



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID : 3NC0
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

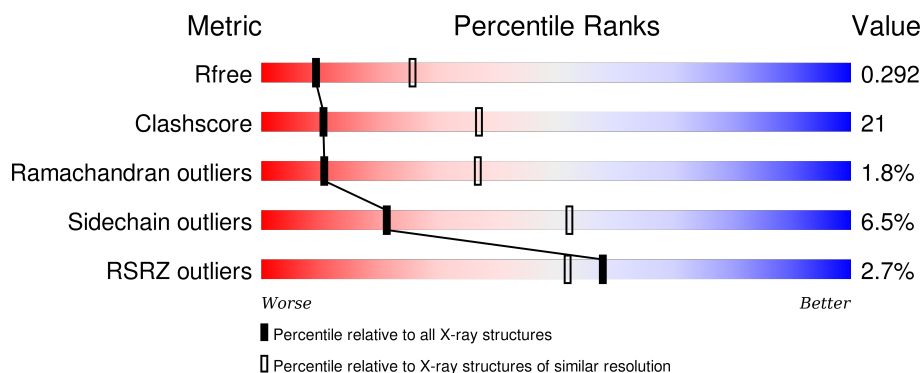
1 Overall quality at a glance

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>60% 33% . .</div> </div>
1	D	1073	<div> <div>3%</div> <div>57% 35% 5% .</div> </div>
2	B	362	<div> <div>4%</div> <div>44% 31% 6% 19%</div> </div>
2	E	362	<div> <div>4%</div> <div>45% 31% 5% 19%</div> </div>
3	C	176	<div> <div>56% 38% . .</div> </div>

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Mol	Chain	Length	Quality of chain
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
4	GOL	C	181	-	-	-	X
5	PEG	A	1075	-	-	X	-
5	PEG	A	1077	-	-	-	X
5	PEG	C	182	-	-	-	X
5	PEG	D	1074	-	-	-	X
5	PEG	D	1075	-	-	-	X
5	PEG	D	1076	-	-	-	X
5	PEG	D	1077	-	-	-	X
5	PEG	D	1078	-	-	-	X
5	PEG	L	29	-	-	-	X

2 Entry composition

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
1	A	1038	Total	C	N	O	S	0	0	0
			8394	5387	1411	1543	53			
1	D	1041	Total	C	N	O	S	0	0	0
			8414	5401	1413	1547	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	293	Total	C	N	O	S	0	0	0
			2350	1498	405	432	15			
2	E	294	Total	C	N	O	S	0	0	0
			2357	1502	406	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	UNP P62826
F	69	LEU	GLN	engineered	UNP P62826

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



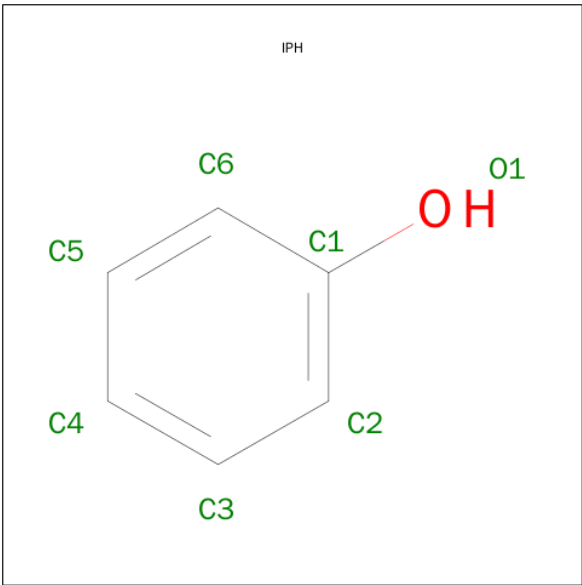
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



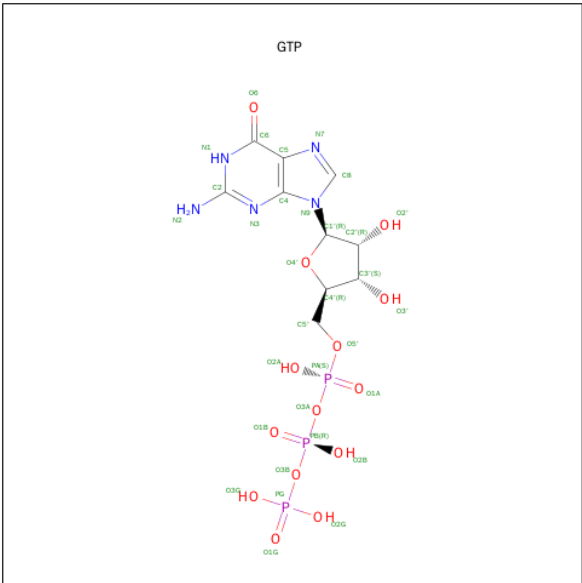
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total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

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

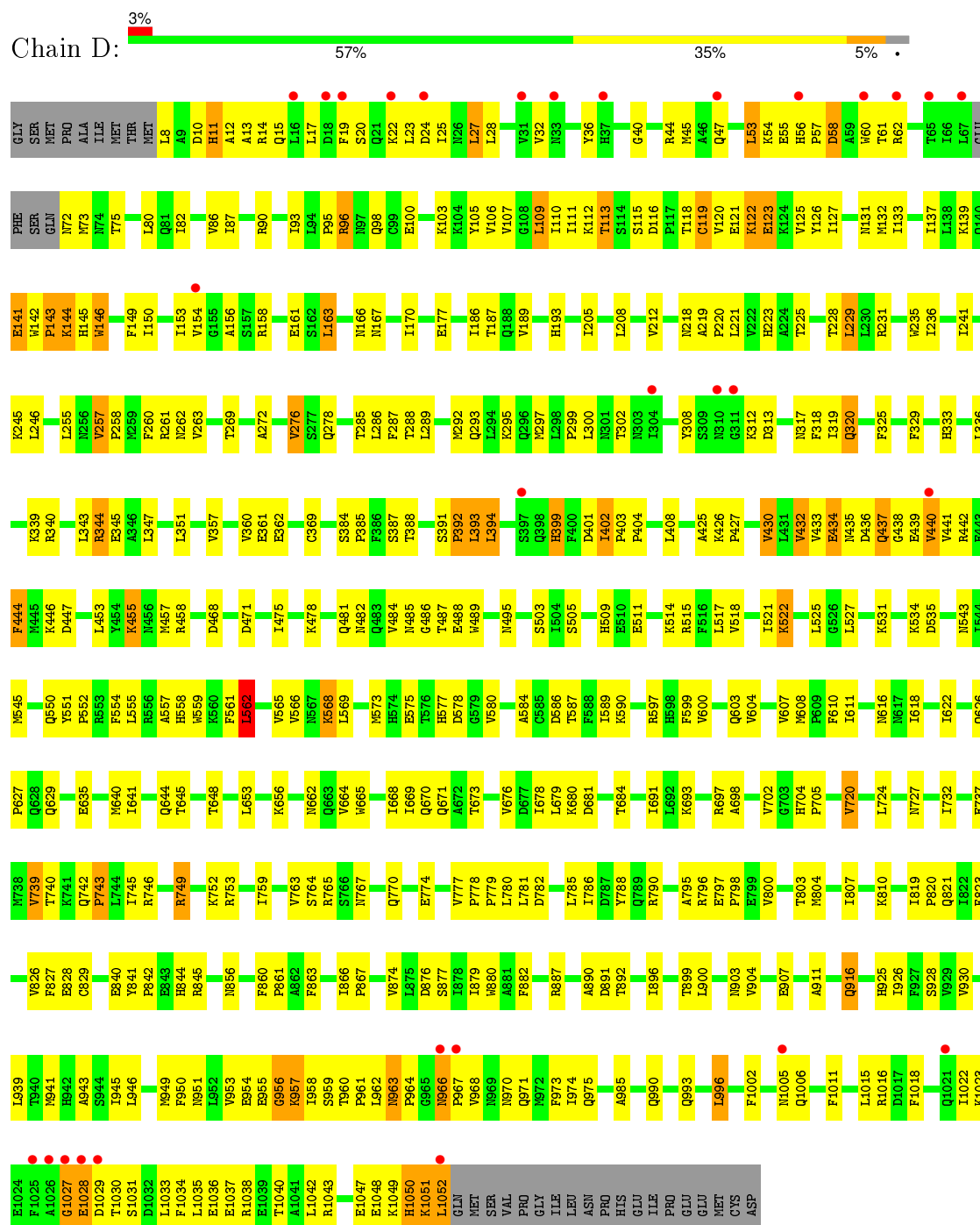
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total 1	Mg 1	0	0
8	F	1	Total 1	Mg 1	0	0

- Molecule 9 is water.

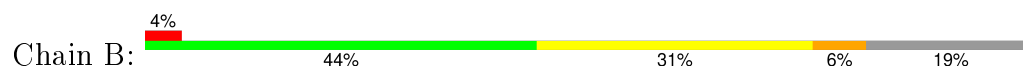
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	230	Total 230	O 230	0	0
9	B	80	Total 80	O 80	0	0
9	C	53	Total 53	O 53	0	0
9	D	183	Total 183	O 183	0	0
9	E	56	Total 56	O 56	0	0
9	F	27	Total 27	O 27	0	0

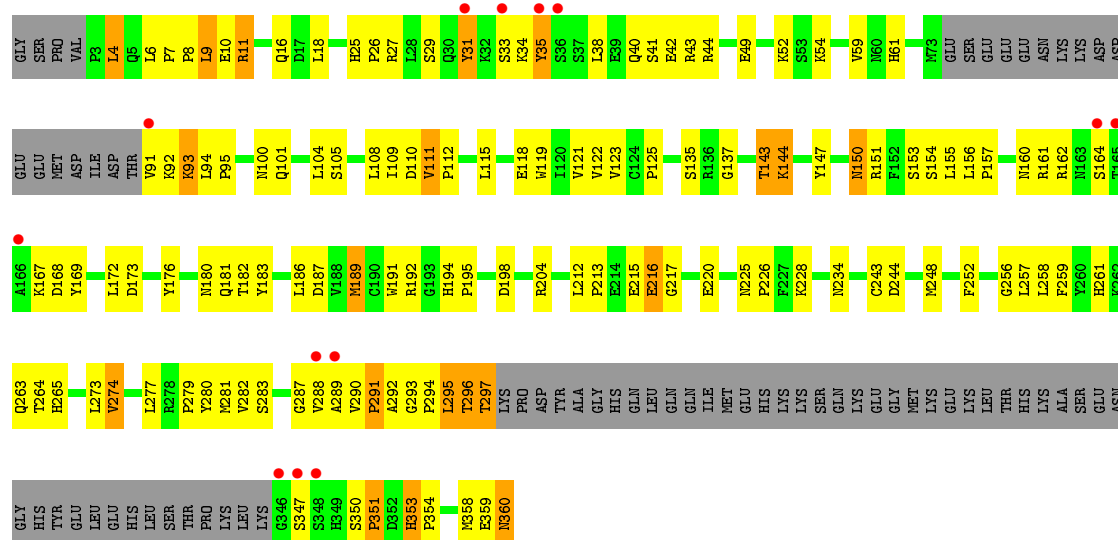
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- Molecule 1: Exportin-1

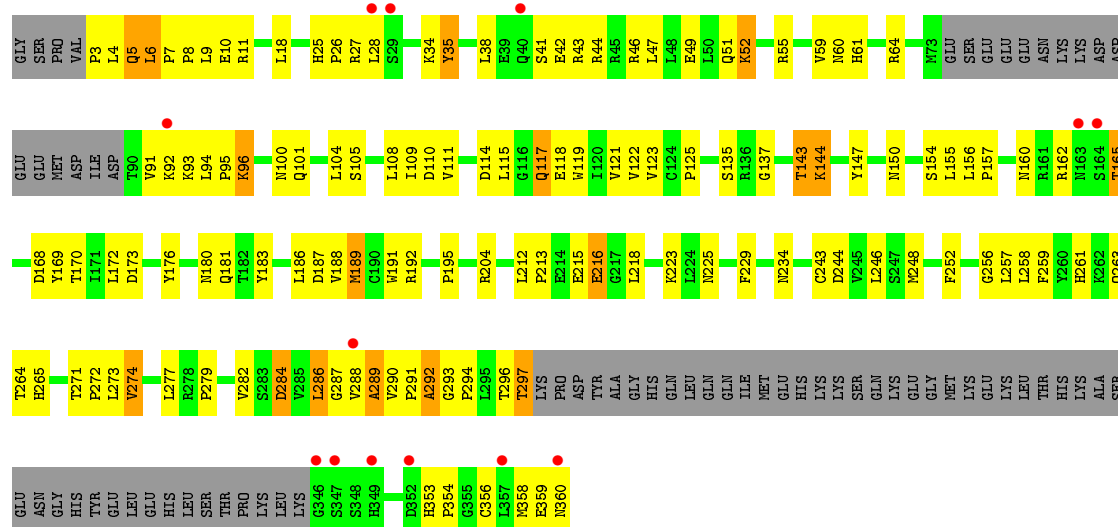


- Molecule 2: Snurportin-1

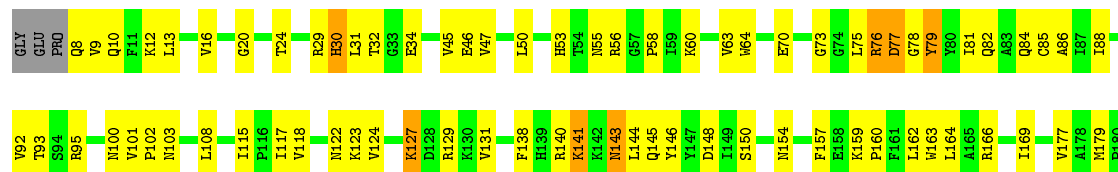




• Molecule 2: Snurportin-1

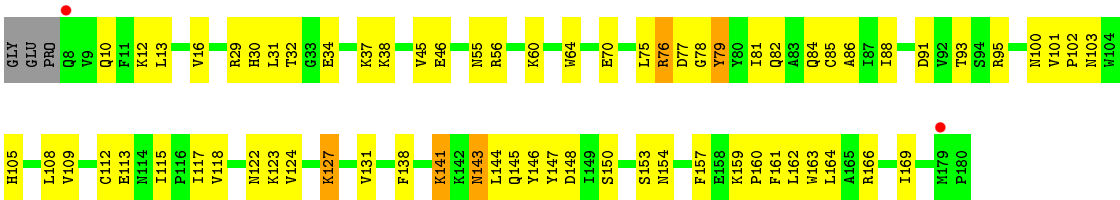


• Molecule 3: GTP-binding nuclear protein Ran



• Molecule 3: GTP-binding nuclear protein Ran





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.26 Å 225.90 Å 163.98 Å 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 2.90 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.242 , 0.295 0.244 , 0.292	Depositor DCC
R_{free} test set	5517 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.136 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 110320 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	25190	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 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: GTP, GOL, MG, PEG, 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	0.25	0/8566	0.42	1/11604 (0.0%)
1	D	0.24	0/8586	0.43	3/11632 (0.0%)
2	B	0.24	0/2415	0.46	0/3278
2	E	0.24	0/2422	0.46	0/3288
3	C	0.32	1/1440 (0.1%)	0.45	0/1945
3	F	0.31	1/1440 (0.1%)	0.44	0/1945
All	All	0.25	2/24869 (0.0%)	0.44	4/33692 (0.0%)

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	8.01	1.52	1.34
3	F	78	GLY	C-N	6.95	1.50	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	562	LEU	CA-CB-CG	5.39	127.71	115.30
1	D	158	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	158	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	D	158	ARG	NE-CZ-NH1	5.17	122.89	120.30

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 ⓘ

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	344	0
1	D	8414	0	8483	356	0
2	B	2350	0	2307	115	0
2	E	2357	0	2314	105	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	1055	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 21.

The worst 5 of 1055 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:A:386:PHE:CZ	5:A:1075:PEG:H31	1.97	0.98
1:D:119:CYS:C	1:D:121:GLU:H	1.63	0.98

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%)	10	35
1	D	1037/1073 (97%)	918 (88%)	103 (10%)	16 (2%)	13	42
2	B	287/362 (79%)	239 (83%)	39 (14%)	9 (3%)	5	21
2	E	288/362 (80%)	247 (86%)	35 (12%)	6 (2%)	9	32
3	C	171/176 (97%)	158 (92%)	12 (7%)	1 (1%)	30	67
3	F	171/176 (97%)	157 (92%)	13 (8%)	1 (1%)	30	67
All	All	2988/3222 (93%)	2638 (88%)	297 (10%)	53 (2%)	11	37

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 ⓘ

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%)	886 (94%)	56 (6%)	24	58
1	D	944/973 (97%)	880 (93%)	64 (7%)	20	49
2	B	264/327 (81%)	245 (93%)	19 (7%)	18	46
2	E	265/327 (81%)	246 (93%)	19 (7%)	18	46
3	C	152/154 (99%)	141 (93%)	11 (7%)	18	46
3	F	152/154 (99%)	143 (94%)	9 (6%)	24	58
All	All	2719/2908 (94%)	2541 (94%)	178 (6%)	21	52

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	93	THR
1	D	163	LEU
2	E	274	VAL
3	C	140	ARG
1	D	61	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	103	ASN
1	D	165	GLN
3	F	53	HIS
3	C	105	HIS
3	C	156	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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[A]	-	5,5,5	0.35	0	5,5,5	0.22	0
4	GOL	A	1072[B]	-	5,5,5	0.34	0	5,5,5	0.24	0
4	GOL	A	1073	-	5,5,5	0.34	0	5,5,5	0.34	0
4	GOL	A	1074	-	5,5,5	0.34	0	5,5,5	0.27	0
5	PEG	A	1075	-	6,6,6	0.46	0	5,5,5	0.59	0
5	PEG	A	1076	-	6,6,6	0.60	0	5,5,5	0.38	0
5	PEG	A	1077	-	6,6,6	0.57	0	5,5,5	0.34	0
5	PEG	A	1078	-	6,6,6	0.54	0	5,5,5	0.58	0
4	GOL	A	1079	-	5,5,5	0.34	0	5,5,5	0.25	0
6	IPH	B	361[A]	-	7,7,7	0.43	0	8,8,8	0.23	0
6	IPH	B	361[B]	-	7,7,7	0.41	0	8,8,8	0.28	0
4	GOL	B	362	-	5,5,5	0.32	0	5,5,5	0.28	0
4	GOL	C	181	-	5,5,5	0.36	0	5,5,5	0.23	0
5	PEG	C	182	-	6,6,6	0.58	0	5,5,5	0.41	0
7	GTP	C	217	8	25,34,34	0.92	1 (4%)	34,54,54	1.72	6 (17%)
4	GOL	D	1072	-	5,5,5	0.30	0	5,5,5	0.23	0
5	PEG	D	1073	-	6,6,6	0.56	0	5,5,5	0.36	0
5	PEG	D	1074	-	6,6,6	0.59	0	5,5,5	0.46	0
5	PEG	D	1075	-	6,6,6	0.55	0	5,5,5	0.39	0
5	PEG	D	1076	-	6,6,6	0.52	0	5,5,5	0.44	0
5	PEG	D	1077	-	6,6,6	0.58	0	5,5,5	0.38	0
5	PEG	D	1078	-	6,6,6	0.55	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	1079	-	5,5,5	0.34	0	5,5,5	0.23	0
4	GOL	E	361[A]	-	5,5,5	0.35	0	5,5,5	0.25	0
4	GOL	E	361[B]	-	5,5,5	0.35	0	5,5,5	0.23	0
4	GOL	E	362	-	5,5,5	0.34	0	5,5,5	0.32	0
7	GTP	F	217	8	25,34,34	0.90	1 (4%)	34,54,54	1.76	7 (20%)
5	PEG	L	29	-	6,6,6	0.38	0	5,5,5	0.81	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[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1072[B]	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1073	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1074	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1075	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1076	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1077	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1078	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1079	-	-	0/4/4/4	0/0/0/0
6	IPH	B	361[A]	-	-	0/0/0/0	0/1/1/1
6	IPH	B	361[B]	-	-	0/0/0/0	0/1/1/1
4	GOL	B	362	-	-	0/4/4/4	0/0/0/0
4	GOL	C	181	-	-	0/4/4/4	0/0/0/0
5	PEG	C	182	-	-	0/4/4/4	0/0/0/0
7	GTP	C	217	8	-	0/18/38/38	0/3/3/3
4	GOL	D	1072	-	-	0/4/4/4	0/0/0/0
5	PEG	D	1073	-	-	0/4/4/4	0/0/0/0
5	PEG	D	1074	-	-	0/4/4/4	0/0/0/0
5	PEG	D	1075	-	-	0/4/4/4	0/0/0/0
5	PEG	D	1076	-	-	0/4/4/4	0/0/0/0
5	PEG	D	1077	-	-	0/4/4/4	0/0/0/0
5	PEG	D	1078	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1079	-	-	0/4/4/4	0/0/0/0
4	GOL	E	361[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	E	361[B]	-	-	0/4/4/4	0/0/0/0
4	GOL	E	362	-	-	0/4/4/4	0/0/0/0
7	GTP	F	217	8	-	0/18/38/38	0/3/3/3
5	PEG	L	29	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	217	GTP	C6-N1	2.73	1.38	1.33
7	C	217	GTP	C6-N1	2.79	1.38	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	217	GTP	N3-C2-N1	-4.90	119.98	127.44
7	F	217	GTP	N3-C2-N1	-4.88	120.02	127.44
7	F	217	GTP	PB-O3B-PG	-3.79	119.94	132.67
7	C	217	GTP	PA-O3A-PB	-3.76	122.18	132.73
7	F	217	GTP	PA-O3A-PB	-3.49	122.93	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1073	GOL	1	0
5	A	1075	PEG	12	0
5	A	1077	PEG	2	0
4	B	362	GOL	1	0
5	C	182	PEG	3	0
7	C	217	GTP	3	0
5	D	1074	PEG	3	0
5	D	1075	PEG	2	0
5	D	1076	PEG	3	0
5	D	1077	PEG	1	0
4	D	1079	GOL	1	0
4	E	362	GOL	1	0
7	F	217	GTP	1	0

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

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, 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%)	-0.03	22 (2%) 67 62	10, 47, 101, 138	0
1	D	1041/1073 (97%)	0.03	30 (2%) 55 49	10, 47, 103, 163	0
2	B	293/362 (80%)	0.10	13 (4%) 38 32	15, 43, 104, 134	0
2	E	294/362 (81%)	0.08	13 (4%) 38 32	13, 43, 107, 145	0
3	C	173/176 (98%)	-0.14	0 100 100	17, 39, 79, 107	0
3	F	173/176 (98%)	-0.10	2 (1%) 81 78	18, 39, 80, 118	0
All	All	3012/3222 (93%)	0.00	80 (2%) 58 52	10, 45, 101, 163	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	PHE	11.1
1	D	967	PRO	8.9
2	B	91	VAL	7.0
1	A	966	ASN	5.9
1	D	966	ASN	5.9

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
5	PEG	D	1076	7/7	0.78	0.47	9.72	50,70,96,100	7
4	GOL	C	181	6/6	0.76	0.44	5.82	48,50,59,63	6
5	PEG	D	1075	7/7	0.85	0.38	5.45	46,54,69,75	7
5	PEG	D	1077	7/7	0.78	0.35	4.76	59,76,82,91	7
5	PEG	A	1077	7/7	0.56	0.49	4.42	44,63,83,84	7
5	PEG	D	1078	7/7	0.80	0.41	2.14	52,65,72,74	7
5	PEG	C	182	7/7	0.75	0.41	1.92	55,60,68,72	7
4	GOL	E	362	6/6	0.78	0.32	1.16	51,59,61,62	6
5	PEG	L	29	7/7	0.66	0.40	1.14	41,69,79,79	7
5	PEG	D	1074	7/7	0.78	0.42	1.09	36,49,54,61	7
4	GOL	E	361[B]	6/6	0.91	0.19	0.85	18,40,57,60	6
4	GOL	E	361[A]	6/6	0.91	0.19	0.27	18,46,56,59	6
8	MG	F	218	1/1	0.59	0.18	-0.03	35,35,35,35	0
7	GTP	F	217	32/32	0.97	0.18	-0.12	5,27,48,65	0
7	GTP	C	217	32/32	0.97	0.17	-0.34	9,21,46,53	1
4	GOL	B	362	6/6	0.83	0.34	-	59,67,72,73	6
6	IPH	B	361[A]	7/7	0.66	0.28	-	14,46,57,57	7
4	GOL	A	1074	6/6	0.77	0.40	-	41,55,66,71	6
6	IPH	B	361[B]	7/7	0.66	0.28	-	43,54,55,56	7
5	PEG	A	1075	7/7	0.51	0.45	-	84,88,95,101	7
4	GOL	A	1079	6/6	0.86	0.41	-	56,72,75,79	6
4	GOL	D	1072	6/6	0.84	0.39	-	45,61,70,77	6
4	GOL	D	1079	6/6	0.77	0.37	-	42,66,72,73	6
5	PEG	A	1076	7/7	0.79	0.34	-	47,59,73,76	7
4	GOL	A	1073	6/6	0.86	0.44	-	37,54,56,59	6
4	GOL	A	1072[B]	6/6	0.89	0.13	-	14,18,51,51	6
8	MG	C	218	1/1	0.89	0.18	-	54,54,54,54	0
4	GOL	A	1072[A]	6/6	0.89	0.13	-	3,27,51,51	6
5	PEG	D	1073	7/7	0.75	0.48	-	47,51,60,68	7
5	PEG	A	1078	7/7	0.69	0.51	-	49,62,74,77	7

6.5 Other polymers [i](#)

There are no such residues in this entry.