



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:30 PM GMT

PDB ID : 4IIJ  
Title : Crystal structure of tubulin-stathmin-TTL-apo complex  
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Deposited on : 2012-12-20  
Resolution : 2.60 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

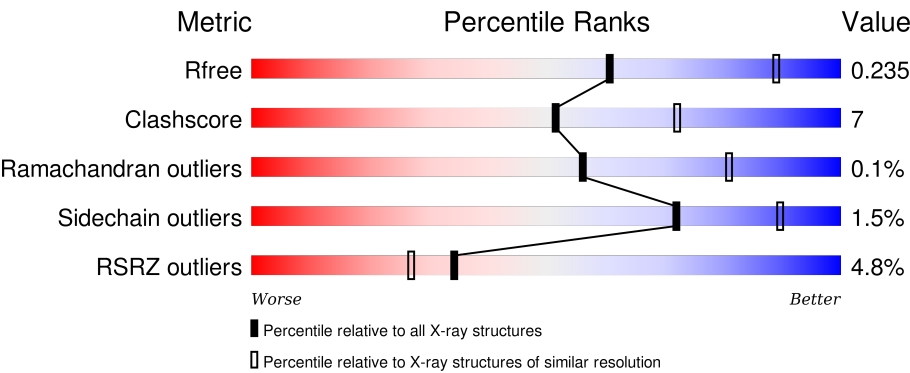
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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></div><div><div></div><div></div><div></div><div></div><div></div></div><div>84%12% . .</div></div>
1	C	451	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>84%14% .</div></div>
2	B	445	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%79%15%6%</div></div>
2	D	445	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%76%18%5%</div></div>
3	E	143	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%80%5% . 15%</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
6	MG	A	502	-	-	-	X
6	MG	C	502	-	-	-	X
7	CA	A	503	-	-	-	X
7	CA	B	503	-	-	-	X
7	CA	C	503	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 33359 atoms, of which 16438 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	H	N	O	S	0	5	0
			6830	2182	3386	586	653	23			
1	C	440	Total	C	H	N	O	S	0	10	0
			6889	2200	3412	587	665	25			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	418	Total	C	H	N	O	S	0	4	0
			6529	2085	3217	564	636	27			
2	D	421	Total	C	H	N	O	S	0	2	0
			6527	2090	3207	563	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	122	Total	C	H	N	O	S	0	2	0
			2063	630	1043	185	200	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	CLONING ARTIFACT	UNP P63043
E	4	ALA	SER	CLONING ARTIFACT	UNP P63043

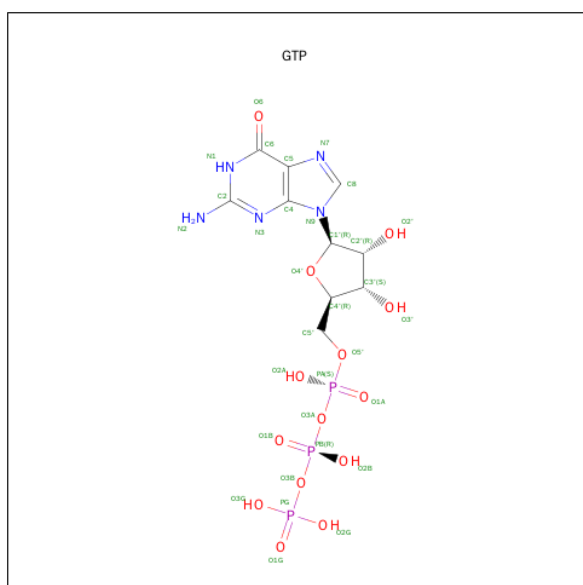
- Molecule 4 is a protein called Tubulin tyrosine ligase, TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	258	Total	C	H	N	O	S	0	0	0
			4235	1367	2120	363	373	12			

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	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	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		
6	C	1	Total	Mg	0	0
			1	1		

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

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7   | B     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 7   | A     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 7   | C     | 1        | Total Ca<br>1 1 | 0       | 0       |

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8   | A     | 1        | Total Cl<br>1 1 | 0       | 0       |

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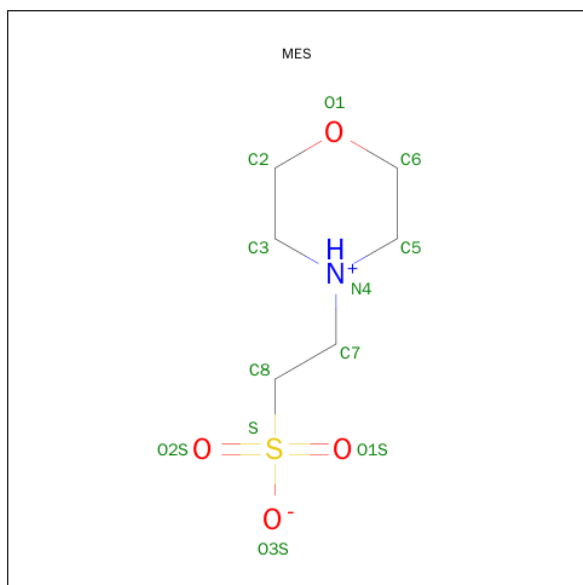
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
								0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	33	Total	O		
			33	33	0	0
11	B	15	Total	O		
			15	15	0	0
11	C	30	Total	O		
			30	30	0	0
11	D	6	Total	O		
			6	6	0	0
11	E	2	Total	O		
			2	2	0	0
11	F	6	Total	O		
			6	6	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.53Å 155.91Å 181.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.27 – 2.60 77.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.27-2.60) 100.0 (77.86-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.62Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.197 , 0.235 0.195 , 0.235	Depositor DCC
$R_{free}$ test set	4511 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 90600 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	33359	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CL, CA, GTP, 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	0.26	0/3537	0.44	0/4800
1	C	0.30	0/3587	0.46	0/4871
2	B	0.28	0/3397	0.44	0/4600
2	D	0.26	0/3401	0.42	0/4609
3	E	0.29	0/1035	0.40	1/1374 (0.1%)
4	F	0.25	0/2168	0.42	0/2930
All	All	0.27	0/17125	0.44	1/23184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	140	LYS	CD-CE-NZ	-5.14	99.87	111.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3444	3386	3374	41	0
1	C	3477	3412	3387	37	0
2	B	3312	3217	3209	47	0
2	D	3320	3207	3197	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1020	1043	1037	9	0
4	F	2115	2120	2110	37	0
5	A	32	10	12	1	0
5	C	32	10	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
6	F	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	10	12	0	0
9	D	28	10	11	1	0
10	B	12	13	13	1	0
11	A	33	0	0	2	0
11	B	15	0	0	0	0
11	C	30	0	0	1	0
11	D	6	0	0	1	0
11	E	2	0	0	0	0
11	F	6	0	0	0	0
All	All	16921	16438	16374	227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (227) 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:D:2:ARG:NH2	2:D:3:GLU:OE1	2.02	0.93
1:C:285:GLN:NE2	1:C:372:GLN:OE1	2.12	0.83
2:D:409:THR:O	3:E:140:LYS:NZ	2.14	0.80
3:E:137:LYS:HA	3:E:140:LYS:HE2	1.66	0.78
2:D:172:MET:SD	2:D:390:ARG:NH2	2.57	0.78
1:C:1:MET:HE1	1:C:51:THR:HG23	1.66	0.77
2:B:334:ASN:OD1	2:B:335:VAL:N	2.22	0.73
4:F:5:VAL:HG13	4:F:32:LYS:HA	1.72	0.71
2:B:1:MET:N	2:B:131:CYS:SG	2.66	0.69
1:A:18:ASN:OD1	1:A:19:ALA:N	2.26	0.69
1:A:97:GLU:OE2	1:A:105:ARG:NH2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ARG:NH2	2:D:130:ASP:HB3	2.09	0.68
2:B:286:LEU:N	2:B:290:GLU:OE1	2.26	0.67
1:A:69:ASP:OD1	11:A:611:HOH:O	2.13	0.67
2:D:12:CYS:SG	2:D:13:GLY:N	2.67	0.66
1:C:1:MET:CE	1:C:51:THR:HG23	2.25	0.65
2:D:2:ARG:NH2	2:D:3:GLU:CD	2.51	0.63
1:A:179:THR:HA	2:B:248:LEU:HD21	1.82	0.62
1:C:357:TYR:CZ	1:C:358[B]:GLN:NE2	2.68	0.62
2:B:199:ASP:OD1	10:B:504:MES:H52	2.00	0.62
2:D:221:THR:HG23	2:D:221:THR:O	2.00	0.61
1:A:5:ILE:HD11	1:A:135:PHE:CE2	2.34	0.61
2:B:39:ASP:OD1	2:B:40:SER:N	2.34	0.61
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.41	0.61
1:C:234:ILE:HD13	1:C:302:MET:SD	2.43	0.59
1:C:71:GLU:OE1	1:C:73:THR:OG1	2.14	0.59
1:A:166:LYS:HE2	1:A:197:HIS:O	2.01	0.59
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.35	0.58
4:F:5:VAL:CG1	4:F:32:LYS:HA	2.34	0.57
2:B:264:ARG:NE	2:B:431:GLU:OE2	2.35	0.57
2:D:311:ARG:NH1	2:D:436:GLN:O	2.37	0.57
4:F:259:GLY:N	4:F:260:ASN:HA	2.19	0.57
2:D:172:MET:HE3	2:D:173:PRO:O	2.05	0.56
2:B:136:GLN:HA	2:B:167:ASN:O	2.05	0.56
4:F:21:LEU:O	4:F:24:THR:HG22	2.05	0.56
1:C:209:ILE:HD11	1:C:302:MET:SD	2.45	0.56
4:F:371:PRO:HA	4:F:372:THR:HB	1.87	0.56
1:A:436:GLY:O	1:A:437:VAL:C	2.45	0.55
2:B:272:PHE:O	2:B:300:ASN:ND2	2.30	0.55
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.55
2:D:172:MET:CG	2:D:205:ASP:HA	2.37	0.55
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.89	0.55
2:D:308:ARG:NH1	11:D:704:HOH:O	2.40	0.54
2:D:172:MET:CE	2:D:390:ARG:NH2	2.71	0.54
1:A:179:THR:HA	2:B:248:LEU:CD2	2.37	0.54
4:F:90:SER:O	4:F:91:CYS:CB	2.55	0.54
4:F:192:LEU:HD13	4:F:193:GLU:N	2.22	0.54
2:B:141:LEU:HD12	2:B:172:MET:SD	2.48	0.54
2:D:172:MET:HG3	2:D:205:ASP:HA	1.90	0.54
2:D:271:GLY:N	2:D:377:PHE:O	2.40	0.53
2:D:205:ASP:OD1	2:D:207:GLU:N	2.41	0.53
2:B:331:GLN:HA	2:B:334:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:371:PRO:CA	4:F:372:THR:HB	2.37	0.53
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.14	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.09	0.53
2:B:274:PRO:C	2:B:275:LEU:HD12	2.29	0.52
2:D:2:ARG:HH22	2:D:130:ASP:HB3	1.74	0.52
2:D:387:LEU:C	2:D:387:LEU:HD23	2.29	0.52
1:A:349:THR:O	1:A:349:THR:OG1	2.26	0.52
1:A:274:PRO:HB2	1:A:276:ILE:CD1	2.40	0.52
1:C:255:PHE:CZ	1:C:318:LEU:CD2	2.93	0.52
4:F:262:MET:HE3	4:F:267:PHE:N	2.24	0.51
2:D:12:CYS:SG	2:D:140:SER:N	2.83	0.51
4:F:1:MET:SD	4:F:28:LYS:HD3	2.50	0.51
4:F:223:THR:O	4:F:260:ASN:CG	2.49	0.51
2:D:286:LEU:O	2:D:286:LEU:HD12	2.11	0.51
4:F:299:GLU:N	4:F:300:PRO:CD	2.74	0.51
2:D:2:ARG:CZ	2:D:2:ARG:HB3	2.41	0.51
2:D:75:MET:SD	2:D:94:PHE:HB3	2.51	0.51
2:D:406:HIS:HA	2:D:409:THR:HG22	1.92	0.50
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.46	0.50
2:D:220:THR:HG23	2:D:221:THR:N	2.27	0.50
1:C:255:PHE:CE2	1:C:318:LEU:HD22	2.46	0.50
1:C:166:LYS:HE2	1:C:197:HIS:O	2.12	0.50
3:E:50:ILE:O	3:E:53:LYS:HG2	2.11	0.50
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.94	0.50
2:D:422:GLU:HG3	2:D:423:SER:N	2.25	0.50
1:C:306:ASP:OD1	1:C:308:ARG:HG2	2.11	0.50
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.42	0.49
2:D:2:ARG:NH2	2:D:130:ASP:CB	2.76	0.49
1:A:97:GLU:HG3	2:B:1:MET:HG2	1.93	0.49
2:D:172:MET:SD	2:D:205:ASP:CG	2.91	0.49
1:A:192:HIS:CG	1:A:421:ALA:HA	2.48	0.49
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.47	0.49
2:D:124:LYS:C	2:D:124:LYS:HD3	2.33	0.49
4:F:90:SER:O	4:F:91:CYS:HB3	2.13	0.49
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.93	0.48
2:B:334:ASN:C	2:B:334:ASN:OD1	2.51	0.48
2:D:9:ALA:HA	2:D:68:VAL:O	2.13	0.48
1:A:18:ASN:OD1	1:A:18:ASN:C	2.52	0.48
3:E:49:GLU:HG3	3:E:52:LYS:HZ2	1.78	0.48
2:B:16[B]:ILE:HG21	2:B:231:VAL:HG11	1.96	0.48
2:D:173:PRO:HG3	2:D:187:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.94	0.48
2:D:293:GLN:N	2:D:293:GLN:OE1	2.44	0.48
1:C:67:PHE:HB2	1:C:92:LEU:HD23	1.95	0.48
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.47
1:A:183:GLU:N	1:A:184:PRO:CD	2.77	0.47
2:D:2:ARG:HB3	2:D:2:ARG:NH1	2.28	0.47
2:D:142:GLY:O	2:D:186:ASN:ND2	2.46	0.47
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.97	0.47
2:D:103:TRP:NE1	2:D:148:GLY:HA2	2.30	0.47
1:A:2:ARG:HB3	1:A:131:GLY:O	2.14	0.47
1:A:164:LYS:N	1:A:164:LYS:HD2	2.30	0.47
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.14	0.47
1:A:413:MET:CE	1:A:418:PHE:CE1	2.98	0.47
1:C:346:TRP:CZ3	1:C:347[B]:CYS:SG	3.08	0.47
2:B:181:VAL:HG21	2:B:404:PHE:CZ	2.49	0.47
4:F:2:TYR:HB3	4:F:27:TRP:CZ3	2.50	0.47
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.55	0.47
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.46	0.47
2:D:69:ASP:OD1	2:D:70:LEU:N	2.47	0.47
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.49	0.47
2:D:143:GLY:HA3	9:D:600:GDP:O3A	2.14	0.47
2:D:192:HIS:CD2	2:D:421:ALA:HA	2.50	0.46
4:F:47:LEU:C	4:F:47:LEU:HD12	2.36	0.46
2:B:192:HIS:CE1	2:B:424[B]:ASN:OD1	2.69	0.46
2:D:287:THR:HB	2:D:289:PRO:HD2	1.97	0.46
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.97	0.46
3:E:52:LYS:HG3	3:E:53:LYS:N	2.31	0.46
2:B:210:TYR:CE2	2:B:222:PRO:HG2	2.50	0.46
2:D:104:ALA:HB2	2:D:413:MET:SD	2.56	0.46
2:D:2:ARG:HH22	2:D:130:ASP:CB	2.29	0.46
2:D:124:LYS:O	2:D:127:GLU:OE1	2.34	0.46
1:A:115:ILE:HG23	1:A:116:ASP:N	2.31	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.50	0.46
2:D:2:ARG:CZ	2:D:130:ASP:HB3	2.46	0.46
1:C:183:GLU:N	1:C:184:PRO:CD	2.79	0.46
2:D:181:VAL:HG13	2:D:182:VAL:HG13	1.96	0.45
1:A:234:ILE:HG12	1:A:302[B]:MET:CE	2.46	0.45
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.45
4:F:221:LEU:HB2	4:F:262:MET:HB3	1.99	0.45
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.52	0.45
2:B:167:ASN:OD1	2:B:200:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:81:ILE:HD12	4:F:94:PHE:CD2	2.51	0.45
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.98	0.45
1:A:74:VAL:HB	11:A:602:HOH:O	2.16	0.44
1:A:343:PHE:HB2	1:A:349:THR:HG22	2.00	0.44
2:B:333:LEU:O	2:B:337:ASN:ND2	2.51	0.44
1:C:313:MET:SD	1:C:435:VAL:HG11	2.58	0.44
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.97	0.44
4:F:192:LEU:HD22	4:F:270:TYR:CZ	2.52	0.44
4:F:87:LEU:O	4:F:88:SER:CB	2.65	0.44
2:D:2:ARG:CB	2:D:2:ARG:NH1	2.81	0.44
4:F:262:MET:HE3	4:F:266:GLU:HB3	1.99	0.44
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.99	0.44
2:D:115:VAL:HG13	2:D:116:ASP:N	2.33	0.44
2:D:5:VAL:HB	2:D:135:PHE:CD2	2.53	0.44
1:A:298:PRO:HA	1:A:301:GLN:CD	2.39	0.43
2:D:172:MET:SD	2:D:205:ASP:OD2	2.75	0.43
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.99	0.43
4:F:341:LYS:HG3	4:F:342:LEU:HD23	1.99	0.43
1:C:75:ILE:O	1:C:78:VAL:N	2.51	0.43
1:A:413:MET:HE2	1:A:418:PHE:CE1	2.54	0.43
1:C:115:ILE:HG23	1:C:116:ASP:N	2.33	0.43
4:F:223:THR:O	4:F:260:ASN:ND2	2.52	0.43
1:A:96:LYS:HG3	1:A:97:GLU:N	2.34	0.43
1:C:357:TYR:OH	1:C:358[B]:GLN:NE2	2.52	0.43
1:C:74:VAL:HB	11:C:624:HOH:O	2.19	0.43
1:C:211[B]:ASP:OD2	1:C:304:LYS:NZ	2.42	0.43
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.43
1:A:5:ILE:HD11	1:A:135:PHE:CD2	2.54	0.43
4:F:259:GLY:HA3	4:F:261:GLU:N	2.34	0.43
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.43
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.32	0.42
2:D:190:SER:O	2:D:194:LEU:HG	2.19	0.42
1:A:262:TYR:HE2	1:A:346:TRP:CZ2	2.37	0.42
1:A:135:PHE:N	1:A:135:PHE:CD1	2.87	0.42
4:F:17:VAL:HG13	4:F:351:VAL:HG12	2.01	0.42
1:A:183:GLU:N	1:A:184:PRO:HD2	2.34	0.42
2:D:109:THR:OG1	2:D:110:GLU:N	2.52	0.42
1:A:276:ILE:HG22	1:A:369:ALA:HB3	2.02	0.42
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.54	0.42
4:F:371:PRO:HA	4:F:372:THR:O	2.19	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:HG12	1:C:348:PRO:HG2	2.02	0.42
2:B:192:HIS:CD2	2:B:424[A]:ASN:ND2	2.88	0.42
2:D:384:ILE:HG21	2:D:432:TYR:CZ	2.53	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.42
2:B:334:ASN:HB2	2:B:338:LYS:NZ	2.34	0.42
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.50	0.42
2:B:387:LEU:C	2:B:387:LEU:HD23	2.40	0.42
4:F:47:LEU:HG	4:F:49:PHE:CZ	2.55	0.42
2:B:36:TYR:OH	2:B:40:SER:O	2.38	0.42
4:F:192:LEU:HD22	4:F:270:TYR:CE1	2.55	0.42
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.55	0.42
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.02	0.42
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.02	0.41
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.55	0.41
2:D:406:HIS:CE1	2:D:407[B]:TRP:CD1	3.09	0.41
1:C:296:PHE:CE2	1:C:341:ILE:HD12	2.55	0.41
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.01	0.41
3:E:49:GLU:HG3	3:E:52:LYS:NZ	2.36	0.41
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.51	0.41
2:B:109:THR:OG1	2:B:110:GLU:N	2.53	0.41
4:F:90:SER:O	4:F:91:CYS:SG	2.78	0.41
4:F:81:ILE:HD12	4:F:94:PHE:CE2	2.55	0.41
4:F:199:PHE:CD1	4:F:199:PHE:C	2.94	0.41
2:B:275:LEU:N	2:B:275:LEU:CD1	2.83	0.41
4:F:47:LEU:HD13	4:F:48:PRO:HD2	2.02	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.02	0.41
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.56	0.41
2:B:16[B]:ILE:CG2	2:B:231:VAL:HG11	2.50	0.41
1:C:141:PHE:CE2	1:C:170:SER:HB3	2.55	0.41
2:D:183:GLU:HB2	2:D:184:PRO:HD3	2.03	0.41
2:B:83:PHE:O	2:B:86:ILE:HG22	2.20	0.41
1:C:76:ASP:O	1:C:80:THR:HG22	2.21	0.41
1:C:282:TYR:CE2	1:C:283:HIS:CE1	3.09	0.41
1:A:399:TYR:CE1	1:A:418:PHE:HB3	2.56	0.41
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.55	0.41
2:D:185:TYR:CE1	2:D:398:MET:HE3	2.56	0.41
4:F:220:VAL:HG11	4:F:339:ALA:HB2	2.02	0.41
2:D:19:LYS:O	2:D:23:VAL:HG23	2.21	0.41
2:B:125:GLU:OE1	2:B:125:GLU:HA	2.21	0.41
1:A:313:MET:O	1:A:314:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:ARG:NH2	2:B:357:ASP:HB3	2.36	0.41
2:D:172:MET:HE1	2:D:205:ASP:OD1	2.20	0.40
1:C:71:GLU:HG2	1:C:72:PRO:HD2	2.03	0.40
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.56	0.40
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.02	0.40
3:E:137:LYS:HG3	3:E:140:LYS:CE	2.51	0.40
4:F:73:ARG:O	4:F:74:LYS:C	2.59	0.40
2:B:347:ILE:HG22	2:B:350:ASN:HB3	2.03	0.40
4:F:7:ARG:HD3	4:F:40:MET:HE3	2.03	0.40
4:F:371:PRO:HA	4:F:372:THR:C	2.41	0.40
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
1	C	448/451 (99%)	434 (97%)	14 (3%)	0	100	100
2	B	418/445 (94%)	399 (96%)	18 (4%)	1 (0%)	52	77
2	D	419/445 (94%)	398 (95%)	20 (5%)	1 (0%)	52	77
3	E	120/143 (84%)	117 (98%)	3 (2%)	0	100	100
4	F	250/384 (65%)	237 (95%)	12 (5%)	1 (0%)	39	65
All	All	2095/2319 (90%)	2008 (96%)	84 (4%)	3 (0%)	56	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	91	CYS

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Mol	Chain	Res	Type
2	B	81	GLY
2	D	73	GLY

### 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	373/379 (98%)	369 (99%)	4 (1%)	80	93
1	C	381/379 (100%)	378 (99%)	3 (1%)	86	95
2	B	366/383 (96%)	363 (99%)	3 (1%)	86	95
2	D	365/383 (95%)	360 (99%)	5 (1%)	74	90
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	234/342 (68%)	221 (94%)	13 (6%)	26	50
All	All	1830/1993 (92%)	1802 (98%)	28 (2%)	72	90

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	120	ASP
1	A	135	PHE
1	A	349	THR
2	B	139	HIS
2	B	325	MET
2	B	345	GLU
1	C	320	ARG
1	C	342	GLN
1	C	381	THR
2	D	96	GLN
2	D	127	GLU
2	D	139	HIS
2	D	158	ARG
2	D	172	MET
4	F	19	ARG

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Mol	Chain	Res	Type
4	F	22	LEU
4	F	44	ARG
4	F	47	LEU
4	F	82	LYS
4	F	86	GLU
4	F	89	GLU
4	F	186	LEU
4	F	191	LEU
4	F	217	ARG
4	F	222	ARG
4	F	275	LEU
4	F	346	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	107	HIS
2	B	192	HIS
1	C	266	HIS
1	C	285	GLN
1	C	372	GLN
2	D	406	HIS
4	F	260	ASN
4	F	379	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 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	25,34,34	1.05	1 (4%)	32,54,54	1.20	4 (12%)
9	GDP	B	501	6	23,30,30	1.41	3 (13%)	28,47,47	1.33	2 (7%)
10	MES	B	504	-	12,12,12	2.14	1 (8%)	16,16,16	2.39	5 (31%)
5	GTP	C	501	6	25,34,34	1.08	1 (4%)	32,54,54	1.15	2 (6%)
9	GDP	D	600	6	23,30,30	1.45	5 (21%)	28,47,47	1.61	5 (17%)

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
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	GDP	D	600	6	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-6.40	1.66	1.78
9	D	600	GDP	C6-N1	-2.04	1.33	1.36
9	D	600	GDP	C2-N3	2.04	1.36	1.33
9	D	600	GDP	C2-N2	2.42	1.35	1.32
9	B	501	GDP	C5-C4	2.68	1.46	1.40
9	B	501	GDP	C2-N2	2.79	1.36	1.32
9	D	600	GDP	C5-C4	2.95	1.47	1.40
9	B	501	GDP	C6-C5	3.58	1.47	1.41
5	A	501	GTP	C2-N3	3.86	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	600	GDP	C6-C5	4.07	1.48	1.41
5	C	501	GTP	C2-N3	4.10	1.38	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	C6-C5-N4	-5.03	103.69	109.98
10	B	504	MES	C8-C7-N4	-4.12	105.11	112.70
5	C	501	GTP	PB-O3B-PG	-3.31	121.58	132.67
10	B	504	MES	O1-C6-C5	-3.30	107.96	111.41
9	D	600	GDP	C4-C5-N7	-3.24	106.50	109.48
5	A	501	GTP	PA-O3A-PB	-3.07	124.10	132.73
9	B	501	GDP	C4-C5-N7	-3.05	106.67	109.48
9	D	600	GDP	PA-O3A-PB	-2.95	122.79	132.67
5	C	501	GTP	PA-O3A-PB	-2.93	124.50	132.73
5	A	501	GTP	PB-O3B-PG	-2.83	123.17	132.67
5	A	501	GTP	C4-C5-N7	-2.02	107.62	109.48
9	D	600	GDP	C4'-O4'-C1'	2.04	111.96	109.72
5	A	501	GTP	N2-C2-N1	2.17	120.17	117.80
10	B	504	MES	C5-N4-C3	3.01	116.09	109.76
10	B	504	MES	O1-C2-C3	3.56	115.14	111.41
9	B	501	GDP	C6-N1-C2	3.91	122.41	120.20
9	D	600	GDP	O2'-C2'-C3'	3.94	124.64	111.83
9	D	600	GDP	C6-N1-C2	4.07	122.50	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
10	B	504	MES	1	0
9	D	600	GDP	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	437/451 (96%)	0.36	4 (0%) 85 83	39, 63, 95, 115	0
1	C	440/451 (97%)	0.39	3 (0%) 89 87	32, 48, 73, 101	0
2	B	418/445 (93%)	0.46	7 (1%) 73 68	34, 55, 90, 126	2 (0%)
2	D	421/445 (94%)	0.53	21 (4%) 32 26	44, 74, 107, 129	5 (1%)
3	E	122/143 (85%)	0.54	6 (4%) 33 26	47, 78, 122, 158	0
4	F	258/384 (67%)	1.21	59 (22%) 1 0	56, 86, 137, 171	0
All	All	2096/2319 (90%)	0.54	100 (4%) 34 27	32, 65, 104, 171	7 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	225	SER	8.6
1	C	1	MET	5.9
4	F	224	SER	5.7
4	F	192	LEU	5.2
2	D	400	ARG	5.1
4	F	226	GLU	5.0
4	F	223	THR	4.9
4	F	320	MET	4.9
2	D	415	GLU	4.6
4	F	259	GLY	4.5
2	B	438	ALA	4.4
4	F	381	HIS	4.1
2	D	177	VAL	4.1
4	F	335	ALA	4.0
4	F	21	LEU	3.9
4	F	262	MET	3.7
2	D	401	ARG	3.7
4	F	26	GLN	3.6
2	D	405	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	263	PHE	3.5
4	F	22	LEU	3.5
4	F	380	HIS	3.5
4	F	330	ILE	3.4
4	F	227	PRO	3.4
4	F	353	VAL	3.4
4	F	260	ASN	3.4
4	F	283	ILE	3.4
4	F	383	HIS	3.3
4	F	319	PHE	3.3
2	D	57	THR	3.3
2	D	285	ALA	3.3
4	F	220	VAL	3.2
4	F	372	THR	3.2
4	F	264	PHE	3.2
2	D	182	VAL	3.0
4	F	267	PHE	3.0
4	F	343	TYR	3.0
1	C	340	SER	2.9
2	D	172	MET	2.9
4	F	199	PHE	2.9
2	B	372	LYS	2.9
2	D	78	VAL	2.9
2	D	399	PHE	2.8
4	F	346	LEU	2.8
4	F	261	GLU	2.8
4	F	325	LEU	2.8
4	F	351	VAL	2.8
4	F	194	PRO	2.8
4	F	27	TRP	2.7
4	F	71	LEU	2.7
4	F	382	HIS	2.7
4	F	73	ARG	2.7
4	F	214	TYR	2.7
4	F	375	PHE	2.7
4	F	197	ARG	2.6
4	F	201	ILE	2.6
2	B	345	GLU	2.6
4	F	20	LEU	2.6
2	D	75	MET	2.5
4	F	384	HIS	2.5
4	F	52	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	79	ARG	2.5
4	F	271	LEU	2.5
1	C	357	TYR	2.5
2	D	403	ALA	2.5
2	D	217	LEU	2.5
2	B	337	ASN	2.5
4	F	3	THR	2.5
1	A	418	PHE	2.5
1	A	93	ILE	2.4
4	F	64	TYR	2.4
3	E	54	LEU	2.4
4	F	371	PRO	2.3
4	F	5	VAL	2.3
3	E	46	SER	2.3
4	F	221	LEU	2.3
3	E	50	ILE	2.3
2	B	358	ILE	2.3
4	F	376	ILE	2.3
4	F	315	PHE	2.3
4	F	31	ARG	2.3
2	D	153	LEU	2.2
1	A	68	VAL	2.2
2	D	404	PHE	2.2
2	B	1	MET	2.2
4	F	284	LEU	2.2
4	F	17	VAL	2.2
4	F	285	LEU	2.2
1	A	390[A]	ARG	2.2
4	F	329	LEU	2.2
2	D	127	GLU	2.2
3	E	24	LEU	2.2
3	E	45	PRO	2.2
2	B	16[A]	ILE	2.1
3	E	116	LEU	2.1
2	D	407[A]	TRP	2.1
2	D	137	LEU	2.1
2	D	204	ILE	2.1
4	F	196	HIS	2.1
4	F	206	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	C	502	1/1	0.96	0.41	6.35	42,42,42,42	0
7	CA	C	503	1/1	0.94	0.30	5.93	68,68,68,68	0
6	MG	A	502	1/1	0.92	0.28	4.14	40,40,40,40	0
7	CA	A	503	1/1	0.93	0.25	3.56	126,126,126,126	0
7	CA	B	503	1/1	0.90	0.33	2.04	87,87,87,87	0
9	GDP	B	501	28/28	0.98	0.23	0.48	21,39,56,61	0
5	GTP	A	501	32/32	0.98	0.21	0.29	29,47,62,64	0
5	GTP	C	501	32/32	0.97	0.21	0.20	25,39,53,59	0
9	GDP	D	600	28/28	0.96	0.17	-0.66	52,73,91,99	0
10	MES	B	504	12/12	0.98	0.18	-0.89	44,59,86,87	0
6	MG	D	601	1/1	0.61	0.18	-	74,74,74,74	0
8	CL	A	504	1/1	0.90	0.09	-	77,77,77,77	0
6	MG	F	401	1/1	0.55	0.83	-	99,99,99,99	0
6	MG	B	502	1/1	0.96	0.40	-	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.