



wwPDB X-ray Structure Validation Summary Report

Mar 9, 2026 – 04:01 AM UTC

PDB ID : 3NC0 / pdb_00003nc0
Title : Crystal structure of the HIV-1 Rev NES-CRM1-RanGTP nuclear export complex (crystal II)
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 : 2.90 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)
Xtrriage (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

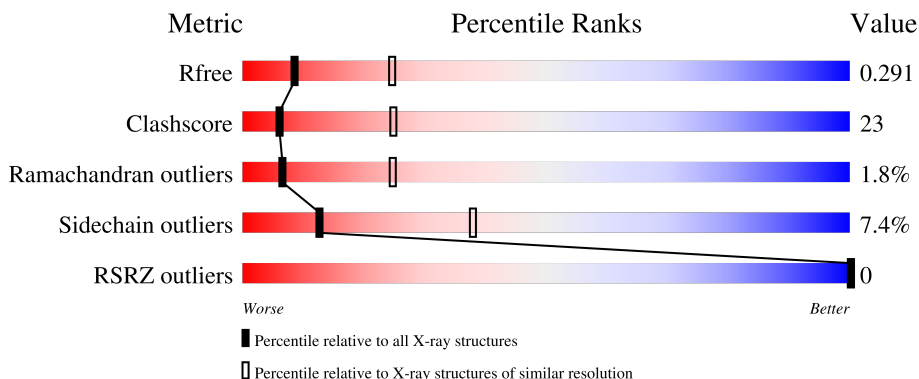
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	57% (green), 35% (yellow), 6% (orange), 2% (red), 0% (grey)
1	D	1073	55% (green), 36% (yellow), 6% (orange), 2% (red), 0% (grey)
2	B	362	41% (green), 34% (yellow), 6% (orange), 19% (grey)
2	E	362	41% (green), 34% (yellow), 6% (orange), 19% (grey)

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Mol	Chain	Length	Quality of chain
3	C	176	
3	F	176	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	1075	-	-	X	-

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 25190 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
			Total	C	N	O	S			
1	A	1038	8394	5387	1411	1543	53	0	0	0
1	D	1041	8414	5401	1413	1547	53	0	0	0

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
			Total	C	N	O	S			
2	B	293	2350	1498	405	432	15	0	0	0
2	E	294	2357	1502	406	434	15	0	0	0

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
			Total	C	N	O	S			
3	C	173	1405	914	246	240	5	0	0	0
3	F	173	1405	914	246	240	5	0	0	0

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 GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



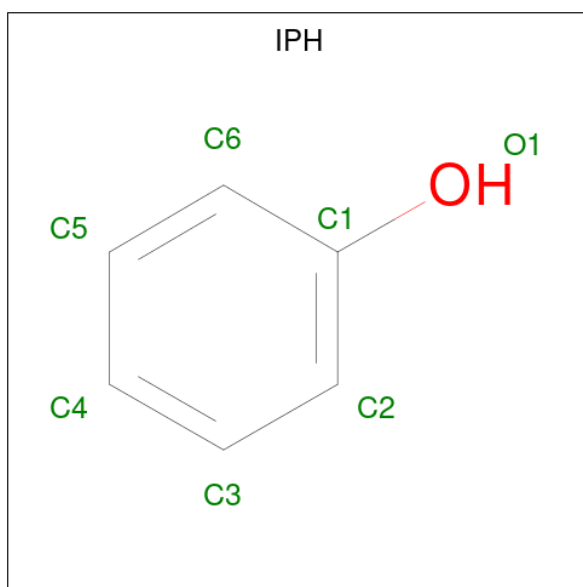
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	1
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 12 6 6	0	1
4	E	1	Total C O 6 3 3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



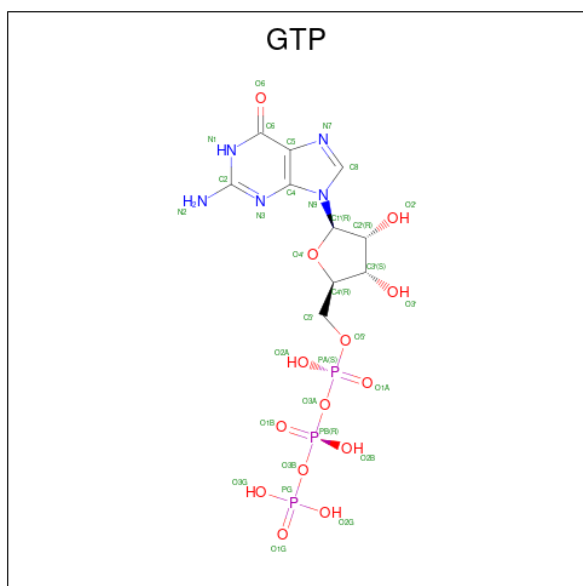
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	L	1	Total C O 7 4 3	0	0

- Molecule 6 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	1
			14	12	2		

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

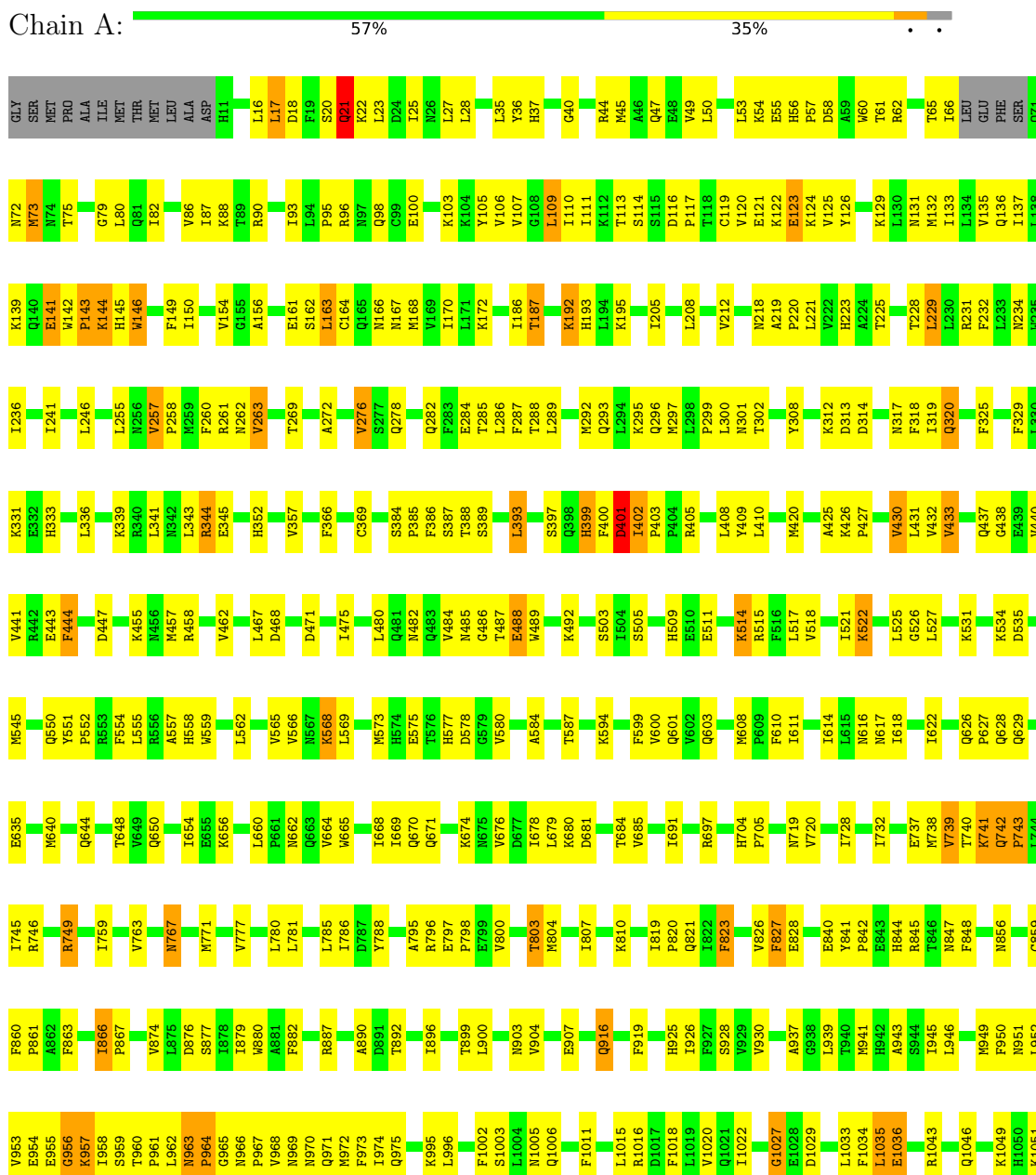
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	230	Total O 230 230	0	0
9	B	80	Total O 80 80	0	0
9	C	53	Total O 53 53	0	0
9	D	183	Total O 183 183	0	0
9	E	56	Total O 56 56	0	0
9	F	27	Total O 27 27	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.

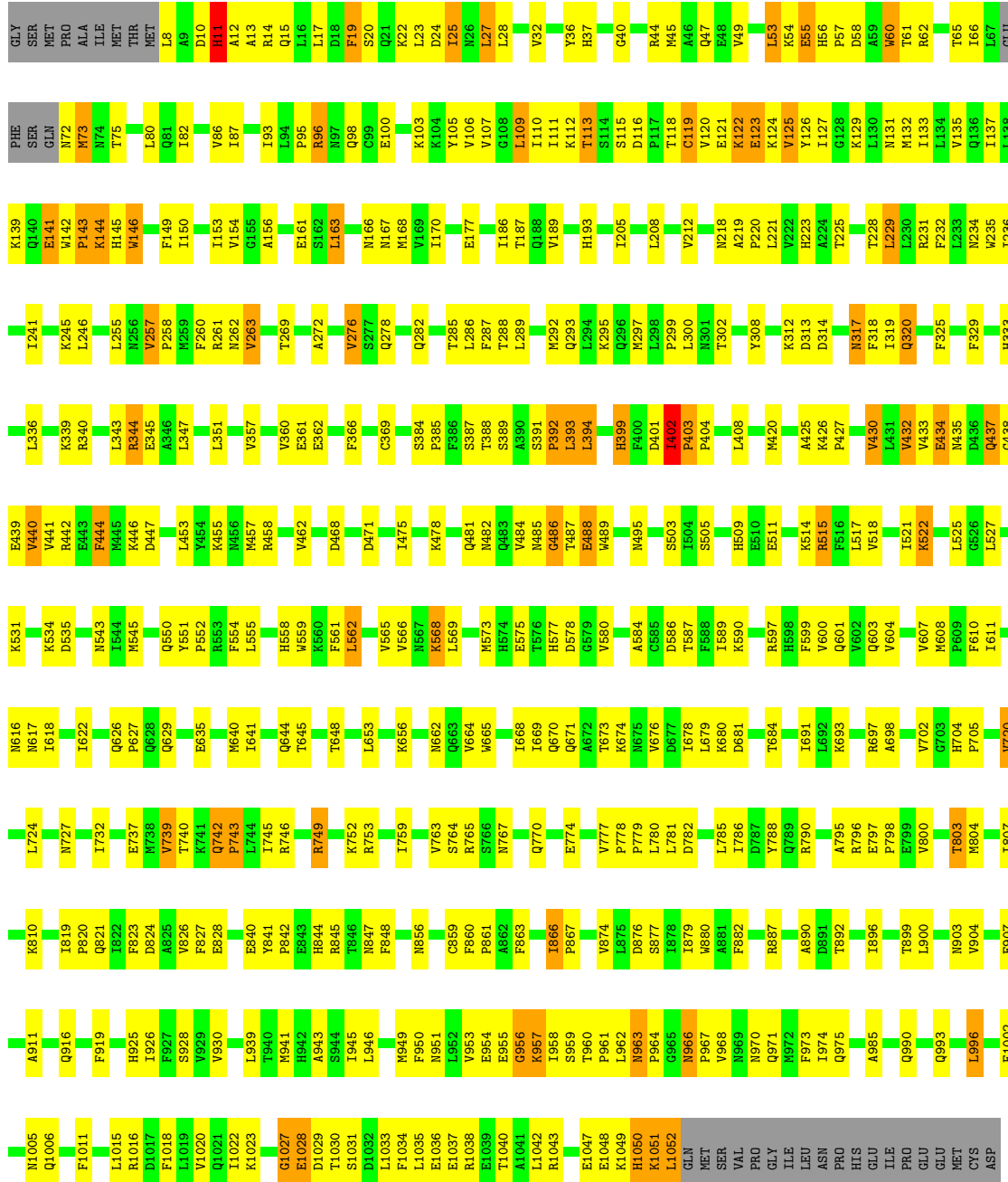
• Molecule 1: Exportin-1



L1052
GLN
MET
SER
PRO
VAL
PRO
ILE
GLY
LEU
ASN
PRO
HIS
GLU
ILE
PRO
GLU
GLU
MET
CYS
ASP

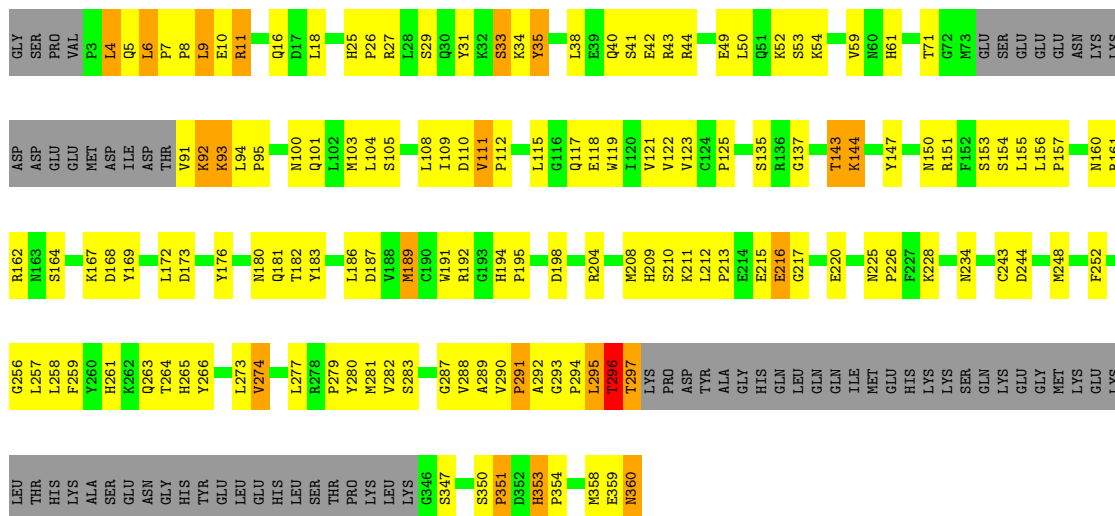
● Molecule 1: Exportin-1

Chain D: 55% 36% 6%

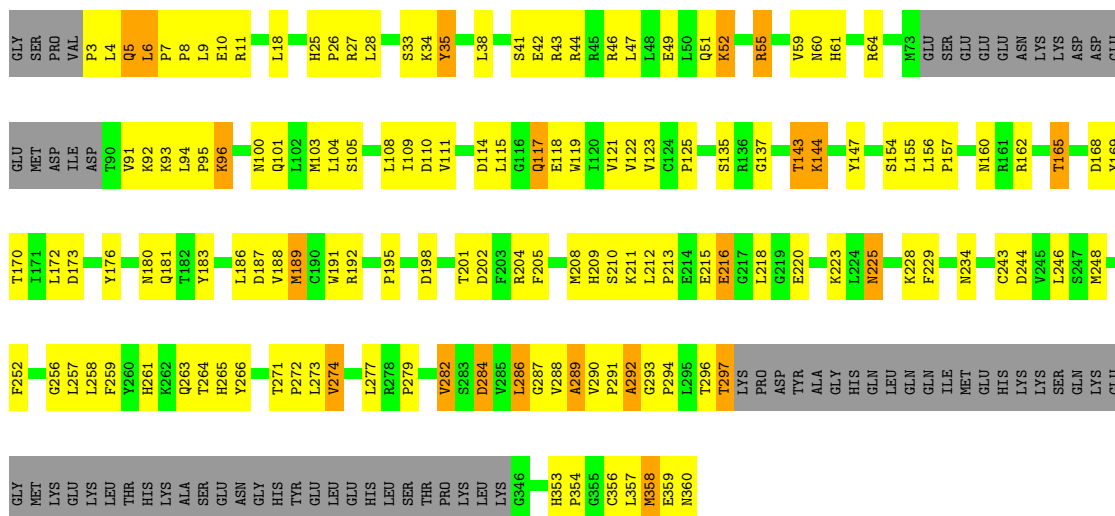


● Molecule 2: Snurportin-1

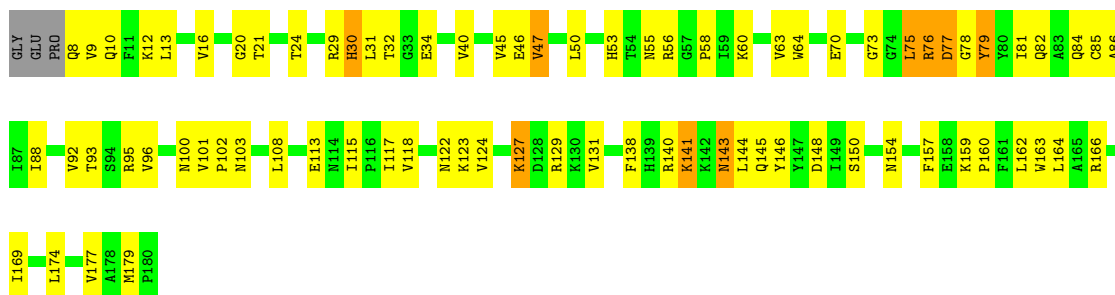
Chain B: 41% 34% 6% 19%



• Molecule 2: Snurportin-1



• Molecule 3: GTP-binding nuclear protein Ran



• Molecule 3: GTP-binding nuclear protein Ran

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.26Å 225.90Å 163.98Å 90.00° 100.75° 90.00°	Depositor
Resolution (Å)	39.05 – 2.90 39.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.5 (39.05-2.90) 85.6 (39.05-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.242 , 0.295 0.241 , 0.291	Depositor DCC
R_{free} test set	5517 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.136 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25190	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, GTP, MG, GOL, IPH

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	0.31	0/8566	0.74	10/11604 (0.1%)
1	D	0.32	0/8586	0.75	16/11632 (0.1%)
2	B	0.31	0/2415	0.82	5/3278 (0.2%)
2	E	0.31	0/2422	0.80	5/3288 (0.2%)
3	C	0.47	1/1440 (0.1%)	0.79	3/1945 (0.2%)
3	F	0.43	1/1440 (0.1%)	0.77	1/1945 (0.1%)
All	All	0.33	2/24869 (0.0%)	0.76	40/33692 (0.1%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	78	GLY	C-N	13.41	1.52	1.34
3	F	78	GLY	C-N	11.65	1.50	1.34

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	75	LEU	N-CA-C	-7.36	100.45	110.68
1	D	124	LYS	N-CA-C	-7.25	103.54	112.38
1	A	403	PRO	CA-C-N	7.12	126.64	119.24
1	A	403	PRO	C-N-CA	7.12	126.64	119.24
1	A	37	HIS	N-CA-C	6.59	119.74	111.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	119	CYS	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8394	0	8460	360	0
1	D	8414	0	8483	375	0
2	B	2350	0	2307	124	0
2	E	2357	0	2314	118	0
3	C	1405	0	1432	82	0
3	F	1405	0	1434	74	0
4	A	30	0	40	1	0
4	B	6	0	8	1	0
4	C	6	0	8	0	0
4	D	12	0	16	1	0
4	E	18	0	24	1	0
5	A	28	0	40	14	0
5	C	7	0	10	3	0
5	D	42	0	60	9	0
5	L	7	0	10	0	0
6	B	14	0	12	0	0
7	C	32	0	12	3	0
7	F	32	0	12	1	0
8	C	1	0	0	0	0
8	F	1	0	0	0	0
9	A	230	0	0	12	0
9	B	80	0	0	2	0
9	C	53	0	0	5	0
9	D	183	0	0	9	0
9	E	56	0	0	3	0
9	F	27	0	0	2	0
All	All	25190	0	24682	1112	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 1112 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:PHE:CZ	5:A:1075:PEG:H21	1.75	1.22
1:D:53:LEU:HG	1:D:54:LYS:H	1.17	1.08
3:C:76:ARG:HD2	5:C:182:PEG:H21	1.39	1.04
1:D:119:CYS:C	1:D:121:GLU:H	1.63	1.02
1:D:119:CYS:C	1:D:121:GLU:N	2.15	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1034/1073 (96%)	919 (89%)	95 (9%)	20 (2%)	6	23
1	D	1037/1073 (97%)	918 (88%)	103 (10%)	16 (2%)	8	28
2	B	287/362 (79%)	239 (83%)	39 (14%)	9 (3%)	3	14
2	E	288/362 (80%)	247 (86%)	35 (12%)	6 (2%)	5	21
3	C	171/176 (97%)	158 (92%)	12 (7%)	1 (1%)	21	51
3	F	171/176 (97%)	157 (92%)	13 (8%)	1 (1%)	21	51
All	All	2988/3222 (93%)	2638 (88%)	297 (10%)	53 (2%)	6	25

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	1029	ASP
1	A	1035	LEU
2	B	29	SER
2	B	216	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	A	942/973 (97%)	881 (94%)	61 (6%)	15	44
1	D	944/973 (97%)	875 (93%)	69 (7%)	13	38
2	B	264/327 (81%)	243 (92%)	21 (8%)	11	34
2	E	265/327 (81%)	247 (93%)	18 (7%)	14	42
3	C	152/154 (99%)	135 (89%)	17 (11%)	6	19
3	F	152/154 (99%)	137 (90%)	15 (10%)	7	24
All	All	2719/2908 (94%)	2518 (93%)	201 (7%)	13	38

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	163	LEU
1	D	531	LYS
3	F	148	ASP
1	D	245	LYS
1	D	402	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	53	HIS
2	E	263	GLN
1	D	167	ASN
2	E	261	HIS
3	F	154	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	GOL	A	1072[B]	-	5,5,5	0.36	0	5,5,5	0.31	0
5	PEG	D	1076	-	6,6,6	0.53	0	5,5,5	0.41	0
5	PEG	C	182	-	6,6,6	0.59	0	5,5,5	0.40	0
4	GOL	A	1079	-	5,5,5	0.38	0	5,5,5	0.33	0
4	GOL	D	1072	-	5,5,5	0.34	0	5,5,5	0.31	0
5	PEG	D	1073	-	6,6,6	0.57	0	5,5,5	0.35	0
4	GOL	A	1072[A]	-	5,5,5	0.37	0	5,5,5	0.28	0
4	GOL	E	361[B]	-	5,5,5	0.37	0	5,5,5	0.32	0
7	GTP	F	217	8	33,34,34	0.98	2 (6%)	50,54,54	1.63	10 (20%)
4	GOL	B	362	-	5,5,5	0.35	0	5,5,5	0.37	0
5	PEG	D	1078	-	6,6,6	0.56	0	5,5,5	0.49	0
4	GOL	A	1073	-	5,5,5	0.38	0	5,5,5	0.40	0
4	GOL	D	1079	-	5,5,5	0.37	0	5,5,5	0.30	0
5	PEG	L	29	-	6,6,6	0.39	0	5,5,5	0.79	0
4	GOL	E	361[A]	-	5,5,5	0.40	0	5,5,5	0.35	0
4	GOL	C	181	-	5,5,5	0.42	0	5,5,5	0.28	0
5	PEG	A	1076	-	6,6,6	0.60	0	5,5,5	0.37	0
5	PEG	A	1075	-	6,6,6	0.47	0	5,5,5	0.58	0
6	IPH	B	361[B]	-	7,7,7	0.42	0	8,8,8	0.35	0
5	PEG	D	1074	-	6,6,6	0.59	0	5,5,5	0.46	0
6	IPH	B	361[A]	-	7,7,7	0.45	0	8,8,8	0.30	0
5	PEG	D	1075	-	6,6,6	0.56	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	1074	-	5,5,5	0.38	0	5,5,5	0.37	0
5	PEG	D	1077	-	6,6,6	0.59	0	5,5,5	0.37	0
4	GOL	E	362	-	5,5,5	0.39	0	5,5,5	0.39	0
7	GTP	C	217	8	33,34,34	0.93	2 (6%)	50,54,54	1.55	8 (16%)
5	PEG	A	1078	-	6,6,6	0.54	0	5,5,5	0.57	0
5	PEG	A	1077	-	6,6,6	0.58	0	5,5,5	0.33	0

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	GOL	A	1072[B]	-	-	2/4/4/4	-
5	PEG	D	1076	-	-	0/4/4/4	-
5	PEG	C	182	-	-	0/4/4/4	-
4	GOL	A	1079	-	-	2/4/4/4	-
4	GOL	D	1072	-	-	3/4/4/4	-
5	PEG	D	1073	-	-	1/4/4/4	-
4	GOL	A	1072[A]	-	-	2/4/4/4	-
4	GOL	E	361[B]	-	-	2/4/4/4	-
7	GTP	F	217	8	-	2/22/38/38	0/3/3/3
4	GOL	B	362	-	-	2/4/4/4	-
5	PEG	D	1078	-	-	0/4/4/4	-
4	GOL	A	1073	-	-	0/4/4/4	-
4	GOL	D	1079	-	-	2/4/4/4	-
5	PEG	L	29	-	-	0/4/4/4	-
4	GOL	E	361[A]	-	-	2/4/4/4	-
4	GOL	C	181	-	-	1/4/4/4	-
5	PEG	A	1076	-	-	1/4/4/4	-
5	PEG	A	1075	-	-	0/4/4/4	-
6	IPH	B	361[B]	-	-	-	0/1/1/1
5	PEG	D	1074	-	-	1/4/4/4	-
6	IPH	B	361[A]	-	-	-	0/1/1/1
5	PEG	D	1075	-	-	0/4/4/4	-
4	GOL	A	1074	-	-	3/4/4/4	-
5	PEG	D	1077	-	-	0/4/4/4	-
4	GOL	E	362	-	-	0/4/4/4	-
7	GTP	C	217	8	-	2/22/38/38	0/3/3/3
5	PEG	A	1078	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	1077	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	217	GTP	PB-O3B	2.77	1.62	1.59
7	C	217	GTP	PB-O3B	2.21	1.61	1.59
7	F	217	GTP	C2-N3	2.15	1.38	1.33
7	C	217	GTP	C2-N3	2.05	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	217	GTP	C5-C4-N3	-5.06	120.34	128.39
7	C	217	GTP	C5-C4-N3	-4.90	120.59	128.39
7	F	217	GTP	C2-N3-C4	4.78	120.54	112.30
7	C	217	GTP	C2-N3-C4	4.70	120.39	112.30
7	C	217	GTP	N9-C4-N3	3.02	131.98	125.95

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1072[A]	GOL	O1-C1-C2-C3
4	A	1072[B]	GOL	O1-C1-C2-C3
4	A	1074	GOL	O1-C1-C2-C3
4	A	1079	GOL	O1-C1-C2-C3
4	B	362	GOL	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 34 short contacts:

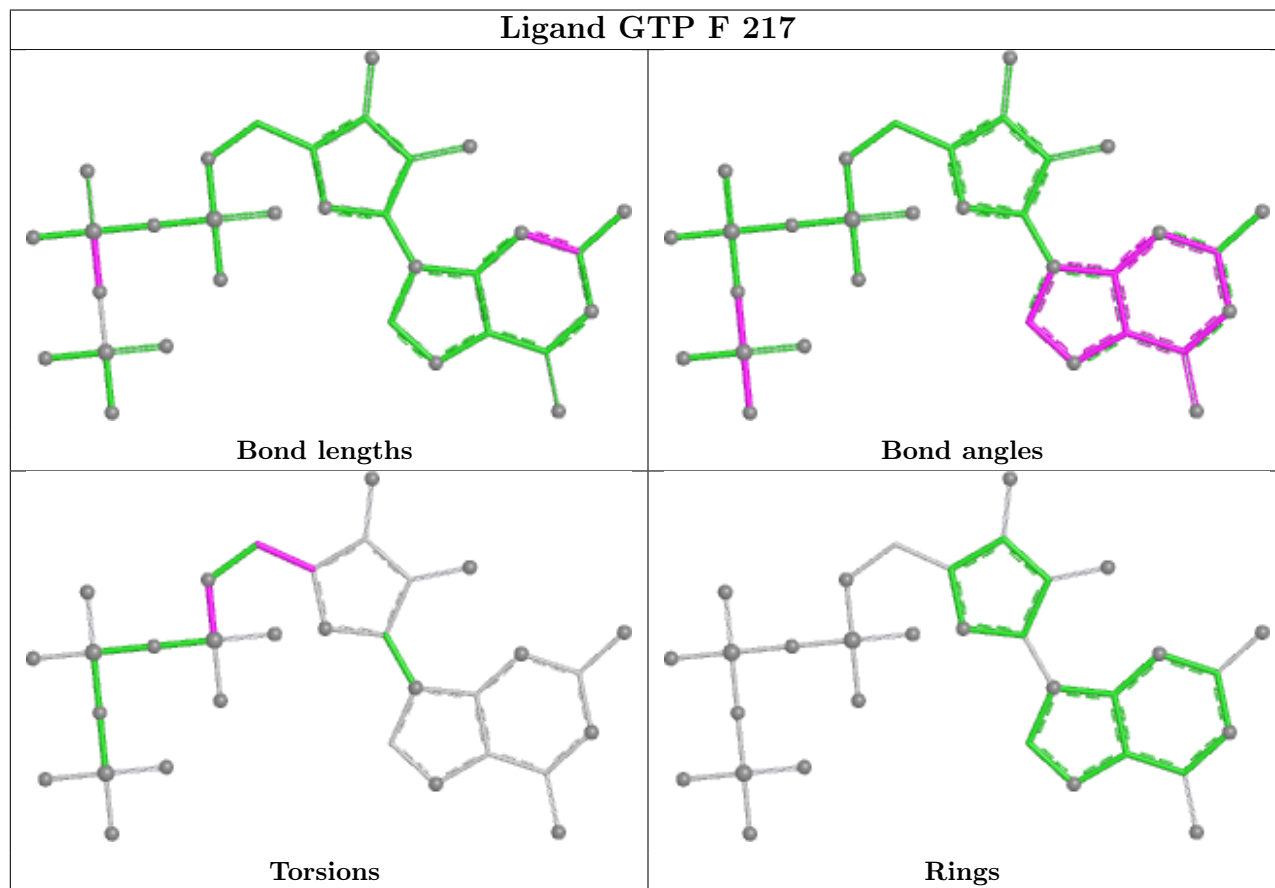
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1076	PEG	3	0
5	C	182	PEG	3	0
7	F	217	GTP	1	0
4	B	362	GOL	1	0
4	A	1073	GOL	1	0
4	D	1079	GOL	1	0
5	A	1075	PEG	12	0
5	D	1074	PEG	3	0

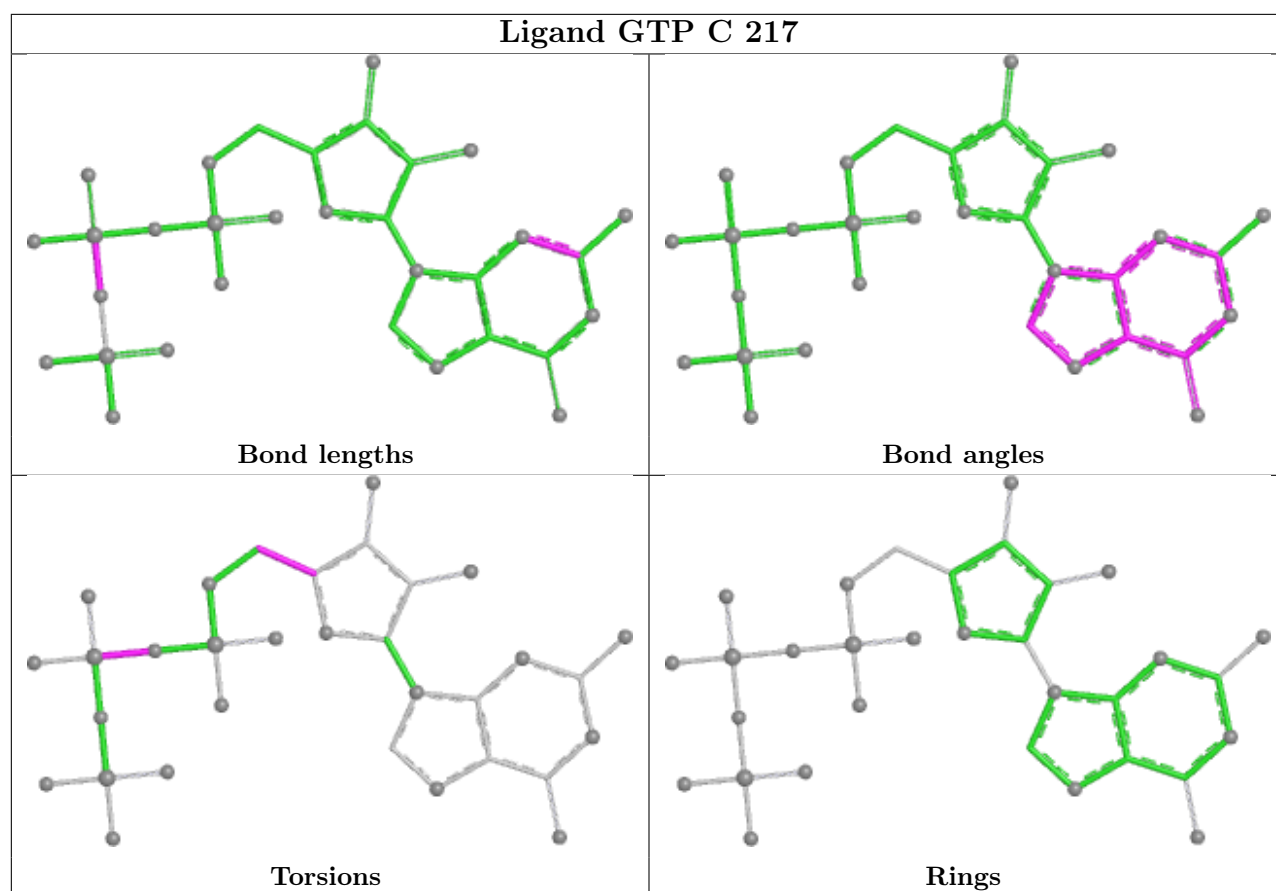
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1075	PEG	2	0
5	D	1077	PEG	1	0
4	E	362	GOL	1	0
7	C	217	GTP	3	0
5	A	1077	PEG	2	0

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 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%)	-1.32	0 100 100	10, 47, 101, 138	0
1	D	1041/1073 (97%)	-1.31	0 100 100	10, 47, 103, 163	0
2	B	293/362 (80%)	-1.36	0 100 100	15, 43, 104, 134	0
2	E	294/362 (81%)	-1.27	0 100 100	13, 43, 107, 145	0
3	C	173/176 (98%)	-1.47	0 100 100	17, 39, 79, 107	0
3	F	173/176 (98%)	-1.49	0 100 100	18, 39, 80, 118	0
All	All	3012/3222 (93%)	-1.34	0 100 100	10, 45, 101, 163	0

There are no RSRZ outliers to report.

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.

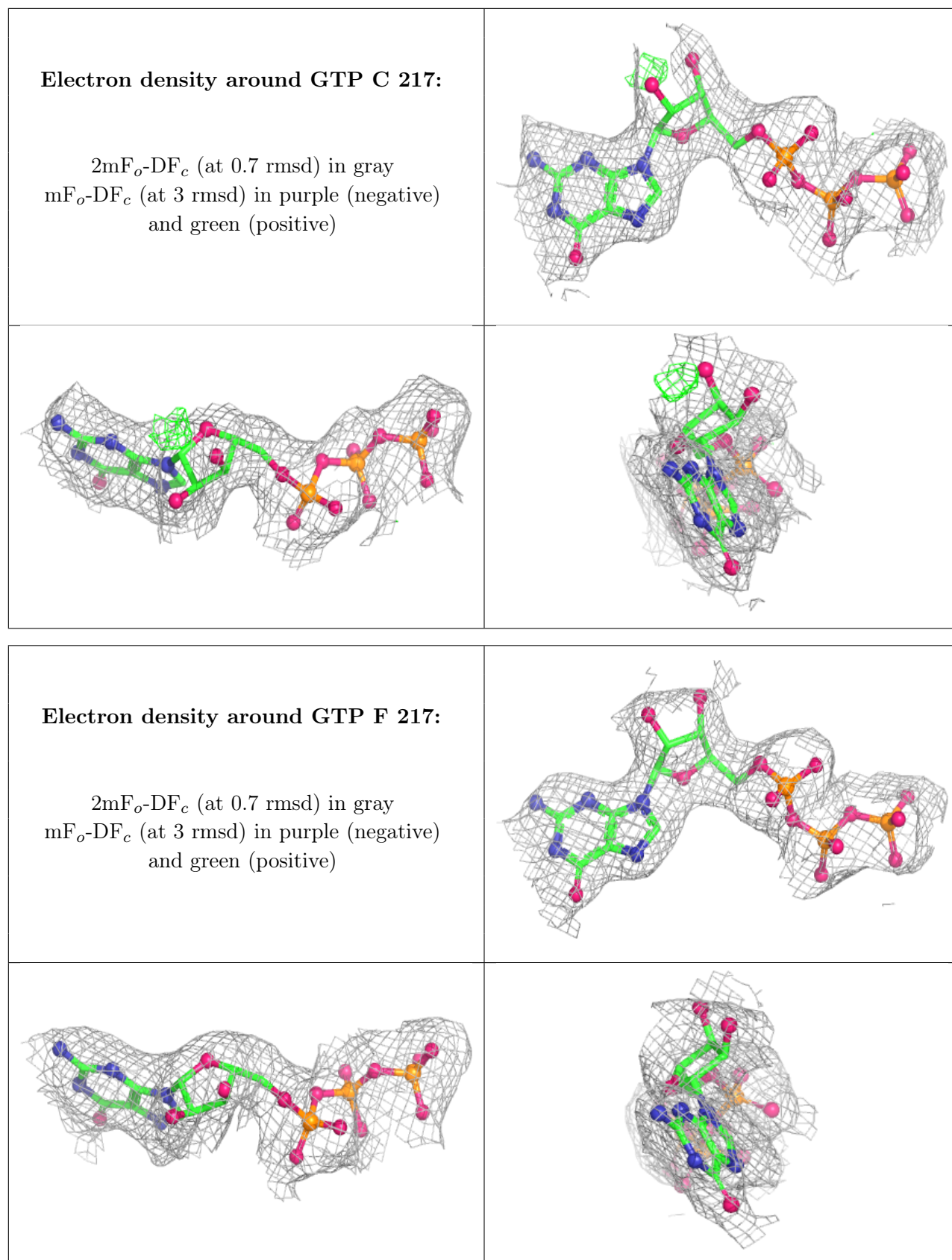
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	D	1077	7/7	0.93	0.19	59,76,82,91	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	1072[B]	6/6	0.94	0.10	14,18,51,51	6
4	GOL	A	1072[A]	6/6	0.94	0.10	3,27,51,51	6
4	GOL	D	1072	6/6	0.95	0.18	45,61,70,77	6
5	PEG	A	1078	7/7	0.95	0.16	49,62,74,77	7
5	PEG	C	182	7/7	0.95	0.16	55,60,68,72	7
4	GOL	A	1073	6/6	0.95	0.17	37,54,56,59	6
5	PEG	L	29	7/7	0.95	0.20	41,69,79,79	7
4	GOL	C	181	6/6	0.96	0.15	48,50,59,63	6
4	GOL	B	362	6/6	0.96	0.13	59,67,72,73	6
5	PEG	A	1075	7/7	0.96	0.09	84,88,95,101	7
5	PEG	A	1077	7/7	0.96	0.21	44,63,83,84	7
4	GOL	D	1079	6/6	0.97	0.14	42,66,72,73	6
4	GOL	E	361[A]	6/6	0.97	0.12	18,46,56,59	6
4	GOL	E	361[B]	6/6	0.97	0.12	18,40,57,60	6
5	PEG	D	1076	7/7	0.97	0.18	50,70,96,100	7
4	GOL	A	1079	6/6	0.97	0.10	56,72,75,79	6
5	PEG	D	1078	7/7	0.97	0.17	52,65,72,74	7
5	PEG	A	1076	7/7	0.97	0.14	47,59,73,76	7
5	PEG	D	1075	7/7	0.98	0.14	46,54,69,75	7
4	GOL	E	362	6/6	0.98	0.12	51,59,61,62	6
4	GOL	A	1074	6/6	0.98	0.14	41,55,66,71	6
5	PEG	D	1073	7/7	0.98	0.13	47,51,60,68	7
5	PEG	D	1074	7/7	0.98	0.10	36,49,54,61	7
6	IPH	B	361[A]	7/7	0.98	0.06	14,46,57,57	7
6	IPH	B	361[B]	7/7	0.98	0.06	43,54,55,56	7
7	GTP	C	217	32/32	1.00	0.02	9,21,46,53	1
7	GTP	F	217	32/32	1.00	0.03	5,27,48,65	0
8	MG	C	218	1/1	1.00	0.03	54,54,54,54	0
8	MG	F	218	1/1	1.00	0.02	35,35,35,35	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.