



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:47 PM UTC

PDB ID : 3NBY / pdb_00003nby
Title : Crystal structure of the PKI NES-CRM1-RanGTP nuclear export complex
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 : 3.42 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

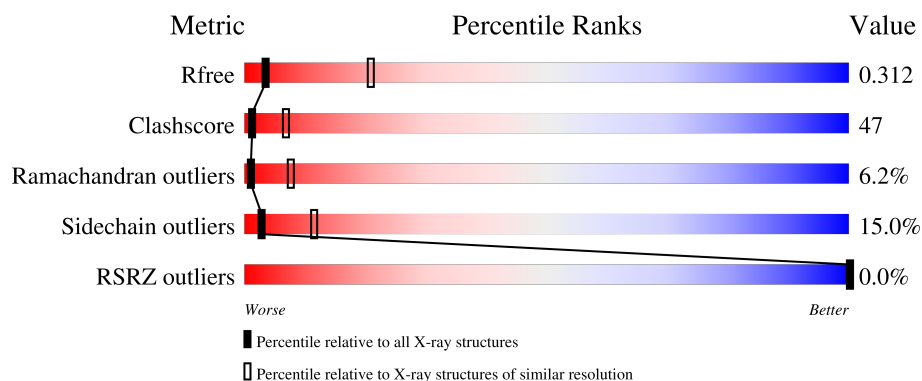
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	B	361	
1	E	361	
2	C	176	
2	F	176	
3	A	1073	

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Mol	Chain	Length	Quality of chain
3	D	1073	29% 52% 16% ••

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24084 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	272	Total	C	N	O	S	0	0	0
			2193	1398	376	405	14			
1	E	277	Total	C	N	O	S	0	0	0
			2221	1416	380	410	15			

There are 30 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	LEU	-	expression tag	UNP O95149
B	2	ASN	-	expression tag	UNP O95149
B	3	GLU	-	expression tag	UNP O95149
B	4	LEU	-	expression tag	UNP O95149
B	5	ALA	-	expression tag	UNP O95149
B	6	LEU	-	expression tag	UNP O95149
B	7	LYS	-	expression tag	UNP O95149
B	8	LEU	-	expression tag	UNP O95149
B	9	ALA	-	expression tag	UNP O95149
B	10	GLY	-	expression tag	UNP O95149
B	11	LEU	-	expression tag	UNP O95149
B	12	ASP	-	expression tag	UNP O95149
B	13	ILE	-	expression tag	UNP O95149
E	-1	GLY	-	expression tag	UNP O95149
E	0	SER	-	expression tag	UNP O95149
E	1	LEU	-	expression tag	UNP O95149
E	2	ASN	-	expression tag	UNP O95149
E	3	GLU	-	expression tag	UNP O95149
E	4	LEU	-	expression tag	UNP O95149
E	5	ALA	-	expression tag	UNP O95149
E	6	LEU	-	expression tag	UNP O95149
E	7	LYS	-	expression tag	UNP O95149
E	8	LEU	-	expression tag	UNP O95149

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Chain	Residue	Modelled	Actual	Comment	Reference
E	9	ALA	-	expression tag	UNP O95149
E	10	GLY	-	expression tag	UNP O95149
E	11	LEU	-	expression tag	UNP O95149
E	12	ASP	-	expression tag	UNP O95149
E	13	ILE	-	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	0	0
			1389	904	243	237	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	0	0
			8413	5397	1413	1549	54			
3	D	1041	Total	C	N	O	S	0	0	0
			8413	5397	1413	1549	54			

There are 4 discrepancies between the modelled and reference sequences:

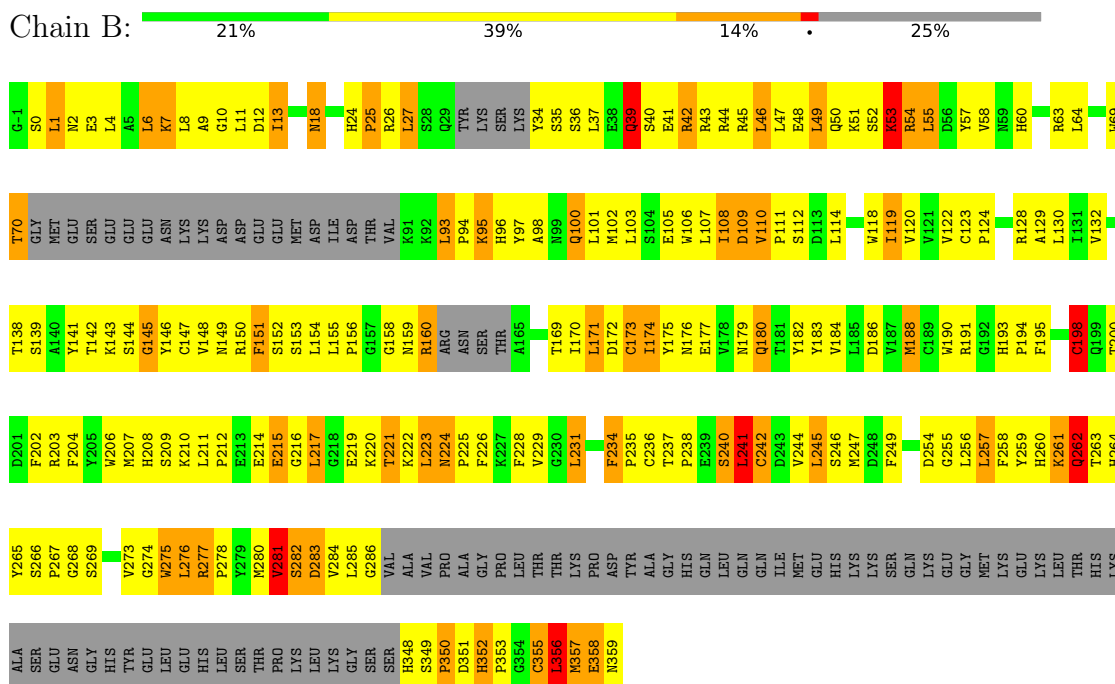
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6P5F9
A	0	SER	-	expression tag	UNP Q6P5F9
D	-1	GLY	-	expression tag	UNP Q6P5F9
D	0	SER	-	expression tag	UNP Q6P5F9

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

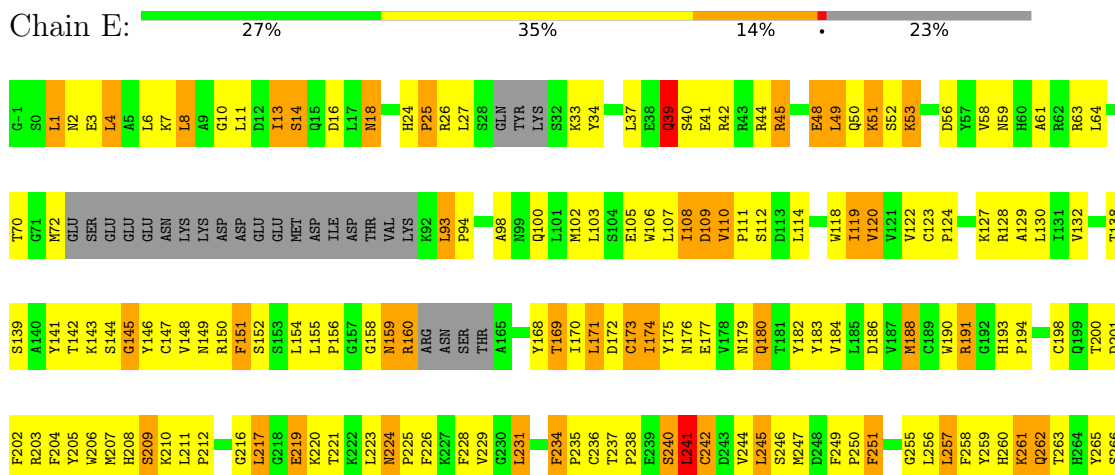
3 Residue-property plots

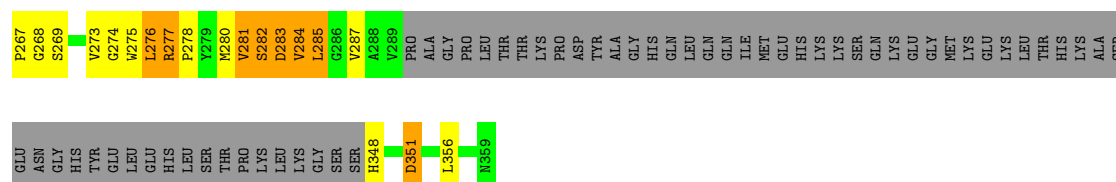
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Snurportin-1



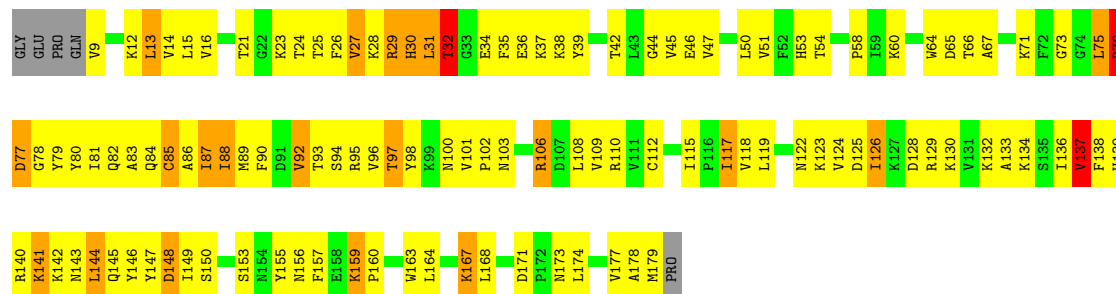
• Molecule 1: Snurportin-1





• Molecule 2: GTP-binding nuclear protein Ran

Chain C: 30% 54% 11% . .



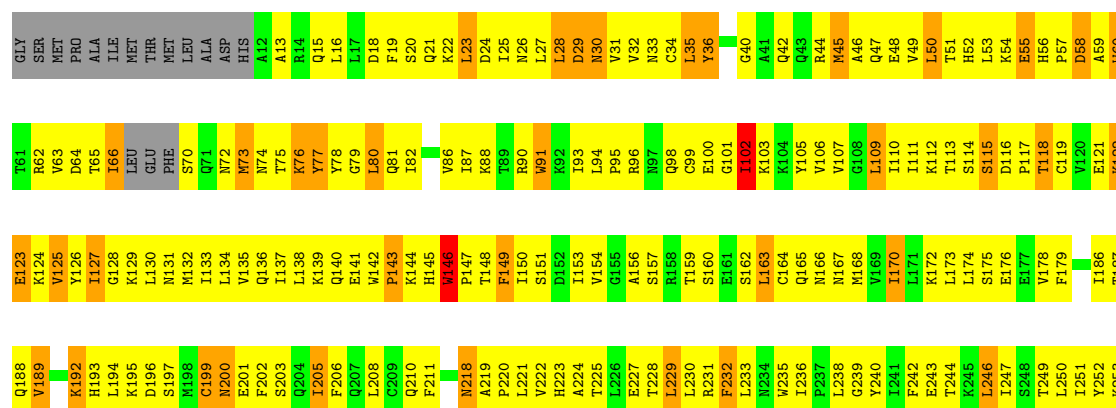
• Molecule 2: GTP-binding nuclear protein Ran

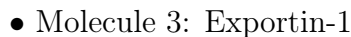
Chain F: 34% 48% 13% . .



• Molecule 3: Exportin-1

Chain A: 28% 53% 15% . .





D1007	T836	K872	T803	K741	Q671	V600	G533	H486	P392	S323	N256	A191	V125
I1008	A937	L873	H804	Q742	A672	E606	K534	L467	L393	L324	V257	K192	Y126
P1009	G938	V874	A895	P743	N675	V607	D535	D468	P258	F325	M259	H193	I127
A1010	L939	L875	T806	L744	V676	M608	N536	Y469	S395	L326	K261	K129	G128
F1011	T940	D876	I807	I745	D677	P609	K537	V470		C327	R261	D196	K130
K1012	M941	S877	K810	R746	D677	F610	A538	D471	H399	T328	R262	S197	L131
E1013	H942	S747	L878	S747	L678	L611	I539	T472	F400	F329	V263	M198	M132
H1014	A943	R748	L879	R748	L679	F612	I540	E473	D401	L330	V264	C199	I133
L1015	S944	W880	G813	R749	D681	D612	I541	E474	L402	K331	K265	N200	L134
R1016	A881	A881	T816	T750	P682	E613	A541	L475	P403	H333	L266	E201	V135
D1017	L946	F882	T816	W751	P682	E614	I544	M476	P404	H332	C267	F202	Q136
	A947		K752	K752	E683	L615			R405	G334	L268	S203	I137
V1020	T885	T885	I819	R753	T684	L616	I547	K479	R406	Q335	L268	Q204	L138
Q1021	H886	F880	F820	E754	V685	N617	V548	L480	Q407	L336	T269	I205	K139
I1022	R887	Q821	T822	L755	K696	L618		Q481	L408	L337	E270	F206	Q140
K1023	N888	L755	K697	K757	Q687		Y551	N482	Y409	E338	I271	Q207	K141
	V889	L756	L692	K757		T620	P552	Q483		K339	A272	L208	W142
G1027	A890	F823	D824	I758	I691	I621	R553	V484	R417	R340	Q273	C209	P143
E1028	D891	A825	A825	I759	L692	I622	F554	N485		L341	Q274	Q210	K144
D1029	V826	V826	F827	S780	K693	G623	L555	Q486	M420	N342	S275	Q211	H145
T1030	G893	G893		G761	T694	D624	L556	T487	S422	L343	Q277		P147
	L894	W762	V696	W762	V696	Q626	H558	W489	R423	R344	Q278	Q217	W146
L1033	T830	T830	R697	R697	R697	S490	W559	S490	M424		Y279	N218	T148
F1034	L831	L831	A698	A698		K560	K560	W491		L347	E280	A219	F149
L1035	H832	H832				Q628	F561		P427	M348	E281	P220	I150
E1036	H833	H833	A701	A701		Q629	L562	T496	E428	A350	Q282	L221	S151
L1037	I834	I834	W702	W702		H631	K563	L497	E429	L351	F283	W222	D152
	D837	D837	G703	G703		T632	T564	C498	V430	E364	E284	H223	I153
A1041	F838	F838	H704	H704		F633	V565	W499	L431	H352	T285	A224	V154
L1042	E839	E839	P705	P705		Y634		A500	V432	Y353	L286	T225	G155
R1043	E840	E840	F706	F706		E635	K568	I501	V433	L366	F287	L226	A156
Q1044	T841	T841	W707	W707		A636	L569	G502	E434		E227	E227	A157
	P842	P842	W708	W708		G638	F570	S503	N435	E362	T290	T228	R158
	E843	E843	Q709	Q709		Y639	E571	I504	D436	T363	M291	L230	L159
	H844	H844					F572	S505	Q437	E364	M292	S160	S160
	T846	T846	E712	E712		M640	M573	G438	E439	I365	Q293	R231	E161
	H847	H847	L715	L715		I641	H509	E510	V440	F366	K295	F232	S162
	F848	F848	D716	D716		A643	T576	E511	R442	I368	Q296	L233	L163
	F849	F849	W717	W717		T644	H577	D512			M297	C164	Q165
	L850	L850	L718	L718		D646	D578	E513	E443		L298	N166	N166
	L851	L851	W719	W719		Q647	G579	K514		E371	P299	M167	M167
	L852	L852	W720	W720		T648	V580	B515	T448	Y372	L300	G239	M168
	Q853	Q853	Y721	Y721		Q648	Q861	F516	D449	N373	K301	Y240	V169
	A854	A854	K722	K722		V649	D582	L517	S450	H375	T302	I241	L170
	V855	V855	G723	G723		Q650	M583	V518	I451	L376	N303	F242	K172
	H856	H856	L724	L724		E651		T519	N452	A377	I304	E243	
	S857	S857					D586	V520	L453	A378	R305	T244	
	H858	H858	W729	W729		K656	T587	I521	Y454	E379	L306	K245	S175
	C859	C859	A730	A730		V657	F588	K522	M457	L380	A307	L246	E176
	F860	F860	A731	A731		M658	I599	L525	R458	Y381	Y308	I247	E177
	P861	P861	T732	T732		L659		G526	E459	R382	F179	S248	F179
	A865	A865	Q733	Q733		P661	A592	L527	T460	E383	D313	T249	
	H866	H866	G736	G736		I662	Q593	C528	L461	S384	L250	L250	I186
	P867	P867	E737	E737			K594	C529	V462		I251	Y252	T187
			W800	W800			G595	E529	Y463	T388	N317	K253	Q188
	Q870	Q870	L801	L801		S667	B596	Q530	Y463	S389	F318	K253	Q188
	F871	F871	W739	W739		T668	R597	K531	L464	A390	F254	V189	V189
			T740	T740				R532	T465	S391	L322	L255	K190

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.09Å 223.73Å 163.06Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	38.63 – 3.42 38.63 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.63-3.42) 89.4 (38.63-3.42)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.258 , 0.315 0.257 , 0.312	Depositor DCC
R_{free} test set	5238 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24084	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: 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	B	0.74	0/2250	1.17	20/3046 (0.7%)
1	E	0.74	0/2278	1.16	16/3084 (0.5%)
2	C	0.74	1/1423 (0.1%)	1.07	3/1921 (0.2%)
2	F	0.71	0/1423	1.10	10/1921 (0.5%)
3	A	0.74	5/8584 (0.1%)	1.12	45/11627 (0.4%)
3	D	0.74	2/8584 (0.0%)	1.13	46/11627 (0.4%)
All	All	0.74	8/24542 (0.0%)	1.13	140/33226 (0.4%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	491	TRP	NE1-CE2	6.63	1.44	1.37
3	A	466	HIS	CD2-NE2	6.09	1.44	1.37
3	D	491	TRP	NE1-CE2	5.96	1.44	1.37
3	A	664	VAL	CA-CB	5.64	1.60	1.54
3	D	521	ILE	CA-CB	5.56	1.61	1.54

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	391	SER	CA-C-N	12.13	135.00	119.84
3	D	391	SER	C-N-CA	12.13	135.00	119.84
3	D	116	ASP	CA-C-N	11.04	133.63	119.84
3	D	116	ASP	C-N-CA	11.04	133.63	119.84
1	B	224	ASN	CA-C-N	10.73	131.09	119.28

There are no chirality outliers.

There are no planarity outliers.

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	B	2193	0	2138	249	0
1	E	2221	0	2170	221	0
2	C	1389	0	1419	133	0
2	F	1389	0	1419	125	0
3	A	8413	0	8480	819	0
3	D	8413	0	8480	799	0
4	C	32	0	12	8	0
4	F	32	0	12	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
All	All	24084	0	24130	2256	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 47.

The worst 5 of 2256 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:328:THR:HA	3:A:331:LYS:HD3	1.27	1.14
3:D:328:THR:HA	3:D:331:LYS:HD3	1.33	1.09
3:D:961:PRO:HG2	3:D:973:PHE:HD2	1.16	1.09
1:B:3:GLU:O	1:B:7:LYS:HB2	1.53	1.07
3:D:996:LEU:HD13	3:D:1035:LEU:HD12	1.37	1.06

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	262/361 (73%)	206 (79%)	38 (14%)	18 (7%)	1	6
1	E	267/361 (74%)	211 (79%)	39 (15%)	17 (6%)	1	7
2	C	169/176 (96%)	139 (82%)	23 (14%)	7 (4%)	2	14
2	F	169/176 (96%)	138 (82%)	24 (14%)	7 (4%)	2	14
3	A	1037/1073 (97%)	760 (73%)	206 (20%)	71 (7%)	1	6
3	D	1037/1073 (97%)	755 (73%)	220 (21%)	62 (6%)	1	8
All	All	2941/3220 (91%)	2209 (75%)	550 (19%)	182 (6%)	1	8

5 of 182 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	GLN
1	B	145	GLY
1	B	180	GLN
1	B	217	LEU
2	C	76	ARG

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	B	244/323 (76%)	197 (81%)	47 (19%)	1	6
1	E	247/323 (76%)	204 (83%)	43 (17%)	2	8
2	C	150/154 (97%)	124 (83%)	26 (17%)	2	8
2	F	150/154 (97%)	120 (80%)	30 (20%)	1	5
3	A	945/973 (97%)	820 (87%)	125 (13%)	4	15
3	D	945/973 (97%)	815 (86%)	130 (14%)	3	14
All	All	2681/2900 (92%)	2280 (85%)	401 (15%)	3	11

5 of 401 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	257	LEU
3	D	80	LEU
3	D	1030	THR
1	E	283	ASP
2	F	108	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1046	GLN
3	D	951	ASN
3	D	43	GLN
3	D	924	GLN
3	D	742	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 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
4	GTP	C	217	5	33,34,34	0.93	1 (3%)	50,54,54	2.01	12 (24%)
4	GTP	F	217	5	33,34,34	0.95	2 (6%)	50,54,54	1.64	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	C	217	5	-	9/22/38/38	0/3/3/3
4	GTP	F	217	5	-	2/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	217	GTP	PB-O3B	2.38	1.62	1.59
4	C	217	GTP	C2-N3	2.30	1.38	1.33
4	F	217	GTP	C2-N3	2.00	1.38	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	217	GTP	C5-C4-N3	-6.27	118.42	128.39
4	C	217	GTP	C2-N3-C4	5.42	121.64	112.30
4	F	217	GTP	C2-N3-C4	4.09	119.34	112.30
4	F	217	GTP	C5-C4-N3	-3.93	122.14	128.39
4	C	217	GTP	C4-C5-N7	-3.69	104.83	110.67

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

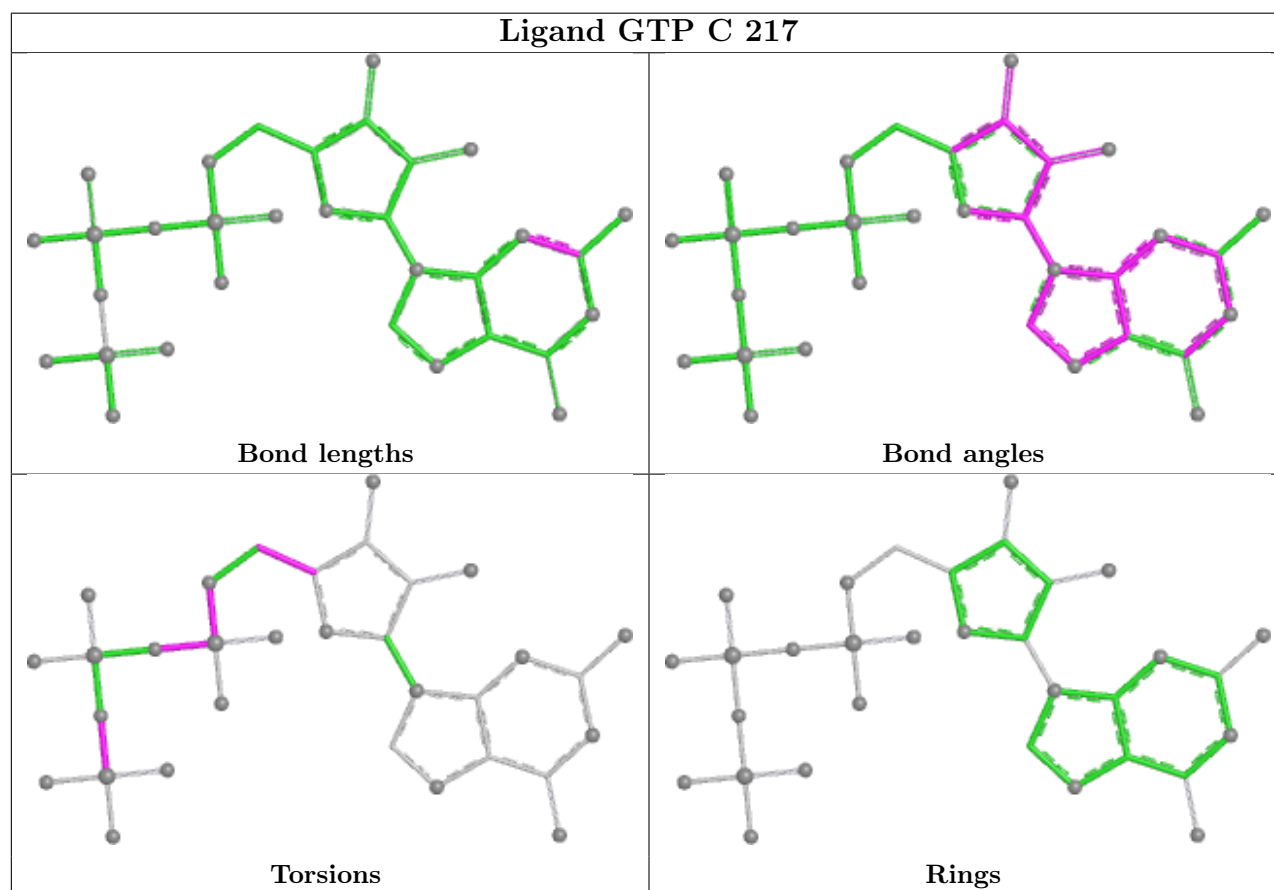
Mol	Chain	Res	Type	Atoms
4	C	217	GTP	PB-O3B-PG-O3G
4	C	217	GTP	C5'-O5'-PA-O3A
4	C	217	GTP	C5'-O5'-PA-O1A
4	C	217	GTP	C5'-O5'-PA-O2A
4	C	217	GTP	O4'-C4'-C5'-O5'

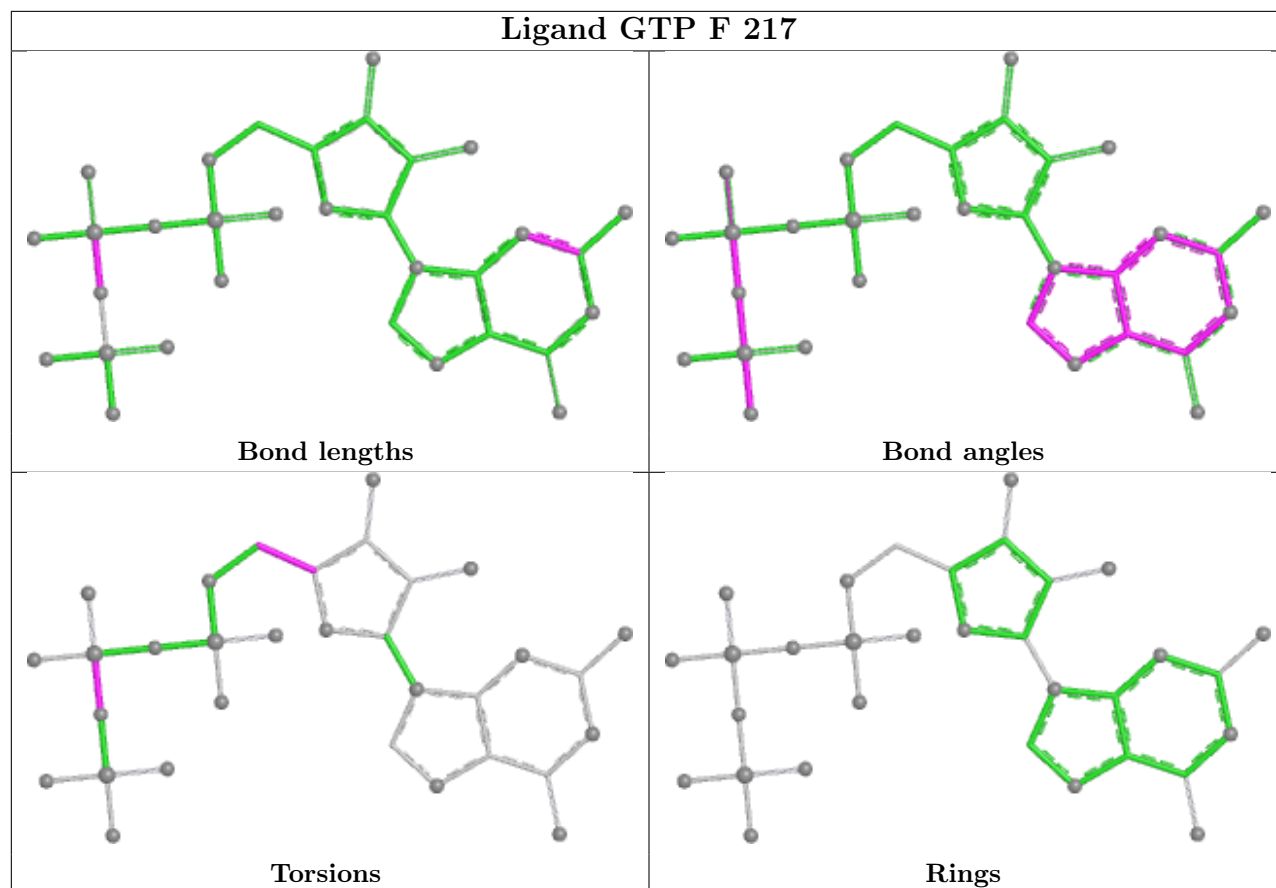
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	217	GTP	8	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	B	272/361 (75%)	-1.35	0 100 100	7, 29, 72, 91	4 (1%)
1	E	277/361 (76%)	-1.36	0 100 100	7, 29, 80, 111	7 (2%)
2	C	171/176 (97%)	-1.43	0 100 100	10, 28, 58, 84	1 (0%)
2	F	171/176 (97%)	-1.45	0 100 100	10, 27, 56, 80	0
3	A	1041/1073 (97%)	-1.35	1 (0%) 92 92	4, 35, 90, 141	6 (0%)
3	D	1041/1073 (97%)	-1.37	0 100 100	5, 35, 89, 147	13 (1%)
All	All	2973/3220 (92%)	-1.37	1 (0%) 100 100	4, 32, 85, 147	31 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	967	PRO	2.5

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](#)

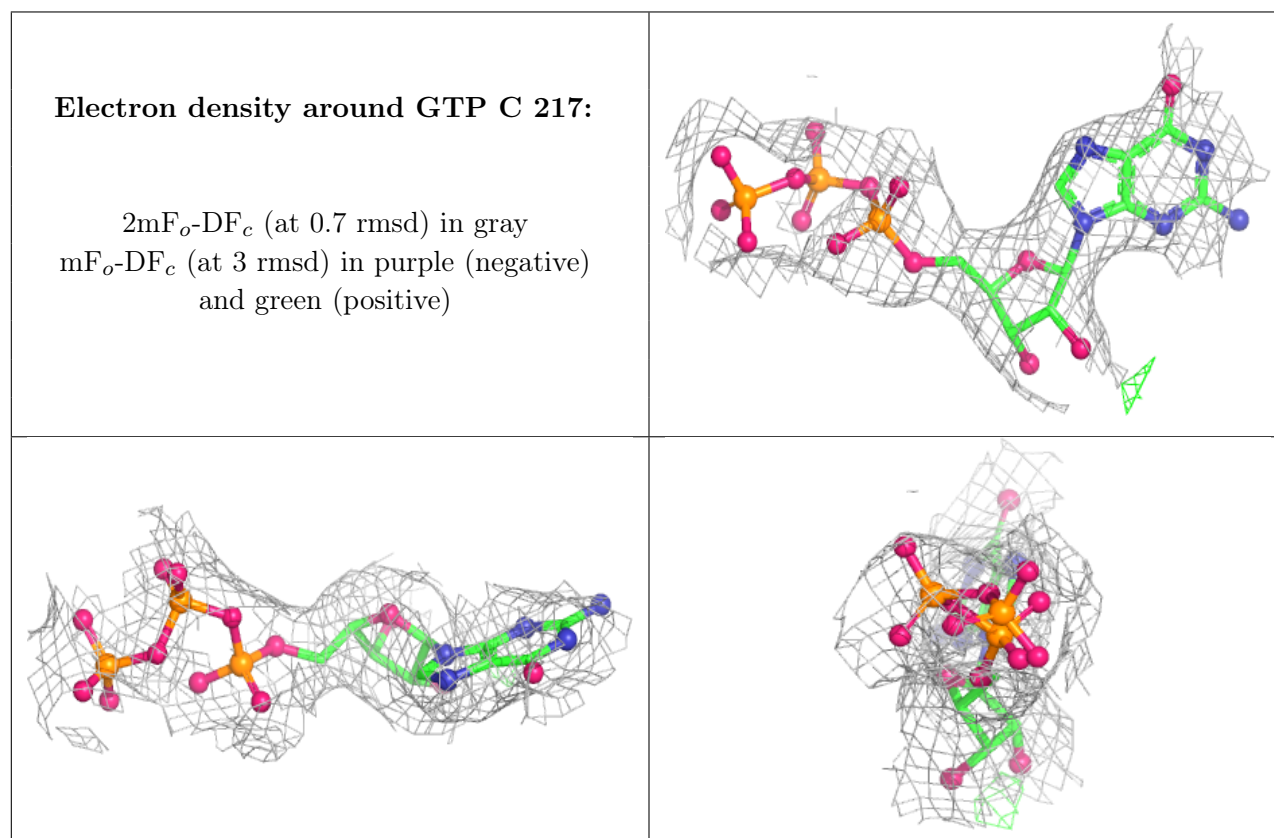
There are no oligosaccharides in this entry.

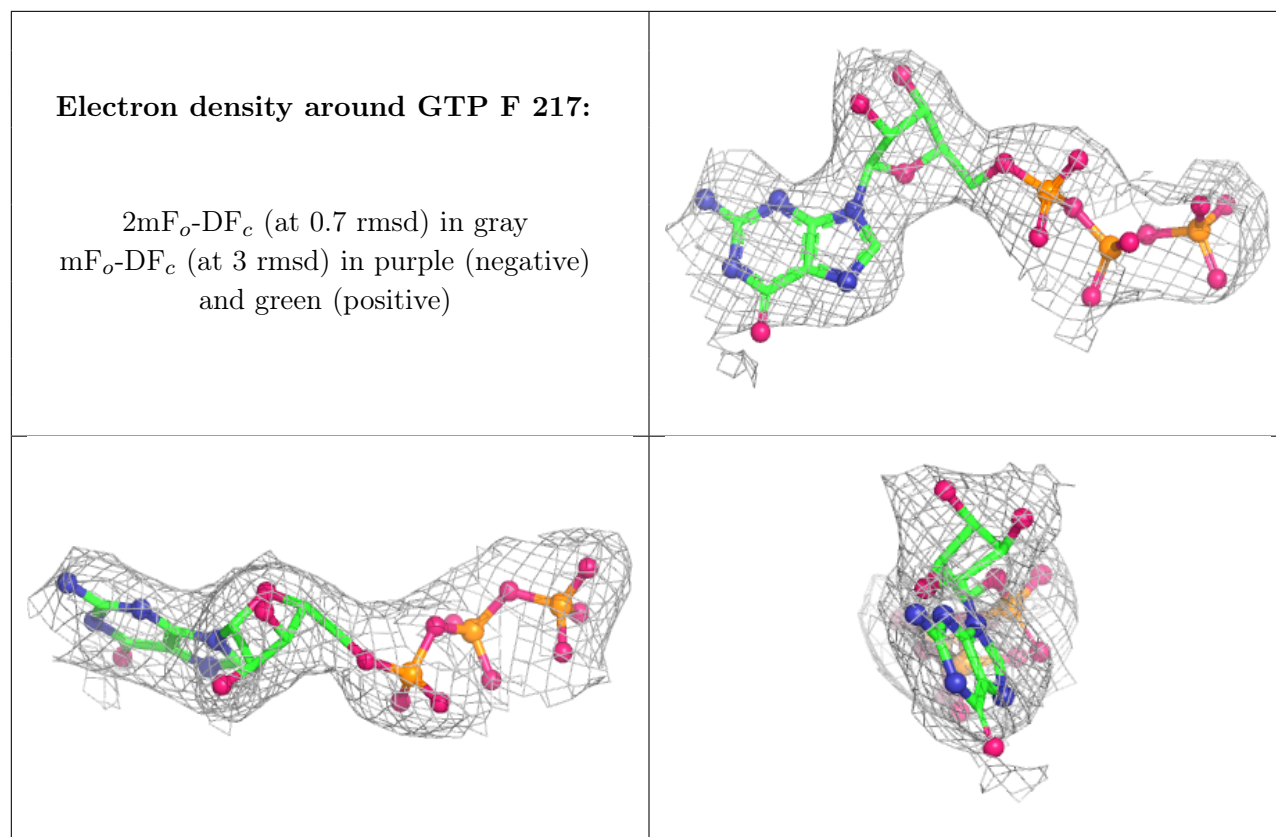
6.4 Ligands [i](#)

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
4	GTP	C	217	32/32	1.00	0.02	10,21,47,63	0
4	GTP	F	217	32/32	1.00	0.02	7,18,30,35	0
5	MG	C	218	1/1	1.00	0.04	0,0,0,0	0
5	MG	F	218	1/1	1.00	0.02	6,6,6,6	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.