



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:18 PM GMT

PDB ID : 3TII  
Title : Tubulin tyrosine ligase  
Authors : Roll-Mecak, A.; Szyk, A.; Deaconescu, A.; Piszczek, G.  
Deposited on : 2011-08-20  
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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

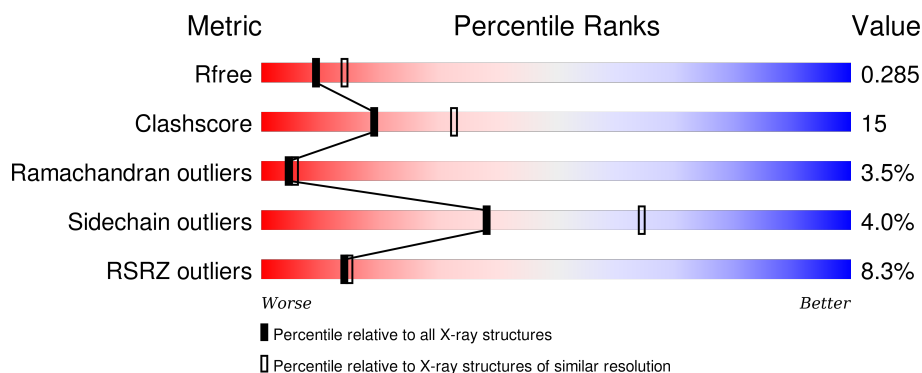
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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	380	
1	B	380	

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
3	MG	A	382	-	-	-	X
3	MG	B	384	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4949 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.

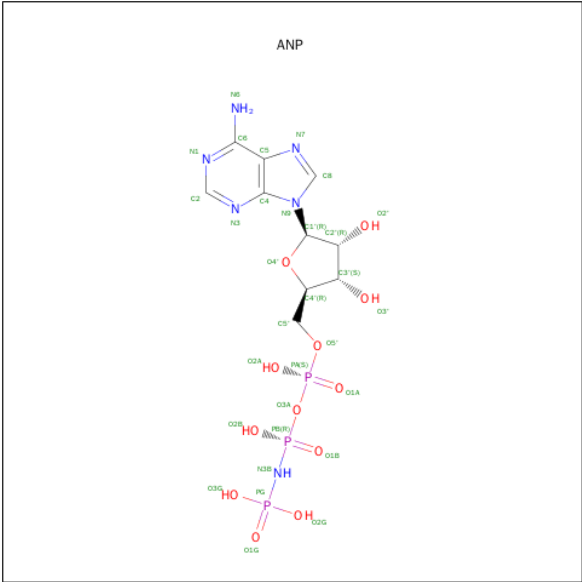
- Molecule 1 is a protein called Ttl protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2396	1556	392	438	10			
1	B	313	Total	C	N	O	S	0	0	0
			2454	1593	404	447	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP A9ULH4
A	-1	SER	-	EXPRESSION TAG	UNP A9ULH4
A	0	PHE	-	EXPRESSION TAG	UNP A9ULH4
A	1	THR	-	EXPRESSION TAG	UNP A9ULH4
B	-2	GLY	-	EXPRESSION TAG	UNP A9ULH4
B	-1	SER	-	EXPRESSION TAG	UNP A9ULH4
B	0	PHE	-	EXPRESSION TAG	UNP A9ULH4
B	1	THR	-	EXPRESSION TAG	UNP A9ULH4

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Mg	0	0
			4	4		
3	A	3	Total	Mg	0	0
			3	3		

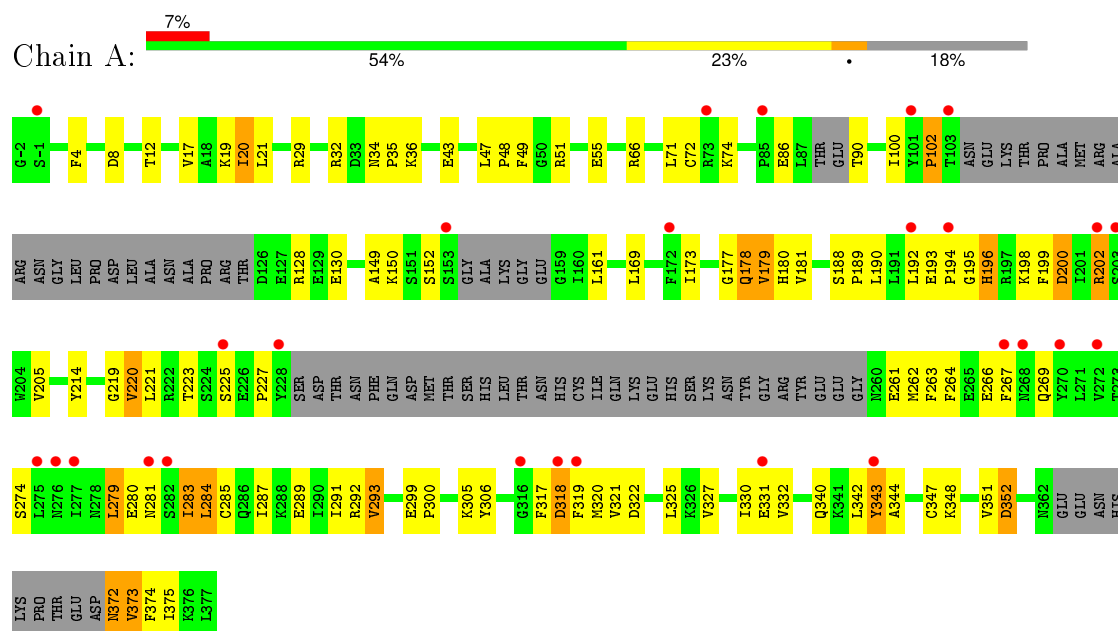
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	13	Total	O	0	0
			13	13		

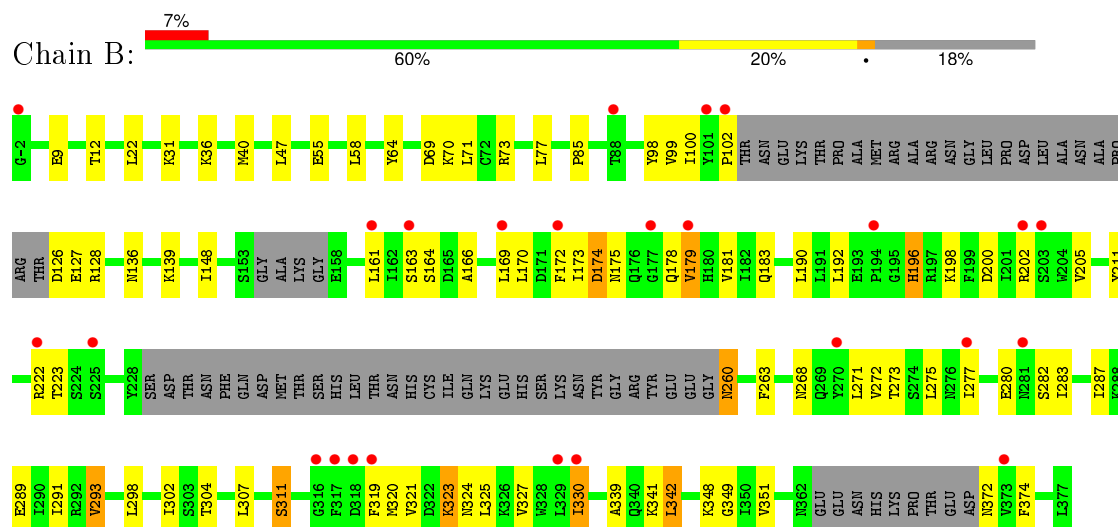
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Ttl protein



#### • Molecule 1: Ttl protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.42Å 74.66Å 117.33Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	29.38 – 2.50 29.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.38-2.50) 98.8 (29.38-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.26 (at 2.51Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.254 , 0.285 0.255 , 0.285	Depositor DCC
$R_{free}$ test set	1317 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.6	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26389 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.57 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6206e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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	0.42	0/2450	0.61	0/3329
1	B	0.39	0/2509	0.62	0/3403
All	All	0.41	0/4959	0.62	0/6732

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2396	0	2247	80	0
1	B	2454	0	2360	65	0
2	A	31	0	13	1	0
2	B	31	0	13	1	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
4	A	17	0	0	0	0
4	B	13	0	0	0	0
All	All	4949	0	4633	145	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 15.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HG	1:A:332:VAL:HG11	1.58	0.86
1:A:161:LEU:HD23	1:A:169:LEU:HD23	1.59	0.84
1:B:289:GLU:O	1:B:293:VAL:HG12	1.79	0.83
1:A:305:LYS:HD3	1:A:306:TYR:CE2	2.14	0.82
1:A:262:MET:HG3	1:A:266:GLU:OE2	1.80	0.80
1:A:173:ILE:HD12	1:A:180:HIS:HB2	1.64	0.79
1:A:289:GLU:CD	1:A:292:ARG:HH21	1.87	0.78
1:B:163:SER:HB3	1:B:169:LEU:HD13	1.65	0.78
1:A:264:PHE:HE2	1:A:284:LEU:HD21	1.49	0.77
1:A:289:GLU:O	1:A:293:VAL:HG12	1.84	0.77
1:A:373:VAL:HG13	1:A:374:PHE:HD2	1.50	0.76
1:A:86:GLU:O	1:A:90:THR:HG22	1.85	0.75
1:A:192:LEU:O	1:A:196:HIS:HA	1.87	0.74
1:B:339:ALA:HB3	1:B:342:LEU:HD22	1.74	0.69
1:A:72:CYS:HA	1:A:332:VAL:HG13	1.76	0.67
1:B:71:LEU:HD12	1:B:77:LEU:HD13	1.76	0.67
1:A:190:LEU:HD22	1:A:325:LEU:HD23	1.77	0.67
1:A:179:VAL:O	1:A:179:VAL:HG13	1.95	0.66
1:B:128:ARG:HH21	1:B:170:LEU:HD13	1.61	0.64
1:A:289:GLU:OE2	1:A:292:ARG:NH2	2.31	0.63
1:B:40:MET:HE3	1:B:47:LEU:HG	1.80	0.63
1:B:200:ASP:OD1	1:B:222:ARG:HB3	1.99	0.62
1:B:161:LEU:HD23	1:B:169:LEU:HD12	1.82	0.61
1:B:173:ILE:C	1:B:175:ASN:H	2.03	0.60
1:A:264:PHE:CE2	1:A:284:LEU:HD21	2.35	0.59
1:A:102:PRO:HG2	1:A:177:GLY:HA2	1.84	0.59
1:B:40:MET:HE1	1:B:47:LEU:HD21	1.85	0.59
1:B:179:VAL:O	1:B:179:VAL:HG13	2.02	0.58
1:A:331:GLU:HG2	1:A:332:VAL:N	2.19	0.57
1:B:98:TYR:HA	1:B:127:GLU:OE2	2.03	0.57
1:B:69:ASP:C	1:B:71:LEU:H	2.07	0.57
1:A:279:LEU:HD22	1:A:284:LEU:CD1	2.34	0.57
1:A:173:ILE:HD12	1:A:180:HIS:CB	2.34	0.57
1:A:372:ASN:O	1:A:374:PHE:N	2.38	0.56
1:B:320:MET:HG3	1:B:330:ILE:HD13	1.87	0.56
1:B:36:LYS:HA	1:B:58:LEU:HD11	1.88	0.55
1:A:280:GLU:HA	1:A:284:LEU:HB2	1.88	0.54
1:B:324:ASN:O	1:B:325:LEU:HB2	2.08	0.54
1:B:304:THR:HG21	1:B:311:SER:HB2	1.89	0.54
1:A:266:GLU:O	1:A:269:GLN:N	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD12	1:A:221:LEU:N	2.24	0.53
1:A:375:ILE:N	1:A:375:ILE:HD12	2.23	0.53
1:A:299:GLU:HB3	1:A:300:PRO:HD3	1.90	0.52
1:A:190:LEU:HB2	1:A:322:ASP:O	2.10	0.52
1:B:372:ASN:N	1:B:372:ASN:OD1	2.41	0.52
1:B:268:ASN:O	1:B:272:VAL:HG12	2.09	0.52
1:B:190:LEU:HA	1:B:323:LYS:HD3	1.91	0.51
1:A:195:GLY:O	1:A:227:PRO:HB3	2.11	0.51
1:B:222:ARG:NH2	2:B:710:ANP:O3'	2.38	0.51
1:B:102:PRO:HD3	1:B:179:VAL:HA	1.92	0.51
1:B:271:LEU:O	1:B:275:LEU:HB2	2.11	0.51
1:A:71:LEU:O	1:A:332:VAL:CG1	2.59	0.51
1:B:298:LEU:HG	1:B:302:ILE:HD13	1.93	0.51
1:A:280:GLU:O	1:A:285:CYS:SG	2.64	0.50
1:A:20:ILE:HD13	1:A:348:LYS:HA	1.94	0.49
1:B:348:LYS:O	1:B:351:VAL:HG22	2.12	0.49
1:A:36:LYS:HD2	1:A:55:GLU:HG2	1.95	0.49
1:A:266:GLU:O	1:A:269:GLN:HB2	2.12	0.49
1:A:74:LYS:HB2	1:A:152:SER:HA	1.95	0.48
1:A:205:VAL:CG2	1:A:291:ILE:HD13	2.43	0.48
1:A:8:ASP:HB2	1:A:43:GLU:HA	1.93	0.48
1:A:12:THR:HB	1:A:343:TYR:OH	2.12	0.48
1:B:148:ILE:HG22	1:B:183:GLN:O	2.13	0.48
1:B:304:THR:HA	1:B:307:LEU:HD12	1.95	0.48
1:B:283:ILE:HG23	1:B:327:VAL:CG2	2.44	0.48
1:B:170:LEU:C	1:B:172:PHE:H	2.16	0.47
1:A:150:LYS:HE3	2:A:700:ANP:O1A	2.14	0.47
1:A:289:GLU:OE1	1:A:289:GLU:HA	2.14	0.47
1:A:17:VAL:HA	1:A:20:ILE:HG22	1.96	0.47
1:A:320:MET:HG3	1:A:330:ILE:HD13	1.96	0.47
1:B:287:ILE:HG23	1:B:319:PHE:CE2	2.49	0.47
1:A:219:GLY:HA3	1:A:264:PHE:CE1	2.50	0.47
1:B:55:GLU:HG2	1:B:58:LEU:HD12	1.96	0.47
1:B:272:VAL:HG13	1:B:273:THR:N	2.29	0.47
1:A:351:VAL:HG23	1:A:352:ASP:N	2.30	0.47
1:B:289:GLU:O	1:B:293:VAL:CG1	2.58	0.47
1:B:99:VAL:N	1:B:127:GLU:OE2	2.39	0.47
1:B:64:TYR:O	1:B:311:SER:OG	2.32	0.47
1:A:202:ARG:HA	1:A:317:PHE:O	2.13	0.47
1:B:321:VAL:HG22	1:B:327:VAL:HG22	1.97	0.47
1:A:205:VAL:HG21	1:A:291:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB1	1:A:173:ILE:HD11	1.97	0.46
1:B:100:ILE:HA	1:B:126:ASP:CB	2.45	0.46
1:A:198:LYS:NZ	1:A:320:MET:CE	2.79	0.46
1:A:348:LYS:HA	1:A:351:VAL:HG22	1.98	0.46
1:A:373:VAL:HG13	1:A:374:PHE:CD2	2.40	0.45
1:A:189:PRO:HA	1:A:322:ASP:HA	1.99	0.45
1:B:283:ILE:HG23	1:B:327:VAL:HG21	1.98	0.45
1:A:130:GLU:N	1:A:130:GLU:OE1	2.49	0.45
1:A:340:GLN:HA	1:A:343:TYR:HD2	1.82	0.44
1:A:283:ILE:HG23	1:A:327:VAL:HG11	1.99	0.44
1:B:173:ILE:C	1:B:175:ASN:N	2.70	0.44
1:A:19:LYS:O	1:A:21:LEU:N	2.50	0.44
1:A:342:LEU:O	1:A:344:ALA:N	2.51	0.44
1:A:178:GLN:O	1:A:179:VAL:C	2.57	0.43
1:B:9:GLU:OE2	1:B:9:GLU:N	2.49	0.43
1:A:279:LEU:HD22	1:A:284:LEU:HG	1.99	0.43
1:B:198:LYS:HE2	1:B:320:MET:HE3	1.99	0.43
1:A:332:VAL:HG13	1:A:332:VAL:O	2.18	0.43
1:B:163:SER:OG	1:B:164:SER:N	2.52	0.43
1:A:4:PHE:CZ	1:A:29:ARG:HB2	2.54	0.43
1:B:100:ILE:HA	1:B:126:ASP:HB2	2.01	0.43
1:B:136:ASN:O	1:B:139:LYS:HB3	2.19	0.43
1:A:220:VAL:HG23	1:A:263:PHE:CD1	2.54	0.43
1:A:192:LEU:HD12	1:A:223:THR:HG22	2.00	0.42
1:A:287:ILE:HG23	1:A:319:PHE:CE2	2.54	0.42
1:A:214:TYR:HB3	1:A:374:PHE:HD1	1.84	0.42
1:B:166:ALA:O	1:B:170:LEU:HG	2.19	0.42
1:B:173:ILE:O	1:B:175:ASN:N	2.52	0.42
1:A:74:LYS:HB3	1:A:181:VAL:HG21	2.01	0.42
1:A:34:ASN:HA	1:A:35:PRO:HD3	1.91	0.42
1:B:73:ARG:HB3	1:B:73:ARG:HH11	1.84	0.42
1:A:198:LYS:NZ	1:A:320:MET:HE3	2.35	0.42
1:B:223:THR:O	1:B:260:ASN:OD1	2.38	0.42
1:A:188:SER:O	1:A:322:ASP:HB2	2.19	0.42
1:B:40:MET:HE3	1:B:47:LEU:CG	2.47	0.42
1:B:40:MET:CE	1:B:47:LEU:HD21	2.48	0.42
1:B:272:VAL:HA	1:B:277:ILE:H	1.84	0.42
1:A:190:LEU:HD22	1:A:325:LEU:CD2	2.46	0.42
1:A:100:ILE:HD12	1:A:128:ARG:CB	2.50	0.42
1:B:272:VAL:HG13	1:B:273:THR:H	1.84	0.42
1:B:325:LEU:HA	1:B:325:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PHE:CZ	1:B:341:LYS:HE2	2.55	0.42
1:A:193:GLU:HA	1:A:194:PRO:C	2.40	0.42
1:B:70:LYS:CG	1:B:70:LYS:O	2.68	0.41
1:B:304:THR:HG22	1:B:307:LEU:HD12	2.01	0.41
1:A:19:LYS:C	1:A:21:LEU:N	2.74	0.41
1:B:192:LEU:O	1:B:196:HIS:HA	2.20	0.41
1:A:47:LEU:C	1:A:47:LEU:HD23	2.41	0.41
1:B:289:GLU:HA	1:B:289:GLU:OE1	2.19	0.41
1:B:205:VAL:CG2	1:B:291:ILE:HD13	2.50	0.41
1:A:48:PRO:O	1:A:51:ARG:HG2	2.19	0.41
1:B:71:LEU:O	1:B:71:LEU:HG	2.20	0.41
1:A:318:ASP:O	1:A:330:ILE:HG12	2.21	0.41
1:B:178:GLN:O	1:B:179:VAL:C	2.59	0.41
1:B:349:GLY:HA3	1:B:374:PHE:CE2	2.55	0.41
1:A:199:PHE:CD1	1:A:200:ASP:N	2.88	0.41
1:A:49:PHE:HB2	1:A:66:ARG:HE	1.86	0.41
1:A:283:ILE:HG23	1:A:327:VAL:CG1	2.51	0.41
1:B:202:ARG:HH11	1:B:202:ARG:HG3	1.86	0.41
1:B:173:ILE:HG13	1:B:174:ASP:N	2.36	0.40
1:A:100:ILE:HD12	1:A:128:ARG:HB3	2.02	0.40
1:A:20:ILE:CD1	1:A:348:LYS:HA	2.52	0.40
1:B:287:ILE:O	1:B:291:ILE:HG13	2.21	0.40
1:A:321:VAL:HG12	1:A:325:LEU:HA	2.04	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	299/380 (79%)	247 (83%)	37 (12%)	15 (5%)	3	3
1	B	303/380 (80%)	269 (89%)	28 (9%)	6 (2%)	9	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	602/760 (79%)	516 (86%)	65 (11%)	21 (4%)	<b>4</b> <b>6</b>

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	179	VAL
1	A	274	SER
1	A	373	VAL
1	B	179	VAL
1	B	280	GLU
1	A	32	ARG
1	A	284	LEU
1	A	343	TYR
1	A	281	ASN
1	B	174	ASP
1	B	211	TYR
1	B	282	SER
1	A	225	SER
1	A	20	ILE
1	A	261	GLU
1	A	102	PRO
1	A	267	PHE
1	A	347	CYS
1	A	283	ILE
1	B	85	PRO

### 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	242/342 (71%)	233 (96%)	9 (4%)	<b>41</b> <b>68</b>
1	B	256/342 (75%)	245 (96%)	11 (4%)	<b>35</b> <b>61</b>
All	All	498/684 (73%)	478 (96%)	20 (4%)	<b>38</b> <b>64</b>

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	200	ASP
1	A	202	ARG
1	A	220	VAL
1	A	279	LEU
1	A	293	VAL
1	A	318	ASP
1	A	352	ASP
1	A	372	ASN
1	B	12	THR
1	B	22	LEU
1	B	31	LYS
1	B	181	VAL
1	B	196	HIS
1	B	260	ASN
1	B	293	VAL
1	B	311	SER
1	B	323	LYS
1	B	330	ILE
1	B	342	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	GLN
1	B	286	GLN
1	B	372	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 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ANP	A	700	3	27,33,33	2.19	6 (22%)	30,52,52	1.32	6 (20%)
2	ANP	B	710	3	27,33,33	2.26	7 (25%)	30,52,52	1.37	4 (13%)

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
2	ANP	A	700	3	-	0/12/38/38	0/3/3/3
2	ANP	B	710	3	-	0/12/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	710	ANP	PB-N3B	-5.75	1.48	1.63
2	A	700	ANP	PB-N3B	-5.70	1.48	1.63
2	B	710	ANP	PB-O3A	-2.83	1.55	1.59
2	B	710	ANP	PB-O2B	-2.68	1.49	1.56
2	A	700	ANP	PB-O2B	-2.34	1.50	1.56
2	B	710	ANP	O2'-C2'	2.42	1.48	1.43
2	A	700	ANP	O2'-C2'	2.44	1.48	1.43
2	B	710	ANP	PB-O1B	2.99	1.49	1.46
2	A	700	ANP	PB-O1B	3.38	1.50	1.46
2	A	700	ANP	O4'-C1'	4.74	1.47	1.41
2	B	710	ANP	PG-O1G	4.89	1.51	1.46
2	A	700	ANP	PG-O1G	5.07	1.51	1.46
2	B	710	ANP	O4'-C1'	5.27	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	710	ANP	O2'-C2'-C3'	-3.49	100.48	111.83
2	A	700	ANP	O2'-C2'-C3'	-3.16	101.55	111.83
2	B	710	ANP	C2'-C1'-N9	-3.07	109.60	114.29
2	B	710	ANP	O1G-PG-N3B	-2.91	107.44	111.90
2	A	700	ANP	O1G-PG-N3B	-2.60	107.92	111.90
2	A	700	ANP	C2'-C1'-N9	-2.03	111.19	114.29
2	A	700	ANP	O2B-PB-O3A	2.07	114.49	105.09
2	A	700	ANP	C4'-O4'-C1'	2.12	112.04	109.72
2	B	710	ANP	PA-O3A-PB	2.46	140.90	132.67
2	A	700	ANP	PA-O3A-PB	2.63	141.47	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	ANP	1	0
2	B	710	ANP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	311/380 (81%)	0.48	27 (8%) 13 13	28, 66, 111, 137	0
1	B	313/380 (82%)	0.28	25 (7%) 15 16	26, 62, 106, 137	0
All	All	624/760 (82%)	0.38	52 (8%) 14 15	26, 64, 110, 137	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	PRO	6.2
1	A	270	TYR	4.5
1	B	88	THR	4.0
1	B	177	GLY	4.0
1	A	272	VAL	3.8
1	B	169	LEU	3.7
1	A	277	ILE	3.7
1	A	276	ASN	3.7
1	B	161	LEU	3.6
1	A	103	THR	3.4
1	A	153	SER	3.3
1	A	316	GLY	3.2
1	B	-2	GLY	3.1
1	A	202	ARG	2.9
1	B	330	ILE	2.9
1	B	225	SER	2.8
1	B	222	ARG	2.7
1	B	373	VAL	2.7
1	A	228	TYR	2.7
1	A	101	TYR	2.7
1	B	318	ASP	2.7
1	A	267	PHE	2.7
1	A	203	SER	2.6
1	B	316	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	172	PHE	2.6
1	B	102	PRO	2.6
1	B	194	PRO	2.6
1	B	270	TYR	2.5
1	B	329	LEU	2.5
1	A	225	SER	2.5
1	B	203	SER	2.5
1	A	172	PHE	2.5
1	A	85	PRO	2.4
1	A	282	SER	2.4
1	A	275	LEU	2.4
1	B	317	PHE	2.3
1	B	202	ARG	2.3
1	B	281	ASN	2.3
1	A	268	ASN	2.3
1	B	179	VAL	2.2
1	A	73	ARG	2.2
1	B	101	TYR	2.1
1	A	192	LEU	2.1
1	A	331	GLU	2.1
1	A	281	ASN	2.1
1	B	319	PHE	2.1
1	B	277	ILE	2.1
1	A	318	ASP	2.1
1	A	319	PHE	2.0
1	A	-1	SER	2.0
1	B	163	SER	2.0
1	A	343	TYR	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
3	MG	A	382	1/1	0.94	0.37	4.47	39,39,39,39	0
3	MG	B	384	1/1	0.89	0.22	3.36	39,39,39,39	0
3	MG	B	382	1/1	0.98	0.22	1.59	36,36,36,36	0
2	ANP	B	710	31/31	0.86	0.17	-0.69	72,88,104,104	0
2	ANP	A	700	31/31	0.88	0.16	-0.88	69,82,107,107	0
3	MG	A	381	1/1	0.95	0.09	-2.05	32,32,32,32	0
3	MG	B	381	1/1	0.99	0.10	-2.56	35,35,35,35	0
3	MG	A	383	1/1	0.98	0.06	-	49,49,49,49	0
3	MG	B	383	1/1	0.93	0.07	-	68,68,68,68	0

## 6.5 Other polymers

There are no such residues in this entry.