



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:37 AM UTC

PDB ID : 3NBZ / pdb_00003nbz
Title : Crystal structure of the HIV-1 Rev NES-CRM1-RanGTP nuclear export complex (crystal I)
Authors : Guttler, T.; Madl, T.; Neumann, P.; Deichsel, D.; Corsini, L.; Monecke, T.; Ficner, R.; Sattler, M.; Gorlich, D.
Deposited on : 2010-06-04
Resolution : 2.80 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 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

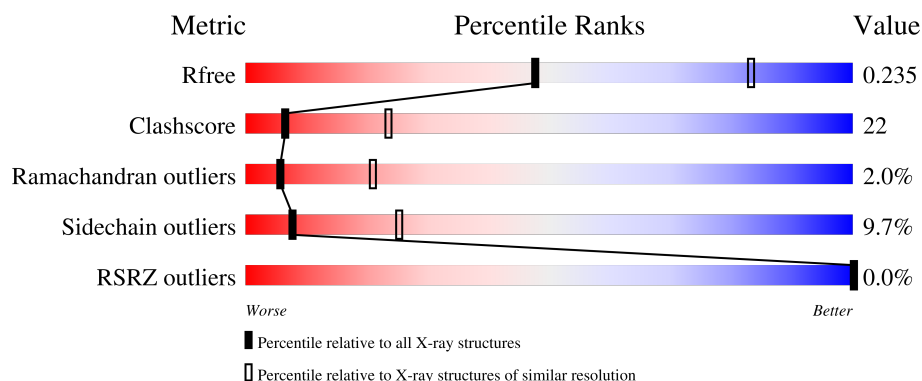
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1073	
1	D	1073	
2	B	362	
2	E	362	

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Mol	Chain	Length	Quality of chain
3	C	176	 60%32%7% •
3	F	176	 55%38%6% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25144 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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0	0
			8394	5387	1411	1543	53			
1	D	1038	Total	C	N	O	S	0	0	0
			8394	5387	1411	1543	53			

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 2 is a protein called Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2339	1491	403	430	15			
2	E	293	Total	C	N	O	S	0	0	0
			2354	1500	405	434	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP O95149
B	0	SER	-	expression tag	UNP O95149
B	1	PRO	-	expression tag	UNP O95149
B	2	VAL	-	expression tag	UNP O95149
B	3	PRO	-	expression tag	UNP O95149
B	4	LEU	-	expression tag	UNP O95149
B	5	GLN	-	expression tag	UNP O95149
B	6	LEU	-	expression tag	UNP O95149

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	PRO	-	expression tag	UNP O95149
B	8	PRO	-	expression tag	UNP O95149
B	9	LEU	-	expression tag	UNP O95149
B	10	GLU	-	expression tag	UNP O95149
B	11	ARG	-	expression tag	UNP O95149
B	12	LEU	-	expression tag	UNP O95149
B	13	THR	-	expression tag	UNP O95149
B	14	LEU	-	expression tag	UNP O95149
E	-1	GLY	-	expression tag	UNP O95149
E	0	SER	-	expression tag	UNP O95149
E	1	PRO	-	expression tag	UNP O95149
E	2	VAL	-	expression tag	UNP O95149
E	3	PRO	-	expression tag	UNP O95149
E	4	LEU	-	expression tag	UNP O95149
E	5	GLN	-	expression tag	UNP O95149
E	6	LEU	-	expression tag	UNP O95149
E	7	PRO	-	expression tag	UNP O95149
E	8	PRO	-	expression tag	UNP O95149
E	9	LEU	-	expression tag	UNP O95149
E	10	GLU	-	expression tag	UNP O95149
E	11	ARG	-	expression tag	UNP O95149
E	12	LEU	-	expression tag	UNP O95149
E	13	THR	-	expression tag	UNP O95149
E	14	LEU	-	expression tag	UNP O95149

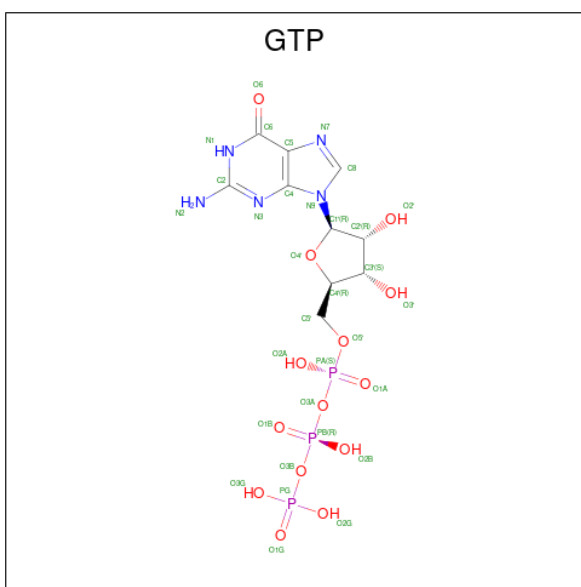
- Molecule 3 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	173	Total	C	N	O	S	0	0	0
			1405	914	246	240	5			
3	F	173	Total	C	N	O	S	0	0	0
			1405	914	246	240	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 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	237	Total	O	0	0
			237	237		

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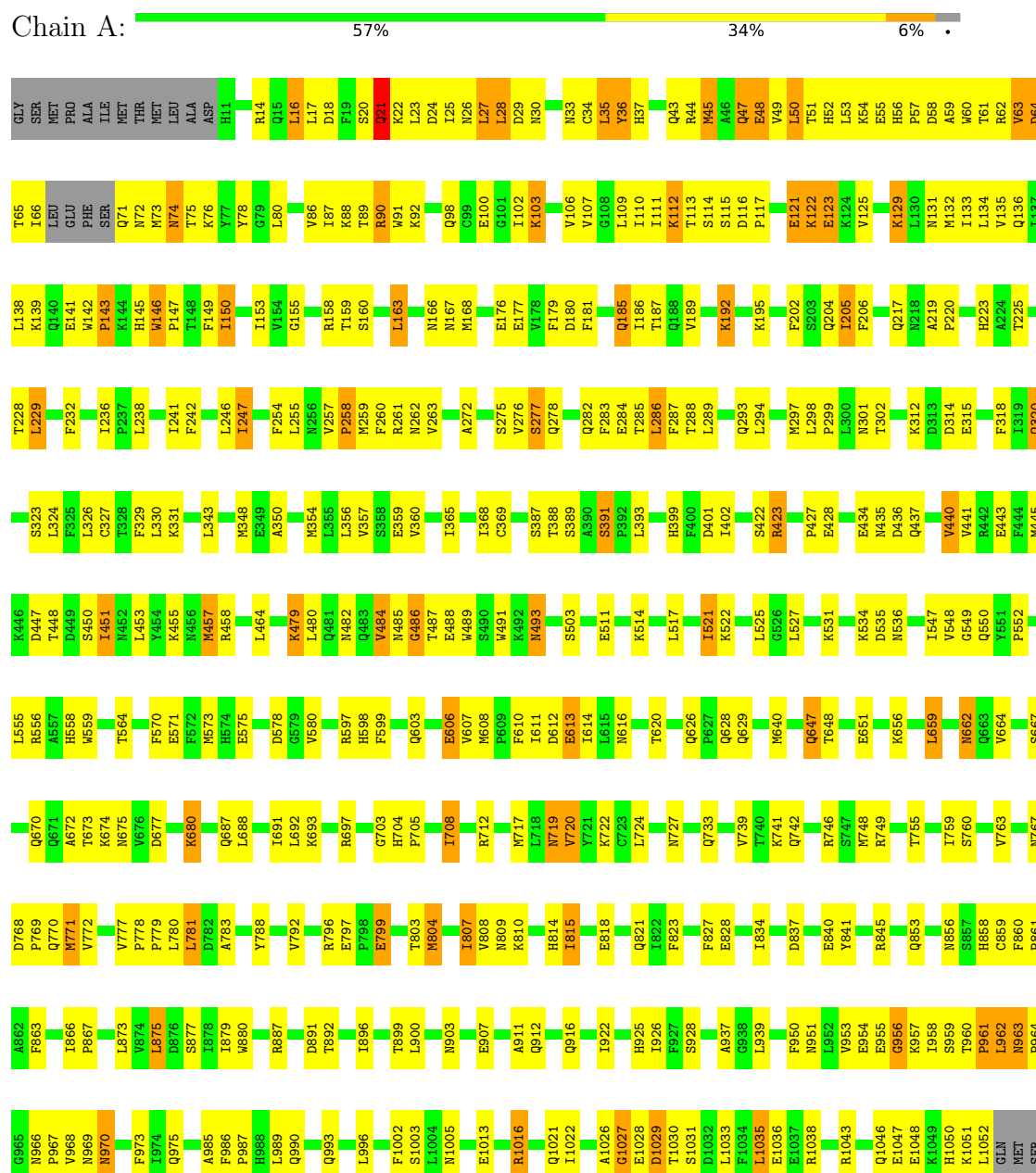
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	94	Total 94	O 94	0	0
7	C	53	Total 53	O 53	0	0
7	D	279	Total 279	O 279	0	0
7	E	71	Total 71	O 71	0	0
7	F	51	Total 51	O 51	0	0

3 Residue-property plots

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: Exportin-1



VAL	PRO	GLY	ILE	LEU	ASN	PRO	HIS	GLU	ILE	PRO	GLU	GLY	MET	CYS	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

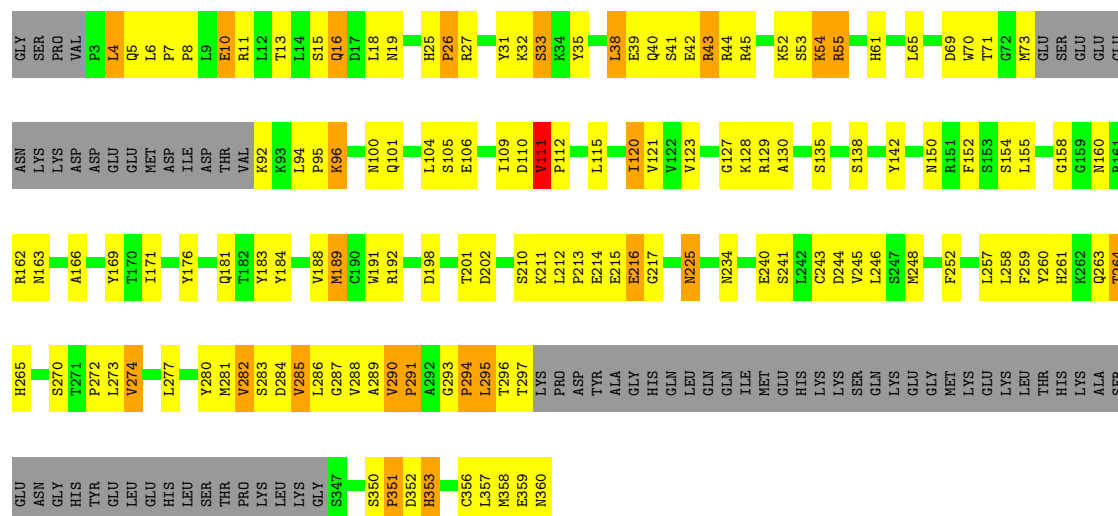
• Molecule 1: Exportin-1

Chain D:  56% 35% 6%

GLY	SER	MET	PRO	ALA	ILE	MET	THR	MET	PHE	LEU	ALA	ASP	H11	R14	Q15	Q16	L17	L18	D18	F19	S20	Q21	K22	L23	D24	I25	N26	L27	L28	D29	N30	V31	V32	N33	C34	L35	Y36	E39	G40	A41	Q42	Q43	R44	M45	A46	Q47	E48	V49	L50	T51	H52	L53	K54	E55	H56	P57	D58	A59	W60
T61	R62	V63	D64	T65	I66	L67	GLU	THR	PHE	SER	Q71	N72	M73	N74	T75	K76	Y77	Y78	G79	L80	V86	I87	K88	T89	R90	W91	K92	I93	L94	P95	R96	N97	Q98	C99	E100	G101	I102	K103	V106	V107	Q110	I111	K112	T113	D116	P117	T118	C119	V120	I205	K121	E123	K124	V125	Y126	I127			
G128	K129	L130	M131	N132	I133	L134	V135	Q136	I137	L138	K139	Q140	E141	W142	P143	K144	W145	W146	F149	I150	I153	V154	G155	R158	K92	S160	S160	L163	M166	N167	M168	E176	E177	V178	F179	D180	F181	T187	Q188	V189	K195	Q203	L294	K295	Q296	M297	F206	N218	A219	T302	N303								
H223	A224	T225	T228	L229	L230	R231	F232	T236	L237	L238	I241	F242	L246	I247	I251	L255	N256	V257	P258	M259	R261	N262	V263	E270	I271	A272	S277	Q278	Y279	Q282	F283	E284	T285	L286	F287	T288	L289	Q293	L294	K295	Q296	M297	L298	P299	L300	N301	T302	N303											
I304	R305	K312	D314	E315	F318	I319	Q320	S323	L324	F325	L326	F329	L330	L343	M348	E349	A350	M354	L355	L356	V357	S358	E359	V360	E361	I368	C369	E379	S387	T388	S391	P392	L393	L394	H399	P400	D401	I402	P403	P404	R405	M420	V421	S422	R423														
K426	P427	E428	V432	N435	D436	Q437	G438	E439	V440	V441	R442	M445	K446	D447	S450	I451	N452	L453	Y454	K455	R458	D468	K479	L480	Q481	N482	Q483	V484	M485	Q486	T487	E488	W489	S490	W491	K492	N493	A500	S503	K514	V518	P521	K522	L525	G526														
L527	C528	E529	Q530	K531	K534	D535	N536	K537	V548	L555	H558	W559	K560	F561	T564	E571	L574	H574	E575	V580	I591	R597	Q603	Q603	E606	V607	M608	P609	F610	I611	D612	E613	L614	L615	N616	N617	L618	N619	T620	D624	L625	Q626	P627	Q628	Q629	H631													
M640	Q647	K656	M657	M658	L659	N662	Q663	V664	A672	T673	K674	N675	M676	D677	L678	L679	K680	L688	G689	S690	L691	L692	K693	R697	G703	H704	P705	F706	Q709	R712	L718	N719	W720	Y721	K722	C723	L724	N727	N735	G736	E737	N738	V739	T740	K741	Q742													
R746	S747	M748	R749	R753	E754	T755	N759	S760	N767	D768	F769	Q770	M771	V772	V777	L780	L781	D782	A783	Y788	A794	R796	E797	V799	W800	T803	M804	T807	V808	N809	L815	E818	Q821	I822	F823	F827	E828	I834	D837	F838	E839	E840																	
Y841	P842	R845	L851	L852	Q853	N856	S857	H858	C859	F860	P861	R863	L875	D876	S877	I878	I879	W880	A881	H884	R887	D891	T892	T896	T899	L899	N903	E907	A911	Q912	Q916	C920	D921	I922	H925	T926	F927	S928	L939	T945																			
M949	F950	N951	L952	E954	E955	G956	K957	L958	S959	T960	P961	N963	P964	V968	N969	N970	F973	I974	Q975	D976	Y977	V978	L981	F986	L989	L996	F997	L1001	F1002	N1005	Q1006	E1013	R1016	I1022	G1027	E1028	D1029	T1030	S1031	D1032	L1033	F1034	L1035	R1038															
R1043	Q1046	E1047	E1048	K1049	L1052	GLN	MET	SER	VAL	PRO	GLY	ILE	LEU	ASN	PRO	HIS	ILE	PRO	GLU	MET	CYS	ASP																																					

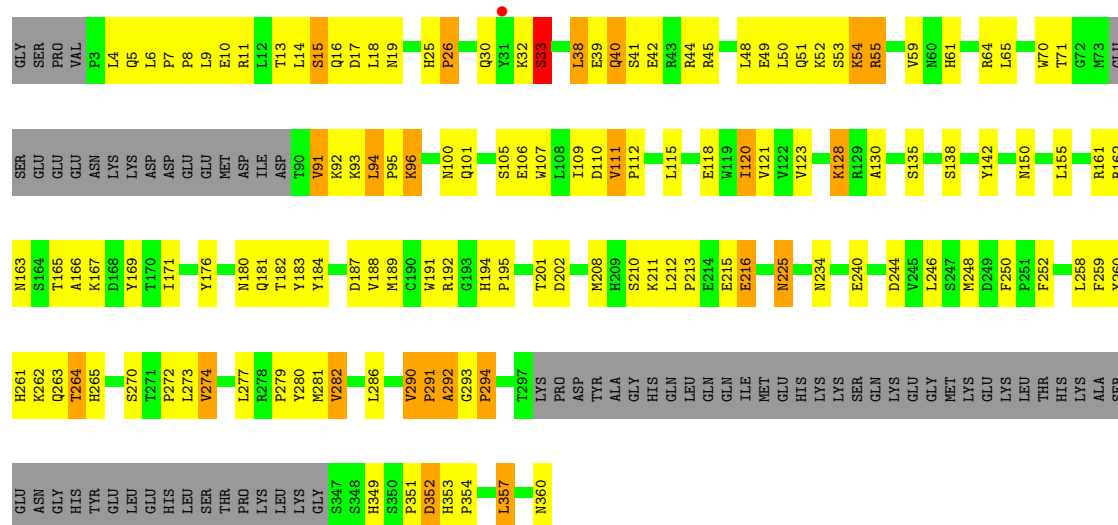
• Molecule 2: Snurportin-1

Chain B:  42% 32% 7% 20%



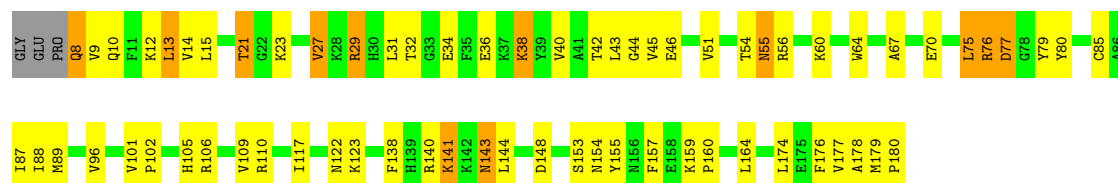
• Molecule 2: Snurportin-1

Chain E: 43% 31% 6% 19%



• Molecule 3: GTP-binding nuclear protein Ran

Chain C: 60% 32% 7%



• Molecule 3: GTP-binding nuclear protein Ran

Chain F: 55% 38% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.66Å 224.62Å 164.02Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	38.90 – 2.80 38.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.1 (38.90-2.80) 81.4 (38.90-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.226 , 0.285 0.226 , 0.235	Depositor DCC
R_{free} test set	5702 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.119 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25144	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: NA, MG, 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	0.41	0/8566	0.80	6/11604 (0.1%)
1	D	0.41	0/8566	0.79	7/11604 (0.1%)
2	B	0.42	0/2404	0.91	8/3263 (0.2%)
2	E	0.42	0/2419	0.91	10/3283 (0.3%)
3	C	0.40	0/1440	0.78	0/1945
3	F	0.40	0/1440	0.79	0/1945
All	All	0.41	0/24835	0.82	31/33644 (0.1%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225	ASN	CA-C-N	9.92	129.71	119.19
2	B	225	ASN	C-N-CA	9.92	129.71	119.19
2	E	225	ASN	CA-C-N	9.07	129.26	119.28
2	E	225	ASN	C-N-CA	9.07	129.26	119.28
1	A	488	GLU	N-CA-C	-8.29	101.32	112.26

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	8394	0	8460	356	0
1	D	8394	0	8460	373	0
2	B	2339	0	2295	122	0
2	E	2354	0	2311	115	0
3	C	1405	0	1434	55	0
3	F	1405	0	1434	68	0
4	C	32	0	12	4	0
4	F	32	0	12	2	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	237	0	0	17	0
7	B	94	0	0	7	0
7	C	53	0	0	6	0
7	D	279	0	0	23	0
7	E	71	0	0	3	0
7	F	51	0	0	6	0
All	All	25144	0	24418	1065	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 22.

The worst 5 of 1065 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)
2:E:290:VAL:H	2:E:291:PRO:HD3	1.09	1.10
2:B:52:LYS:HZ3	2:B:264:THR:HA	1.03	1.06
2:E:52:LYS:HZ3	2:E:264:THR:HA	1.19	1.01
1:A:131:ASN:HD21	1:A:166:ASN:HD21	1.12	0.95
1:D:964:PRO:HG2	1:D:968:VAL:HB	1.49	0.94

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	1034/1073 (96%)	931 (90%)	85 (8%)	18 (2%)	7	25
1	D	1034/1073 (96%)	933 (90%)	83 (8%)	18 (2%)	7	25
2	B	285/362 (79%)	251 (88%)	23 (8%)	11 (4%)	2	8
2	E	287/362 (79%)	249 (87%)	28 (10%)	10 (4%)	3	10
3	C	171/176 (97%)	157 (92%)	13 (8%)	1 (1%)	21	51
3	F	171/176 (97%)	154 (90%)	16 (9%)	1 (1%)	21	51
All	All	2982/3222 (93%)	2675 (90%)	248 (8%)	59 (2%)	6	21

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	963	ASN
2	B	216	GLU
1	D	123	GLU
1	D	963	ASN

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	942/973 (97%)	851 (90%)	91 (10%)	8	25
1	D	942/973 (97%)	857 (91%)	85 (9%)	9	28
2	B	263/327 (80%)	237 (90%)	26 (10%)	7	24
2	E	265/327 (81%)	242 (91%)	23 (9%)	9	30
3	C	152/154 (99%)	133 (88%)	19 (12%)	4	15
3	F	152/154 (99%)	132 (87%)	20 (13%)	4	14
All	All	2716/2908 (93%)	2452 (90%)	264 (10%)	8	25

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	128	LYS
2	E	264	THR
3	F	113	GLU
2	B	96	LYS
2	B	33	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	916	GLN
1	D	970	ASN
2	E	163	ASN
1	A	1006	GLN
1	A	990	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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
4	GTP	F	217	5	33,34,34	0.90	0	50,54,54	1.52	9 (18%)
4	GTP	C	217	5	33,34,34	0.87	1 (3%)	50,54,54	1.57	10 (20%)

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
4	GTP	F	217	5	-	7/22/38/38	0/3/3/3
4	GTP	C	217	5	-	2/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	217	GTP	O4'-C4'	-2.04	1.40	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	217	GTP	C5-C4-N3	-4.98	120.46	128.39
4	C	217	GTP	C2-N3-C4	4.75	120.48	112.30
4	F	217	GTP	C2-N3-C4	4.70	120.39	112.30
4	C	217	GTP	C5-C4-N3	-4.35	121.47	128.39
4	C	217	GTP	N9-C8-N7	-3.10	107.66	113.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

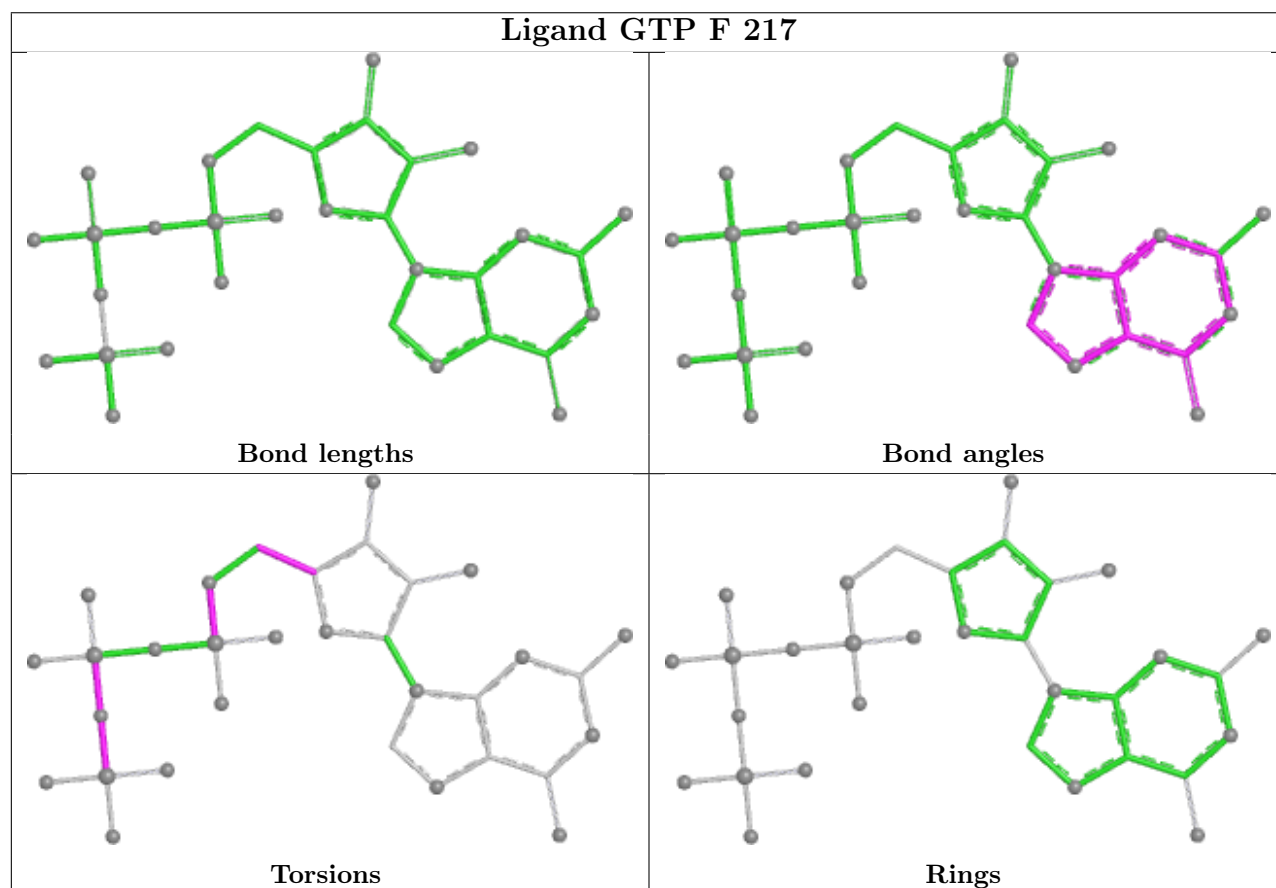
Mol	Chain	Res	Type	Atoms
4	C	217	GTP	PB-O3B-PG-O3G
4	F	217	GTP	PB-O3B-PG-O2G
4	F	217	GTP	C5'-O5'-PA-O2A
4	F	217	GTP	O4'-C4'-C5'-O5'
4	F	217	GTP	C3'-C4'-C5'-O5'

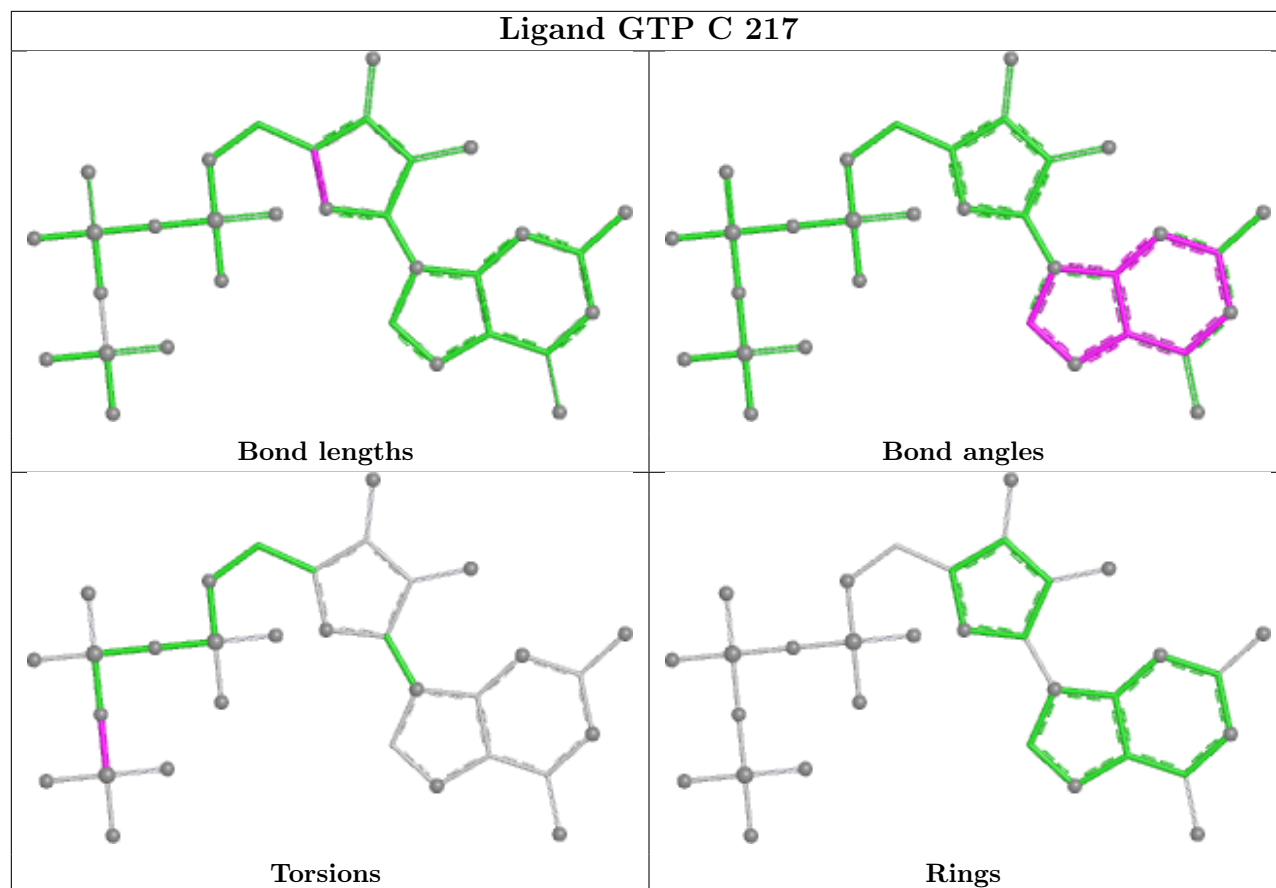
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	217	GTP	2	0
4	C	217	GTP	4	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 [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	1038/1073 (96%)	-1.22	0 100 100	14, 47, 107, 152	0
1	D	1038/1073 (96%)	-1.23	0 100 100	14, 47, 103, 176	0
2	B	291/362 (80%)	-1.23	0 100 100	15, 44, 116, 167	0
2	E	293/362 (80%)	-1.18	1 (0%) 90 86	15, 45, 123, 167	0
3	C	173/176 (98%)	-1.35	0 100 100	21, 39, 79, 132	0
3	F	173/176 (98%)	-1.41	0 100 100	20, 39, 79, 106	0
All	All	3006/3222 (93%)	-1.24	1 (0%) 100 100	14, 45, 106, 176	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	31	TYR	2.6

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](#)

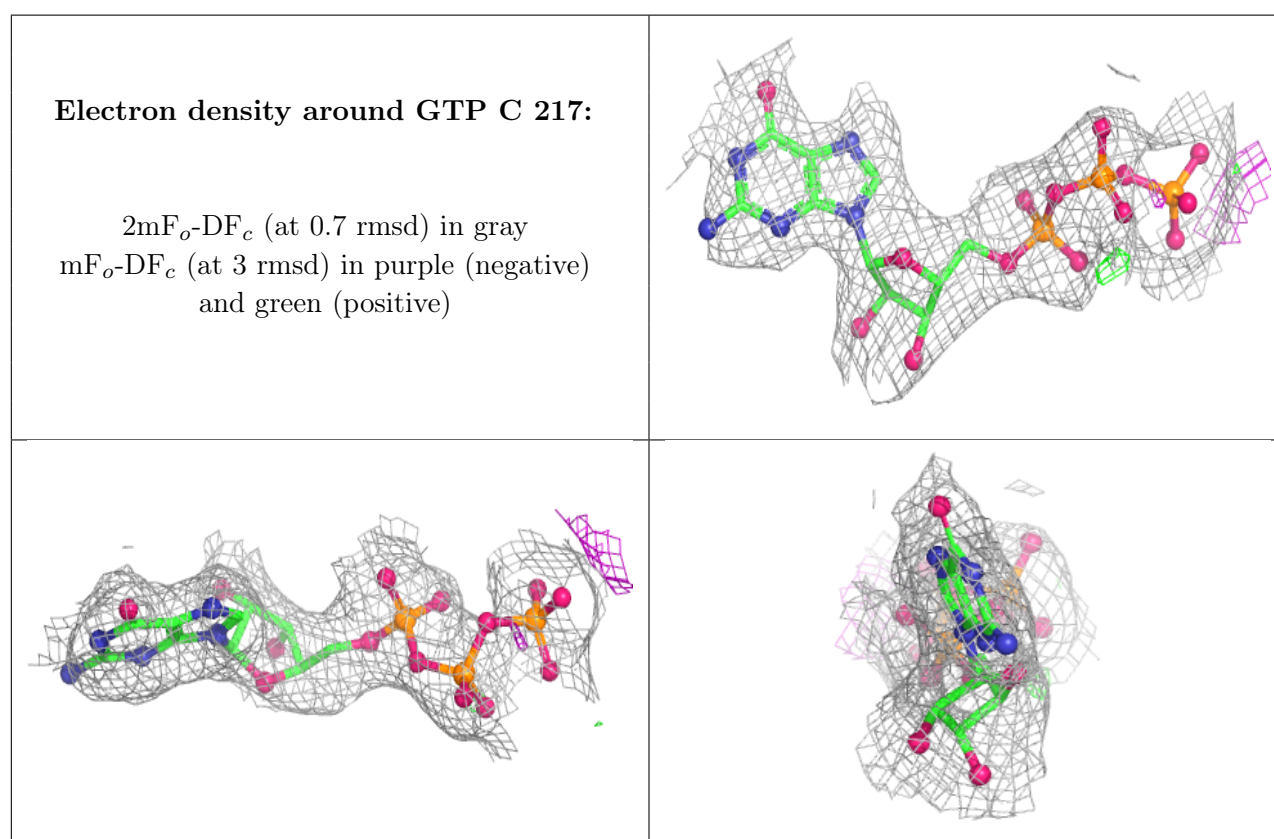
There are no oligosaccharides in this entry.

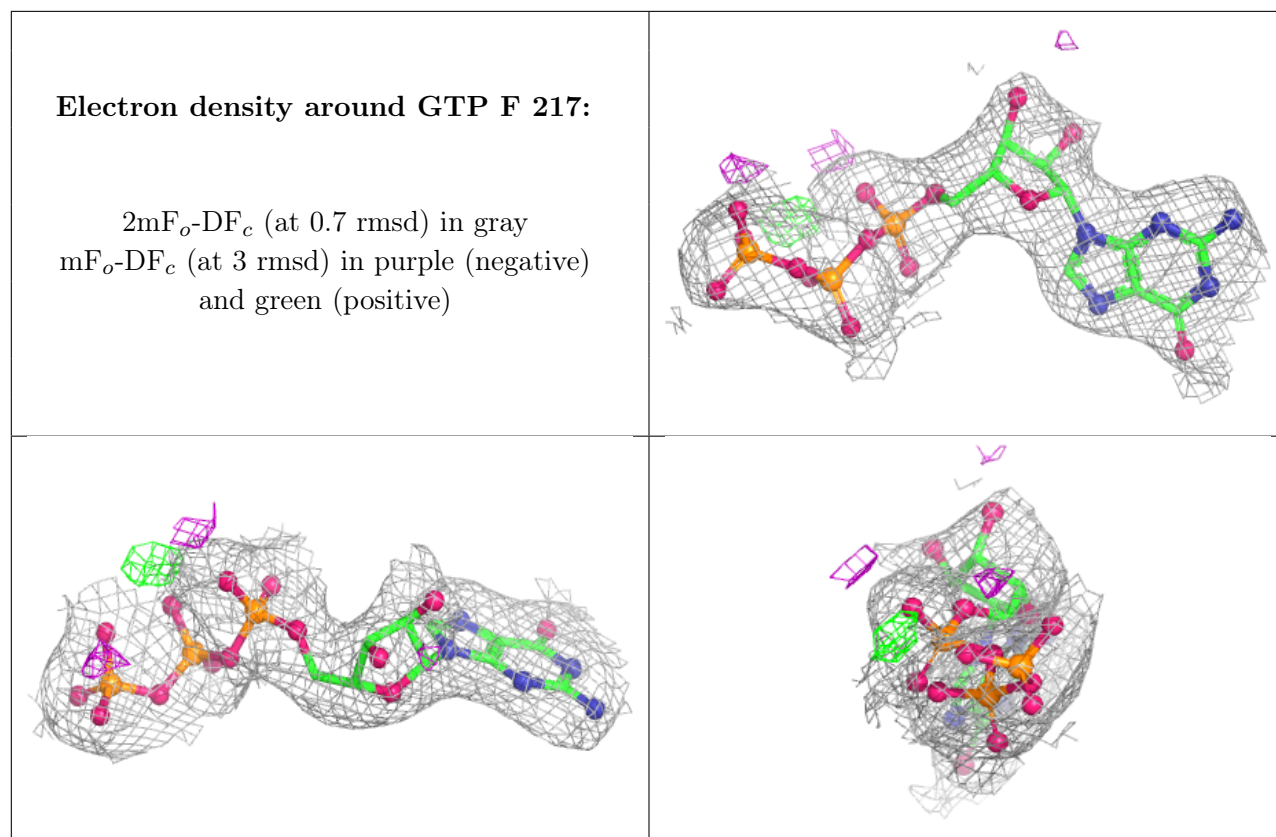
6.4 Ligands [i](#)

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
6	NA	C	1	1/1	0.99	0.05	42,42,42,42	0
6	NA	D	1072	1/1	0.99	0.09	52,52,52,52	0
5	MG	C	218	1/1	1.00	0.01	14,14,14,14	0
5	MG	F	218	1/1	1.00	0.02	26,26,26,26	0
4	GTP	C	217	32/32	1.00	0.03	12,29,37,71	0
4	GTP	F	217	32/32	1.00	0.03	16,34,50,56	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.