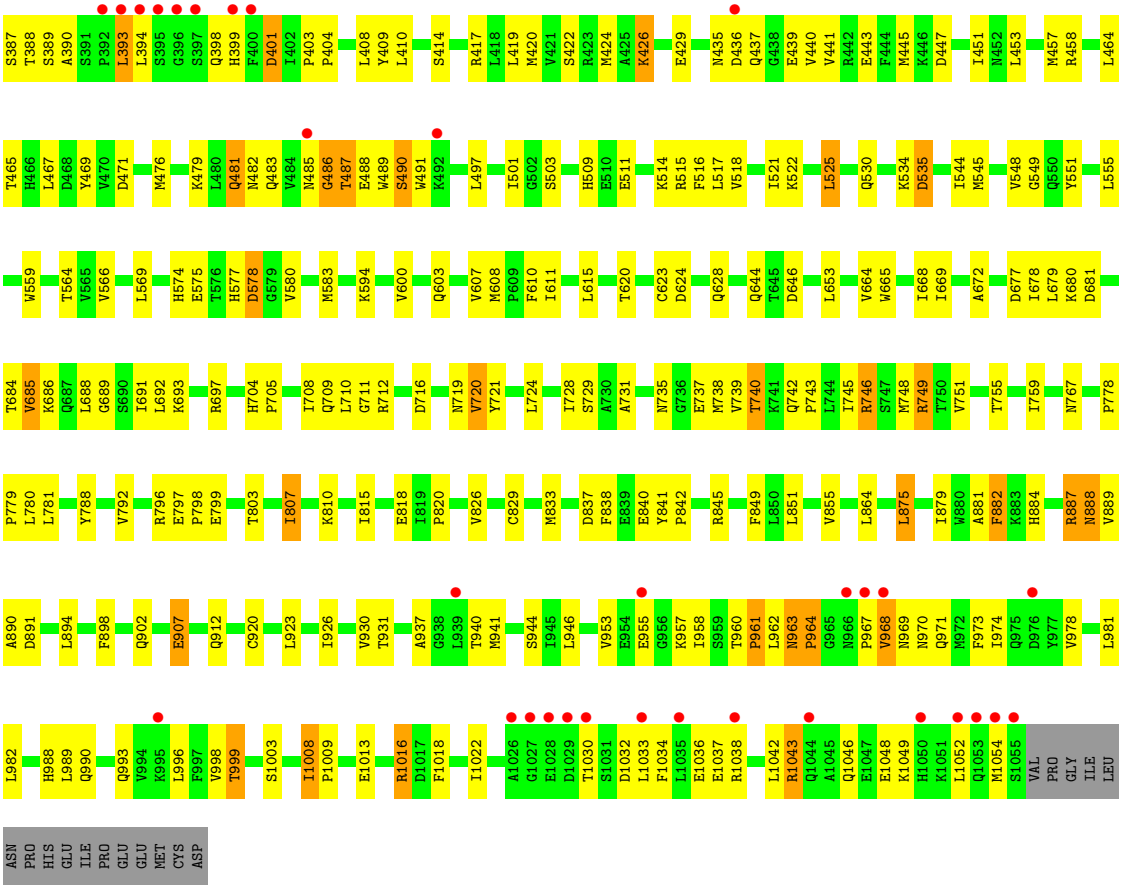
Chain F:



• Molecule 3: Exportin-1

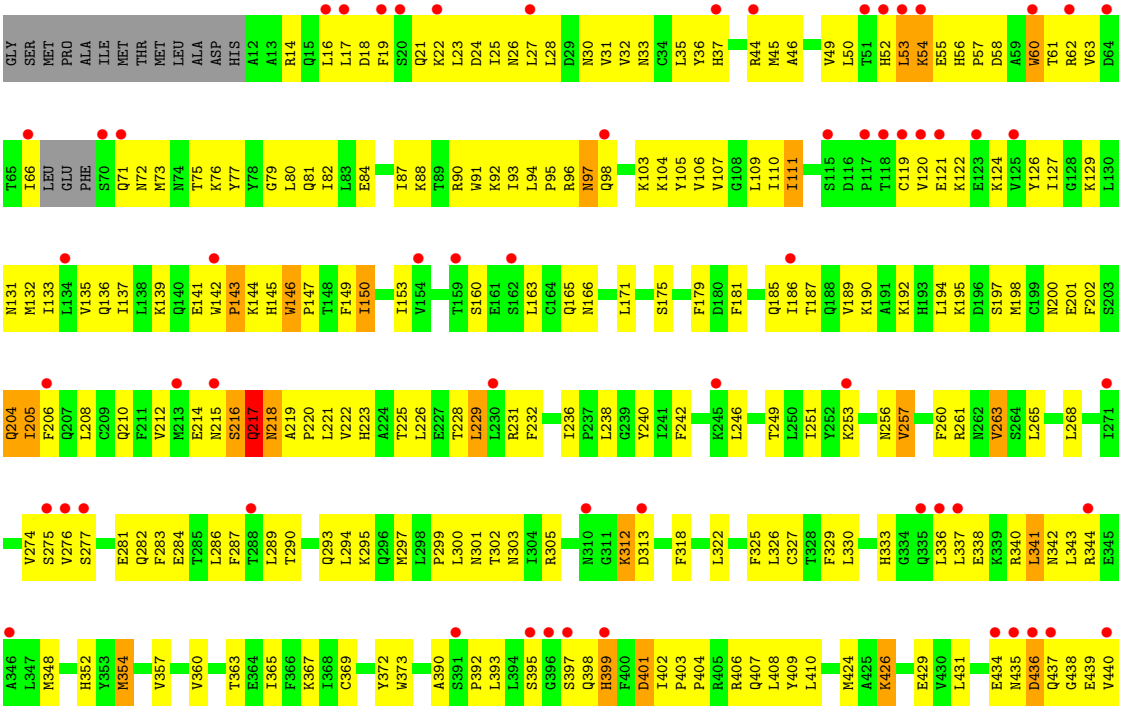
Chain A:

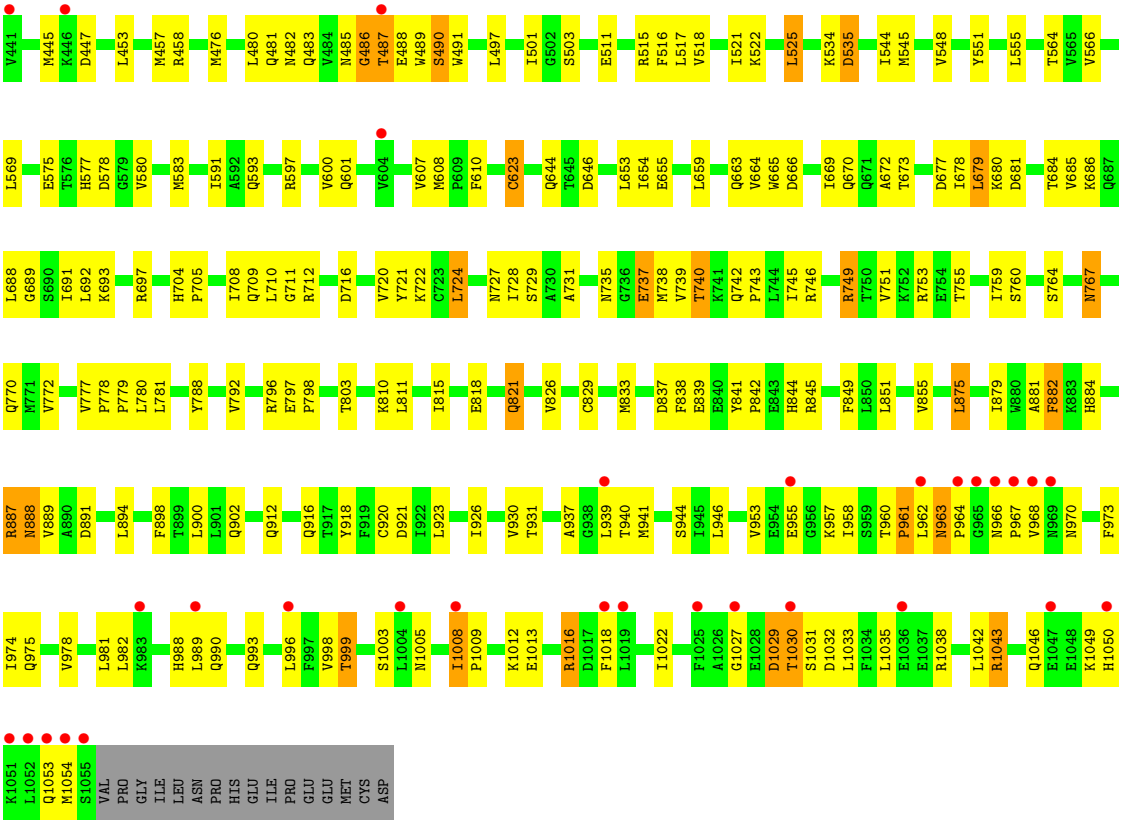




• Molecule 3: Exportin-1

Chain D:




V441 M445 K446 D447 L453 M457 R458 M476 L480 Q481 N482 Q483 V484 N485 G486 T487 E488 W489 S490 W491 L497 I501 G502 S503 E511 R515 F516 L517 V518 I521 K522 L525 K534 D535 I544 M545 V548 Y551 L555 T564 V565 V566
L569 E575 T576 H577 D578 G579 V580 M583 I591 A592 Q593 R597 V600 Q601 V604 V607 M608 P609 F610 C623 Q644 T645 D646 L653 I654 E655 L659 Q663 V664 W665 D666 I669 Q670 Q671 A672 T673 D677 I678 L679 K680 D681 T684 V685 K686 Q687
L688 G689 S690 I691 L692 K693 R697 H704 P705 I708 Q709 L710 G711 R712 D716 V720 Y721 K722 C723 L724 N727 I728 S729 A730 A731 N735 G736 E737 M738 V739 T740 K741 Q742 P743 L744 I745 R746 R749 T750 V751 K752 R753 E754 T755 I759 S760 S764 N767
Q770 M771 V772 V777 P778 P779 L780 L781 Y788 V792 R796 E797 P798 T803 K810 L811 I815 E818 Q821 V826 C829 M833 D837 F838 E839 E840 Y841 P842 E843 H844 R845 F849 L850 L851 V855 L875 I879 W880 A881 F882 K883 H884
R887 N888 V889 A890 D891 L894 F898 T899 L900 L901 Q902 Q912 Q916 T917 Y918 F919 C920 D921 I922 L923 I926 V930 T931 A937 G938 L939 T940 M941 S944 I945 L946 V953 E954 E955 G956 K957 I958 S959 T960 P961 L962 N963 P964 G965 N966 P967 V968 N969 N970 F973
I974 Q975 V978 L981 L982 K983 H988 L989 Q990 Q993 L996 F997 V998 T999 S1003 L1004 N1005 I1008 P1009 K1012 E1013 R1016 D1017 F1018 L1019 I1022 F1025 A1026 G1027 E1028 D1029 T1030 S1031 D1032 L1033 F1034 L1035 E1036 E1037 R1038 L1042 R1043 Q1046 E1047 E1048 K1049 H1050
K1051 L1052 Q1053 M1054 S1055 VAL PRO GLY ILE LEU ASN PRO HIS GLU ILE PRO GLU GLU MET CYS ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.17Å 225.74Å 163.45Å 90.00° 100.56° 90.00°	Depositor
Resolution (Å)	38.84 – 2.50 47.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.84-2.50) 86.9 (47.81-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.51Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, R_{free}	0.244 , 0.281 0.246 , 0.282	Depositor DCC
R_{free} test set	8606 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.147 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	25280	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: MG, NA, GTP, CL

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	B	0.42	0/2283	0.74	3/3090 (0.1%)
1	E	0.40	0/2364	0.64	0/3202
2	C	0.34	0/1434	0.52	0/1936
2	F	0.33	0/1423	0.56	2/1921 (0.1%)
3	A	0.36	0/8628	0.51	0/11687
3	D	0.36	0/8656	0.51	0/11724
All	All	0.37	0/24788	0.55	5/33560 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	351	PRO	CA-N-CD	-10.95	96.18	111.50
1	B	352	ASP	N-CA-C	6.65	128.97	111.00
2	F	13	LEU	CA-CB-CG	5.79	128.61	115.30
1	B	215	GLU	N-CA-C	-5.18	97.00	111.00
2	F	13	LEU	CB-CG-CD1	5.02	119.54	111.00

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	B	2222	0	2151	107	0
1	E	2303	0	2223	105	0
2	C	1399	0	1425	60	0
2	F	1389	0	1419	52	0
3	A	8456	0	8516	419	0
3	D	8483	0	8530	417	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	C	32	0	12	2	0
5	F	32	0	12	2	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	E	1	0	0	1	0
8	A	258	0	0	15	0
8	B	134	0	0	8	0
8	C	58	0	0	3	0
8	D	333	0	0	9	0
8	E	130	0	0	7	0
8	F	46	0	0	2	0
All	All	25280	0	24288	1137	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 23.

The worst 5 of 1137 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)
3:A:476:MET:HE3	3:A:501:ILE:HG12	1.18	1.13
2:F:54:THR:HG22	2:F:176:PHE:HB3	1.19	1.11
3:D:33:ASN:HB2	3:D:44:ARG:HG3	1.33	1.09
3:A:1008:ILE:HG23	3:A:1009:PRO:HD3	1.35	1.07
1:E:350:SER:HB3	1:E:351:PRO:HD2	1.37	1.05

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	B	266/365 (73%)	241 (91%)	20 (8%)	5 (2%)	8 13
1	E	277/365 (76%)	253 (91%)	16 (6%)	8 (3%)	4 6
2	C	170/216 (79%)	157 (92%)	11 (6%)	2 (1%)	13 24
2	F	169/216 (78%)	157 (93%)	9 (5%)	3 (2%)	8 14
3	A	1042/1073 (97%)	945 (91%)	79 (8%)	18 (2%)	9 16
3	D	1045/1073 (97%)	952 (91%)	71 (7%)	22 (2%)	7 11
All	All	2969/3308 (90%)	2705 (91%)	206 (7%)	58 (2%)	8 12

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	ASN
1	B	216	GLU
1	B	351	PRO
2	C	169	ILE
3	A	123	GLU

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	B	249/327 (76%)	229 (92%)	20 (8%)	12 23
1	E	257/327 (79%)	242 (94%)	15 (6%)	20 38
2	C	151/185 (82%)	138 (91%)	13 (9%)	10 20
2	F	150/185 (81%)	139 (93%)	11 (7%)	14 27
3	A	950/973 (98%)	889 (94%)	61 (6%)	17 33
3	D	953/973 (98%)	894 (94%)	59 (6%)	18 35
All	All	2710/2970 (91%)	2531 (93%)	179 (7%)	16 32

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	134	LYS
3	D	263	VAL
2	F	177	VAL
3	D	146	TRP
3	D	436	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	261	HIS
3	D	204	GLN
1	E	353	HIS
3	D	30	ASN
3	D	218	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 5 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	$\#\|Z\|>2$
5	GTP	C	217	-	26,34,34	0.98	1 (3%)	33,54,54	1.84	8 (24%)
5	GTP	F	217	-	26,34,34	0.97	1 (3%)	33,54,54	1.81	7 (21%)

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
5	GTP	C	217	-	-	2/18/38/38	0/3/3/3
5	GTP	F	217	-	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	217	GTP	C6-N1	2.98	1.38	1.33
5	F	217	GTP	C6-N1	2.72	1.37	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	217	GTP	N3-C2-N1	-5.12	120.39	127.22
5	F	217	GTP	N3-C2-N1	-4.92	120.65	127.22
5	C	217	GTP	C2-N3-C4	3.99	119.91	115.36
5	F	217	GTP	C2-N3-C4	3.74	119.63	115.36
5	C	217	GTP	PA-O3A-PB	-3.65	120.32	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	217	GTP	PG-O3B-PB-O1B
5	C	217	GTP	PG-O3B-PB-O1B
5	C	217	GTP	O4'-C4'-C5'-O5'
5	F	217	GTP	O4'-C4'-C5'-O5'

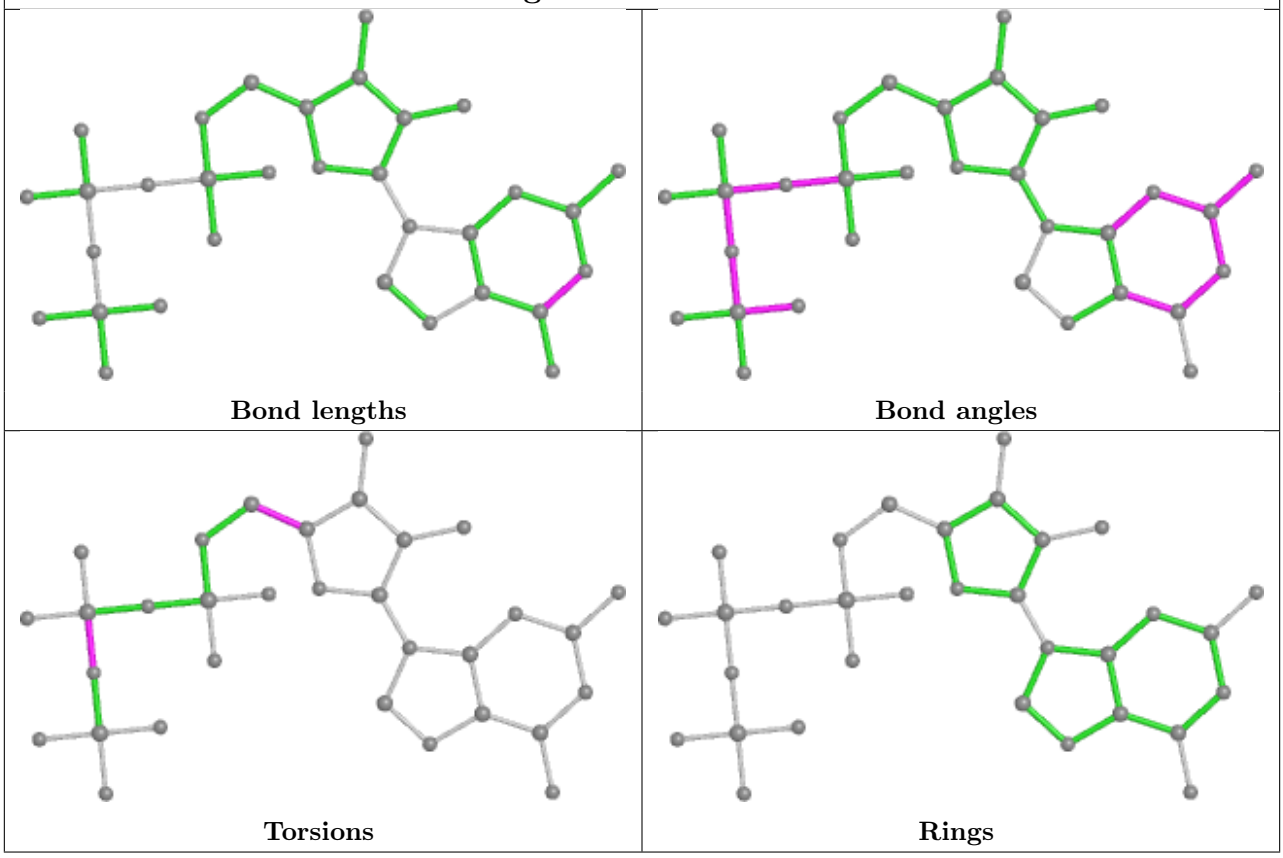
There are no ring outliers.

2 monomers are involved in 4 short contacts:

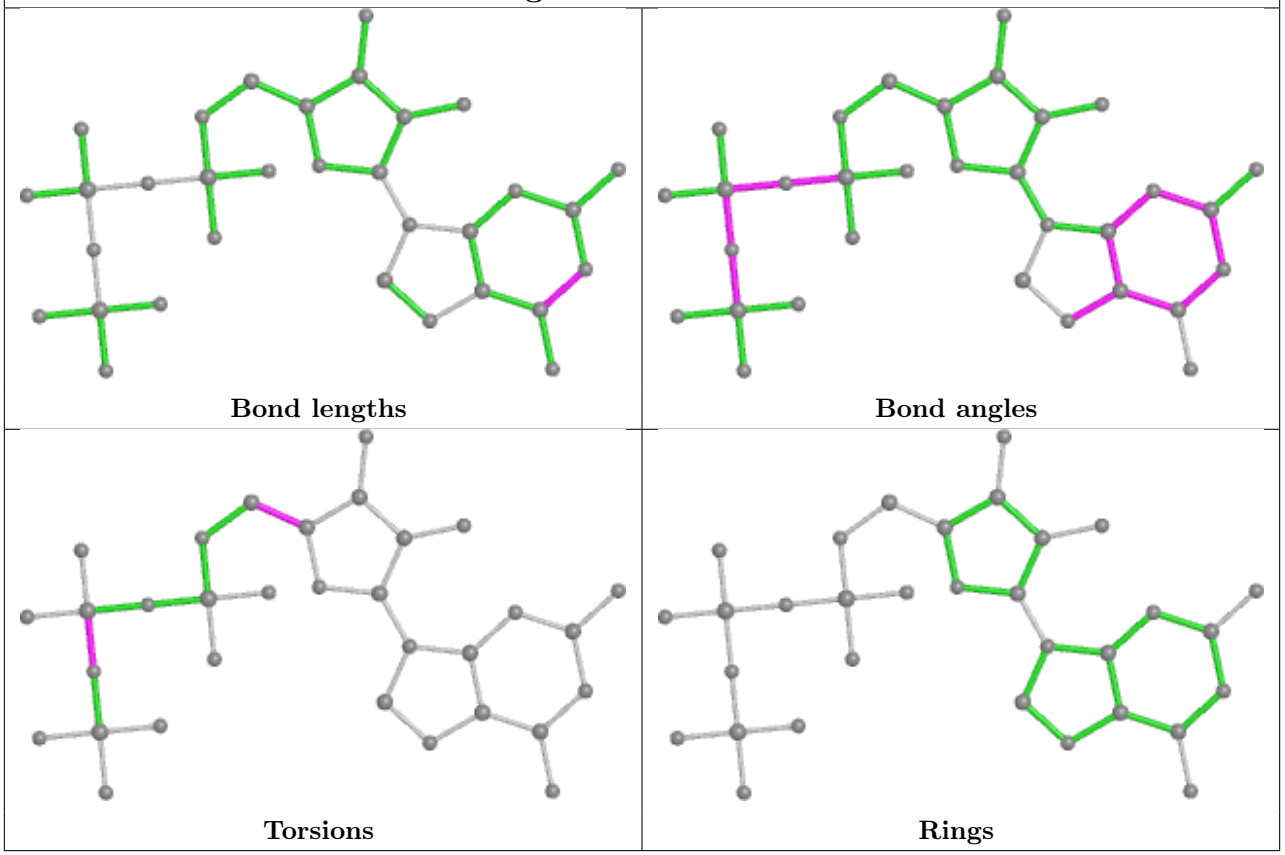
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	217	GTP	2	0
5	F	217	GTP	2	0

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 C 217



Ligand GTP F 217



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^{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	B	274/365 (75%)	0.23	8 (2%) 51 55	19, 36, 78, 112	3 (1%)
1	E	279/365 (76%)	0.27	9 (3%) 47 51	19, 37, 85, 126	0
2	C	171/216 (79%)	0.21	2 (1%) 79 80	20, 43, 73, 99	0
2	F	171/216 (79%)	0.19	0 100 100	20, 42, 77, 99	0
3	A	1041/1073 (97%)	0.43	65 (6%) 20 21	14, 46, 100, 152	1 (0%)
3	D	1041/1073 (97%)	0.53	92 (8%) 10 10	16, 46, 107, 156	5 (0%)
All	All	2977/3308 (89%)	0.40	176 (5%) 22 23	14, 43, 96, 156	9 (0%)

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1053	GLN	10.0
3	A	1053	GLN	9.0
3	D	967	PRO	8.0
3	D	1055	SER	7.8
3	D	19	PHE	7.7

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 monosaccharides in this entry.

6.4 Ligands (i)

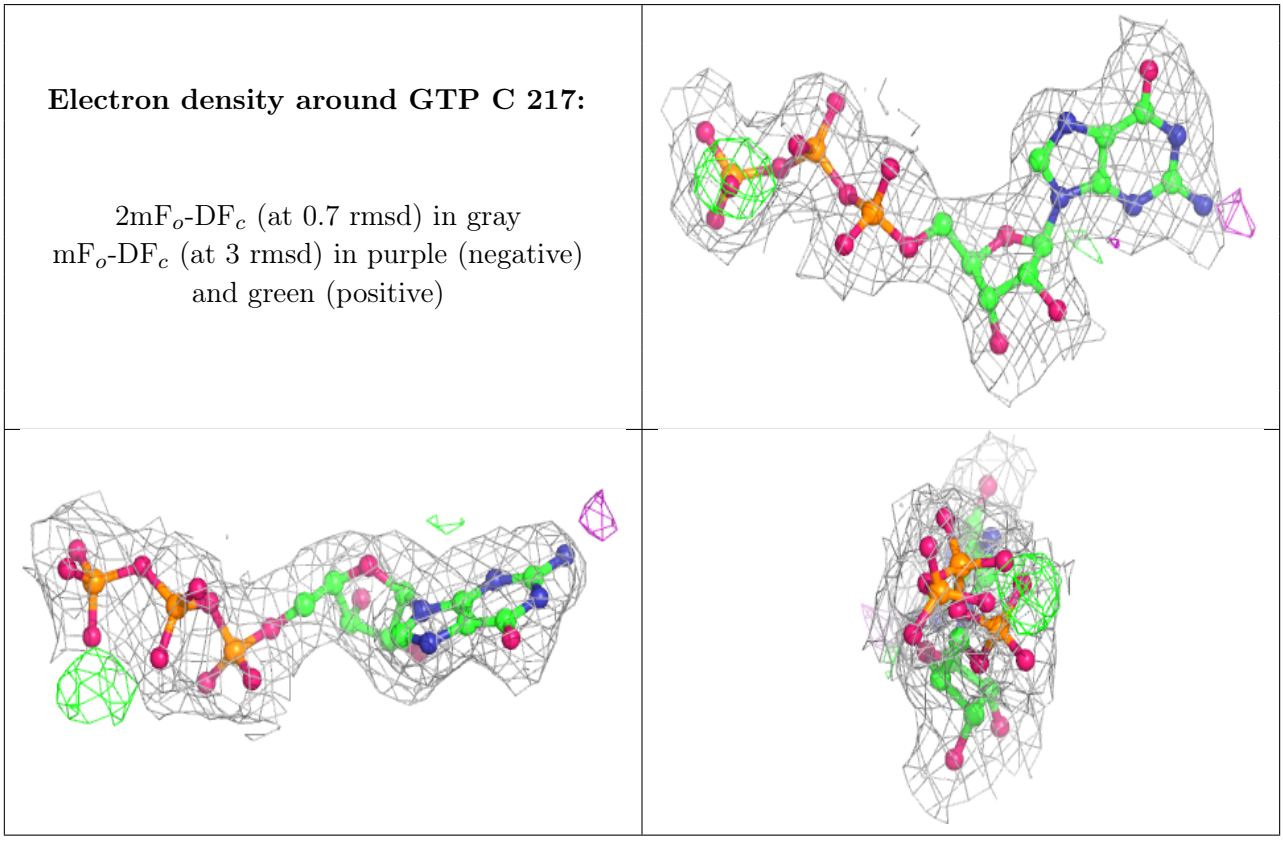
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	MG	C	218	1/1	0.77	0.17	40,40,40,40	0
4	NA	E	361	1/1	0.83	0.19	64,64,64,64	0
4	NA	B	361	1/1	0.92	0.18	34,34,34,34	0
6	MG	F	218	1/1	0.95	0.15	33,33,33,33	0
7	CL	E	362	1/1	0.95	0.11	49,49,49,49	0
5	GTP	C	217	32/32	0.97	0.14	13,27,39,52	0
5	GTP	F	217	32/32	0.98	0.15	14,27,40,50	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.

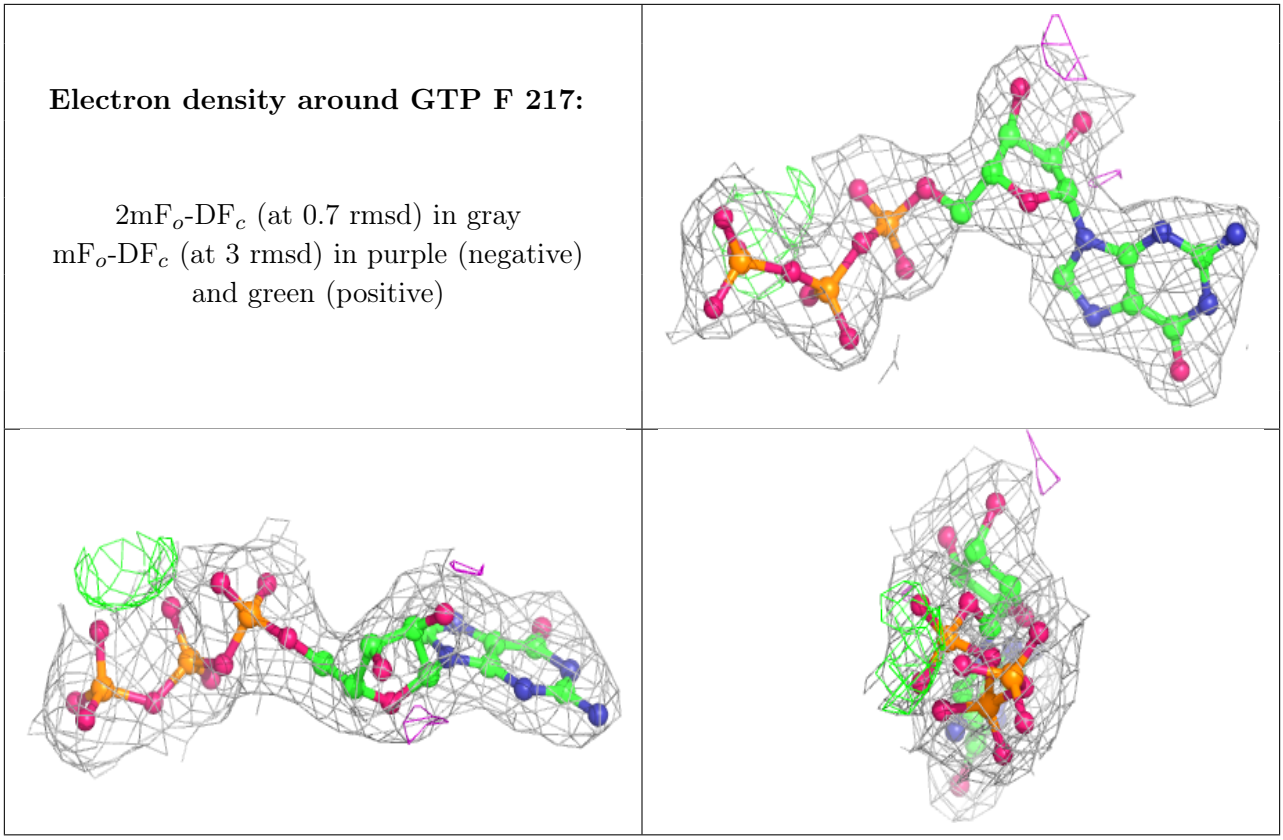
Electron density around GTP C 217:

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



Electron density around GTP F 217:

$2mF_o$-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.