



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:22 PM GMT

PDB ID : 3WYF  
Title : Crystal structure of Xpo1p-Yrb2p-Gsp1p-GTP complex  
Authors : Koyama, M.; Shirai, N.; Matsuura, Y.  
Deposited on : 2014-08-26  
Resolution : 2.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

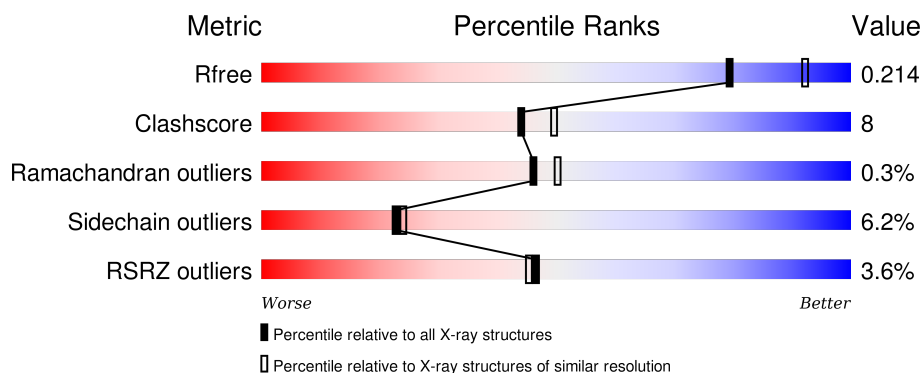
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.22 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.



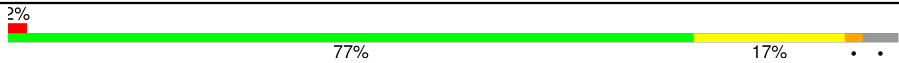
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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  $\geq 3$ , 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	219	<div> <div>4%</div> <div>68% 16% • 14%</div> </div>
1	D	219	<div> <div>•</div> <div>65% 18% • 16%</div> </div>
2	B	238	<div> <div>11%</div> <div>43% 14% • 39%</div> </div>
2	E	238	<div> <div>7%</div> <div>35% 19% • • 40%</div> </div>
3	C	1049	<div> <div>3%</div> <div>81% 17% ••</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	1049	 A horizontal bar chart showing the quality of chain F. The bar is divided into segments: a small red segment at the beginning labeled '2%', followed by a long green segment labeled '77%', then a yellow segment labeled '17%', and a small grey segment at the end. Two small black dots are visible at the far right of the bar.

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22420 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 Gsp1p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1492	973	252	262	5			
1	D	185	Total	C	N	O	S	0	0	0
			1459	953	245	257	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LEU	GLN	ENGINEERED MUTATION	UNP E7KFU1
D	71	LEU	GLN	ENGINEERED MUTATION	UNP E7KFU1

- Molecule 2 is a protein called Ran-specific GTPase-activating protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1073	691	180	200	2			
2	E	142	Total	C	N	O	S	0	0	0
			1074	690	181	201	2			

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1040	Total	C	N	O	S	0	0	0
			8322	5348	1361	1573	40			
3	F	1005	Total	C	N	O	S	0	0	0
			8046	5179	1316	1512	39			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P30822
C	0	ALA	-	EXPRESSION TAG	UNP P30822

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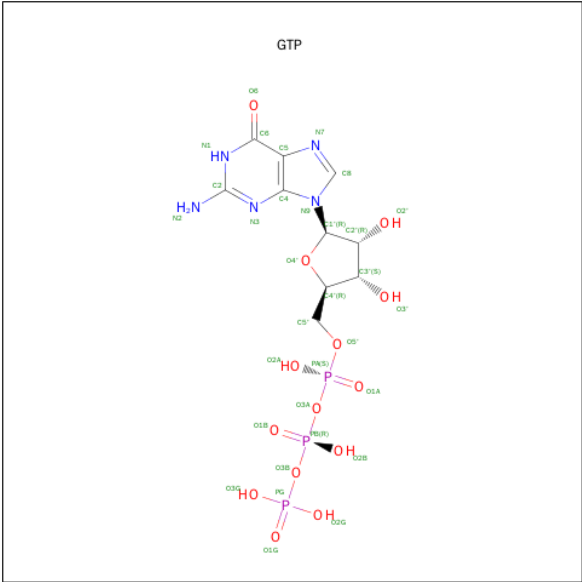
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	DELETION	UNP P30822
C	?	-	GLN	DELETION	UNP P30822
C	?	-	ARG	DELETION	UNP P30822
C	?	-	LEU	DELETION	UNP P30822
C	?	-	PRO	DELETION	UNP P30822
C	?	-	ALA	DELETION	UNP P30822
C	?	-	THR	DELETION	UNP P30822
C	?	-	GLU	DELETION	UNP P30822
C	?	-	MET	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	PRO	DELETION	UNP P30822
C	?	-	LEU	DELETION	UNP P30822
C	?	-	ILE	DELETION	UNP P30822
C	?	-	GLN	DELETION	UNP P30822
C	?	-	LEU	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	VAL	DELETION	UNP P30822
C	?	-	GLY	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	GLN	DELETION	UNP P30822
C	?	-	ALA	DELETION	UNP P30822
C	?	-	ILE	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	THR	DELETION	UNP P30822
C	?	-	GLY	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	GLY	DELETION	UNP P30822
C	?	-	ALA	DELETION	UNP P30822
C	?	-	LEU	DELETION	UNP P30822
C	?	-	ASN	DELETION	UNP P30822
C	?	-	PRO	DELETION	UNP P30822
C	?	-	GLU	DELETION	UNP P30822
C	?	-	TYR	DELETION	UNP P30822
C	?	-	MET	DELETION	UNP P30822
C	?	-	LYS	DELETION	UNP P30822
C	?	-	ARG	DELETION	UNP P30822
C	?	-	PHE	DELETION	UNP P30822
F	-1	GLY	-	EXPRESSION TAG	UNP P30822
F	0	ALA	-	EXPRESSION TAG	UNP P30822
F	?	-	VAL	DELETION	UNP P30822
F	?	-	GLN	DELETION	UNP P30822
F	?	-	ARG	DELETION	UNP P30822

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	LEU	DELETION	UNP P30822
F	?	-	PRO	DELETION	UNP P30822
F	?	-	ALA	DELETION	UNP P30822
F	?	-	THR	DELETION	UNP P30822
F	?	-	GLU	DELETION	UNP P30822
F	?	-	MET	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	PRO	DELETION	UNP P30822
F	?	-	LEU	DELETION	UNP P30822
F	?	-	ILE	DELETION	UNP P30822
F	?	-	GLN	DELETION	UNP P30822
F	?	-	LEU	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	VAL	DELETION	UNP P30822
F	?	-	GLY	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	GLN	DELETION	UNP P30822
F	?	-	ALA	DELETION	UNP P30822
F	?	-	ILE	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	THR	DELETION	UNP P30822
F	?	-	GLY	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	GLY	DELETION	UNP P30822
F	?	-	ALA	DELETION	UNP P30822
F	?	-	LEU	DELETION	UNP P30822
F	?	-	ASN	DELETION	UNP P30822
F	?	-	PRO	DELETION	UNP P30822
F	?	-	GLU	DELETION	UNP P30822
F	?	-	TYR	DELETION	UNP P30822
F	?	-	MET	DELETION	UNP P30822
F	?	-	LYS	DELETION	UNP P30822
F	?	-	ARG	DELETION	UNP P30822
F	?	-	PHE	DELETION	UNP P30822

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total	O	0	0
			84	84		
6	B	11	Total	O	0	0
			11	11		
6	C	351	Total	O	0	0
			351	351		
6	D	86	Total	O	0	0
			86	86		
6	E	10	Total	O	0	0
			10	10		

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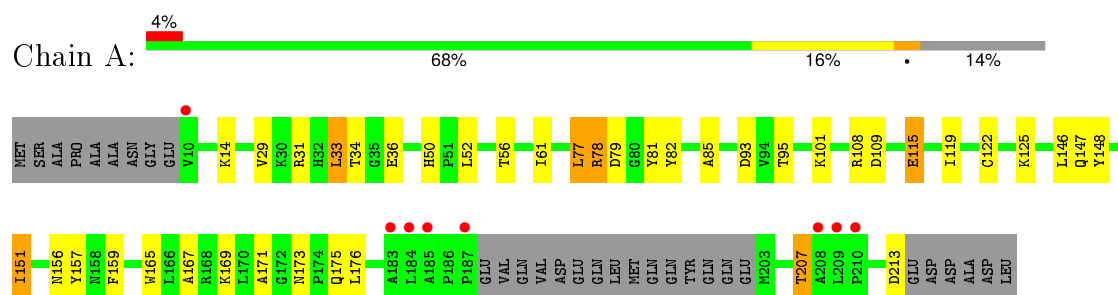
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	346	Total	O	0	0
			346	346		



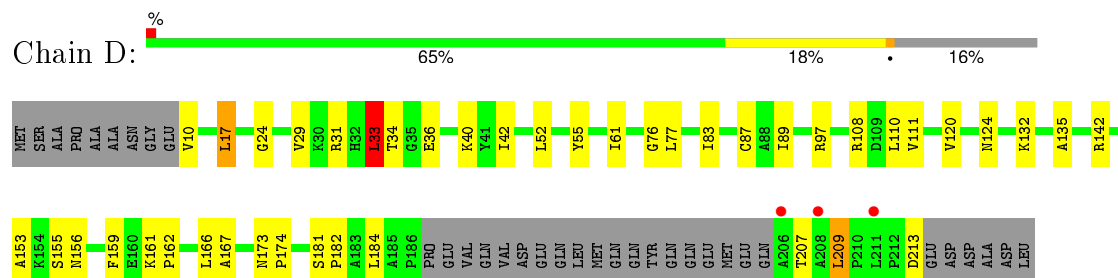
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

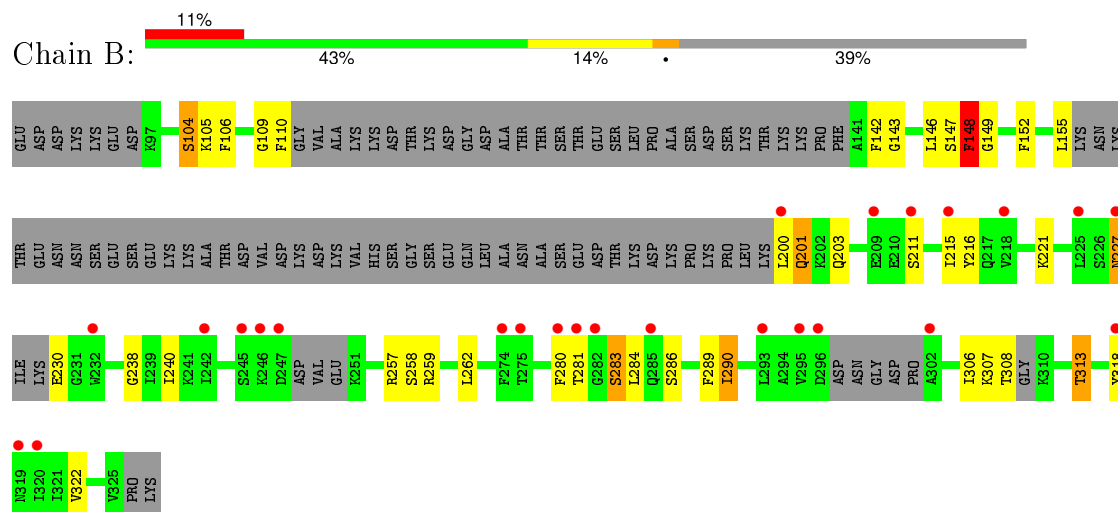
#### • Molecule 1: Gsp1p



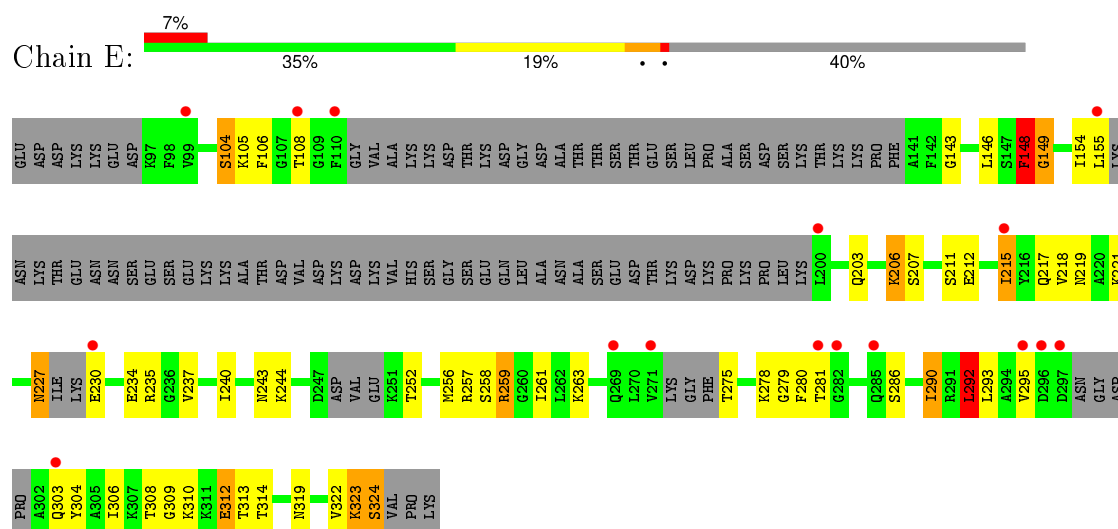
#### • Molecule 1: Gsp1p



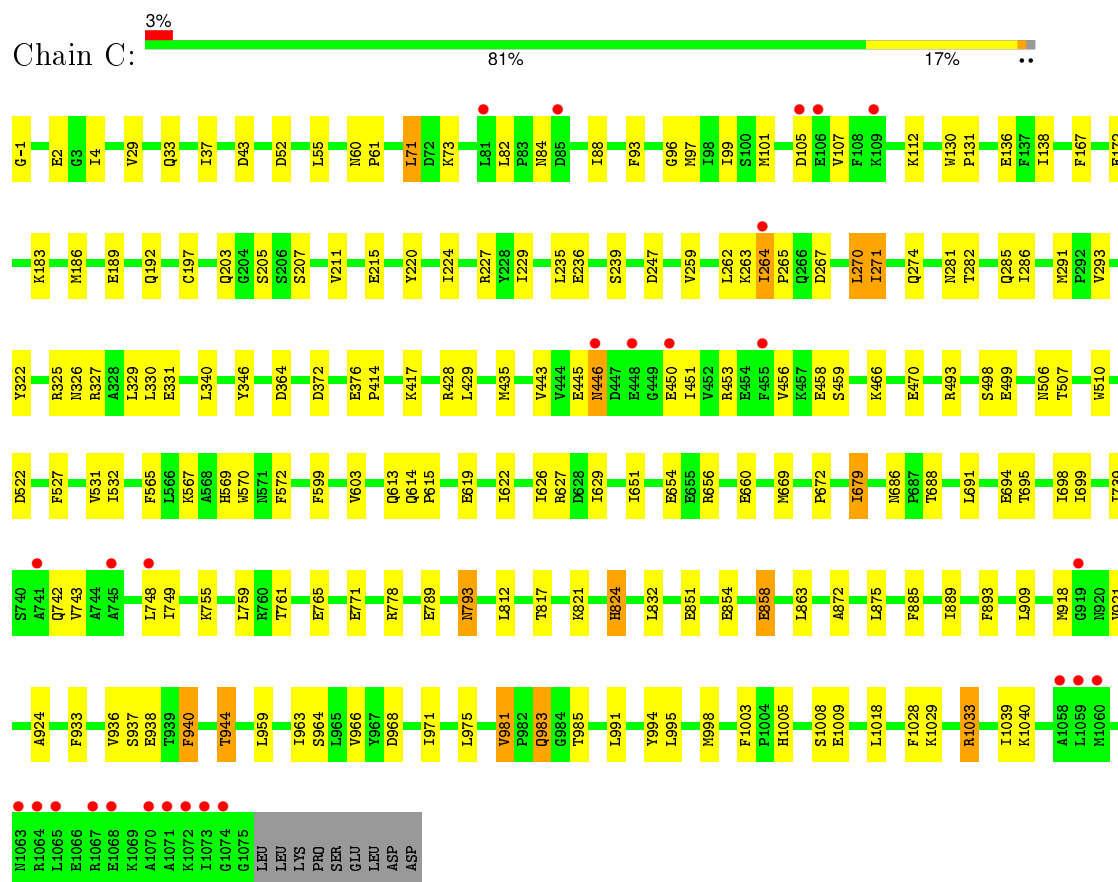
#### • Molecule 2: Ran-specific GTPase-activating protein 2



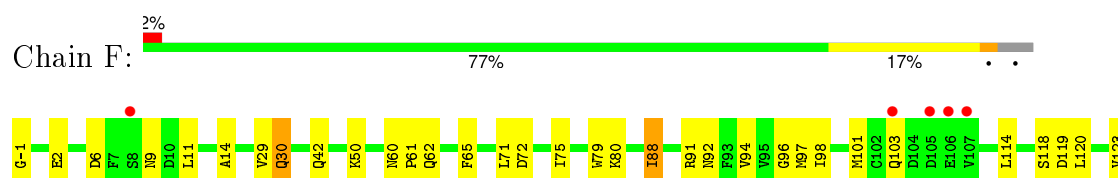
#### • Molecule 2: Ran-specific GTPase-activating protein 2

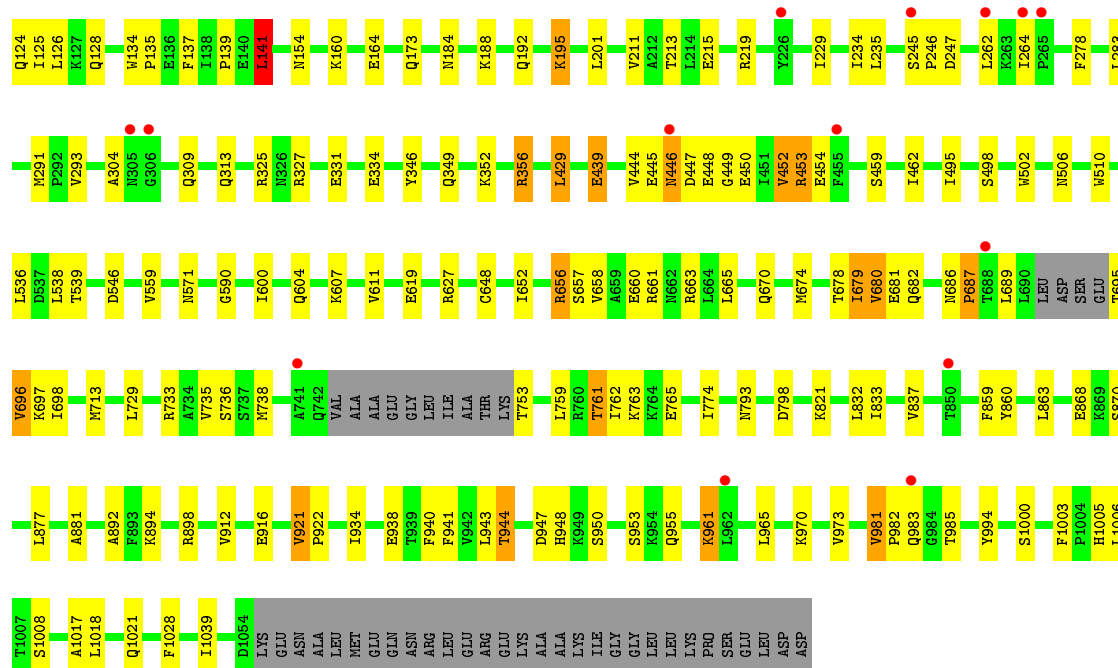


• Molecule 3: Exportin-1



• Molecule 3: Exportin-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.49Å 155.95Å 149.82Å 90.00° 106.91° 90.00°	Depositor
Resolution (Å)	33.69 – 2.22 33.69 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.69-2.22) 99.0 (33.69-2.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.175 , 0.214 0.175 , 0.214	Depositor DCC
$R_{free}$ test set	9411 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.3	EDS
Estimated twinning fraction	0.776 for H, K, L 0.224 for H, -K, -H-L 0.226 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.776 for H, K, L 0.224 for H, -K, -H-L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 187295 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, MG

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	0.73	0/1531	0.87	1/2079 (0.0%)
1	D	0.72	0/1497	0.88	5/2033 (0.2%)
2	B	0.48	0/1082	0.75	0/1449
2	E	0.52	0/1082	0.85	3/1444 (0.2%)
3	C	0.68	0/8480	0.82	6/11503 (0.1%)
3	F	0.64	0/8202	0.78	1/11129 (0.0%)
All	All	0.66	0/21874	0.81	16/29637 (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
2	B	0	1
2	E	0	2
3	C	0	1
3	F	0	1
All	All	0	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	149	GLY	N-CA-C	-6.59	96.63	113.10
2	E	279	GLY	N-CA-C	-6.58	96.64	113.10
3	F	141	LEU	CA-CB-CG	6.50	130.26	115.30
1	D	142	ARG	NE-CZ-NH1	-6.12	117.24	120.30
2	E	292	LEU	CA-CB-CG	5.98	129.05	115.30
3	C	71	LEU	CA-CB-CG	5.90	128.86	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	D	17	LEU	CA-CB-CG	5.84	128.73	115.30
1	D	110	LEU	CB-CG-CD2	-5.59	101.50	111.00
3	C	428	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	108	ARG	NE-CZ-NH1	5.41	123.00	120.30
3	C	893	PHE	N-CA-CB	5.41	120.33	110.60
1	D	33	LEU	CA-CB-CG	5.29	127.48	115.30
3	C	428	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	C	748	LEU	CA-CB-CG	5.17	127.19	115.30
3	C	567	LYS	CD-CE-NZ	-5.16	99.83	111.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	148	PHE	Peptide
3	C	376	GLU	Mainchain
2	E	148	PHE	Peptide
2	E	278	LYS	Peptide
3	F	687	PRO	Peptide

## 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	1492	0	1486	33	0
1	D	1459	0	1453	29	0
2	B	1073	0	1044	28	0
2	E	1074	0	1064	47	0
3	C	8322	0	8330	115	0
3	F	8046	0	8052	122	0
4	A	32	0	12	1	0
4	D	32	0	12	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	84	0	0	2	0
6	B	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	351	0	0	8	1
6	D	86	0	0	1	0
6	E	10	0	0	2	0
6	F	346	0	0	5	1
All	All	22420	0	21453	342	1

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 8.

All (342) 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:B:280:PHE:O	2:B:286:SER:HB2	1.19	1.28
2:E:308:THR:HG21	2:E:313:THR:OG1	1.48	1.12
2:B:280:PHE:O	2:B:286:SER:CB	2.05	1.02
1:A:34:THR:OG1	1:A:36:GLU:HG2	1.65	0.97
3:C:1033:ARG:HG3	3:C:1033:ARG:HH11	1.30	0.96
1:D:209:LEU:HD23	1:D:209:LEU:H	1.28	0.96
1:A:207:THR:HG22	2:B:281:THR:H	1.33	0.92
1:D:55:TYR:HD1	2:E:206:LYS:HD3	1.34	0.91
1:D:174:PRO:HG3	3:F:304:ALA:HB3	1.53	0.91
2:E:308:THR:CG2	2:E:313:THR:OG1	2.20	0.89
3:C:264:ILE:HG22	3:C:325:ARG:NH2	1.88	0.87
2:B:283:SER:O	2:B:286:SER:HB3	1.78	0.84
3:F:-1:GLY:N	3:F:2:GLU:OE2	2.12	0.83
2:E:308:THR:HG21	2:E:313:THR:CB	2.10	0.81
3:F:763:LYS:NZ	3:F:798:ASP:OD2	2.14	0.81
3:F:695:THR:HA	3:F:698:ILE:HD13	1.60	0.81
2:B:152:PHE:O	2:B:155:LEU:HB2	1.80	0.80
3:C:236:GLU:HG2	6:C:1429:HOH:O	1.81	0.79
3:C:239:SER:HB2	3:C:281:ASN:HB2	1.67	0.77
2:B:290:ILE:HD11	2:B:318:TYR:HB2	1.65	0.77
3:C:270:LEU:O	3:C:274:GLN:HG3	1.85	0.77
3:C:981:VAL:HG11	3:C:985:THR:HB	1.66	0.76
3:C:446:ASN:HD21	3:C:450:GLU:H	1.33	0.76
1:D:34:THR:OG1	1:D:36:GLU:HG2	1.87	0.75
3:C:940:PHE:O	3:C:944:THR:HB	1.87	0.74
2:E:234:GLU:HB2	6:E:408:HOH:O	1.87	0.73
3:C:55:LEU:HB3	3:C:97:MET:HE3	1.69	0.73
2:E:308:THR:HG22	2:E:309:GLY:N	2.03	0.73
1:A:93:ASP:OD1	1:A:95:THR:HB	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:445:GLU:OE2	3:F:449:GLY:HA2	1.90	0.71
3:F:619:GLU:OE1	3:F:627:ARG:NH2	2.24	0.70
1:D:209:LEU:CD2	1:D:209:LEU:H	2.04	0.70
3:F:894:LYS:O	3:F:948:HIS:HE1	1.75	0.70
2:E:308:THR:CG2	2:E:309:GLY:N	2.55	0.70
1:D:55:TYR:CD1	2:E:206:LYS:HD3	2.22	0.70
1:D:61:ILE:HD13	1:D:167:ALA:HB1	1.75	0.69
1:A:56:THR:CG2	1:A:61:ILE:HD12	2.22	0.69
1:A:122:CYS:HB3	1:A:151:ILE:HD13	1.74	0.68
3:F:679:ILE:HD13	3:F:682:GLN:OE1	1.94	0.68
3:C:414:PRO:O	3:C:417:LYS:HB2	1.94	0.67
3:C:679:ILE:HD11	3:C:695:THR:HG23	1.76	0.67
3:F:940:PHE:O	3:F:944:THR:HB	1.94	0.67
3:C:446:ASN:ND2	3:C:450:GLU:H	1.93	0.67
3:F:184:ASN:O	3:F:188:LYS:HD3	1.94	0.66
1:D:209:LEU:HD23	1:D:209:LEU:N	2.06	0.66
2:E:275:THR:HG21	2:E:293:LEU:HD23	1.76	0.66
3:F:657:SER:OG	3:F:660:GLU:OE1	2.09	0.66
3:C:293:VAL:HG12	3:C:346:TYR:CE2	2.32	0.65
3:F:944:THR:HG23	3:F:1003:PHE:HZ	1.60	0.65
3:C:679:ILE:HD12	3:C:699:ILE:HD11	1.79	0.65
3:F:120:LEU:O	3:F:124:GLN:HG2	1.97	0.65
1:A:14:LYS:HG2	1:A:85:ALA:HA	1.79	0.64
3:C:981:VAL:CG1	3:C:985:THR:HB	2.26	0.64
1:D:155:SER:O	1:D:156:ASN:HB2	1.98	0.63
3:C:936:VAL:HG11	3:C:995:LEU:HD21	1.78	0.63
3:C:29:VAL:O	3:C:33:GLN:HG3	1.99	0.63
3:C:227:ARG:HG2	6:C:1422:HOH:O	1.98	0.63
1:A:56:THR:HG21	1:A:61:ILE:HD12	1.79	0.63
3:F:981:VAL:HG23	6:F:1255:HOH:O	1.98	0.62
3:C:918:MET:HE3	3:C:924:ALA:HB2	1.82	0.62
3:C:429:LEU:HD22	3:F:498:SER:HB2	1.81	0.62
3:F:264:ILE:HG22	3:F:325:ARG:NH2	2.15	0.61
1:D:31:ARG:HD3	1:D:156:ASN:OD1	2.00	0.61
3:F:30:GLN:HE21	3:F:30:GLN:H	1.47	0.61
3:F:88:ILE:HG23	3:F:92:ASN:ND2	2.15	0.61
2:B:142:PHE:CE2	3:C:52:ASP:HB3	2.36	0.61
3:C:981:VAL:HG11	3:C:985:THR:CB	2.31	0.61
3:F:912:VAL:HG13	3:F:965:LEU:HD11	1.84	0.60
3:C:981:VAL:CG1	3:C:985:THR:CB	2.80	0.60
2:E:219:ASN:HD21	2:E:259:ARG:HH21	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:VAL:HG12	1:D:33:LEU:HD22	1.84	0.59
3:F:453:ARG:NH1	3:F:454:GLU:O	2.36	0.58
3:F:14:ALA:O	6:F:1268:HOH:O	2.17	0.58
3:F:698:ILE:H	3:F:698:ILE:HD12	1.67	0.58
3:C:619:GLU:OE1	3:C:627:ARG:NH2	2.34	0.58
3:C:936:VAL:CG1	3:C:995:LEU:HD21	2.33	0.58
3:F:921:VAL:HG22	3:F:922:PRO:HD2	1.85	0.58
2:E:106:PHE:CD2	3:F:941:PHE:HD1	2.21	0.58
3:C:622:ILE:O	3:C:626:ILE:HG13	2.04	0.58
1:D:207:THR:CG2	2:E:281:THR:H	2.17	0.58
3:C:981:VAL:HG13	3:C:985:THR:OG1	2.04	0.57
3:F:309:GLN:O	3:F:313:GLN:HG3	2.04	0.57
3:C:211:VAL:O	3:C:215:GLU:HG2	2.05	0.57
2:E:308:THR:CG2	2:E:309:GLY:H	2.18	0.57
3:F:446:ASN:HD21	3:F:450:GLU:HB2	1.69	0.57
1:A:207:THR:HG22	2:B:281:THR:N	2.12	0.57
3:F:916:GLU:OE1	3:F:961:LYS:NZ	2.38	0.57
3:C:264:ILE:CG2	3:C:325:ARG:NH2	2.64	0.56
3:C:694:GLU:O	3:C:698:ILE:HG13	2.05	0.56
2:E:104:SER:C	2:E:106:PHE:H	2.07	0.56
2:B:148:PHE:O	3:C:96:GLY:HA3	2.06	0.56
2:E:143:GLY:HA2	2:E:146:LEU:HD12	1.86	0.56
3:C:959:LEU:O	3:C:963:ILE:HG13	2.06	0.56
3:F:898:ARG:NH1	3:F:950:SER:O	2.39	0.56
3:C:778:ARG:NH1	6:C:1356:HOH:O	2.39	0.55
3:F:944:THR:CG2	3:F:1003:PHE:HZ	2.19	0.55
1:A:29:VAL:HG12	1:A:33:LEU:HD22	1.89	0.55
3:F:119:ASP:OD2	3:F:154:ASN:ND2	2.39	0.55
2:B:240:ILE:CD1	2:B:306:ILE:HD13	2.37	0.55
1:D:181:SER:OG	6:D:456:HOH:O	2.11	0.55
3:F:445:GLU:HB3	6:F:1358:HOH:O	2.07	0.54
3:F:859:PHE:CE2	3:F:863:LEU:HD11	2.41	0.54
2:E:308:THR:HB	2:E:314:THR:OG1	2.07	0.54
3:F:439:GLU:HB3	3:F:462:ILE:HG12	1.90	0.54
3:C:1033:ARG:HG3	3:C:1033:ARG:NH1	2.09	0.54
3:C:55:LEU:HD22	3:C:97:MET:HE1	1.90	0.54
1:A:147:GLN:HE21	1:A:148:TYR:H	1.56	0.53
3:F:453:ARG:HG3	3:F:590:GLY:HA2	1.90	0.53
3:F:229:ILE:HD13	3:F:262:LEU:HD13	1.90	0.53
1:D:174:PRO:HG3	3:F:304:ALA:CB	2.33	0.53
3:C:944:THR:CG2	3:C:1003:PHE:HZ	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1033:ARG:CG	3:C:1033:ARG:HH11	2.12	0.53
3:C:235:LEU:HD21	3:C:259:VAL:HG11	1.91	0.53
3:C:570:TRP:CE2	3:C:614:GLN:HG3	2.43	0.52
1:A:157:TYR:CE2	3:C:458:GLU:HG2	2.45	0.52
3:F:506:ASN:HB3	3:F:510:TRP:CZ2	2.44	0.52
3:C:229:ILE:HD13	3:C:262:LEU:HD13	1.91	0.52
3:F:75:ILE:HD13	3:F:125:ILE:HG13	1.89	0.52
3:C:944:THR:HG23	3:C:1003:PHE:HZ	1.74	0.52
3:C:192:GLN:HG3	6:C:1395:HOH:O	2.07	0.52
2:E:146:LEU:O	2:E:149:GLY:HA3	2.09	0.52
3:C:264:ILE:HG22	3:C:325:ARG:HH22	1.72	0.52
3:C:-1:GLY:N	3:C:2:GLU:OE1	2.43	0.52
3:F:446:ASN:HD22	3:F:446:ASN:C	2.12	0.51
3:F:229:ILE:HG22	3:F:235:LEU:HG	1.92	0.51
3:F:349:GLN:HE22	3:F:352:LYS:NZ	2.08	0.51
1:A:56:THR:HG21	1:A:61:ILE:CD1	2.39	0.51
3:C:669:MET:O	3:C:672:PRO:HD2	2.10	0.51
3:F:446:ASN:ND2	3:F:450:GLU:H	2.09	0.51
3:C:282:THR:O	3:C:286:ILE:HG12	2.10	0.51
2:E:155:LEU:HD13	3:F:103:GLN:HE22	1.75	0.51
2:B:216:TYR:OH	2:B:313:THR:HG22	2.11	0.51
3:C:691:LEU:HD11	3:C:742:GLN:HE22	1.76	0.51
2:E:293:LEU:HD13	2:E:303:GLN:HG3	1.92	0.51
1:A:56:THR:HG23	1:A:61:ILE:HD12	1.91	0.51
3:F:446:ASN:ND2	3:F:450:GLU:HB2	2.26	0.50
3:C:614:GLN:HE21	3:C:615:PRO:HD2	1.76	0.50
3:F:11:LEU:HB2	3:F:50:LYS:HD2	1.92	0.50
1:A:165:TRP:CZ2	1:A:169:LYS:HE2	2.46	0.50
1:A:176:LEU:HD23	1:A:176:LEU:C	2.32	0.50
2:B:142:PHE:CZ	3:C:52:ASP:HB3	2.46	0.50
3:F:94:VAL:O	3:F:98:ILE:HG13	2.11	0.50
2:B:149:GLY:H	3:C:93:PHE:HA	1.75	0.50
2:E:308:THR:HG22	2:E:310:LYS:H	1.76	0.50
3:F:264:ILE:CG2	3:F:325:ARG:NH2	2.74	0.50
3:C:327:ARG:O	3:C:331:GLU:HG3	2.11	0.50
3:C:443:VAL:HG13	3:C:451:ILE:CG2	2.41	0.50
2:B:109:GLY:O	2:B:110:PHE:HB2	2.11	0.50
2:E:146:LEU:O	2:E:149:GLY:CA	2.60	0.50
3:F:160:LYS:HD2	3:F:219:ARG:CZ	2.41	0.50
2:B:238:GLY:HA3	2:B:257:ARG:O	2.12	0.50
3:C:964:SER:O	3:C:968:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:275:THR:HB	2:E:293:LEU:HB2	1.94	0.49
2:B:104:SER:C	2:B:106:PHE:H	2.16	0.49
1:A:213:ASP:OD1	2:B:221:LYS:NZ	2.43	0.49
3:C:565:PHE:HE2	3:C:572:PHE:CD2	2.30	0.49
2:E:308:THR:HG21	2:E:313:THR:HB	1.93	0.49
3:C:565:PHE:O	3:C:569:HIS:HD2	1.95	0.49
3:F:201:LEU:HD12	3:F:234:ILE:HD11	1.93	0.49
3:F:211:VAL:O	3:F:215:GLU:HG2	2.13	0.49
3:F:658:VAL:HG22	3:F:661:ARG:HH22	1.78	0.49
3:F:101:MET:HE1	3:F:114:LEU:HD21	1.95	0.49
2:E:275:THR:O	2:E:292:LEU:HB2	2.13	0.48
1:A:33:LEU:HD13	1:A:52:LEU:HD12	1.95	0.48
1:A:101:LYS:HG2	1:A:101:LYS:O	2.12	0.48
3:C:466:LYS:O	3:C:470:GLU:HG3	2.13	0.48
3:F:454:GLU:HG3	3:F:454:GLU:O	2.12	0.48
3:F:1018:LEU:HD22	3:F:1028:PHE:CE1	2.48	0.48
3:C:651:ILE:O	3:C:654:GLU:HB3	2.13	0.48
3:C:43:ASP:OD2	3:C:73:LYS:NZ	2.47	0.48
3:F:134:TRP:N	3:F:135:PRO:CD	2.76	0.48
1:A:31:ARG:HD3	1:A:156:ASN:OD1	2.14	0.48
1:A:61:ILE:HD11	1:A:176:LEU:HD11	1.95	0.48
3:F:600:ILE:O	3:F:604:GLN:HG3	2.13	0.48
3:C:885:PHE:O	3:C:889:ILE:HG13	2.13	0.48
3:C:789:GLU:O	3:C:793:ASN:HB2	2.14	0.48
3:F:264:ILE:HG23	3:F:264:ILE:O	2.14	0.48
2:E:148:PHE:O	3:F:96:GLY:HA3	2.14	0.48
3:C:372:ASP:HB2	6:C:1169:HOH:O	2.14	0.48
3:F:6:ASP:OD2	3:F:9:ASN:ND2	2.47	0.48
2:E:257:ARG:HA	2:E:263:LYS:O	2.14	0.48
3:C:599:PHE:O	3:C:603:VAL:HG13	2.13	0.48
3:F:160:LYS:O	3:F:164:GLU:HG3	2.13	0.47
3:C:4:ILE:HD11	3:C:37:ILE:HG22	1.96	0.47
3:F:859:PHE:CZ	3:F:863:LEU:HD11	2.48	0.47
3:C:443:VAL:HG13	3:C:451:ILE:HG23	1.96	0.47
3:F:79:TRP:CD1	3:F:128:GLN:HB3	2.50	0.47
3:C:112:LYS:HB2	6:C:1154:HOH:O	2.15	0.47
2:E:206:LYS:HE3	2:E:206:LYS:HA	1.95	0.47
3:C:570:TRP:CD2	3:C:614:GLN:HG3	2.49	0.47
1:D:213:ASP:N	1:D:213:ASP:OD2	2.47	0.47
2:E:319:ASN:O	2:E:323:LYS:HB2	2.14	0.47
3:F:860:TYR:CE1	3:F:892:ALA:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:613:GLN:HE21	3:C:619:GLU:HA	1.79	0.47
3:F:349:GLN:HE22	3:F:352:LYS:HZ2	1.62	0.47
3:C:1018:LEU:HD22	3:C:1028:PHE:CE1	2.50	0.47
3:F:686:ASN:HB3	3:F:689:LEU:HD12	1.97	0.47
1:D:182:PRO:HB3	2:E:207:SER:O	2.15	0.46
2:B:143:GLY:HA2	2:B:146:LEU:HD12	1.96	0.46
3:C:130:TRP:CD1	3:C:131:PRO:HA	2.51	0.46
2:B:216:TYR:HH	2:B:313:THR:HG22	1.81	0.46
3:C:322:TYR:O	3:C:326:ASN:HB2	2.16	0.46
3:C:981:VAL:CG1	3:C:985:THR:OG1	2.63	0.46
3:F:860:TYR:CZ	3:F:892:ALA:HB2	2.51	0.46
3:F:934:ILE:O	3:F:938:GLU:HG2	2.15	0.46
3:C:739:ILE:O	3:C:743:VAL:HG23	2.16	0.46
3:C:220:TYR:O	3:C:224:ILE:HG23	2.16	0.46
3:F:648:CYS:O	3:F:652:ILE:HG13	2.15	0.46
1:D:97:ARG:NH1	1:D:132:LYS:HD3	2.31	0.46
3:F:679:ILE:CG2	3:F:680:VAL:N	2.79	0.46
3:F:139:PRO:HG3	3:F:192:GLN:HE22	1.81	0.46
3:F:674:MET:O	3:F:678:THR:HG23	2.16	0.46
3:C:937:SER:HB2	3:C:998:MET:SD	2.56	0.46
3:F:735:VAL:HG21	3:F:762:ILE:HD12	1.98	0.45
2:E:227:ASN:ND2	2:E:230:GLU:O	2.49	0.45
3:C:167:PHE:CE1	3:C:183:LYS:HG2	2.51	0.45
3:F:447:ASP:HA	6:F:1349:HOH:O	2.16	0.45
2:B:155:LEU:HD13	3:C:99:ILE:HD13	1.99	0.45
3:C:498:SER:HB2	3:F:429:LEU:HD22	1.97	0.45
2:E:292:LEU:HD22	2:E:304:TYR:HB2	1.98	0.45
3:F:981:VAL:CG1	3:F:985:THR:OG1	2.65	0.45
3:F:736:SER:HB3	3:F:798:ASP:OD1	2.16	0.45
3:F:91:ARG:HG3	3:F:134:TRP:CH2	2.51	0.45
1:A:125:LYS:HE2	4:A:301:GTP:C4	2.51	0.45
1:D:87:CYS:HB2	1:D:166:LEU:HD22	1.98	0.45
3:C:265:PRO:HD2	3:C:271:ILE:HD12	1.98	0.45
1:A:61:ILE:HD13	1:A:167:ALA:HB1	1.99	0.45
1:D:17:LEU:HD13	1:D:89:ILE:HB	1.99	0.45
3:F:445:GLU:N	6:F:1358:HOH:O	2.35	0.45
2:B:149:GLY:N	3:C:93:PHE:HA	2.31	0.45
2:E:148:PHE:CE2	3:F:97:MET:HG3	2.52	0.45
1:D:24:GLY:HA3	1:D:124:ASN:ND2	2.32	0.45
3:F:195:LYS:HB2	3:F:195:LYS:HE2	1.71	0.45
3:C:669:MET:C	3:C:672:PRO:HD2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ASP:OD1	2:E:221:LYS:NZ	2.45	0.45
3:F:774:ILE:O	3:F:821:LYS:HG2	2.17	0.45
3:F:1005:HIS:CD2	3:F:1005:HIS:H	2.35	0.45
1:A:171:ALA:CB	2:B:201:GLN:HG3	2.47	0.45
2:E:290:ILE:HG22	2:E:306:ILE:HB	1.99	0.45
3:C:138:ILE:HB	3:C:189:GLU:OE2	2.17	0.45
3:F:729:LEU:O	3:F:733:ARG:HG3	2.16	0.44
3:C:55:LEU:HB3	3:C:97:MET:CE	2.44	0.44
2:B:258:SER:O	2:B:262:LEU:HA	2.17	0.44
3:F:293:VAL:HG12	3:F:346:TYR:CE2	2.53	0.44
2:E:308:THR:HG23	2:E:309:GLY:H	1.82	0.44
1:A:77:LEU:HB2	1:A:81:TYR:CE1	2.53	0.44
1:A:78:ARG:NH2	1:A:78:ARG:HG2	2.32	0.44
3:F:502:TRP:CZ2	3:F:546:ASP:HB3	2.52	0.44
3:C:872:ALA:HA	3:C:875:LEU:HD12	2.00	0.44
3:F:665:LEU:HD13	3:F:713:MET:SD	2.56	0.44
3:F:761:THR:O	3:F:765:GLU:HG2	2.18	0.44
3:F:445:GLU:HA	3:F:450:GLU:O	2.16	0.44
3:C:1005:HIS:CE1	3:C:1039:ILE:O	2.70	0.44
3:C:527:PHE:O	3:C:531:VAL:HG23	2.18	0.44
3:F:536:LEU:O	3:F:539:THR:HB	2.17	0.44
3:F:495:ILE:HD13	3:F:538:LEU:HG	2.00	0.44
3:C:971:ILE:HD13	3:C:975:LEU:HD21	2.00	0.44
3:F:1017:ALA:O	3:F:1021:GLN:HG3	2.18	0.44
1:A:115:GLU:HG3	6:A:452:HOH:O	2.17	0.44
3:C:1009:GLU:OE1	3:C:1009:GLU:N	2.51	0.44
3:C:824:HIS:CD2	3:C:824:HIS:H	2.35	0.43
3:F:994:TYR:C	3:F:994:TYR:CD2	2.91	0.43
3:F:696:VAL:CG2	3:F:759:LEU:HD23	2.48	0.43
2:E:217:GLN:HA	2:E:240:ILE:O	2.18	0.43
2:E:215:ILE:HD11	2:E:244:LYS:CB	2.48	0.43
3:C:493:ARG:HB3	3:C:499:GLU:HG3	2.00	0.43
3:C:1029:LYS:O	3:C:1033:ARG:HG2	2.18	0.43
3:F:733:ARG:O	3:F:736:SER:HB2	2.18	0.43
3:C:445:GLU:N	6:C:1334:HOH:O	2.37	0.43
3:F:88:ILE:HG23	3:F:92:ASN:HD22	1.84	0.43
1:A:33:LEU:HD21	1:A:50:HIS:HB3	2.00	0.43
2:E:155:LEU:CD1	3:F:103:GLN:NE2	2.82	0.43
3:C:326:ASN:O	3:C:329:LEU:HB2	2.18	0.43
3:C:966:VAL:HG21	3:C:991:LEU:HD22	2.01	0.43
3:F:229:ILE:HD13	3:F:262:LEU:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ILE:HD11	3:F:65:PHE:CG	2.53	0.43
3:F:916:GLU:OE2	3:F:970:LYS:HE2	2.18	0.43
3:C:691:LEU:HD11	3:C:742:GLN:NE2	2.33	0.43
2:B:240:ILE:CD1	2:B:306:ILE:CD1	2.97	0.43
3:C:686:ASN:ND2	3:C:688:THR:OG1	2.46	0.43
3:F:679:ILE:HG22	3:F:680:VAL:N	2.33	0.43
1:D:29:VAL:HG12	1:D:33:LEU:CD2	2.47	0.43
3:C:101:MET:HG2	3:C:107:VAL:HG11	2.01	0.43
1:A:78:ARG:HH21	1:A:78:ARG:HG2	1.84	0.42
3:F:877:LEU:HB3	3:F:881:ALA:HB3	2.01	0.42
1:A:82:TYR:CD1	1:A:82:TYR:N	2.86	0.42
2:B:227:ASN:HD22	2:B:230:GLU:N	2.17	0.42
3:F:981:VAL:HG13	3:F:982:PRO:O	2.18	0.42
1:A:78:ARG:HB3	1:A:79:ASP:H	1.49	0.42
1:D:40:LYS:HE2	1:D:42:ILE:HD11	2.01	0.42
3:F:123:VAL:HA	3:F:126:LEU:HD12	2.00	0.42
1:D:76:GLY:O	3:F:42:GLN:NE2	2.52	0.42
3:C:983:GLN:H	3:C:983:GLN:HG3	1.44	0.42
3:C:1033:ARG:CG	3:C:1033:ARG:NH1	2.78	0.42
3:F:327:ARG:O	3:F:331:GLU:HG3	2.20	0.42
3:F:60:ASN:HA	3:F:61:PRO:HD2	1.74	0.42
3:C:235:LEU:HA	3:C:235:LEU:HD23	1.71	0.41
3:C:435:MET:O	3:C:507:THR:HG22	2.20	0.41
3:C:755:LYS:O	3:C:759:LEU:HG	2.20	0.41
3:F:448:GLU:HG3	3:F:450:GLU:OE1	2.19	0.41
3:C:863:LEU:HA	3:C:863:LEU:HD23	1.87	0.41
3:C:771:GLU:HG2	3:C:817:THR:OG1	2.20	0.41
3:F:444:VAL:O	3:F:452:VAL:N	2.42	0.41
1:D:161:LYS:N	1:D:162:PRO:CD	2.84	0.41
2:E:322:VAL:C	2:E:324:SER:N	2.74	0.41
3:C:812:LEU:HB2	3:C:858:GLU:HB3	2.02	0.41
3:C:532:ILE:HD13	3:C:532:ILE:HA	1.83	0.41
1:A:173:ASN:OD1	1:A:175:GLN:HB2	2.19	0.41
3:C:506:ASN:HB3	3:C:510:TRP:CZ2	2.55	0.41
3:C:330:LEU:HB2	3:C:340:LEU:HD13	2.02	0.41
3:F:137:PHE:CZ	3:F:141:LEU:HG	2.56	0.41
3:F:283:LEU:HD13	3:F:283:LEU:HA	1.89	0.41
3:F:245:SER:HA	3:F:246:PRO:HD3	1.84	0.41
2:E:148:PHE:CZ	3:F:97:MET:HG3	2.55	0.41
3:C:1040:LYS:HE3	6:C:1297:HOH:O	2.21	0.41
3:F:833:ILE:O	3:F:837:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:PHE:CE2	2:B:307:LYS:HD2	2.56	0.41
3:F:656:ARG:HA	3:F:656:ARG:HD2	1.74	0.41
3:C:1018:LEU:HD22	3:C:1028:PHE:CZ	2.55	0.41
3:F:293:VAL:HG12	3:F:346:TYR:CZ	2.55	0.41
2:E:108:THR:HB	6:E:405:HOH:O	2.20	0.41
1:A:119:ILE:HB	1:A:146:LEU:HD22	2.02	0.41
2:E:240:ILE:HG13	2:E:256:MET:HB2	2.03	0.41
1:A:108:ARG:NH1	6:A:463:HOH:O	2.54	0.41
3:C:761:THR:O	3:C:765:GLU:HG2	2.21	0.41
3:C:322:TYR:C	3:C:322:TYR:CD2	2.94	0.40
3:C:60:ASN:HA	3:C:61:PRO:HD3	1.94	0.40
2:E:155:LEU:CD1	3:F:103:GLN:HE22	2.33	0.40
3:F:1006:LEU:HD11	3:F:1039:ILE:HG22	2.02	0.40
3:F:356:ARG:HB2	3:F:356:ARG:HE	1.65	0.40
1:D:34:THR:O	2:E:235:ARG:HD2	2.21	0.40
3:F:982:PRO:O	3:F:985:THR:HG23	2.20	0.40
2:B:104:SER:HB2	3:C:938:GLU:OE2	2.22	0.40
2:E:148:PHE:HB2	3:F:96:GLY:C	2.42	0.40
2:E:212:GLU:OE2	2:E:243:ASN:HB3	2.21	0.40
3:C:933:PHE:CD1	3:C:994:TYR:CD2	3.10	0.40
1:D:173:ASN:HA	1:D:174:PRO:HD3	1.81	0.40
3:F:687:PRO:HB2	3:F:738:MET:SD	2.61	0.40
2:E:258:SER:OG	2:E:261:ILE:HG23	2.22	0.40
1:D:31:ARG:HD2	1:D:153:ALA:O	2.22	0.40
2:B:146:LEU:O	2:B:149:GLY:HA3	2.21	0.40
3:F:943:LEU:HA	3:F:955:GLN:OE1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1274:HOH:O	6:F:1158:HOH:O[1_656]	2.17	0.03

## 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	185/219 (84%)	179 (97%)	6 (3%)	0	100	100
1	D	181/219 (83%)	171 (94%)	9 (5%)	1 (1%)	30	29
2	B	130/238 (55%)	115 (88%)	13 (10%)	2 (2%)	13	9
2	E	128/238 (54%)	112 (88%)	13 (10%)	3 (2%)	8	4
3	C	1038/1049 (99%)	1008 (97%)	29 (3%)	1 (0%)	56	64
3	F	999/1049 (95%)	958 (96%)	40 (4%)	1 (0%)	56	64
All	All	2661/3012 (88%)	2543 (96%)	110 (4%)	8 (0%)	46	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	312	GLU
2	E	323	LYS
3	F	681	GLU
2	B	105	LYS
2	E	105	LYS
3	C	172	GLU
1	D	135	ALA
2	B	215	ILE

### 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	157/188 (84%)	150 (96%)	7 (4%)	34	40
1	D	153/188 (81%)	144 (94%)	9 (6%)	24	26
2	B	107/205 (52%)	92 (86%)	15 (14%)	4	3
2	E	109/205 (53%)	90 (83%)	19 (17%)	2	1
3	C	927/955 (97%)	882 (95%)	45 (5%)	31	35
3	F	900/955 (94%)	850 (94%)	50 (6%)	26	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2353/2696 (87%)	2208 (94%)	145 (6%)	23	24

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	77	LEU
1	A	78	ARG
1	A	115	GLU
1	A	151	ILE
1	A	159	PHE
1	A	207	THR
2	B	104	SER
2	B	147	SER
2	B	148	PHE
2	B	200	LEU
2	B	201	GLN
2	B	203	GLN
2	B	211	SER
2	B	227	ASN
2	B	259	ARG
2	B	283	SER
2	B	284	LEU
2	B	290	ILE
2	B	308	THR
2	B	313	THR
2	B	322	VAL
3	C	71	LEU
3	C	82	LEU
3	C	84	ASN
3	C	88	ILE
3	C	105	ASP
3	C	136	GLU
3	C	186	MET
3	C	197	CYS
3	C	203	GLN
3	C	205	SER
3	C	207	SER
3	C	247	ASP
3	C	263	LYS
3	C	264	ILE
3	C	267	ASP

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Mol	Chain	Res	Type
3	C	270	LEU
3	C	271	ILE
3	C	285	GLN
3	C	291	MET
3	C	364	ASP
3	C	446	ASN
3	C	453	ARG
3	C	456	VAL
3	C	459	SER
3	C	522	ASP
3	C	629	ILE
3	C	656	ARG
3	C	660	GLU
3	C	679	ILE
3	C	749	ILE
3	C	793	ASN
3	C	821	LYS
3	C	824	HIS
3	C	832	LEU
3	C	851	GLU
3	C	854	GLU
3	C	858	GLU
3	C	909	LEU
3	C	921	VAL
3	C	940	PHE
3	C	944	THR
3	C	981	VAL
3	C	983	GLN
3	C	1008	SER
3	C	1033	ARG
1	D	10	VAL
1	D	33	LEU
1	D	52	LEU
1	D	77	LEU
1	D	111	VAL
1	D	120	VAL
1	D	159	PHE
1	D	184	LEU
1	D	209	LEU
2	E	104	SER
2	E	148	PHE
2	E	154	ILE

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Mol	Chain	Res	Type
2	E	203	GLN
2	E	206	LYS
2	E	211	SER
2	E	215	ILE
2	E	218	VAL
2	E	227	ASN
2	E	237	VAL
2	E	252	THR
2	E	259	ARG
2	E	280	PHE
2	E	286	SER
2	E	290	ILE
2	E	292	LEU
2	E	295	VAL
2	E	312	GLU
2	E	324	SER
3	F	29	VAL
3	F	30	GLN
3	F	62	GLN
3	F	71	LEU
3	F	72	ASP
3	F	80	LYS
3	F	88	ILE
3	F	118	SER
3	F	141	LEU
3	F	173	GLN
3	F	195	LYS
3	F	213	THR
3	F	247	ASP
3	F	278	PHE
3	F	291	MET
3	F	334	GLU
3	F	356	ARG
3	F	429	LEU
3	F	439	GLU
3	F	446	ASN
3	F	452	VAL
3	F	453	ARG
3	F	459	SER
3	F	559	VAL
3	F	571	ASN
3	F	607	LYS

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Mol	Chain	Res	Type
3	F	611	VAL
3	F	656	ARG
3	F	663	ARG
3	F	670	GLN
3	F	679	ILE
3	F	680	VAL
3	F	696	VAL
3	F	697	LYS
3	F	753	THR
3	F	761	THR
3	F	793	ASN
3	F	832	LEU
3	F	868	GLU
3	F	870	SER
3	F	921	VAL
3	F	944	THR
3	F	947	ASP
3	F	953	SER
3	F	961	LYS
3	F	973	VAL
3	F	981	VAL
3	F	983	GLN
3	F	1000	SER
3	F	1008	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	147	GLN
1	A	158	ASN
2	B	201	GLN
2	B	203	GLN
2	B	269	GLN
3	C	35	GLN
3	C	49	GLN
3	C	192	GLN
3	C	285	GLN
3	C	446	ASN
3	C	569	HIS
3	C	613	GLN
3	C	614	GLN

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Mol	Chain	Res	Type
3	C	639	GLN
3	C	686	ASN
3	C	742	GLN
3	C	824	HIS
3	C	867	ASN
3	C	948	HIS
3	C	983	GLN
3	C	1005	HIS
3	C	1057	ASN
3	C	1063	ASN
1	D	147	GLN
2	E	201	GLN
2	E	203	GLN
2	E	219	ASN
2	E	227	ASN
2	E	269	GLN
2	E	285	GLN
3	F	9	ASN
3	F	18	GLN
3	F	30	GLN
3	F	35	GLN
3	F	49	GLN
3	F	92	ASN
3	F	103	GLN
3	F	116	ASN
3	F	173	GLN
3	F	176	GLN
3	F	192	GLN
3	F	349	GLN
3	F	446	ASN
3	F	639	GLN
3	F	824	HIS
3	F	867	ASN
3	F	948	HIS
3	F	983	GLN
3	F	1005	HIS

### 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 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	A	301	5	25,34,34	1.47	4 (16%)	34,54,54	2.40	9 (26%)
4	GTP	D	301	5	25,34,34	1.43	4 (16%)	34,54,54	1.73	9 (26%)

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	A	301	5	-	0/18/38/38	0/3/3/3
4	GTP	D	301	5	-	0/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	GTP	PA-O2A	-2.60	1.43	1.54
4	A	301	GTP	PG-O3G	-2.12	1.47	1.54
4	A	301	GTP	O4'-C1'	2.43	1.44	1.41
4	D	301	GTP	C5-C4	3.00	1.47	1.40
4	D	301	GTP	O4'-C1'	3.10	1.45	1.41
4	A	301	GTP	C5-C4	3.40	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GTP	C6-C5	3.65	1.48	1.41
4	D	301	GTP	C6-C5	3.68	1.48	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	GTP	C5-C6-N1	-6.57	114.60	123.59
4	A	301	GTP	C4-C5-N7	-5.05	104.83	109.48
4	D	301	GTP	C4-C5-N7	-4.00	105.80	109.48
4	D	301	GTP	PA-O3A-PB	-3.92	121.73	132.73
4	A	301	GTP	C2'-C1'-N9	-3.70	108.64	114.29
4	D	301	GTP	C1'-N9-C4	-3.45	121.73	126.94
4	D	301	GTP	C5-C6-N1	-3.04	119.44	123.59
4	D	301	GTP	C6-C5-C4	-3.00	117.32	120.90
4	A	301	GTP	PA-O3A-PB	-2.90	124.58	132.73
4	A	301	GTP	N3-C2-N1	-2.90	123.03	127.44
4	D	301	GTP	O3G-PG-O2G	2.01	115.03	107.38
4	D	301	GTP	O2A-PA-O3A	2.09	114.56	105.09
4	D	301	GTP	C6-N1-C2	2.18	118.97	115.94
4	A	301	GTP	O2B-PB-O3B	2.44	116.18	105.09
4	D	301	GTP	O3G-PG-O1G	2.68	119.21	110.58
4	A	301	GTP	O3G-PG-O2G	3.13	119.31	107.38
4	A	301	GTP	O2G-PG-O1G	3.81	122.86	110.58
4	A	301	GTP	C6-N1-C2	6.36	124.77	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GTP	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	189/219 (86%)	0.13	8 (4%) 40 39	19, 32, 80, 108	0
1	D	185/219 (84%)	0.06	3 (1%) 74 73	22, 34, 61, 76	0
2	B	144/238 (60%)	1.12	25 (17%) 2 2	41, 69, 90, 104	0
2	E	142/238 (59%)	0.76	16 (11%) 7 6	34, 62, 91, 105	0
3	C	1040/1049 (99%)	0.01	27 (2%) 59 59	17, 36, 60, 98	0
3	F	1005/1049 (95%)	0.03	19 (1%) 70 68	18, 39, 65, 101	0
All	All	2705/3012 (89%)	0.13	98 (3%) 46 45	17, 39, 73, 108	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	271	VAL	8.2
1	A	187	PRO	7.0
2	B	281	THR	6.8
2	E	200	LEU	6.7
2	E	295	VAL	6.0
3	C	455	PHE	5.5
2	B	295	VAL	5.4
2	B	225	LEU	5.1
2	B	200	LEU	5.1
3	F	741	ALA	4.9
3	F	264	ILE	4.8
1	D	208	ALA	4.5
3	C	1065	LEU	4.5
1	A	208	ALA	4.4
2	B	302	ALA	4.4
3	C	448	GLU	4.4
2	B	245	SER	4.2
3	C	1068	GLU	3.8
2	B	296	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	1059	LEU	3.7
1	A	209	LEU	3.7
1	A	185	ALA	3.7
3	C	264	ILE	3.6
2	E	296	ASP	3.6
2	E	155	LEU	3.6
1	A	183	ALA	3.5
3	F	103	GLN	3.5
3	F	8	SER	3.4
3	F	226	TYR	3.4
1	D	211	LEU	3.4
2	B	282	GLY	3.3
2	E	110	PHE	3.3
3	C	1073	ILE	3.3
3	C	81	LEU	3.3
3	C	1064	ARG	3.2
3	C	1060	MET	3.2
3	F	265	PRO	3.1
3	F	262	LEU	3.1
2	B	232	TRP	3.1
2	B	274	PHE	3.0
1	A	210	PRO	3.0
2	B	218	VAL	3.0
3	C	109	LYS	2.9
1	A	184	LEU	2.8
2	B	285	GLN	2.8
2	E	281	THR	2.8
3	C	1070	ALA	2.8
2	B	227	ASN	2.7
2	E	99	VAL	2.7
2	B	275	THR	2.7
2	B	320	ILE	2.7
2	E	108	THR	2.7
3	C	748	LEU	2.7
3	F	446	ASN	2.7
3	F	983	GLN	2.7
2	E	230	GLU	2.7
3	F	688	THR	2.7
2	B	211	SER	2.6
2	B	215	ILE	2.6
3	F	106	GLU	2.6
3	C	1058	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	215	ILE	2.5
1	D	206	ALA	2.5
2	E	297	ASP	2.5
3	C	1072	LYS	2.5
2	E	303	GLN	2.5
3	C	1074	GLY	2.5
3	F	105	ASP	2.4
3	C	1067	ARG	2.4
2	B	293	LEU	2.4
2	B	209	GLU	2.4
3	F	107	VAL	2.4
3	C	85	ASP	2.4
3	C	106	GLU	2.4
2	B	280	PHE	2.4
2	E	285	GLN	2.4
2	E	282	GLY	2.3
2	B	242	ILE	2.3
3	C	446	ASN	2.3
3	F	306	GLY	2.3
3	F	455	PHE	2.3
3	F	850	THR	2.3
2	B	247	ASP	2.3
3	C	105	ASP	2.2
3	F	245	SER	2.2
1	A	10	VAL	2.2
3	C	1071	ALA	2.2
2	B	318	TYR	2.1
3	C	450	GLU	2.1
3	C	919	GLY	2.1
3	F	305	ASN	2.1
2	B	319	ASN	2.1
2	E	269	GLN	2.1
2	B	246	LYS	2.1
3	C	745	ALA	2.1
3	C	1063	ASN	2.0
3	C	741	ALA	2.0
3	F	962	LEU	2.0

## 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 [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	GTP	A	301	32/32	0.98	0.11	-0.51	21,27,30,31	0
4	GTP	D	301	32/32	0.98	0.10	-0.76	23,28,34,38	0
5	MG	A	302	1/1	0.98	0.06	-2.81	24,24,24,24	0
5	MG	D	302	1/1	0.97	0.05	-4.01	27,27,27,27	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.