



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:36 am GMT

PDB ID : 5J2U  
Title : Tubulin-MMAF complex  
Authors : Waight, A.B.; Bargsten, K.; Doronina, S.; Steinmetz, M.O.; Sussman, D.;  
Prota, A.E.  
Deposited on : 2016-03-30  
Resolution : 2.50 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 : trunk28620  
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) : recalc28949

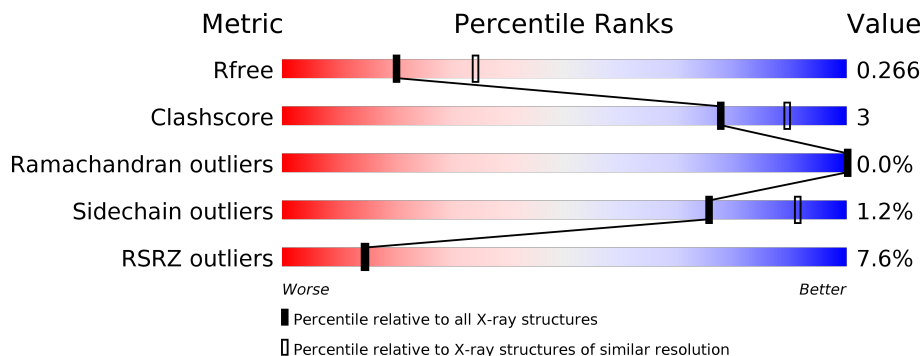
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> </div>
1	C	451	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> </div>
2	B	445	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div></div> </div> </div>
2	D	445	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
3	E	143	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div></div> </div> </div>
4	F	384	<div> <div>26%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div></div> </div> </div>

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
6	MG	A	502	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 35242 atoms, of which 17311 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	439	Total	C	H	N	O	S	0	6	0
			6834	2194	3377	584	657	22			
1	C	440	Total	C	H	N	O	S	0	12	0
			6894	2212	3407	585	666	24			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	428	Total	C	H	N	O	S	9	10	0
			6690	2137	3290	580	656	27			
2	D	422	Total	C	H	N	O	S	0	4	0
			6532	2093	3204	563	645	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	6	0
			2106	644	1064	186	206	6			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	344	Total	C	H	N	O	S	0	2	0
			5605	1808	2787	479	517	14			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP Q6B856
F	2	TYR	-	expression tag	UNP Q6B856
F	3	THR	-	expression tag	UNP Q6B856
F	4	PHE	-	expression tag	UNP Q6B856
F	5	VAL	-	expression tag	UNP Q6B856
F	6	VAL	-	expression tag	UNP Q6B856
F	7	ARG	-	expression tag	UNP Q6B856
F	8	ASP	-	expression tag	UNP Q6B856
F	9	GLU	-	expression tag	UNP Q6B856
F	10	ASN	-	expression tag	UNP Q6B856
F	11	SER	-	expression tag	UNP Q6B856
F	12	SER	-	expression tag	UNP Q6B856
F	13	VAL	-	expression tag	UNP Q6B856
F	14	TYR	-	expression tag	UNP Q6B856
F	15	ALA	-	expression tag	UNP Q6B856
F	16	GLU	MET	conflict	UNP Q6B856
F	17	VAL	ARG	conflict	UNP Q6B856
F	18	SER	GLU	conflict	UNP Q6B856
F	19	ARG	ILE	conflict	UNP Q6B856
F	20	LEU	VAL	conflict	UNP Q6B856
F	21	LEU	HIS	conflict	UNP Q6B856
F	22	LEU	ILE	conflict	UNP Q6B856
F	23	ALA	GLN	conflict	UNP Q6B856
F	24	THR	ALA	conflict	UNP Q6B856
F	27	TRP	CYS	conflict	UNP Q6B856
F	28	LYS	GLY	conflict	UNP Q6B856
F	29	ARG	ASN	conflict	UNP Q6B856
F	30	LEU	GLN	conflict	UNP Q6B856
F	31	ARG	ILE	conflict	UNP Q6B856
F	32	LYS	GLY	conflict	UNP Q6B856
F	33	ASP	ALA	conflict	UNP Q6B856
F	34	ASN	LYS	conflict	UNP Q6B856
F	35	PRO	PHE	conflict	UNP Q6B856
F	36	ARG	TRP	conflict	UNP Q6B856
F	37	PHE	GLU	conflict	UNP Q6B856
F	38	ASN	VAL	conflict	UNP Q6B856
F	39	LEU	ILE	conflict	UNP Q6B856
F	40	MET	SER	conflict	UNP Q6B856
F	41	LEU	ASP	conflict	UNP Q6B856
F	42	GLY	GLU	conflict	UNP Q6B856
F	43	GLU	HIS	conflict	UNP Q6B856
F	44	ARG	GLY	conflict	UNP Q6B856
F	45	ASN	ILE	conflict	UNP Q6B856

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Chain	Residue	Modelled	Actual	Comment	Reference
F	46	ARG	ASP	conflict	UNP Q6B856
F	47	LEU	PRO	conflict	UNP Q6B856
F	48	PRO	THR	conflict	UNP Q6B856
F	49	PHE	GLY	conflict	UNP Q6B856
F	50	GLY	SER	conflict	UNP Q6B856
F	51	ARG	TYR	conflict	UNP Q6B856
F	52	LEU	HIS	conflict	UNP Q6B856
F	54	HIS	ASP	conflict	UNP Q6B856
F	55	GLU	SER	conflict	UNP Q6B856
F	56	PRO	ASP	conflict	UNP Q6B856
F	57	GLY	LEU	conflict	UNP Q6B856
F	58	LEU	GLN	conflict	UNP Q6B856
F	59	VAL	LEU	conflict	UNP Q6B856
F	60	GLN	GLU	conflict	UNP Q6B856
F	61	LEU	ARG	conflict	UNP Q6B856
F	62	VAL	ILE	conflict	UNP Q6B856
F	64	TYR	VAL	conflict	UNP Q6B856
F	66	ARG	TYR	conflict	UNP Q6B856
F	67	GLY	ASN	conflict	UNP Q6B856
F	68	ALA	GLU	conflict	UNP Q6B856
F	69	ASP	ALA	conflict	UNP Q6B856
F	70	LYS	THR	conflict	UNP Q6B856
F	71	LEU	GLY	conflict	UNP Q6B856
F	72	CYS	ASN	conflict	UNP Q6B856
F	73	ARG	LYS	conflict	UNP Q6B856
F	74	LYS	TYR	conflict	UNP Q6B856
F	75	ALA	VAL	conflict	UNP Q6B856
F	76	SER	PRO	conflict	UNP Q6B856
F	77	LEU	ARG	conflict	UNP Q6B856
F	78	VAL	ALA	conflict	UNP Q6B856
F	79	LYS	ILE	conflict	UNP Q6B856
F	81	ILE	VAL	conflict	UNP Q6B856
F	82	LYS	ASP	conflict	UNP Q6B856
F	83	THR	LEU	conflict	UNP Q6B856
F	84	SER	GLU	conflict	UNP Q6B856
F	86	GLU	GLY	conflict	UNP Q6B856
F	87	LEU	THR	conflict	UNP Q6B856
F	88	SER	MET	conflict	UNP Q6B856
F	89	GLU	ASP	conflict	UNP Q6B856
F	91	CYS	VAL	conflict	UNP Q6B856
F	92	THR	ARG	conflict	UNP Q6B856
F	93	TRP	SER	conflict	UNP Q6B856

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Chain	Residue	Modelled	Actual	Comment	Reference
F	94	PHE	GLY	conflict	UNP Q6B856
F	96	GLU	PHE	conflict	UNP Q6B856
F	97	SER	GLY	conflict	UNP Q6B856
F	98	TYR	GLN	conflict	UNP Q6B856
F	99	VAL	ILE	conflict	UNP Q6B856
F	100	ILE	PHE	conflict	UNP Q6B856
F	101	TYR	ARG	conflict	UNP Q6B856
F	103	THR	ASP	conflict	UNP Q6B856
F	105	LEU	PHE	conflict	UNP Q6B856
F	106	LYS	VAL	conflict	UNP Q6B856
F	107	THR	PHE	conflict	UNP Q6B856
F	108	PRO	GLY	conflict	UNP Q6B856
F	109	VAL	GLN	conflict	UNP Q6B856
F	110	ALA	SER	conflict	UNP Q6B856
F	111	PRO	GLY	conflict	UNP Q6B856
F	113	GLN	GLY	conflict	UNP Q6B856
F	115	GLY	ASN	conflict	UNP Q6B856
F	116	ILE	TRP	conflict	UNP Q6B856
F	117	ARG	ALA	conflict	UNP Q6B856
F	118	HIS	LYS	conflict	UNP Q6B856
F	119	LEU	GLY	conflict	UNP Q6B856
F	120	ILE	HIS	conflict	UNP Q6B856
F	121	ASN	TYR	conflict	UNP Q6B856
F	122	ASN	THR	conflict	UNP Q6B856
F	123	THR	GLU	conflict	UNP Q6B856
F	124	ARG	GLY	conflict	UNP Q6B856
F	125	THR	ALA	conflict	UNP Q6B856
F	126	ASP	GLU	conflict	UNP Q6B856
F	127	GLU	LEU	conflict	UNP Q6B856
F	128	ARG	VAL	conflict	UNP Q6B856
F	129	GLU	ASP	conflict	UNP Q6B856
F	130	VAL	SER	conflict	UNP Q6B856
F	131	PHE	VAL	conflict	UNP Q6B856
F	133	ALA	ASP	conflict	UNP Q6B856
F	134	ALA	VAL	conflict	UNP Q6B856
F	135	TYR	VAL	conflict	UNP Q6B856
F	136	ASN	ARG	conflict	UNP Q6B856
F	137	ARG	LYS	conflict	UNP Q6B856
F	138	ARG	GLU	conflict	UNP Q6B856
F	139	ARG	SER	conflict	UNP Q6B856
F	141	GLY	SER	conflict	UNP Q6B856
F	142	ARG	CYS	conflict	UNP Q6B856

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Chain	Residue	Modelled	Actual	Comment	Reference
F	143	GLU	ASP	conflict	UNP Q6B856
F	144	GLY	CYS	conflict	UNP Q6B856
F	145	ASN	LEU	conflict	UNP Q6B856
F	146	VAL	GLN	conflict	UNP Q6B856
F	147	TRP	GLY	conflict	UNP Q6B856
F	148	ILE	PHE	conflict	UNP Q6B856
F	149	ALA	GLN	conflict	UNP Q6B856
F	150	LYS	LEU	conflict	UNP Q6B856
F	151	SER	THR	conflict	UNP Q6B856
F	152	SER	HIS	conflict	UNP Q6B856
F	153	ALA	SER	conflict	UNP Q6B856
F	154	GLY	LEU	conflict	UNP Q6B856
F	155	ALA	GLY	conflict	UNP Q6B856
F	156	LYS	GLY	conflict	UNP Q6B856
F	158	GLU	THR	conflict	UNP Q6B856
F	160	ILE	LEU	conflict	UNP Q6B856
F	164	SER	LYS	conflict	UNP Q6B856
F	165	GLU	ILE	conflict	UNP Q6B856
F	166	ALA	ARG	conflict	UNP Q6B856
F	167	SER	GLU	conflict	UNP Q6B856
F	169	LEU	TYR	conflict	UNP Q6B856
F	170	LEU	PRO	conflict	UNP Q6B856
F	172	PHE	ARG	conflict	UNP Q6B856
F	174	ASP	MET	conflict	UNP Q6B856
F	175	GLU	ASN	conflict	UNP Q6B856
F	176	GLN	THR	conflict	UNP Q6B856
F	177	GLY	PHE	conflict	UNP Q6B856
F	178	GLN	SER	conflict	UNP Q6B856
F	180	HIS	MET	conflict	UNP Q6B856
F	181	VAL	PRO	conflict	UNP Q6B856
F	182	ILE	SER	conflict	UNP Q6B856
F	183	GLN	PRO	conflict	UNP Q6B856
F	185	TYR	THR	conflict	UNP Q6B856
F	187	GLU	SER	conflict	UNP Q6B856
F	188	LYS	VAL	conflict	UNP Q6B856
F	189	PRO	HIS	conflict	UNP Q6B856
F	190	LEU	GLN	conflict	UNP Q6B856
F	192	LEU	VAL	conflict	UNP Q6B856
F	194	PRO	ASN	conflict	UNP Q6B856
F	195	GLY	THR	conflict	UNP Q6B856
F	196	HIS	ASP	conflict	UNP Q6B856
F	197	ARG	GLU	conflict	UNP Q6B856

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Chain	Residue	Modelled	Actual	Comment	Reference
F	198	LYS	THR	conflict	UNP Q6B856
F	199	PHE	TYR	conflict	UNP Q6B856
F	200	ASP	CYS	conflict	UNP Q6B856
F	202	ARG	ASP	conflict	UNP Q6B856
F	203	SER	ASN	conflict	UNP Q6B856
F	204	TRP	GLU	conflict	UNP Q6B856
F	205	VAL	ALA	conflict	UNP Q6B856
F	207	VAL	TYR	conflict	UNP Q6B856
F	209	HIS	ILE	conflict	UNP Q6B856
F	210	LEU	CYS	conflict	UNP Q6B856
F	211	TYR	PHE	conflict	UNP Q6B856
F	212	ASN	ARG	conflict	UNP Q6B856
F	213	ILE	THR	conflict	UNP Q6B856
F	214	TYR	LEU	conflict	UNP Q6B856
F	215	LEU	LYS	conflict	UNP Q6B856
F	216	TYR	LEU	conflict	UNP Q6B856
F	217	ARG	THR	conflict	UNP Q6B856
F	218	GLU	THR	conflict	UNP Q6B856
F	219	GLY	PRO	conflict	UNP Q6B856
F	220	VAL	THR	conflict	UNP Q6B856
F	221	LEU	TYR	conflict	UNP Q6B856
F	222	ARG	GLY	conflict	UNP Q6B856
F	223	THR	ASP	conflict	UNP Q6B856
F	224	SER	LEU	conflict	UNP Q6B856
F	225	SER	ASN	conflict	UNP Q6B856
F	226	GLU	HIS	conflict	UNP Q6B856
F	227	PRO	LEU	conflict	UNP Q6B856
F	228	TYR	VAL	conflict	UNP Q6B856
F	229	ASN	SER	conflict	UNP Q6B856
F	230	SER	ALA	conflict	UNP Q6B856
F	231	ALA	THR	conflict	UNP Q6B856
F	232	ASN	MET	conflict	UNP Q6B856
F	233	PHE	SER	conflict	UNP Q6B856
F	234	GLN	GLY	conflict	UNP Q6B856
F	235	ASP	VAL	conflict	UNP Q6B856
F	236	LYS	THR	conflict	UNP Q6B856
F	239	HIS	LEU	conflict	UNP Q6B856
F	240	LEU	ARG	conflict	UNP Q6B856
F	241	THR	PHE	conflict	UNP Q6B856
F	242	ASN	PRO	conflict	UNP Q6B856
F	243	HIS	GLY	conflict	UNP Q6B856
F	244	CYS	GLN	conflict	UNP Q6B856

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Chain	Residue	Modelled	Actual	Comment	Reference
F	245	ILE	LEU	conflict	UNP Q6B856
F	246	GLN	ASN	conflict	UNP Q6B856
F	247	LYS	ALA	conflict	UNP Q6B856
F	248	GLU	ASP	conflict	UNP Q6B856
F	249	TYR	LEU	conflict	UNP Q6B856
F	250	SER	ARG	conflict	UNP Q6B856
F	252	ASN	LEU	conflict	UNP Q6B856
F	253	TYR	ALA	conflict	UNP Q6B856
F	254	GLY	VAL	conflict	UNP Q6B856
F	255	ARG	ASN	conflict	UNP Q6B856
F	256	TYR	MET	conflict	UNP Q6B856
F	257	GLU	VAL	conflict	UNP Q6B856
F	258	GLU	PRO	conflict	UNP Q6B856
F	259	GLY	PHE	conflict	UNP Q6B856
F	260	ASN	PRO	conflict	UNP Q6B856
F	261	GLU	ARG	conflict	UNP Q6B856
F	262	MET	LEU	conflict	UNP Q6B856
F	263	PHE	HIS	conflict	UNP Q6B856
F	265	GLU	PHE	conflict	UNP Q6B856
F	266	GLU	MET	conflict	UNP Q6B856
F	267	PHE	PRO	conflict	UNP Q6B856
F	268	ASN	GLY	conflict	UNP Q6B856
F	269	GLN	PHE	conflict	UNP Q6B856
F	270	TYR	ALA	conflict	UNP Q6B856
F	271	LEU	PRO	conflict	UNP Q6B856
F	272	MET	LEU	conflict	UNP Q6B856
F	273	ASP	THR	conflict	UNP Q6B856
F	274	ALA	SER	conflict	UNP Q6B856
F	275	LEU	ARG	conflict	UNP Q6B856
F	276	ASN	GLY	conflict	UNP Q6B856
F	277	THR	SER	conflict	UNP Q6B856
F	278	THR	GLN	conflict	UNP Q6B856
F	279	LEU	GLN	conflict	UNP Q6B856
F	280	GLU	TYR	conflict	UNP Q6B856
F	281	ASN	ARG	conflict	UNP Q6B856
F	282	SER	ALA	conflict	UNP Q6B856
F	283	ILE	LEU	conflict	UNP Q6B856
F	284	LEU	THR	conflict	UNP Q6B856
F	285	LEU	VAL	conflict	UNP Q6B856
F	286	GLN	PRO	conflict	UNP Q6B856
F	287	ILE	GLU	conflict	UNP Q6B856
F	288	LYS	LEU	conflict	UNP Q6B856

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Chain	Residue	Modelled	Actual	Comment	Reference
F	289	HIS	THR	conflict	UNP Q6B856
F	290	ILE	GLN	conflict	UNP Q6B856
F	291	ILE	GLN	conflict	UNP Q6B856
F	292	ARG	MET	conflict	UNP Q6B856
F	293	SER	PHE	conflict	UNP Q6B856
F	294	CYS	ASP	conflict	UNP Q6B856
F	295	LEU	SER	conflict	UNP Q6B856
F	296	MET	LYS	conflict	UNP Q6B856
F	297	CYS	ASN	conflict	UNP Q6B856
F	298	ILE	MET	conflict	UNP Q6B856
F	299	GLU	MET	conflict	UNP Q6B856
F	300	PRO	ALA	conflict	UNP Q6B856
F	302	ILE	CYS	conflict	UNP Q6B856
F	303	SER	ASP	conflict	UNP Q6B856
F	304	THR	PRO	conflict	UNP Q6B856
F	305	LYS	ARG	conflict	UNP Q6B856
F	307	LEU	GLY	conflict	UNP Q6B856
F	308	HIS	ARG	conflict	UNP Q6B856
F	310	GLN	LEU	conflict	UNP Q6B856
F	311	SER	THR	conflict	UNP Q6B856
F	312	PHE	VAL	conflict	UNP Q6B856
F	313	GLN	ALA	conflict	UNP Q6B856
F	314	LEU	ALA	conflict	UNP Q6B856
F	315	PHE	ILE	conflict	UNP Q6B856
F	316	GLY	PHE	conflict	UNP Q6B856
F	317	PHE	ARG	conflict	UNP Q6B856
F	318	ASP	GLY	conflict	UNP Q6B856
F	319	PHE	ARG	conflict	UNP Q6B856
F	321	VAL	SER	conflict	UNP Q6B856
F	322	ASP	MET	conflict	UNP Q6B856
F	323	GLU	LYS	conflict	UNP Q6B856
F	325	LEU	VAL	conflict	UNP Q6B856
F	326	LYS	ASP	conflict	UNP Q6B856
F	327	VAL	GLU	conflict	UNP Q6B856
F	328	TRP	GLN	conflict	UNP Q6B856
F	329	LEU	MET	conflict	UNP Q6B856
F	330	ILE	LEU	conflict	UNP Q6B856
F	331	GLU	ASN	conflict	UNP Q6B856
F	333	ASN	-	insertion	UNP Q6B856
F	334	GLY	-	insertion	UNP Q6B856
F	335	ALA	-	insertion	UNP Q6B856
F	336	PRO	GLN	conflict	UNP Q6B856

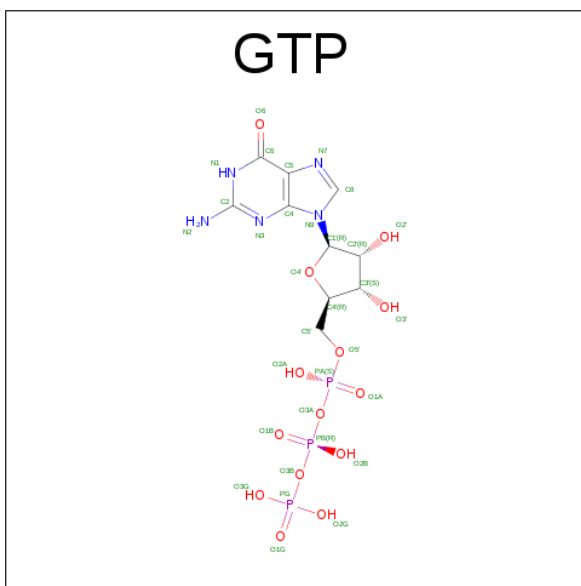
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Chain	Residue	Modelled	Actual	Comment	Reference
F	337	ALA	ASN	conflict	UNP Q6B856
F	338	CYS	LYS	conflict	UNP Q6B856
F	339	ALA	ASN	conflict	UNP Q6B856
F	340	GLN	SER	conflict	UNP Q6B856
F	341	LYS	SER	conflict	UNP Q6B856
F	342	LEU	TYR	conflict	UNP Q6B856
F	343	TYR	PHE	conflict	UNP Q6B856
F	344	ALA	VAL	conflict	UNP Q6B856
F	346	LEU	TRP	conflict	UNP Q6B856
F	347	CYS	ILE	conflict	UNP Q6B856
F	348	GLN	PRO	conflict	UNP Q6B856
F	349	GLY	ASN	conflict	UNP Q6B856
F	350	ILE	ASN	conflict	UNP Q6B856
F	352	ASP	LYS	conflict	UNP Q6B856
F	353	VAL	THR	conflict	UNP Q6B856
F	355	ILE	VAL	conflict	UNP Q6B856
F	356	SER	CYS	conflict	UNP Q6B856
F	357	SER	ASP	conflict	UNP Q6B856
F	358	VAL	ILE	conflict	UNP Q6B856
F	359	PHE	PRO	conflict	UNP Q6B856
F	361	LEU	ARG	conflict	UNP Q6B856
F	362	ALA	GLY	conflict	UNP Q6B856
F	363	ASP	LEU	conflict	UNP Q6B856
F	364	THR	LYS	conflict	UNP Q6B856
F	365	GLY	MET	conflict	UNP Q6B856
F	366	GLN	SER	conflict	UNP Q6B856
F	367	LYS	ALA	conflict	UNP Q6B856
F	369	SER	PHE	conflict	UNP Q6B856
F	370	GLN	ILE	conflict	UNP Q6B856
F	371	PRO	GLY	conflict	UNP Q6B856
F	372	THR	ASN	conflict	UNP Q6B856
F	374	ILE	THR	conflict	UNP Q6B856
F	375	PHE	ALA	conflict	UNP Q6B856
F	377	LYS	GLN	conflict	UNP Q6B856
F	378	LEU	GLU	conflict	UNP Q6B856
F	379	HIS	LEU	conflict	UNP Q6B856
F	380	HIS	PHE	conflict	UNP Q6B856
F	381	HIS	-	expression tag	UNP Q6B856
F	382	HIS	-	expression tag	UNP Q6B856
F	383	HIS	-	expression tag	UNP Q6B856
F	384	HIS	-	expression tag	UNP Q6B856

- 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	H	N	O	P	0	0
			41	10	9	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			41	10	9	5	14	3		

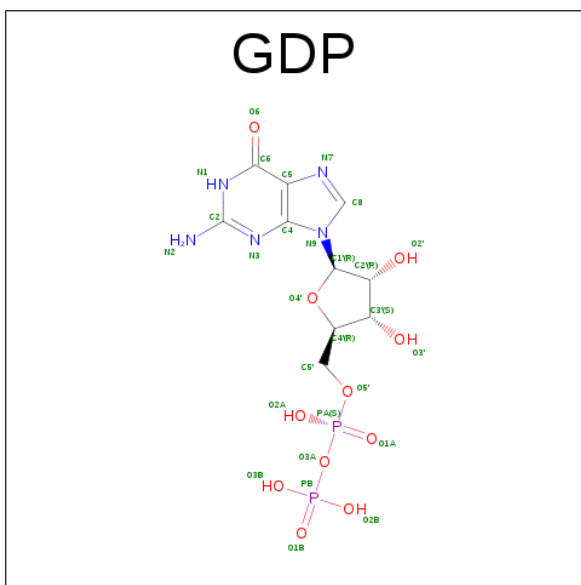
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Mg	0	0
			2	2		
6	A	1	Total	Mg	0	0
			1	1		
6	C	2	Total	Mg	0	0
			2	2		

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

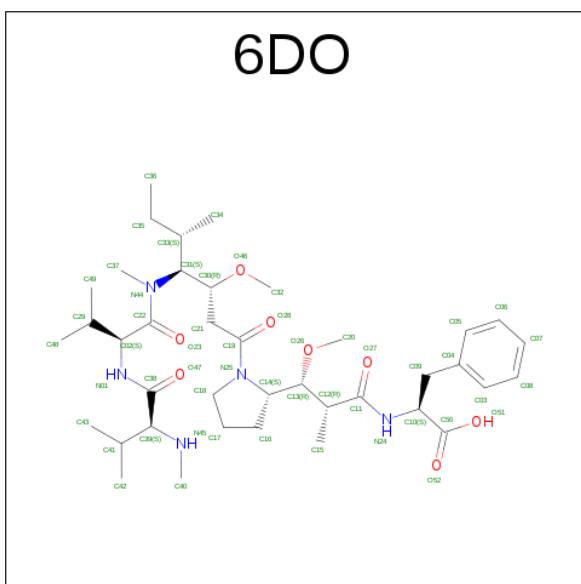
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



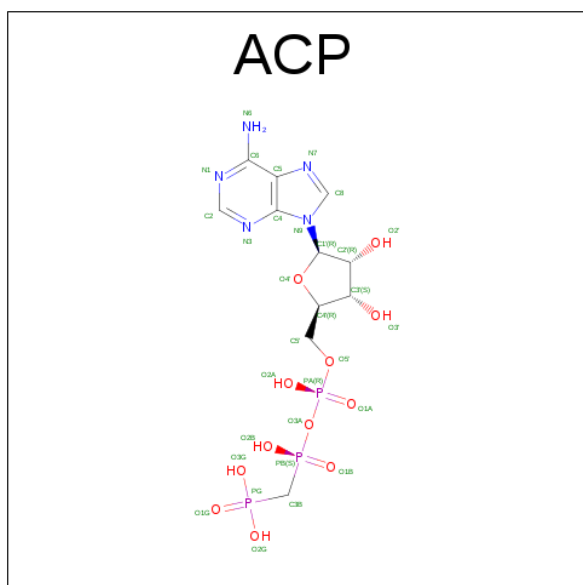
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
8	D	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0

- Molecule 9 is (2 {S})-2-[[[(2 {R},3 {R})-3-methoxy-3-[(2 {S})-1-[(3 {R},4 {S},5 {S})-3-methoxy-5-methyl-4-[methyl-[(2 {S})-3-methyl-2-[[[(2 {S})-3-methyl-2-(methylamino)butanoyl]amino]butanoyl]amino]heptanoyl]pyrrolidin-2-yl]-2-methyl-propanoyl]amino]-3-phenyl-propanoic acid (three-letter code: 6DO) (formula: C<sub>39</sub>H<sub>65</sub>N<sub>5</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			117	39	65	5	8		
9	D	1	Total	C	H	N	O	0	0
			117	39	65	5	8		

- Molecule 10 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
10	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

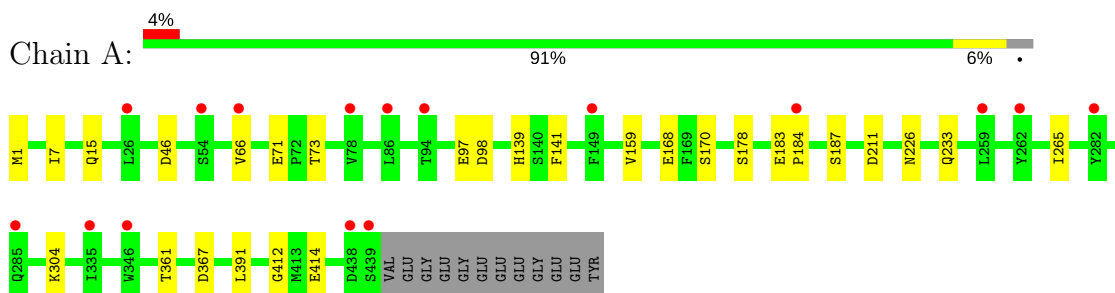
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	12	Total	O	0	0
			12	12		
11	B	52	Total	O	0	0
			52	52		
11	C	47	Total	O	0	0
			47	47		
11	D	9	Total	O	0	0
			9	9		
11	E	9	Total	O	0	0
			9	9		
11	F	9	Total	O	0	0
			9	9		

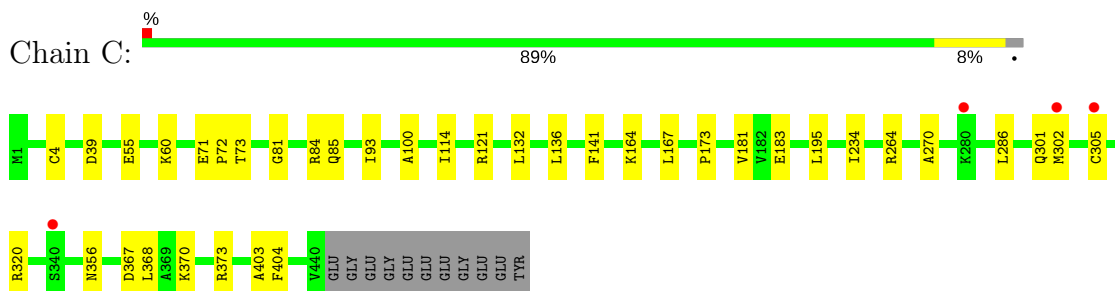
### 3 Residue-property plots [i](#)

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.

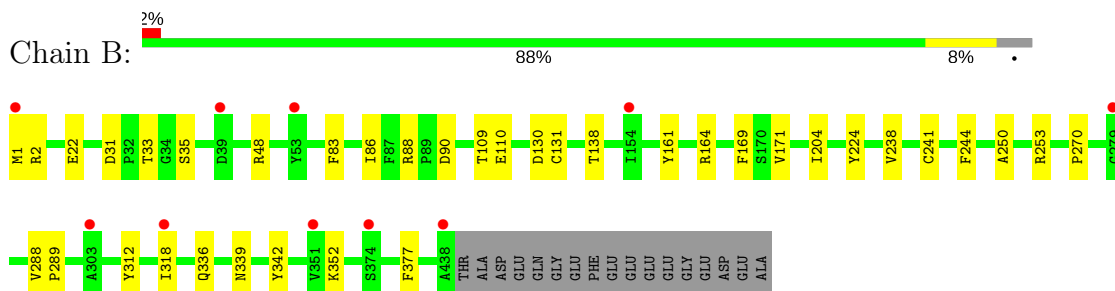
- Molecule 1: Tubulin alpha-1B chain



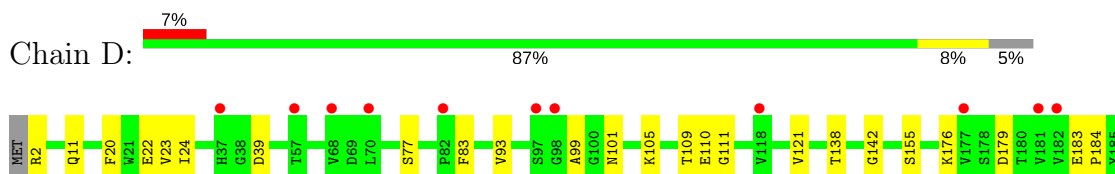
- Molecule 1: Tubulin alpha-1B chain



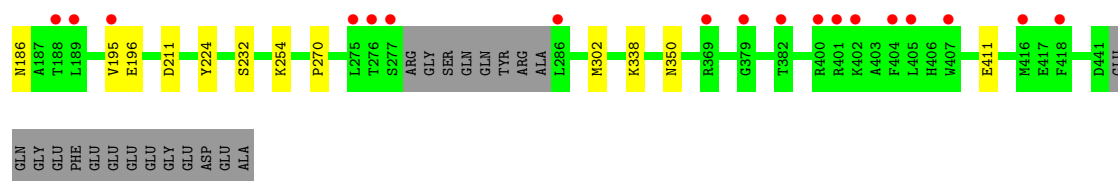
- Molecule 2: Tubulin beta-2B chain



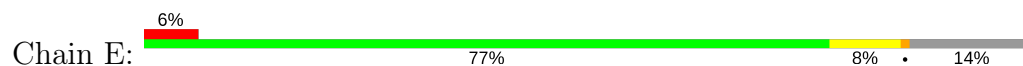
- Molecule 2: Tubulin beta-2B chain



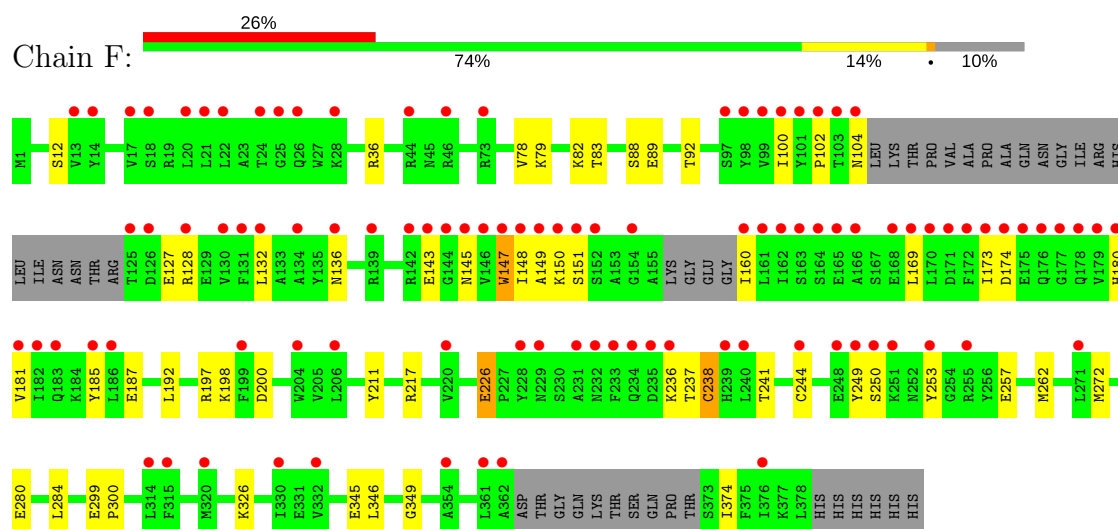




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin beta-2B chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.57Å 155.39Å 182.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.65 – 2.50 56.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (56.65-2.50) 86.4 (56.65-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.216 , 0.250 0.236 , 0.266	Depositor DCC
$R_{free}$ test set	2000 reflections (2.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.6	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	0.93	EDS
Total number of atoms	35242	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, CA, GTP, ACP, 6DO

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	0.29	0/3554	0.47	0/4826
1	C	0.35	0/3601	0.47	0/4892
2	B	0.28	0/3503	0.44	0/4743
2	D	0.27	0/3413	0.48	3/4624 (0.1%)
3	E	0.25	0/1068	0.41	0/1418
4	F	0.28	0/2886	0.48	0/3899
All	All	0.29	0/18025	0.46	3/24402 (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
4	F	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	109	THR	N-CA-C	7.57	131.43	111.00
2	D	110	GLU	N-CA-CB	5.40	120.32	110.60
2	D	109	THR	CB-CA-C	-5.37	97.11	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	149	ALA	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	3457	3377	3390	20	0
1	C	3487	3407	3424	23	0
2	B	3400	3290	3273	24	0
2	D	3328	3204	3215	21	1
3	E	1042	1064	1070	12	0
4	F	2818	2787	2796	29	1
5	A	32	9	12	1	0
5	C	32	9	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
7	A	1	0	0	0	0
8	B	28	10	12	0	0
8	D	28	10	12	1	0
9	B	52	65	0	0	0
9	D	52	65	0	2	0
10	F	31	14	14	0	0
11	A	12	0	0	0	0
11	B	52	0	0	3	0
11	C	47	0	0	2	0
11	D	9	0	0	1	0
11	E	9	0	0	1	0
11	F	9	0	0	1	0
All	All	17931	17311	17230	120	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 3.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:46:SER:OG	3:E:49:GLU:HB2	1.29	1.29
4:F:82:LYS:NZ	4:F:127:GLU:OE2	1.92	1.02
3:E:46:SER:HG	3:E:49:GLU:HB2	1.26	0.98
3:E:46:SER:OG	3:E:49:GLU:CB	2.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LYS:NZ	1:C:85:GLN:O	2.09	0.86
4:F:151:SER:OG	4:F:180:HIS:CE1	2.29	0.86
2:B:241:CYS:SG	2:B:318:ILE:HG12	2.29	0.73
4:F:102:PRO:O	4:F:104:ASN:ND2	2.24	0.70
2:B:1:MET:N	2:B:131:CYS:SG	2.65	0.70
2:B:224:TYR:OH	11:B:601:HOH:O	2.13	0.67
2:D:99:ALA:O	2:D:101:ASN:N	2.28	0.66
1:C:370:LYS:NZ	11:C:601:HOH:O	2.28	0.65
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.29	0.65
4:F:197:ARG:NH2	4:F:257:GLU:OE1	2.29	0.65
1:C:132:LEU:O	1:C:164:LYS:NZ	2.29	0.65
4:F:217:ARG:NH2	4:F:345:GLU:OE2	2.30	0.64
1:C:286:LEU:O	1:C:373:ARG:NH1	2.32	0.62
1:A:233:GLN:NE2	1:A:361:THR:O	2.34	0.61
2:D:142:GLY:O	2:D:186:ASN:ND2	2.33	0.60
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.35	0.60
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.84	0.59
1:C:121:ARG:NH2	11:C:603:HOH:O	2.35	0.59
2:D:11:GLN:N	8:D:501:GDP:O2B	2.37	0.57
2:B:48:ARG:NH2	2:B:250:ALA:O	2.39	0.55
1:A:265:ILE:HG22	1:A:265:ILE:O	2.06	0.55
3:E:44:ASP:HB3	3:E:45:PRO:HD3	1.89	0.55
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.26	0.54
2:D:176:LYS:NZ	2:D:211:ASP:OD1	2.38	0.53
4:F:192:LEU:HD11	4:F:262:MET:CE	2.39	0.53
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.90	0.53
4:F:36:ARG:NH1	11:F:501:HOH:O	2.41	0.52
2:B:339:ASN:ND2	11:B:605:HOH:O	2.42	0.52
2:D:224:TYR:N	9:D:502:6DO:O28	2.39	0.52
3:E:6:MET:N	11:E:201:HOH:O	2.41	0.52
4:F:79:LYS:O	4:F:83:THR:OG1	2.19	0.52
1:C:81:GLY:O	1:C:84:ARG:NH2	2.38	0.51
2:D:155[A]:SER:HB2	3:E:126:LYS:HZ3	1.75	0.51
1:A:414:GLU:OE1	3:E:60:ARG:NH1	2.44	0.51
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG23	1.93	0.51
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.91	0.51
4:F:150:LYS:HA	4:F:160:ILE:HG22	1.92	0.51
2:B:48:ARG:NH1	2:B:244:PHE:O	2.40	0.51
4:F:151:SER:OG	4:F:180:HIS:ND1	2.44	0.50
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.94	0.50
1:C:181[B]:VAL:HG11	1:C:404:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:CYS:SG	2:B:318:ILE:CG1	3.00	0.49
1:C:301:GLN:NE2	1:C:305:CYS:SG	2.86	0.48
1:C:71:GLU:OE2	1:C:73:THR:N	2.44	0.48
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.95	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.96	0.48
1:C:71:GLU:OE2	1:C:73:THR:HB	2.13	0.48
1:C:71:GLU:OE2	1:C:73:THR:CB	2.61	0.48
2:D:179:ASP:OD1	9:D:502:6DO:N45	2.47	0.48
4:F:100:ILE:HG22	4:F:128:ARG:NH1	2.29	0.48
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.43	0.47
1:C:234:ILE:HG21	1:C:302:MET:SD	2.55	0.47
2:D:39:ASP:N	2:D:39:ASP:OD1	2.40	0.47
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.33	0.47
4:F:346:LEU:O	4:F:349:GLY:N	2.48	0.46
2:B:336:GLN:OE1	4:F:36:ARG:NH2	2.47	0.46
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.97	0.46
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.34	0.45
1:C:39:ASP:OD2	1:C:55:GLU:OE2	2.34	0.45
4:F:192:LEU:HD11	4:F:262:MET:HE2	1.98	0.45
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.52	0.45
1:A:178:SER:OG	2:B:352:LYS:NZ	2.49	0.45
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.31	0.45
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.48	0.45
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.56	0.45
2:B:83:PHE:O	2:B:86:ILE:HG22	2.16	0.45
1:C:173:PRO:HB3	1:C:183:GLU:OE2	2.18	0.44
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.99	0.44
4:F:236:LYS:O	4:F:238:CYS:N	2.50	0.44
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.53	0.44
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.53	0.44
4:F:226:GLU:OE1	4:F:250:SER:OG	2.23	0.44
2:B:31:ASP:OD2	2:B:35:SER:HB2	2.18	0.44
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.82	0.44
2:B:110:GLU:OE2	11:B:602:HOH:O	2.21	0.43
2:B:2:ARG:NH2	2:B:130:ASP:OD2	2.51	0.43
4:F:145:ASN:HA	4:F:187:GLU:OE2	2.18	0.43
2:D:22:GLU:HG2	2:D:83:PHE:CE1	2.53	0.43
2:D:93:VAL:HG21	2:D:121:VAL:HG21	2.01	0.43
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.51	0.43
2:D:105:LYS:O	2:D:111:GLY:N	2.52	0.43
1:A:139:HIS:NE2	1:A:168:GLU:OE1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:280:GLU:HA	4:F:284:LEU:HB2	2.01	0.42
4:F:299:GLU:N	4:F:300:PRO:HD2	2.34	0.42
3:E:9:ILE:HG22	3:E:10:GLU:HG3	2.02	0.42
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.01	0.42
2:D:411:GLU:HA	3:E:137:LYS:HD3	2.01	0.42
2:D:195:VAL:HG13	2:D:196:GLU:HG2	2.01	0.42
1:A:412:GLY:O	3:E:60:ARG:NE	2.40	0.42
1:A:98:ASP:C	1:A:98:ASP:OD1	2.58	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.19	0.42
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.31	0.42
4:F:92:THR:O	4:F:326:LYS:NZ	2.48	0.42
2:D:254:LYS:NZ	11:D:601:HOH:O	2.52	0.41
1:C:403:ALA:O	1:C:404:PHE:HB2	2.20	0.41
4:F:249:TYR:O	4:F:250:SER:OG	2.37	0.41
1:C:320:ARG:HA	1:C:356:ASN:O	2.20	0.41
1:A:1:MET:CB	1:A:46:ASP:OD1	2.68	0.41
1:A:183:GLU:N	1:A:184:PRO:CD	2.84	0.41
1:C:195:LEU:HD23	1:C:264:ARG:NH1	2.35	0.41
1:C:71:GLU:HG2	1:C:72:PRO:HD2	2.02	0.41
2:D:2:ARG:NH1	2:D:2:ARG:HB2	2.36	0.41
1:A:97:GLU:HG3	2:B:1:MET:HG2	2.03	0.41
1:A:1:MET:HB2	1:A:46:ASP:OD1	2.20	0.41
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.56	0.41
4:F:169:LEU:O	4:F:173:ILE:N	2.52	0.41
2:B:109:THR:OG1	2:B:110:GLU:N	2.53	0.41
2:B:161:TYR:HB3	2:B:164:ARG:CG	2.51	0.41
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.03	0.41
2:D:183:GLU:HB2	2:D:184:PRO:HD3	2.03	0.41
1:A:159:VAL:HG11	3:E:47:LEU:HB2	2.02	0.41
1:C:100:ALA:HA	2:D:254:LYS:HG3	2.03	0.41
2:D:350:ASN:OD1	2:D:350:ASN:N	2.52	0.41
2:D:270:PRO:HG2	2:D:302:MET:HB2	2.03	0.40
4:F:147:TRP:CD1	4:F:147:TRP:N	2.89	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:338:LYS:NZ	4:F:88:SER:OG[3_545]	2.08	0.12

## 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	443/451 (98%)	421 (95%)	22 (5%)	0	100	100
1	C	450/451 (100%)	431 (96%)	19 (4%)	0	100	100
2	B	433/445 (97%)	418 (96%)	15 (4%)	0	100	100
2	D	422/445 (95%)	400 (95%)	22 (5%)	0	100	100
3	E	125/143 (87%)	123 (98%)	2 (2%)	0	100	100
4	F	338/384 (88%)	316 (94%)	21 (6%)	1 (0%)	44	66
All	All	2211/2319 (95%)	2109 (95%)	101 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	237	THR

### 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	376/379 (99%)	376 (100%)	0	100	100
1	C	383/379 (101%)	380 (99%)	3 (1%)	85	95
2	B	377/383 (98%)	374 (99%)	3 (1%)	85	95
2	D	369/383 (96%)	367 (100%)	2 (0%)	91	97
3	E	116/127 (91%)	113 (97%)	3 (3%)	51	78
4	F	310/342 (91%)	298 (96%)	12 (4%)	37	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1931/1993 (97%)	1908 (99%)	23 (1%)	75 91

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	238[B]	VAL
2	B	253	ARG
2	B	270	PRO
1	C	141	PHE
1	C	367	ASP
1	C	368	LEU
2	D	77	SER
2	D	138	THR
3	E	60	ARG
3	E	90[A]	ASN
3	E	90[B]	ASN
4	F	12	SER
4	F	89	GLU
4	F	132	LEU
4	F	136	ASN
4	F	143	GLU
4	F	147	TRP
4	F	148	ILE
4	F	226	GLU
4	F	238	CYS
4	F	244	CYS
4	F	253	TYR
4	F	272	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	139	HIS
2	B	192	HIS
2	B	385	GLN
1	C	301	GLN
4	F	104	ASN
4	F	180	HIS
4	F	243	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 13 ligands modelled in this entry, 6 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	1.11	1 (3%)	24,54,54	1.21	1 (4%)
8	GDP	B	501	-	25,30,30	1.35	4 (16%)	23,47,47	1.37	3 (13%)
9	6DO	B	504	-	49,53,53	2.64	12 (24%)	48,73,73	1.54	3 (6%)
5	GTP	C	501	6	27,34,34	1.08	1 (3%)	24,54,54	1.13	1 (4%)
8	GDP	D	501	-	25,30,30	1.39	4 (16%)	23,47,47	1.31	3 (13%)
9	6DO	D	502	-	49,53,53	2.67	12 (24%)	48,73,73	1.59	4 (8%)
10	ACP	F	401	-	27,33,33	1.94	8 (29%)	30,52,52	1.69	5 (16%)

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
8	GDP	B	501	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	6DO	B	504	-	-	0/72/86/86	0/2/2/2
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GDP	D	501	-	-	0/12/32/32	0/3/3/3
9	6DO	D	502	-	-	0/72/86/86	0/2/2/2
10	ACP	F	401	-	-	0/15/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	401	ACP	PB-O2B	-3.73	1.47	1.56
10	F	401	ACP	PG-O3G	-3.14	1.47	1.54
9	D	502	6DO	C18-N25	-2.76	1.42	1.47
9	B	504	6DO	C10-N24	-2.71	1.42	1.46
8	B	501	GDP	C6-N1	-2.54	1.33	1.36
9	B	504	6DO	C16-C14	-2.49	1.49	1.53
9	D	502	6DO	C16-C14	-2.47	1.49	1.53
9	B	504	6DO	C18-N25	-2.42	1.43	1.47
8	D	501	GDP	C6-N1	-2.38	1.33	1.36
9	D	502	6DO	C10-N24	-2.15	1.43	1.46
10	F	401	ACP	C2'-C1'	-2.02	1.50	1.53
9	B	504	6DO	C09-C04	2.17	1.56	1.51
9	D	502	6DO	C09-C04	2.21	1.56	1.51
10	F	401	ACP	PG-O2G	2.33	1.60	1.54
8	B	501	GDP	C2-N2	2.56	1.36	1.32
8	D	501	GDP	C2-N2	2.60	1.36	1.32
8	B	501	GDP	C5-C4	2.71	1.46	1.40
9	D	502	6DO	C21-C19	2.75	1.56	1.51
8	D	501	GDP	C5-C4	2.79	1.46	1.40
9	B	504	6DO	C21-C19	2.97	1.56	1.51
10	F	401	ACP	C5-C4	3.11	1.47	1.40
10	F	401	ACP	PB-O3A	3.23	1.62	1.58
8	B	501	GDP	C6-C5	3.67	1.47	1.41
8	D	501	GDP	C6-C5	3.69	1.47	1.41
10	F	401	ACP	PB-O1B	3.81	1.61	1.51
5	A	501	GTP	C2-N3	4.20	1.38	1.33
5	C	501	GTP	C2-N3	4.25	1.38	1.33
10	F	401	ACP	PG-O1G	4.86	1.60	1.50
9	B	504	6DO	C11-N24	5.18	1.45	1.34
9	B	504	6DO	C38-N01	5.26	1.45	1.34
9	D	502	6DO	C11-N24	5.52	1.46	1.34
9	D	502	6DO	C19-N25	5.74	1.49	1.35
9	D	502	6DO	C38-N01	5.80	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	6DO	C19-N25	5.94	1.49	1.35
9	B	504	6DO	C07-C06	6.38	1.53	1.38
9	D	502	6DO	C07-C06	6.53	1.53	1.38
9	B	504	6DO	C22-N44	6.66	1.51	1.35
9	D	502	6DO	C22-N44	6.76	1.51	1.35
9	B	504	6DO	C05-C04	6.95	1.53	1.38
9	D	502	6DO	C05-C04	7.04	1.53	1.38
9	D	502	6DO	C08-C03	7.30	1.52	1.38
9	B	504	6DO	C08-C03	7.32	1.52	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	401	ACP	N3-C2-N1	-5.44	124.12	128.86
10	F	401	ACP	C4'-O4'-C1'	-3.75	105.78	109.77
8	B	501	GDP	C1'-N9-C4	-3.13	121.23	126.64
8	B	501	GDP	C4-C5-N7	-2.93	106.58	109.41
8	D	501	GDP	C4-C5-N7	-2.82	106.68	109.41
8	D	501	GDP	C1'-N9-C4	-2.42	122.46	126.64
9	B	504	6DO	O23-C22-C02	-2.19	115.92	120.09
10	F	401	ACP	PA-O3A-PB	-2.06	125.76	132.39
10	F	401	ACP	O1G-PG-C3B	-2.03	106.75	111.22
9	D	502	6DO	O26-C13-C12	2.09	110.83	105.81
9	D	502	6DO	C12-C11-N24	2.20	120.23	116.65
10	F	401	ACP	O3G-PG-C3B	2.46	112.36	106.40
9	D	502	6DO	C02-C22-N44	2.49	123.82	118.61
9	B	504	6DO	C02-C22-N44	3.31	125.54	118.61
8	B	501	GDP	C2-N3-C4	3.98	119.81	115.16
5	C	501	GTP	C2-N3-C4	4.21	120.07	115.16
8	D	501	GDP	C2-N3-C4	4.31	120.19	115.16
5	A	501	GTP	C2-N3-C4	4.51	120.42	115.16
9	B	504	6DO	C16-C14-N25	7.64	109.04	102.68
9	D	502	6DO	C16-C14-N25	8.41	109.69	102.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	1	0
9	D	502	6DO	2	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, 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	439/451 (97%)	0.49	16 (3%) 43 45	46, 68, 103, 154	0
1	C	440/451 (97%)	0.27	4 (0%) 84 85	37, 50, 73, 106	0
2	B	428/445 (96%)	0.34	10 (2%) 61 63	36, 56, 83, 131	1 (0%)
2	D	422/445 (94%)	0.58	29 (6%) 18 18	49, 71, 101, 127	2 (0%)
3	E	123/143 (86%)	0.57	8 (6%) 20 20	47, 74, 114, 138	0
4	F	344/384 (89%)	1.61	99 (28%) 1 0	61, 97, 163, 245	0
All	All	2196/2319 (94%)	0.61	166 (7%) 15 14	36, 66, 127, 245	3 (0%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	150	LYS	10.8
4	F	233	PHE	9.4
4	F	151	SER	9.2
4	F	173	ILE	9.0
4	F	161	LEU	8.7
4	F	148	ILE	8.7
4	F	149	ALA	7.8
4	F	160	ILE	7.3
4	F	234	GLN	7.1
4	F	99	VAL	6.7
4	F	142	ARG	6.5
4	F	176	GLN	6.5
4	F	147	TRP	6.4
4	F	239	HIS	6.3
4	F	177	GLY	6.2
4	F	162	ILE	6.2
4	F	143	GLU	6.2
4	F	182	ILE	6.0
4	F	361	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
4	F	235	ASP	5.9
4	F	169	LEU	5.9
2	D	405	LEU	5.8
4	F	330	ILE	5.6
4	F	132	LEU	5.6
4	F	240	LEU	5.5
4	F	101	TYR	5.2
4	F	163	SER	5.1
4	F	181	VAL	5.0
4	F	104	ASN	4.9
4	F	103	THR	4.9
4	F	180	HIS	4.8
4	F	178	GLN	4.6
4	F	100	ILE	4.4
4	F	13	VAL	4.3
4	F	172	PHE	4.3
4	F	232	ASN	4.3
2	D	401	ARG	4.2
4	F	139	ARG	4.2
1	A	438	ASP	4.2
4	F	146	VAL	4.2
2	D	57	THR	4.1
4	F	244	CYS	4.1
4	F	128	ARG	4.1
4	F	186	LEU	4.0
4	F	102	PRO	3.9
4	F	249	TYR	3.9
4	F	22	LEU	3.8
4	F	251	LYS	3.8
4	F	14	TYR	3.8
4	F	231	ALA	3.7
1	C	340	SER	3.7
4	F	165	GLU	3.6
3	E	24	LEU	3.6
1	A	439	SER	3.5
4	F	152	SER	3.5
4	F	166	ALA	3.5
4	F	125	THR	3.5
4	F	28	LYS	3.5
2	D	404	PHE	3.4
2	B	438	ALA	3.4
4	F	168	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	346	TRP	3.3
4	F	255	ARG	3.3
4	F	229	ASN	3.3
4	F	236	LYS	3.2
4	F	131	PHE	3.2
4	F	228	TYR	3.2
2	D	195	VAL	3.2
4	F	376	ILE	3.2
4	F	248	GLU	3.2
1	A	335	ILE	3.1
2	D	277	SER	3.1
2	D	407	TRP	3.1
4	F	145	ASN	3.1
4	F	362	ALA	3.1
1	A	262	TYR	3.1
4	F	126	ASP	3.1
4	F	253	TYR	3.1
4	F	206	LEU	3.1
4	F	320	MET	3.0
2	D	400	ARG	3.0
4	F	332	VAL	3.0
1	A	66[A]	VAL	2.9
4	F	134	ALA	2.9
4	F	21	LEU	2.9
1	A	149	PHE	2.9
2	D	276	THR	2.9
3	E	45	PRO	2.9
3	E	48	GLU	2.9
4	F	185	TYR	2.9
4	F	73	ARG	2.9
4	F	315	PHE	2.9
2	D	286	LEU	2.9
4	F	175	GLU	2.8
2	D	418	PHE	2.8
1	A	78	VAL	2.8
2	B	303	ALA	2.8
4	F	136	ASN	2.7
2	B	1	MET	2.7
4	F	17	VAL	2.7
2	D	70	LEU	2.7
2	D	188	THR	2.7
4	F	98	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	97	SER	2.6
2	D	182	VAL	2.6
4	F	24	THR	2.6
3	E	54	LEU	2.6
2	D	37	HIS	2.5
4	F	25	GLY	2.5
4	F	183	GLN	2.5
4	F	130	VAL	2.5
1	A	259	LEU	2.5
2	D	68	VAL	2.5
4	F	171	ASP	2.5
4	F	164	SER	2.5
1	A	282	TYR	2.5
1	C	305	CYS	2.5
4	F	314	LEU	2.4
4	F	220[A]	VAL	2.4
4	F	174	ASP	2.4
4	F	179	VAL	2.4
3	E	15[A]	THR	2.4
4	F	20	LEU	2.4
1	A	54	SER	2.4
2	D	82	PRO	2.4
3	E	28	SER	2.4
4	F	144	GLY	2.3
2	D	118	VAL	2.3
3	E	27	PRO	2.3
2	D	402	LYS	2.3
2	D	98	GLY	2.3
4	F	44	ARG	2.3
1	A	94	THR	2.3
2	B	351	VAL	2.3
2	B	318	ILE	2.3
1	A	26	LEU	2.3
3	E	139	LEU	2.3
2	B	279	GLY	2.2
2	D	379	GLY	2.2
2	D	97	SER	2.2
2	D	369	ARG	2.2
2	D	189	LEU	2.2
1	C	280	LYS	2.2
1	A	86	LEU	2.2
4	F	18	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	302	MET	2.1
4	F	154	GLY	2.1
1	A	285	GLN	2.1
4	F	26	GLN	2.1
4	F	199	PHE	2.1
4	F	271	LEU	2.1
2	B	374	SER	2.1
2	B	39	ASP	2.1
2	B	154	ILE	2.1
4	F	204	TRP	2.1
2	D	416	MET	2.1
1	A	184	PRO	2.1
4	F	46	ARG	2.1
4	F	354	ALA	2.1
2	D	181	VAL	2.0
2	D	382	THR	2.0
4	F	250	SER	2.0
2	B	53	TYR	2.0
2	D	177	VAL	2.0
2	D	275	LEU	2.0
4	F	170	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no 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
6	MG	A	502	1/1	0.87	0.40	5.76	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GTP	A	501	32/32	0.96	0.26	1.75	49,57,69,79	0
9	6DO	D	502	52/52	0.85	0.26	1.37	76,105,139,152	0
8	GDP	B	501	28/28	0.97	0.20	0.91	33,40,55,57	0
6	MG	C	503	1/1	0.88	0.17	0.79	87,87,87,87	0
5	GTP	C	501	32/32	0.96	0.20	0.62	37,46,57,72	0
9	6DO	B	504	52/52	0.94	0.19	0.27	33,47,60,64	0
6	MG	C	502	1/1	0.96	0.15	-0.20	39,39,39,39	0
8	GDP	D	501	28/28	0.93	0.17	-0.31	63,75,96,109	0
10	ACP	F	401	31/31	0.80	0.22	-0.68	121,145,169,178	0
6	MG	B	503	1/1	0.97	0.13	-0.94	52,52,52,52	0
7	CA	A	503	1/1	0.90	0.09	-1.35	123,123,123,123	0
6	MG	B	502	1/1	0.84	0.35	-	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.