



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2017 – 12:27 PM EDT

PDB ID : 5JQG  
Title : An apo tubulin-RB-TTL complex structure used for side-by-side comparison  
Authors : Wang, Y.X.; Naismith, J.H.; Zhu, X.  
Deposited on : unknown  
Resolution : 2.24 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

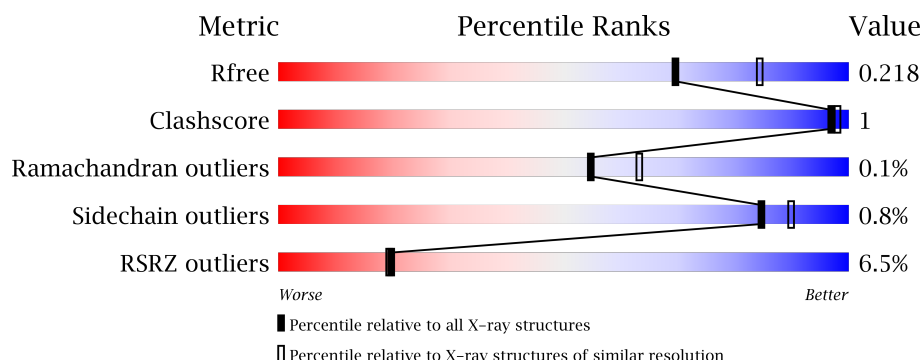
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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))
$R_{free}$	100719	1804 (2.26-2.22)
Clashscore	112137	1957 (2.26-2.22)
Ramachandran outliers	110173	1916 (2.26-2.22)
Sidechain outliers	110143	1917 (2.26-2.22)
RSRZ outliers	101464	1809 (2.26-2.22)

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	451	<div> <div>4%</div> <div>93%</div> <div>7%</div> <div>• •</div> </div>
1	C	451	<div> <div>%</div> <div>90%</div> <div>7%</div> <div>•</div> </div>
2	B	445	<div> <div>4%</div> <div>90%</div> <div>5%</div> <div>•</div> </div>
2	D	445	<div> <div>11%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>
3	E	143	<div> <div>7%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

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
10	MES	B	505	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17646 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	3	0
			3430	2173	582	651	24			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2200	589	668	25			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	4	0
			3353	2107	575	646	25			
2	D	420	Total	C	N	O	S	0	1	0
			3296	2073	561	637	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	3	0
			1012	627	182	197	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	309	Total	C	N	O	S	0	3	0
			2553	1645	438	455	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

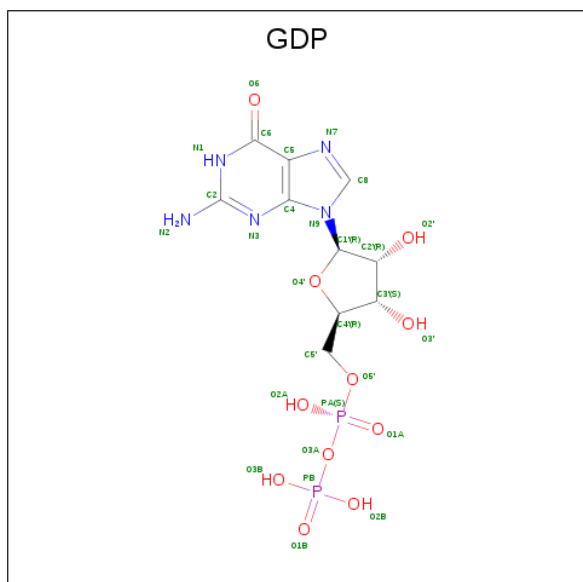
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

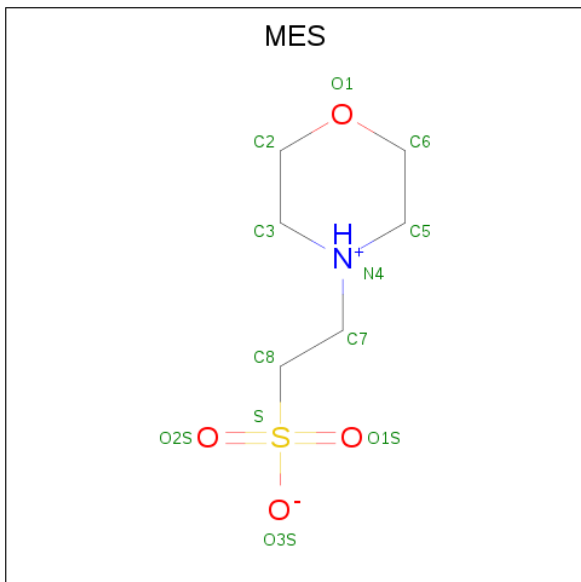
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



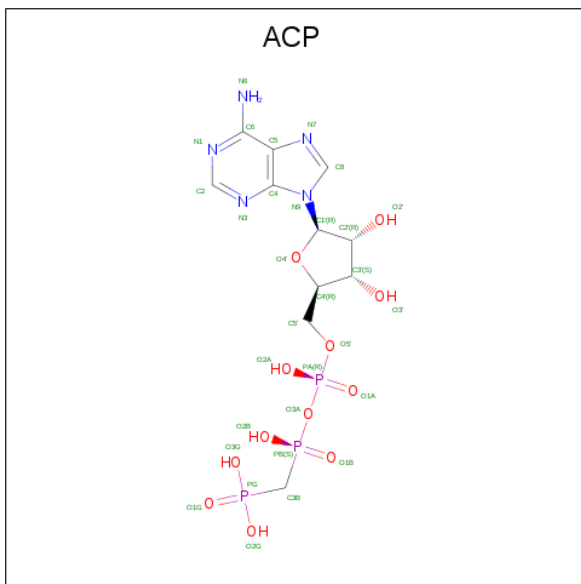
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

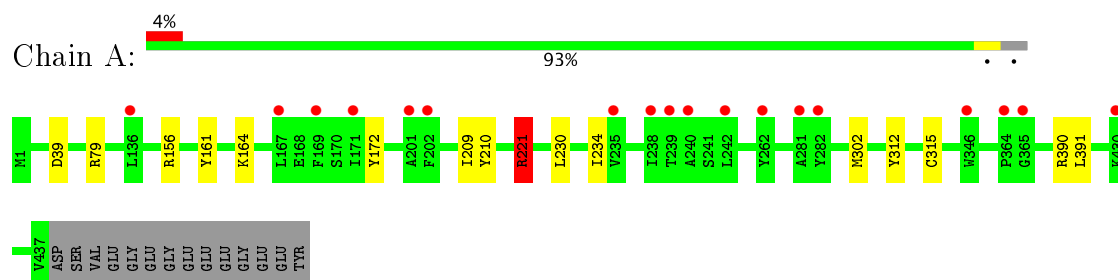
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	78	Total	O	0	0
			78	78		
12	B	62	Total	O	0	0
			62	62		
12	C	131	Total	O	0	0
			131	131		
12	D	35	Total	O	0	0
			35	35		
12	E	6	Total	O	0	0
			6	6		
12	F	21	Total	O	0	0
			21	21		



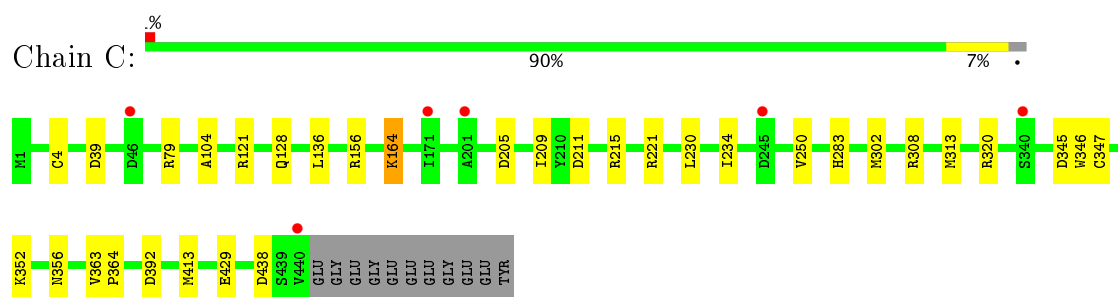
### 3 Residue-property plots [i](#)

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

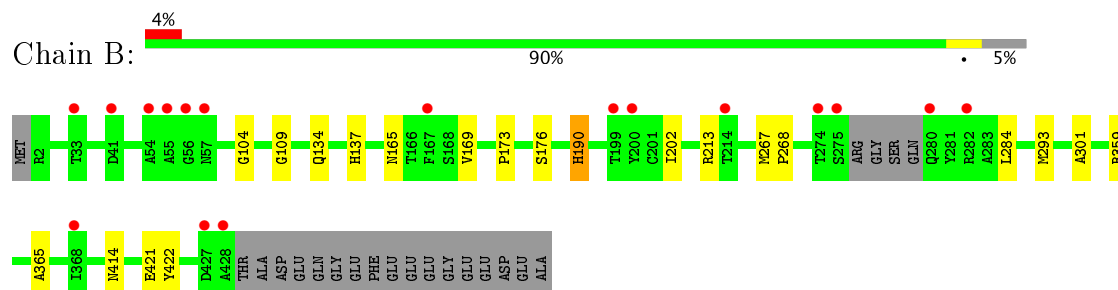
- Molecule 1: Tubulin alpha-1B chain



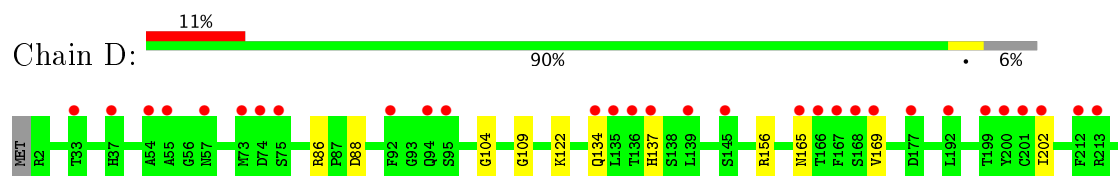
- Molecule 1: Tubulin alpha-1B chain

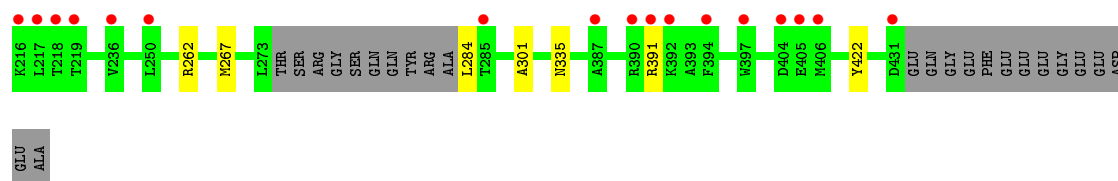


- Molecule 2: Tubulin beta chain

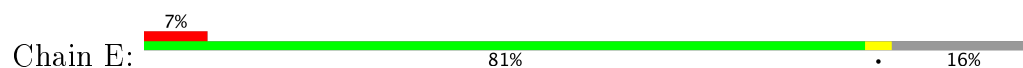


- Molecule 2: Tubulin beta chain

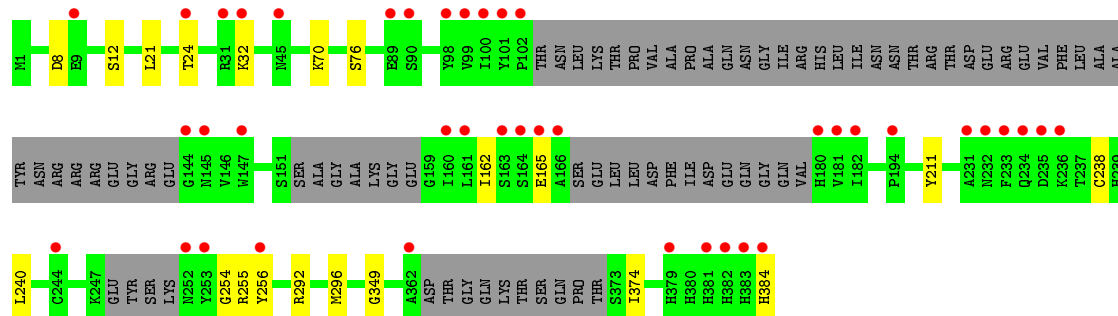
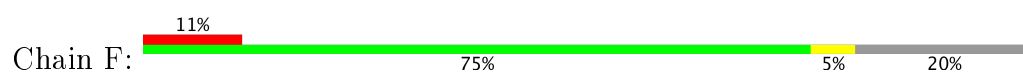




● Molecule 3: Stathmin-4



● Molecule 4: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.05Å 158.12Å 180.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.22 – 2.24 35.22 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.22-2.24) 100.0 (35.22-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.181 , 0.212 0.190 , 0.218	Depositor DCC
$R_{free}$ test set	7246 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17646	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CL, CA, GTP, ACP, MES

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	0.74	0/3514	0.87	6/4770 (0.1%)
1	C	0.84	0/3572	0.91	12/4850 (0.2%)
2	B	0.81	2/3433 (0.1%)	0.82	4/4651 (0.1%)
2	D	0.72	0/3369	0.81	4/4566 (0.1%)
3	E	0.82	1/1026 (0.1%)	0.87	2/1361 (0.1%)
4	F	0.72	1/2618 (0.0%)	0.78	1/3537 (0.0%)
All	All	0.77	4/17532 (0.0%)	0.85	29/23735 (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
4	F	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	55	GLU	CD-OE1	8.19	1.34	1.25
2	B	422	TYR	CZ-OH	6.15	1.48	1.37
4	F	254	GLY	C-O	6.11	1.33	1.23
2	B	421	GLU	CD-OE2	5.74	1.31	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211[A]	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	A	221	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	D	156	ARG	NE-CZ-NH1	6.45	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211[A]	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	79	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	390	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	D	422	TYR	CB-CG-CD2	6.00	124.60	121.00
4	F	8	ASP	CB-CG-OD1	5.97	123.67	118.30
2	D	262	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	156	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	205	ASP	CB-CG-OD2	-5.89	113.00	118.30
2	B	422	TYR	CB-CG-CD2	5.87	124.52	121.00
2	B	213	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	D	156	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	345	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	39	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	215	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	79	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	390	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	205	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	308	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	E	60	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	C	39	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	121	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	B	359	ARG	NE-CZ-NH1	5.18	122.89	120.30
3	E	122	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	156	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	B	421	GLU	CG-CD-OE1	-5.03	108.23	118.30
1	C	438	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	165	GLU	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	3430	0	3350	7	0
1	C	3482	0	3384	12	0
2	B	3353	0	3233	7	0
2	D	3296	0	3173	7	1
3	E	1012	0	1038	0	0
4	F	2553	0	2519	6	1
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	12	0	0
10	B	24	0	26	0	0
11	F	31	0	14	0	0
12	A	78	0	0	0	0
12	B	62	0	0	0	0
12	C	131	0	0	1	0
12	D	35	0	0	0	0
12	E	6	0	0	0	0
12	F	21	0	0	0	0
All	All	17646	0	16785	39	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 1.

All (39) 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:C:234:ILE:HD13	1:C:302:MET:SD	2.24	0.77
1:C:128:GLN:OE1	12:C:601:HOH:O	2.05	0.75
1:A:234:ILE:HD13	1:A:302:MET:SD	2.29	0.73
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.32	0.70
1:A:209:ILE:HD11	1:A:302:MET:SD	2.35	0.67
1:C:209:ILE:HD11	1:C:302:MET:SD	2.36	0.66
1:C:346:TRP:CZ3	1:C:347[A]:CYS:SG	2.89	0.65
1:C:313:MET:O	1:C:347[B]:CYS:SG	2.59	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:HIS:CE1	2:B:414[B]:ASN:OD1	2.56	0.58
1:C:104:ALA:HB2	1:C:413:MET:SD	2.43	0.58
2:B:173:PRO:HA	2:B:176:SER:HB2	1.93	0.51
2:D:104:GLY:O	2:D:109:GLY:HA3	2.13	0.49
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.94	0.48
2:D:86:ARG:NH1	2:D:122:LYS:HE2	2.28	0.48
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.95	0.47
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.95	0.47
2:D:86:ARG:NH1	2:D:88:ASP:HB2	2.29	0.47
2:B:104:GLY:O	2:B:109:GLY:HA3	2.16	0.46
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.98	0.45
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.52	0.45
2:B:293:MET:HE3	2:B:365:ALA:HB1	1.99	0.45
4:F:292:ARG:NH1	4:F:296[B]:MET:SD	2.90	0.45
1:A:312:TYR:CD2	1:A:315[B]:CYS:SG	3.10	0.45
2:B:134:GLN:HA	2:B:165:ASN:O	2.18	0.44
4:F:162:ILE:HD11	4:F:240:LEU:HD11	2.00	0.44
2:D:134:GLN:HA	2:D:165:ASN:O	2.17	0.44
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.00	0.43
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.99	0.43
1:C:320:ARG:HA	1:C:356:ASN:O	2.19	0.42
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.36	0.42
4:F:255:ARG:HD3	4:F:256:TYR:CZ	2.55	0.42
1:A:210:TYR:OH	1:A:221:ARG:HD3	2.20	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.42
4:F:21:LEU:O	4:F:24:THR:HB	2.20	0.42
4:F:70:LYS:O	4:F:76:SER:HB3	2.20	0.42
2:B:169:VAL:HA	2:B:202:ILE:O	2.21	0.41
1:C:363:VAL:HG12	1:C:364:PRO:O	2.22	0.40
2:D:122:LYS:HB3	2:D:122:LYS:HE3	1.95	0.40
2:D:169:VAL:HA	2:D:202:ILE:O	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)
2:D:335:ASN:OD1	4:F:384:HIS:NE2[3_545]	2.13	0.07

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
1	C	446/451 (99%)	437 (98%)	7 (2%)	2 (0%)	38	40
2	B	423/445 (95%)	416 (98%)	7 (2%)	0	100	100
2	D	416/445 (94%)	411 (99%)	5 (1%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	300/384 (78%)	290 (97%)	10 (3%)	0	100	100
All	All	2142/2319 (92%)	2100 (98%)	40 (2%)	2 (0%)	55	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	LYS
1	C	283	HIS

### 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	371/379 (98%)	370 (100%)	1 (0%)	94	96
1	C	379/379 (100%)	377 (100%)	2 (0%)	91	94
2	B	368/381 (97%)	364 (99%)	4 (1%)	78	85
2	D	361/381 (95%)	358 (99%)	3 (1%)	85	90
3	E	111/127 (87%)	110 (99%)	1 (1%)	82	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	281/342 (82%)	277 (99%)	4 (1%)	71	80
All	All	1871/1989 (94%)	1856 (99%)	15 (1%)	85	90

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
2	B	137	HIS
2	B	190	HIS
2	B	268	PRO
2	B	284	LEU
1	C	164	LYS
1	C	221	ARG
2	D	137	HIS
2	D	284	LEU
2	D	391	ARG
3	E	77	GLU
4	F	12	SER
4	F	32	LYS
4	F	211	TYR
4	F	238	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	F	229	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 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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$
5	GTP	A	501	6	27,34,34	1.21	3 (11%)	27,54,54	2.04	7 (25%)
9	GDP	B	501	6	25,30,30	1.20	3 (12%)	26,47,47	2.30	7 (26%)
10	MES	B	504	-	12,12,12	1.89	1 (8%)	14,16,16	1.90	4 (28%)
10	MES	B	505	-	12,12,12	2.12	1 (8%)	14,16,16	1.43	2 (14%)
5	GTP	C	501	6	27,34,34	1.14	4 (14%)	27,54,54	2.16	6 (22%)
5	GTP	D	501	6	27,34,34	1.28	3 (11%)	27,54,54	2.08	7 (25%)
11	ACP	F	401	-	27,33,33	1.69	8 (29%)	30,52,52	1.59	2 (6%)

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
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
5	GTP	D	501	6	-	0/18/38/38	0/3/3/3
11	ACP	F	401	-	-	0/15/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-6.93	1.67	1.77
10	B	504	MES	C8-S	-6.17	1.68	1.77
11	F	401	ACP	PB-O2B	-3.25	1.48	1.56
11	F	401	ACP	C2-N3	2.03	1.35	1.32
11	F	401	ACP	O4'-C1'	2.03	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C5-C4	2.08	1.45	1.40
9	B	501	GDP	O4'-C1'	2.26	1.44	1.41
11	F	401	ACP	PB-O3A	2.29	1.61	1.58
5	C	501	GTP	O4'-C1'	2.51	1.44	1.41
11	F	401	ACP	PG-O3G	2.57	1.61	1.54
5	A	501	GTP	C5-C4	2.62	1.46	1.40
5	C	501	GTP	C6-C5	2.77	1.46	1.41
9	B	501	GDP	C5-C4	2.77	1.46	1.40
5	D	501	GTP	C5-C4	2.81	1.46	1.40
5	C	501	GTP	PG-O3B	2.93	1.64	1.60
11	F	401	ACP	PG-O2G	2.96	1.61	1.54
9	B	501	GDP	C6-C5	3.01	1.47	1.41
5	A	501	GTP	PG-O3B	3.02	1.64	1.60
11	F	401	ACP	C5-C4	3.18	1.47	1.40
5	D	501	GTP	PG-O3B	3.39	1.65	1.60
5	D	501	GTP	C6-C5	3.48	1.48	1.41
5	A	501	GTP	C6-C5	3.52	1.48	1.41
11	F	401	ACP	PB-O1B	4.23	1.62	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N3-C2-N1	-6.77	122.96	128.86
9	B	501	GDP	C6-C5-C4	-5.99	114.89	120.84
5	C	501	GTP	C6-C5-C4	-4.99	115.88	120.84
5	D	501	GTP	C6-C5-C4	-4.97	115.90	120.84
5	A	501	GTP	C6-C5-C4	-4.61	116.26	120.84
5	C	501	GTP	C5-C6-N1	-4.04	117.73	123.48
5	C	501	GTP	N3-C2-N1	-3.93	121.72	127.46
5	A	501	GTP	C5-C6-N1	-3.91	117.92	123.48
9	B	501	GDP	N3-C2-N1	-3.90	121.77	127.46
5	D	501	GTP	N3-C2-N1	-3.60	122.20	127.46
5	D	501	GTP	C5-C6-N1	-3.41	118.63	123.48
10	B	504	MES	O1S-S-C8	-3.41	103.86	106.79
9	B	501	GDP	C5-C6-N1	-3.36	118.71	123.48
5	A	501	GTP	N3-C2-N1	-2.94	123.16	127.46
5	D	501	GTP	C1'-N9-C4	-2.90	121.62	126.64
9	B	501	GDP	C1'-N9-C4	-2.89	121.63	126.64
5	A	501	GTP	C1'-N9-C4	-2.57	122.19	126.64
5	D	501	GTP	C4-C5-N7	-2.48	107.01	109.41
11	F	401	ACP	C4-C5-N7	-2.34	107.15	109.41
10	B	505	MES	O2S-S-C8	2.20	108.68	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O3G-PG-O1G	2.22	119.19	110.50
10	B	504	MES	C5-N4-C3	2.24	113.94	108.87
10	B	504	MES	O3S-S-C8	2.65	109.32	106.06
9	B	501	GDP	O2A-PA-O1A	2.70	126.23	112.28
5	A	501	GTP	O3G-PG-O1G	2.93	121.98	110.50
5	A	501	GTP	C2-N3-C4	3.40	119.12	115.16
5	C	501	GTP	C2-N3-C4	3.44	119.17	115.16
10	B	505	MES	O3S-S-C8	3.84	110.78	106.06
10	B	504	MES	O2S-S-C8	3.96	110.20	106.79
9	B	501	GDP	C2-N3-C4	4.12	119.97	115.16
5	D	501	GTP	C6-N1-C2	4.33	122.29	116.06
5	A	501	GTP	C6-N1-C2	4.49	122.52	116.06
5	D	501	GTP	C2-N3-C4	4.64	120.58	115.16
9	B	501	GDP	C6-N1-C2	5.01	123.27	116.06
5	C	501	GTP	C6-N1-C2	5.62	124.14	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	437/451 (96%)	0.07	18 (4%)	38 38	29, 43, 71, 92	0
1	C	440/451 (97%)	-0.20	6 (1%)	75 77	23, 35, 59, 90	1 (0%)
2	B	423/445 (95%)	0.08	17 (4%)	39 39	25, 43, 72, 97	1 (0%)
2	D	420/445 (94%)	0.36	47 (11%)	6 5	30, 53, 86, 111	4 (0%)
3	E	120/143 (83%)	0.44	10 (8%)	12 12	32, 56, 91, 105	0
4	F	309/384 (80%)	0.31	41 (13%)	4 3	35, 59, 96, 123	0
All	All	2149/2319 (92%)	0.13	139 (6%)	20 19	23, 46, 82, 123	6 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	6.4
4	F	101	TYR	5.8
4	F	165	GLU	5.6
4	F	100	ILE	5.6
4	F	161	LEU	5.3
2	D	390	ARG	5.1
2	B	57	ASN	4.9
3	E	139	LEU	4.6
3	E	26	PRO	4.6
4	F	231	ALA	4.5
4	F	233	PHE	4.4
4	F	99	VAL	4.4
2	D	73	MET	4.2
1	A	346	TRP	4.2
1	A	365	GLY	4.2
2	D	167	PHE	4.1
4	F	102	PRO	4.1
1	A	282	TYR	4.1
4	F	381	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	56	GLY	4.0
2	D	95	SER	3.9
2	D	219	THR	3.9
2	B	55	ALA	3.9
2	D	135	LEU	3.8
4	F	163	SER	3.8
4	F	362	ALA	3.7
2	D	216	LYS	3.7
2	D	218	THR	3.6
1	A	364	PRO	3.6
2	B	282	ARG	3.6
1	C	340	SER	3.6
1	C	440	VAL	3.5
4	F	234	GLN	3.5
2	D	212	PHE	3.5
4	F	180	HIS	3.4
3	E	45	PRO	3.4
2	B	427	ASP	3.4
2	D	394	PHE	3.4
4	F	164	SER	3.4
2	D	55	ALA	3.4
2	D	200	TYR	3.4
2	B	428	ALA	3.3
2	D	94	GLN	3.3
4	F	232	ASN	3.3
2	D	145[A]	SER	3.2
2	D	217	LEU	3.2
2	D	387	ALA	3.2
2	B	41	ASP	3.2
2	B	274	THR	3.1
4	F	181	VAL	3.1
2	D	139	LEU	3.1
4	F	253	TYR	3.0
2	D	137	HIS	3.0
4	F	147	TRP	3.0
2	D	168	SER	3.0
4	F	24	THR	2.9
2	D	177	ASP	2.9
4	F	45	ASN	2.9
1	A	262	TYR	2.9
4	F	145	ASN	2.9
2	B	33	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	7	GLU	2.9
2	D	391	ARG	2.9
4	F	32	LYS	2.8
4	F	98	TYR	2.8
1	A	281	ALA	2.8
3	E	140	LYS	2.7
4	F	89	GLU	2.7
1	A	242	LEU	2.7
2	D	92	PHE	2.7
3	E	25	LYS	2.7
1	A	235	VAL	2.7
4	F	166	ALA	2.7
4	F	379	HIS	2.7
2	D	54	ALA	2.6
4	F	31	ARG	2.6
2	B	167	PHE	2.6
1	A	201	ALA	2.6
2	D	165	ASN	2.6
4	F	90	SER	2.6
2	D	431	ASP	2.5
4	F	194	PRO	2.5
2	D	37	HIS	2.5
1	A	238	ILE	2.5
2	D	192	LEU	2.5
3	E	48	GLU	2.5
4	F	382	HIS	2.5
1	A	202	PHE	2.5
2	D	405	GLU	2.5
2	D	406	MET	2.4
2	D	202	ILE	2.4
2	D	75	SER	2.4
4	F	244	CYS	2.4
1	A	171	ILE	2.4
4	F	383	HIS	2.4
1	C	171	ILE	2.4
2	D	392	LYS	2.4
2	B	54	ALA	2.4
3	E	46	SER	2.4
2	D	285	THR	2.4
2	D	57	ASN	2.3
2	D	404	ASP	2.3
2	B	199	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	252	ASN	2.3
2	B	214	THR	2.3
2	D	136	THR	2.3
1	A	239	THR	2.2
4	F	384	HIS	2.2
1	A	169	PHE	2.2
1	C	201	ALA	2.2
1	A	167	LEU	2.2
2	D	213	ARG	2.2
2	D	74	ASP	2.2
4	F	235	ASP	2.2
3	E	132	GLU	2.2
4	F	160	ILE	2.2
4	F	236	LYS	2.2
2	D	236	VAL	2.2
4	F	144	GLY	2.2
2	B	200	TYR	2.1
4	F	256	TYR	2.1
2	D	33	THR	2.1
1	C	46	ASP	2.1
1	A	136	LEU	2.1
2	B	275	SER	2.1
2	D	166	THR	2.1
2	D	199	THR	2.1
2	D	201	CYS	2.1
1	A	240	ALA	2.1
2	D	250	LEU	2.1
2	D	397	TRP	2.1
1	C	245	ASP	2.1
2	B	368	ILE	2.0
2	B	280	GLN	2.0
3	E	138	GLU	2.0
4	F	9	GLU	2.0
1	A	430	LYS	2.0
2	D	169	VAL	2.0
2	D	134	GLN	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(Å <sup>2</sup> )	Q<0.9
10	MES	B	505	12/12	0.90	0.23	2.89	58,66,93,94	0
5	GTP	C	501	32/32	0.98	0.12	-0.39	22,26,30,31	0
9	GDP	B	501	28/28	0.99	0.13	-0.45	25,29,34,38	0
10	MES	B	504	12/12	0.93	0.12	-0.51	38,46,54,58	0
5	GTP	A	501	32/32	0.97	0.12	-0.64	25,30,33,33	0
7	CA	C	503	1/1	0.97	0.09	-0.92	39,39,39,39	0
5	GTP	D	501	32/32	0.96	0.10	-1.12	37,46,58,60	0
7	CA	A	503	1/1	0.91	0.07	-1.30	50,50,50,50	0
11	ACP	F	401	31/31	0.93	0.09	-1.54	55,65,84,94	0
8	CL	A	504	1/1	0.86	0.06	-	69,69,69,69	0
6	MG	C	502	1/1	0.95	0.10	-	28,28,28,28	0
6	MG	A	502	1/1	0.86	0.08	-	32,32,32,32	0
6	MG	D	502	1/1	0.84	0.07	-	54,54,54,54	0
7	CA	B	503	1/1	0.62	0.09	-	81,81,81,81	0
6	MG	B	502	1/1	0.90	0.09	-	29,29,29,29	0

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

There are no such residues in this entry.